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WHIZARD¹

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¹The original meaning of the acronym is *W, Higgs, Z, And Respective Decays*. The current program is much more than that, however.

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Abstract

WHIZARD is an application of the VAMP algorithm: Adaptive multi-channel integration and event generation. The bare VAMP library is augmented by modules for Lorentz algebra, particles, phase space, etc., such that physical processes with arbitrary complex final states [well, in principle. . .] can be integrated and *unweighted* events be generated.

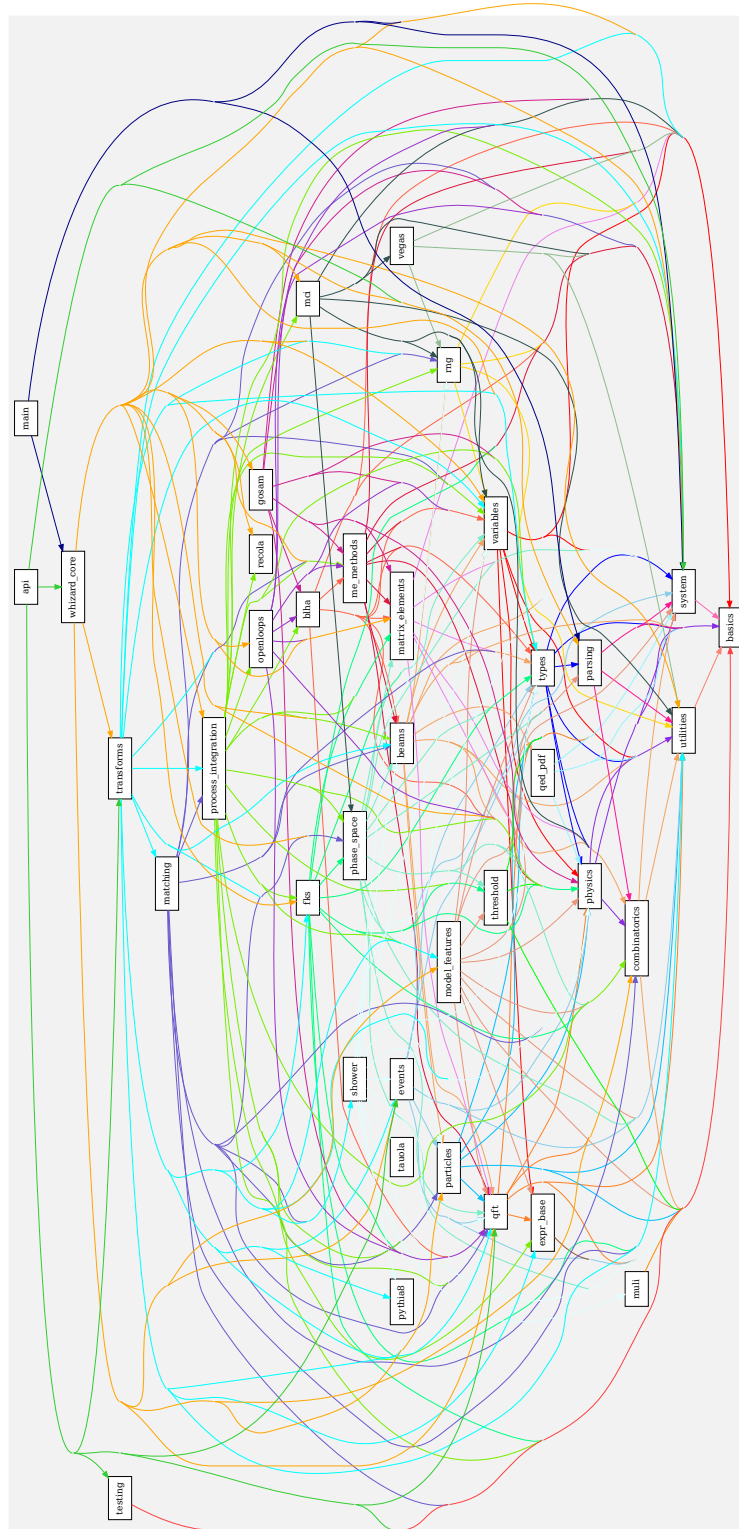


Figure 1: Overall folder structure

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Chapter 1

Changes

For a comprehensive list of changes confer the ChangeLog file or the subversion log.

Chapter 2

Preliminaries

The WHIZARD file header:

```
<File header>≡
! WHIZARD <Version> <Date>
!
! Copyright (C) 1999-2023 by
!   Wolfgang Kilian <kilian@physik.uni-siegen.de>
!   Thorsten Ohl <ohl@physik.uni-wuerzburg.de>
!   Juergen Reuter <juergen.reuter@desy.de>
!
!   with contributions from
!   cf. main AUTHORS file
!
! WHIZARD is free software; you can redistribute it and/or modify it
! under the terms of the GNU General Public License as published by
! the Free Software Foundation; either version 2, or (at your option)
! any later version.
!
! WHIZARD is distributed in the hope that it will be useful, but
! WITHOUT ANY WARRANTY; without even the implied warranty of
! MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
! GNU General Public License for more details.
!
! You should have received a copy of the GNU General Public License
! along with this program; if not, write to the Free Software
! Foundation, Inc., 675 Mass Ave, Cambridge, MA 02139, USA.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! This file has been stripped of most comments. For documentation, refer
! to the source 'whizard.nw'
```

We are strict with our names:

```
<Standard module head>≡
  implicit none
  private
```

This is the way to invoke the kinds module (not contained in this source)

```
<Use kinds>≡
  use kinds, only: default
```

<Use kinds with double>≡

```
use kinds, only: default, double
```

And we make heavy use of variable-length strings

<Use strings>≡

```
use iso_varying_string, string_t => varying_string
```

Access to the `debug_on` master switch

<Use debug>≡

```
use debug_master, only: debug_on
```

And we need the Fortran 2008 MPI module, if compiled with MPI.

<Use mpi f08>≡

<MPI: Use mpi f08>≡

```
use mpi_f08 !NODEP!
```

Chapter 3

Utilities

These modules are intended as part of WHIZARD, but in fact they are generic and could be useful for any purpose.

The modules depend only on modules from the **basics** set.

file_utils Procedures that deal with external files, if not covered by Fortran built-ins.

file_registries Manage files that are accessed by their name.

string_utils Some string-handling utilities. Includes conversion to C string.

format_utils Utilities for pretty-printing.

format_defs Predefined format strings.

numeric_utils Utilities for comparing numerical values.

data_utils Utilities for data structures, i.e. a fixed size queue, polymorphic binary tree and dynamic array list.



No internal dependencies

Figure 3.1: Module dependencies in **src/utilities**.

3.1 File Utilities

This module provides miscellaneous tools associated with named external files. Currently only:

- Delete a named file

```
<file_utils.f90>≡  
  <File header>  
  
  module file_utils  
  
    <Standard module head>  
  
    <File utils: public>  
  
    interface  
      <File utils: sub interfaces>  
    end interface  
  
  end module file_utils  
  
<file_utils_sub.f90>≡  
  <File header>  
  
  submodule (file_utils) file_utils_s  
  
    use io_units  
  
    implicit none  
  
    contains  
  
    <File utils: procedures>  
  
  end submodule file_utils_s
```

3.1.1 Deleting a file

Fortran does not contain a command for deleting a file. Here, we provide a subroutine that deletes a file if it exists. We do not handle the subtleties, so we assume that it is writable if it exists.

```
<File utils: public>≡  
  public :: delete_file  
  
<File utils: sub interfaces>≡  
    module subroutine delete_file (name)  
      character(*), intent(in) :: name  
    end subroutine delete_file  
  
<File utils: procedures>≡  
    module subroutine delete_file (name)  
      character(*), intent(in) :: name  
      logical :: exist
```

```

integer :: u
inquire (file = name, exist = exist)
if (exist) then
    u = free_unit ()
    open (unit = u, file = name)
    close (u, status = "delete")
end if
end subroutine delete_file

```

3.2 File Registries

This module provides a file-registry facility. We can open and close files multiple times without inadvertently accessing a single file by two different I/O unit numbers. Opening a file the first time enters it into the registry. Opening again just returns the associated I/O unit. The registry maintains a reference count, so closing a file does not actually complete until the last reference is released.

File access will always be sequential, however. The file can't be opened at different positions simultaneously.

```

<file_registries.f90>≡
  <File header>

  module file_registries

    <Use strings>

    <Standard module head>

    <File registries: public>

    <File registries: types>

    interface
    <File registries: sub interfaces>
    end interface

  end module file_registries

<file_registries_sub.f90>≡
  <File header>

  submodule (file_registries) file_registries_s

    use io_units

    implicit none

    contains

    <File registries: procedures>

  end submodule file_registries_s

```


3.2.1 File handle

This object holds a filename (fully qualified), the associated unit, and a reference count. The idea is that the object should be deleted when the reference count drops to zero.

```
<File registries: types>≡
  type :: file_handle_t
    type(string_t) :: file
    integer :: unit = 0
    integer :: refcount = 0
  contains
    <File registries: file handle: TBP>
  end type file_handle_t
```

Debugging output:

```
<File registries: file handle: TBP>≡
  procedure :: write => file_handle_write

<File registries: sub interfaces>≡
  module subroutine file_handle_write (handle, u, show_unit)
    class(file_handle_t), intent(in) :: handle
    integer, intent(in) :: u
    logical, intent(in), optional :: show_unit
  end subroutine file_handle_write

<File registries: procedures>≡
  module subroutine file_handle_write (handle, u, show_unit)
    class(file_handle_t), intent(in) :: handle
    integer, intent(in) :: u
    logical, intent(in), optional :: show_unit
    logical :: show_u
    show_u = .false.; if (present (show_unit)) show_u = show_unit
    if (show_u) then
      write (u, "(3x,A,1x,I0,1x,'(,I0,')')") &
        char (handle%file), handle%unit, handle%refcount
    else
      write (u, "(3x,A,1x,'(,I0,')')") &
        char (handle%file), handle%refcount
    end if
  end subroutine file_handle_write
```

Initialize with a file name, don't open the file yet:

```
<File registries: file handle: TBP>+≡
  procedure :: init => file_handle_init

<File registries: sub interfaces>+≡
  module subroutine file_handle_init (handle, file)
    class(file_handle_t), intent(out) :: handle
    type(string_t), intent(in) :: file
  end subroutine file_handle_init

<File registries: procedures>+≡
  module subroutine file_handle_init (handle, file)
    class(file_handle_t), intent(out) :: handle
    type(string_t), intent(in) :: file
```

```

        handle%file = file
    end subroutine file_handle_init

```

We check the refcount before actually opening the file.

```

<File registries: file handle: TBP>+≡
    procedure :: open => file_handle_open

<File registries: sub interfaces>+≡
    module subroutine file_handle_open (handle)
        class(file_handle_t), intent(inout) :: handle
    end subroutine file_handle_open

<File registries: procedures>+≡
    module subroutine file_handle_open (handle)
        class(file_handle_t), intent(inout) :: handle
        if (handle%refcount == 0) then
            handle%unit = free_unit ()
            open (unit = handle%unit, file = char (handle%file), action = "read", &
                status = "old")
        end if
        handle%refcount = handle%refcount + 1
    end subroutine file_handle_open

```

Analogously, close if the refcount drops to zero. The caller may then delete the object.

```

<File registries: file handle: TBP>+≡
    procedure :: close => file_handle_close

<File registries: sub interfaces>+≡
    module subroutine file_handle_close (handle)
        class(file_handle_t), intent(inout) :: handle
    end subroutine file_handle_close

<File registries: procedures>+≡
    module subroutine file_handle_close (handle)
        class(file_handle_t), intent(inout) :: handle
        handle%refcount = handle%refcount - 1
        if (handle%refcount == 0) then
            close (handle%unit)
            handle%unit = 0
        end if
    end subroutine file_handle_close

```

The I/O unit will be nonzero when the file is open.

```

<File registries: file handle: TBP>+≡
    procedure :: is_open => file_handle_is_open

<File registries: sub interfaces>+≡
    module function file_handle_is_open (handle) result (flag)
        class(file_handle_t), intent(in) :: handle
        logical :: flag
    end function file_handle_is_open

```

```

<File registries: procedures>+≡
  module function file_handle_is_open (handle) result (flag)
    class(file_handle_t), intent(in) :: handle
    logical :: flag
    flag = handle%unit /= 0
  end function file_handle_is_open

```

Return the filename, so we can identify the entry.

```

<File registries: file handle: TBP>+≡
  procedure :: get_file => file_handle_get_file

<File registries: sub interfaces>+≡
  module function file_handle_get_file (handle) result (file)
    class(file_handle_t), intent(in) :: handle
    type(string_t) :: file
  end function file_handle_get_file

<File registries: procedures>+≡
  module function file_handle_get_file (handle) result (file)
    class(file_handle_t), intent(in) :: handle
    type(string_t) :: file
    file = handle%file
  end function file_handle_get_file

```

For debugging, return the I/O unit number.

```

<File registries: file handle: TBP>+≡
  procedure :: get_unit => file_handle_get_unit

<File registries: sub interfaces>+≡
  module function file_handle_get_unit (handle) result (unit)
    class(file_handle_t), intent(in) :: handle
    integer :: unit
  end function file_handle_get_unit

<File registries: procedures>+≡
  module function file_handle_get_unit (handle) result (unit)
    class(file_handle_t), intent(in) :: handle
    integer :: unit
    unit = handle%unit
  end function file_handle_get_unit

```

3.2.2 File handles registry

This is implemented as a doubly-linked list. The list exists only once in the program, as a private module variable.

Extend the handle type to become a list entry:

```

<File registries: types>+≡
  type, extends (file_handle_t) :: file_entry_t
    type(file_entry_t), pointer :: prev => null ()
    type(file_entry_t), pointer :: next => null ()
  end type file_entry_t

```

The actual registry. We need only the pointer to the first entry.

```

<File registries: public>≡
    public :: file_registry_t

<File registries: types>+≡
    type :: file_registry_t
        type(file_entry_t), pointer :: first => null ()
    contains
        <File registries: file registry: TBP>
    end type file_registry_t

```

Debugging output.

```

<File registries: file registry: TBP>≡
    procedure :: write => file_registry_write

<File registries: sub interfaces>+≡
    module subroutine file_registry_write (registry, unit, show_unit)
        class(file_registry_t), intent(in) :: registry
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_unit
    end subroutine file_registry_write

<File registries: procedures>+≡
    module subroutine file_registry_write (registry, unit, show_unit)
        class(file_registry_t), intent(in) :: registry
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_unit
        type(file_entry_t), pointer :: entry
        integer :: u
        u = given_output_unit (unit)
        if (associated (registry%first)) then
            write (u, "(1x,A)") "File registry:"
            entry => registry%first
            do while (associated (entry))
                call entry%write (u, show_unit)
                entry => entry%next
            end do
        else
            write (u, "(1x,A)") "File registry: [empty]"
        end if
    end subroutine file_registry_write

```

Open a file: find the appropriate entry. Create a new entry and add to the list if necessary. The list is extended at the beginning. Return the I/O unit number for the records.

```

<File registries: file registry: TBP>+≡
    procedure :: open => file_registry_open

<File registries: sub interfaces>+≡
    module subroutine file_registry_open (registry, file, unit)
        class(file_registry_t), intent(inout) :: registry
        type(string_t), intent(in) :: file
        integer, intent(out), optional :: unit
    end subroutine file_registry_open

```

```

<File registries: procedures>+=
module subroutine file_registry_open (registry, file, unit)
  class(file_registry_t), intent(inout) :: registry
  type(string_t), intent(in) :: file
  integer, intent(out), optional :: unit
  type(file_entry_t), pointer :: entry
  entry => registry%first
  FIND_ENTRY: do while (associated (entry))
    if (entry%get_file () == file) exit FIND_ENTRY
    entry => entry%next
  end do FIND_ENTRY
  if (.not. associated (entry)) then
    allocate (entry)
    call entry%init (file)
    if (associated (registry%first)) then
      registry%first%prev => entry
      entry%next => registry%first
    end if
    registry%first => entry
  end if
  call entry%open ()
  if (present (unit)) unit = entry%get_unit ()
end subroutine file_registry_open

```

Close a file: find the appropriate entry. Delete the entry if there is no file connected to it anymore.

```

<File registries: file registry: TBP>+=
procedure :: close => file_registry_close

<File registries: sub interfaces>+=
module subroutine file_registry_close (registry, file)
  class(file_registry_t), intent(inout) :: registry
  type(string_t), intent(in) :: file
end subroutine file_registry_close

<File registries: procedures>+=
module subroutine file_registry_close (registry, file)
  class(file_registry_t), intent(inout) :: registry
  type(string_t), intent(in) :: file
  type(file_entry_t), pointer :: entry
  entry => registry%first
  FIND_ENTRY: do while (associated (entry))
    if (entry%get_file () == file) exit FIND_ENTRY
    entry => entry%next
  end do FIND_ENTRY
  if (associated (entry)) then
    call entry%close ()
    if (.not. entry%is_open ()) then
      if (associated (entry%prev)) then
        entry%prev%next => entry%next
      else
        registry%first => entry%next
      end if
    end if
    if (associated (entry%next)) then
      entry%next%prev => entry%prev
    end if
  end if
end subroutine file_registry_close

```

```

        end if
        deallocate (entry)
    end if
end if
end subroutine file_registry_close

```

3.3 String Utilities

This module provides tools associated with strings (built-in and variable). Currently:

- Upper and lower case for strings
- Convert to null-terminated C string

```

⟨string_utils.f90⟩≡
⟨File header⟩

module string_utils

    use, intrinsic :: iso_c_binding

    ⟨Use kinds⟩
    ⟨Use strings⟩

    ⟨Standard module head⟩

    ⟨String utils: public⟩

    ⟨String utils: interfaces⟩

    interface
    ⟨String utils: sub interfaces⟩
    end interface

end module string_utils

⟨string_utils_sub.f90⟩≡
⟨File header⟩

submodule (string_utils) string_utils_s

    implicit none

contains

    ⟨String utils: procedures⟩

end submodule string_utils_s

```

3.3.1 Upper and Lower Case

These are, unfortunately, not part of Fortran.

```
<String utils: public>≡
    public :: upper_case
    public :: lower_case

<String utils: interfaces>≡
    interface upper_case
        module procedure upper_case_char, upper_case_string
    end interface
    interface lower_case
        module procedure lower_case_char, lower_case_string
    end interface

<String utils: sub interfaces>≡
    module function upper_case_char (string) result (new_string)
        character(*), intent(in) :: string
        character(len(string)) :: new_string
    end function upper_case_char
    module function lower_case_char (string) result (new_string)
        character(*), intent(in) :: string
        character(len(string)) :: new_string
    end function lower_case_char
    module function upper_case_string (string) result (new_string)
        type(string_t), intent(in) :: string
        type(string_t) :: new_string
    end function upper_case_string
    module function lower_case_string (string) result (new_string)
        type(string_t), intent(in) :: string
        type(string_t) :: new_string
    end function lower_case_string

<String utils: procedures>≡
    module function upper_case_char (string) result (new_string)
        character(*), intent(in) :: string
        character(len(string)) :: new_string
        integer :: pos, code
        integer, parameter :: offset = ichar('A')-ichar('a')
        do pos = 1, len (string)
            code = ichar (string(pos:pos))
            select case (code)
            case (ichar('a'):ichar('z'))
                new_string(pos:pos) = char (code + offset)
            case default
                new_string(pos:pos) = string(pos:pos)
            end select
        end do
    end function upper_case_char

    module function lower_case_char (string) result (new_string)
        character(*), intent(in) :: string
        character(len(string)) :: new_string
        integer :: pos, code
        integer, parameter :: offset = ichar('a')-ichar('A')
        do pos = 1, len (string)
```

```

        code = ichar (string(pos:pos))
        select case (code)
        case (ichar('A'):ichar('Z'))
            new_string(pos:pos) = char (code + offset)
        case default
            new_string(pos:pos) = string(pos:pos)
        end select
    end do
end function lower_case_char

module function upper_case_string (string) result (new_string)
    type(string_t), intent(in) :: string
    type(string_t) :: new_string
    new_string = upper_case_char (char (string))
end function upper_case_string

module function lower_case_string (string) result (new_string)
    type(string_t), intent(in) :: string
    type(string_t) :: new_string
    new_string = lower_case_char (char (string))
end function lower_case_string

```

3.3.2 C-Fortran String Conversion

Convert a FORTRAN string to a null-terminated C string.

```

<String utils: public>+≡
    public :: string_f2c

<String utils: interfaces>+≡
    interface string_f2c
        module procedure string_f2c_char, string_f2c_var_str
    end interface string_f2c

<String utils: sub interfaces>+≡
    pure module function string_f2c_char (i) result (o)
        character(*), intent(in) :: i
        character(kind=c_char, len=len (i) + 1) :: o
    end function string_f2c_char
    pure module function string_f2c_var_str (i) result (o)
        type(string_t), intent(in) :: i
        character(kind=c_char, len=len (i) + 1) :: o
    end function string_f2c_var_str

<String utils: procedures>+≡
    pure module function string_f2c_char (i) result (o)
        character(*), intent(in) :: i
        character(kind=c_char, len=len (i) + 1) :: o
        o = i // c_null_char
    end function string_f2c_char

    pure module function string_f2c_var_str (i) result (o)
        type(string_t), intent(in) :: i
        character(kind=c_char, len=len (i) + 1) :: o
        o = char (i) // c_null_char
    end function string_f2c_var_str

```



```
end function string_f2c_var_str
```

The same task done by a subroutine, analogous to the C `strcpy` function. We append a null char and copy the characters to the output string, given by a character array – which is equal to a `c_char` character string by the rule of sequence association.

Note: Just like with the `strcpy` function, there is no bounds check.

```
<String utils: public>+≡
  public :: strcpy_f2c

<String utils: sub interfaces>+≡
  module subroutine strcpy_f2c (fstring, cstring)
    character(*), intent(in) :: fstring
    character(c_char), dimension(*), intent(inout) :: cstring
  end subroutine strcpy_f2c

<String utils: procedures>+≡
  module subroutine strcpy_f2c (fstring, cstring)
    character(*), intent(in) :: fstring
    character(c_char), dimension(*), intent(inout) :: cstring

    integer :: i

    do i = 1, len (fstring)
      cstring(i) = fstring(i:i)
    end do
    cstring(len(fstring)+1) = c_null_char

  end subroutine strcpy_f2c
```

Convert a null-terminated C string to a Fortran string. The C-string argument is sequence-associated to a one-dimensional array of C characters, where we do not know the dimension.

To convert this to a `string_t` object, we need to assign it or to wrap it by another `var_str` conversion.

```
<String utils: public>+≡
  public :: string_c2f

<String utils: sub interfaces>+≡
  module function string_c2f (cstring) result (fstring)
    character(c_char), dimension(*), intent(in) :: cstring
    character(:), allocatable :: fstring
  end function string_c2f

<String utils: procedures>+≡
  module function string_c2f (cstring) result (fstring)
    character(c_char), dimension(*), intent(in) :: cstring
    character(:), allocatable :: fstring

    integer :: i, n

    n = 0
    do while (cstring(n+1) /= c_null_char)
      n = n + 1
```

```

end do

allocate (character(n) :: fstring)
do i = 1, n
    fstring(i:i) = cstring(i)
end do

end function string_c2f

```

3.3.3 Number Conversion

Create a string from a number. We use fixed format for the reals and variable format for integers.

```

<String utils: public>+≡
    public :: str

<String utils: interfaces>+≡
    interface str
        module procedure str_log, str_logs, str_int, str_ints, &
            str_real, str_reals, str_complex, str_complexs
    end interface

<String utils: sub interfaces>+≡
    module function str_log (l) result (s)
        logical, intent(in) :: l
        type(string_t) :: s
    end function str_log
    module function str_logs (x) result (s)
        logical, dimension(:), intent(in) :: x
        type(string_t) :: s
    end function str_logs
    module function str_int (i) result (s)
        integer, intent(in) :: i
        type(string_t) :: s
    end function str_int
    module function str_ints (x) result (s)
        integer, dimension(:), intent(in) :: x
        type(string_t) :: s
    end function str_ints
    module function str_real (x) result (s)
        real(default), intent(in) :: x
        type(string_t) :: s
    end function str_real
    module function str_reals (x) result (s)
        real(default), dimension(:), intent(in) :: x
        type(string_t) :: s
    end function str_reals
    module function str_complex (x) result (s)
        complex(default), intent(in) :: x
        type(string_t) :: s
    end function str_complex
    module function str_complexs (x) result (s)
        complex(default), dimension(:), intent(in) :: x

```

```

        type(string_t) :: s
    end function str_complexs

<String utils: procedures>+≡
module function str_log (l) result (s)
    logical, intent(in) :: l
    type(string_t) :: s
    if (l) then
        s = "True"
    else
        s = "False"
    end if
end function str_log

module function str_logs (x) result (s)
    logical, dimension(:), intent(in) :: x
    <concatenate strings>
end function str_logs

module function str_int (i) result (s)
    integer, intent(in) :: i
    type(string_t) :: s
    character(32) :: buffer
    write (buffer, "(I0)") i
    s = var_str (trim (adjustl (buffer)))
end function str_int

module function str_ints (x) result (s)
    integer, dimension(:), intent(in) :: x
    <concatenate strings>
end function str_ints

module function str_real (x) result (s)
    real(default), intent(in) :: x
    type(string_t) :: s
    character(32) :: buffer
    write (buffer, "(ES17.10)") x
    s = var_str (trim (adjustl (buffer)))
end function str_real

module function str_reals (x) result (s)
    real(default), dimension(:), intent(in) :: x
    <concatenate strings>
end function str_reals

module function str_complex (x) result (s)
    complex(default), intent(in) :: x
    type(string_t) :: s
    s = str_real (real (x)) // " + i " // str_real (aimag (x))
end function str_complex

module function str_complexs (x) result (s)
    complex(default), dimension(:), intent(in) :: x
    <concatenate strings>
end function str_complexs

```

```

⟨concatenate strings⟩≡
  type(string_t) :: s
  integer :: i
  s = '['
  do i = 1, size(x) - 1
    s = s // str(x(i)) // ', '
  end do
  s = s // str(x(size(x))) // ']'

```

Auxiliary: Read real, integer, string value.

```

⟨String utils: public⟩+≡
  public :: read_rval
  public :: read_ival

```

```

⟨String utils: sub interfaces⟩+≡
  module function read_rval (s) result (rval)
    real(default) :: rval
    type(string_t), intent(in) :: s
  end function read_rval
  module function read_ival (s) result (ival)
    integer :: ival
    type(string_t), intent(in) :: s
  end function read_ival

```

```

⟨String utils: procedures⟩+≡
  module function read_rval (s) result (rval)
    real(default) :: rval
    type(string_t), intent(in) :: s
    character(80) :: buffer
    buffer = s
    read (buffer, *) rval
  end function read_rval

  module function read_ival (s) result (ival)
    integer :: ival
    type(string_t), intent(in) :: s
    character(80) :: buffer
    buffer = s
    read (buffer, *) ival
  end function read_ival

```

3.3.4 String splitting

```

⟨String utils: public⟩+≡
  public :: string_contains_word

```

```

⟨String utils: sub interfaces⟩+≡
  pure module function string_contains_word &
    (str, word, include_identical) result (val)
    logical :: val
    type(string_t), intent(in) :: str, word
    logical, intent(in), optional :: include_identical
  end function string_contains_word

```

```

<String utils: procedures>+≡
  pure module function string_contains_word &
    (str, word, include_identical) result (val)
    logical :: val
    type(string_t), intent(in) :: str, word
    type(string_t) :: str_tmp, str_out
    logical, intent(in), optional :: include_identical
    logical :: yorn
    str_tmp = str
    val = .false.
    yorn = .false.; if (present (include_identical)) yorn = include_identical
    if (yorn) val = str == word
    call split (str_tmp, str_out, word)
    val = val .or. (str_out /= "")
  end function string_contains_word

```

Create an array of strings using a separator.

```

<String utils: public>+≡
  public :: split_string

<String utils: sub interfaces>+≡
  pure module subroutine split_string (str, separator, str_array)
    type(string_t), dimension(:), allocatable, intent(out) :: str_array
    type(string_t), intent(in) :: str, separator
  end subroutine split_string

<String utils: procedures>+≡
  pure module subroutine split_string (str, separator, str_array)
    type(string_t), dimension(:), allocatable, intent(out) :: str_array
    type(string_t), intent(in) :: str, separator
    type(string_t) :: str_tmp, str_out
    integer :: n_str
    n_str = 0; str_tmp = str
    do while (string_contains_word (str_tmp, separator))
      n_str = n_str + 1
      call split (str_tmp, str_out, separator)
    end do
    allocate (str_array (n_str))
    n_str = 1; str_tmp = str
    do while (string_contains_word (str_tmp, separator))
      call split (str_tmp, str_array (n_str), separator)
      n_str = n_str + 1
    end do
  end subroutine split_string

```

3.4 Format Utilities

This module provides miscellaneous tools associated with formatting and pretty-printing.

- Horizontal separator lines in output
- Indenting an output line

- Formatting a number for T_EX output.
- Formatting a number for MetaPost output.
- Alternate numeric formats.

```

⟨format_utils.f90⟩≡
  ⟨File header⟩

  module format_utils

    ⟨Use kinds⟩
    ⟨Use strings⟩

    ⟨Standard module head⟩

    ⟨Format utils: public⟩

    interface
    ⟨Format utils: sub interfaces⟩
    end interface

  end module format_utils

⟨format_utils_sub.f90⟩≡
  ⟨File header⟩

  submodule (format_utils) format_utils_s

    use string_utils, only: lower_case
    use io_units, only: given_output_unit

    implicit none

  contains

    ⟨Format utils: procedures⟩

  end submodule format_utils_s

```

3.4.1 Line Output

Write a separator line.

```

⟨Format utils: public⟩≡
  public :: write_separator

⟨Format utils: sub interfaces⟩≡
  module subroutine write_separator (u, mode)
    integer, intent(in) :: u
    integer, intent(in), optional :: mode
  end subroutine write_separator

```

```

<Format utils: procedures>+=
module subroutine write_separator (u, mode)
  integer, intent(in) :: u
  integer, intent(in), optional :: mode
  integer :: m
  m = 1; if (present (mode)) m = mode
  select case (m)
  case default
    write (u, "(A)") repeat("-", 72)
  case (1)
    write (u, "(A)") repeat("-", 72)
  case (2)
    write (u, "(A)") repeat("=", 72)
  end select
end subroutine write_separator

```

Indent the line with given number of blanks.

```

<Format utils: public>+=
public :: write_indent

<Format utils: sub interfaces>+=
module subroutine write_indent (unit, indent)
  integer, intent(in) :: unit
  integer, intent(in), optional :: indent
end subroutine write_indent

<Format utils: procedures>+=
module subroutine write_indent (unit, indent)
  integer, intent(in) :: unit
  integer, intent(in), optional :: indent
  if (present (indent)) then
    write (unit, "(1x,A)", advance="no") repeat(" ", indent)
  end if
end subroutine write_indent

```

3.4.2 Array Output

Write an array of integers.

```

<Format utils: public>+=
public :: write_integer_array

<Format utils: sub interfaces>+=
module subroutine write_integer_array (array, unit, n_max, no_skip)
  integer, intent(in), dimension(:) :: array
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: n_max
  logical, intent(in), optional :: no_skip
end subroutine write_integer_array

<Format utils: procedures>+=
module subroutine write_integer_array (array, unit, n_max, no_skip)
  integer, intent(in), dimension(:) :: array
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: n_max

```

```

logical, intent(in), optional :: no_skip
integer :: u, i, n
logical :: yorn
u = given_output_unit (unit)
yorn = .false.; if (present (no_skip)) yorn = no_skip
if (present (n_max)) then
    n = n_max
else
    n = size (array)
end if
do i = 1, n
    if (i < n .or. yorn) then
        write (u, "(IO, A)", advance = "no") array(i), ", "
    else
        write (u, "(IO)") array(i)
    end if
end do
end subroutine write_integer_array

```

3.4.3 T_EX-compatible Output

Quote underscore characters for use in T_EX output.

```

<Format utils: public>+≡
    public :: quote_underscore

<Format utils: sub interfaces>+≡
    module function quote_underscore (string) result (quoted)
        type(string_t) :: quoted
        type(string_t), intent(in) :: string
    end function quote_underscore

<Format utils: procedures>+≡
    module function quote_underscore (string) result (quoted)
        type(string_t) :: quoted
        type(string_t), intent(in) :: string
        type(string_t) :: part
        type(string_t) :: buffer
        buffer = string
        quoted = ""
    do
        call split (part, buffer, "_")
        quoted = quoted // part
        if (buffer == "") exit
        quoted = quoted // "\"
    end do
    end function quote_underscore

```

Format a number with n significant digits for use in T_EX documents.

```

<Format utils: public>+≡
    public :: tex_format

```


<Format utils: sub interfaces>+≡

```

module function tex_format (rval, n_digits) result (string)
  type(string_t) :: string
  real(default), intent(in) :: rval
  integer, intent(in) :: n_digits
end function tex_format

```

<Format utils: procedures>+≡

```

module function tex_format (rval, n_digits) result (string)
  type(string_t) :: string
  real(default), intent(in) :: rval
  integer, intent(in) :: n_digits
  integer :: e, n, w, d
  real(default) :: absval
  real(default) :: mantissa
  character :: sign
  character(20) :: format
  character(80) :: cstr
  n = min (abs (n_digits), 16)
  if (rval == 0) then
    string = "0"
  else
    absval = abs (rval)
    e = int (log10 (absval))
    if (rval < 0) then
      sign = "-"
    else
      sign = ""
    end if
    select case (e)
    case (:-3)
      d = max (n - 1, 0)
      w = max (d + 2, 2)
      write (format, "('(F',IO,'.',IO,'A,IO,A)')") w, d
      mantissa = absval * 10._default ** (1 - e)
      write (cstr, fmt=format) mantissa, "\times 10^{", e - 1, "}"
    case (-2:0)
      d = max (n - e, 1 - e)
      w = max (d + e + 2, d + 2)
      write (format, "('(F',IO,'.',IO,')')") w, d
      write (cstr, fmt=format) absval
    case (1:2)
      d = max (n - e - 1, -e, 0)
      w = max (d + e + 2, d + 2, e + 2)
      write (format, "('(F',IO,'.',IO,')')") w, d
      write (cstr, fmt=format) absval
    case default
      d = max (n - 1, 0)
      w = max (d + 2, 2)
      write (format, "('(F',IO,'.',IO,'A,IO,A)')") w, d
      mantissa = absval * 10._default ** (- e)
      write (cstr, fmt=format) mantissa, "\times 10^{", e, "}"
    end select
    string = sign // trim (cstr)
  end if
end if

```

```
end function tex_format
```

3.4.4 Metapost-compatible Output

Write a number for use in Metapost code:

```
<Format utils: public>+≡
  public :: mp_format

<Format utils: sub interfaces>+≡
  module function mp_format (rval) result (string)
    type(string_t) :: string
    real(default), intent(in) :: rval
  end function mp_format

<Format utils: procedures>+≡
  module function mp_format (rval) result (string)
    type(string_t) :: string
    real(default), intent(in) :: rval
    character(16) :: tmp
    write (tmp, "(G16.8)") rval
    string = lower_case (trim (adjustl (trim (tmp))))
  end function mp_format
```

3.4.5 Conditional Formatting

Conditional format string, intended for switchable numeric precision.

```
<Format utils: public>+≡
  public :: pac_fmt

<Format utils: sub interfaces>+≡
  module subroutine pac_fmt (fmt, fmt_orig, fmt_pac, pacify)
    character(*), intent(in) :: fmt_orig, fmt_pac
    character(*), intent(out) :: fmt
    logical, intent(in), optional :: pacify
  end subroutine pac_fmt

<Format utils: procedures>+≡
  module subroutine pac_fmt (fmt, fmt_orig, fmt_pac, pacify)
    character(*), intent(in) :: fmt_orig, fmt_pac
    character(*), intent(out) :: fmt
    logical, intent(in), optional :: pacify
    logical :: pacified
    pacified = .false.
    if (present (pacify)) pacified = pacify
    if (pacified) then
      fmt = fmt_pac
    else
      fmt = fmt_orig
    end if
  end subroutine pac_fmt
```

3.4.6 Guard tiny values

This function can be applied if values smaller than 10^{-99} would cause an underflow in the output format. We know that Fortran fixed-format can handle this by omitting the exponent letter, but we should expect non-Fortran or Fortran list-directed input, which would fail. We reset such values to $\pm 10^{-99}$, assuming that such tiny values would not matter, except for being non-zero.

```
<Format utils: public>+≡
    public :: refmt_tiny

<Format utils: sub interfaces>+≡
    elemental module function refmt_tiny (val) result (trunc_val)
        real(default), intent(in) :: val
        real(default) :: trunc_val
    end function refmt_tiny

<Format utils: procedures>+≡
    elemental module function refmt_tiny (val) result (trunc_val)
        real(default), intent(in) :: val
        real(default) :: trunc_val
        real(default), parameter :: tiny_val = 1.e-99_default

        if (val /= 0) then
            if (abs (val) < tiny_val) then
                trunc_val = sign (tiny_val, val)
            else
                trunc_val = val
            end if
        else
            trunc_val = val
        end if

    end function refmt_tiny
```

3.4.7 Compressed output of integer arrays

```
<Format utils: public>+≡
    public :: write_compressed_integer_array

<Format utils: sub interfaces>+≡
    module subroutine write_compressed_integer_array (chars, array)
        character(len=*), intent(out) :: chars
        integer, intent(in), allocatable, dimension(:) :: array
    end subroutine write_compressed_integer_array

<Format utils: procedures>+≡
    module subroutine write_compressed_integer_array (chars, array)
        character(len=*), intent(out) :: chars
        integer, intent(in), allocatable, dimension(:) :: array
        logical, dimension(:), allocatable :: used
        character(len=16) :: tmp
        type(string_t) :: string
        integer :: i, j, start_chain, end_chain
        chars = '[none]'
        string = ""
```

```

if (allocated (array)) then
  if (size (array) > 0) then
    allocate (used (size (array)))
    used = .false.
    do i = 1, size (array)
      if (.not. used(i)) then
        start_chain = array(i)
        end_chain = array(i)
        used(i) = .true.
        EXTEND: do
          do j = 1, size (array)
            if (array(j) == end_chain + 1) then
              end_chain = array(j)
              used(j) = .true.
              cycle EXTEND
            end if
            if (array(j) == start_chain - 1) then
              start_chain = array(j)
              used(j) = .true.
              cycle EXTEND
            end if
          end do
        end do EXTEND
      if (end_chain - start_chain > 0) then
        write (tmp, "(I0,A,I0)") start_chain, "-", end_chain
      else
        write (tmp, "(I0)") start_chain
      end if
      string = string // trim (tmp)
      if (any (.not. used)) then
        string = string // ', '
      end if
    end if
  end do
  chars = string
end if
chars = adjustr (chars)
end subroutine write_compressed_integer_array

```

3.5 Format Definitions

This module provides named integer parameters that specify certain format strings, used for numerical output.

<format_defs.f90>≡

<File header>

module format_defs

<Standard module head>

⟨Format defs: public parameters⟩

```
end module format_defs
```

We collect format strings for various numerical output formats here.

⟨Format defs: public parameters⟩≡

```
character(*), parameter, public :: FMT_19 = "ES19.12"  
character(*), parameter, public :: FMT_18 = "ES18.11"  
character(*), parameter, public :: FMT_17 = "ES17.10"  
character(*), parameter, public :: FMT_16 = "ES16.9"  
character(*), parameter, public :: FMT_15 = "ES15.8"  
character(*), parameter, public :: FMT_14 = "ES14.7"  
character(*), parameter, public :: FMT_13 = "ES13.6"  
character(*), parameter, public :: FMT_12 = "ES12.5"  
character(*), parameter, public :: FMT_11 = "ES11.4"  
character(*), parameter, public :: FMT_10 = "ES10.3"
```

Fixed-point formats for better readability, where appropriate.

⟨Format defs: public parameters⟩+≡

```
character(*), parameter, public :: FMT_12 = "F12.9"
```

3.6 Numeric Utilities

⟨numeric_utils.f90⟩≡

⟨File header⟩

```
module numeric_utils
```

⟨Use kinds⟩

⟨Use strings⟩

⟨Standard module head⟩

⟨Numeric utils: public⟩

⟨Numeric utils: parameters⟩

⟨Numeric utils: types⟩

⟨Numeric utils: interfaces⟩

```
interface
```

⟨Numeric utils: sub interfaces⟩

```
end interface
```

```
end module numeric_utils
```

⟨numeric_utils_sub.f90⟩≡

⟨File header⟩

```
submodule (numeric_utils) numeric_utils_s
```

```

    use string_utils
    use constants
    use format_defs

    implicit none

contains

    <Numeric utils: procedures>

    end submodule numeric_utils_s

```

Probably, there needs to be a single, global workspace for the whole calculations and not one local to the integration routine.

```

    <Numeric utils: types>≡
    type :: int_workspace_t
    private
    integer :: limit
    integer :: size = 0
    integer :: nrmax = 1
    integer :: i = 1
    integer :: maximum_level = 0
    real(default), dimension(:), allocatable :: alist
    real(default), dimension(:), allocatable :: blist
    real(default), dimension(:), allocatable :: rlist
    real(default), dimension(:), allocatable :: elist
    integer, dimension(:), allocatable :: order
    integer, dimension(:), allocatable :: level
contains
    <Numeric utils: workspace: TBP>
end type int_workspace_t

    <Numeric utils: workspace: TBP>≡
    procedure :: init => int_workspace_init

    <Numeric utils: sub interfaces>≡
    module subroutine int_workspace_init (work, a, b, limit)
    class(int_workspace_t), intent(out) :: work
    real(default), intent(in) :: a, b
    integer, intent(in) :: limit
    end subroutine int_workspace_init

    <Numeric utils: procedures>≡
    module subroutine int_workspace_init (work, a, b, limit)
    class(int_workspace_t), intent(out) :: work
    real(default), intent(in) :: a, b
    integer, intent(in) :: limit
    work%limit = limit
    allocate (work%alist (limit), work%blist (limit), &
    work%rlist (limit), work%elist(limit), &
    work%order(limit), work%level(limit))
    work%alist(1) = a
    work%blist(1) = b
end subroutine int_workspace_init

```

```

<Numeric utils: workspace: TBP>+≡
    procedure :: set_initial => int_workspace_set_initial

<Numeric utils: sub interfaces>+≡
    module subroutine int_workspace_set_initial (work, res, err)
        class(int_workspace_t), intent(inout) :: work
        real(default), intent(in) :: res, err
    end subroutine int_workspace_set_initial

<Numeric utils: procedures>+≡
    module subroutine int_workspace_set_initial (work, res, err)
        class(int_workspace_t), intent(inout) :: work
        real(default), intent(in) :: res, err
        work%size = 1
        work%order(1) = 1
        work%rlist(1) = res
        work%elist(1) = err
    end subroutine int_workspace_set_initial

<Numeric utils: workspace: TBP>+≡
    procedure :: update => int_workspace_update

<Numeric utils: sub interfaces>+≡
    module subroutine int_workspace_update (work, a1, b1, area1, error1, &
        a2, b2, area2, error2)
        class(int_workspace_t), intent(inout) :: work
        real(default), intent(in) :: a1, b1, area1, error1, &
            a2, b2, area2, error2
    end subroutine int_workspace_update

<Numeric utils: procedures>+≡
    module subroutine int_workspace_update (work, a1, b1, area1, error1, &
        a2, b2, area2, error2)
        class(int_workspace_t), intent(inout) :: work
        real(default), intent(in) :: a1, b1, area1, error1, &
            a2, b2, area2, error2
        integer :: i_max, i_new, new_level
        i_max = work%i
        i_new = work%size + 1
        new_level = work%level(i_max) + 1
        ! append the newly-created intervals to the list
        if (error2 > error1) then
            ! work%blist(maxerr) is already b2
            work%alist(i_max) = a2
            work%rlist(i_max) = area2
            work%elist(i_max) = error2
            work%level(i_max) = new_level
            work%alist(i_new) = a1
            work%blist(i_new) = b1
            work%rlist(i_new) = area1
            work%elist(i_new) = error1
            work%level(i_new) = new_level
        else
            ! work%alist(maxerr) is already a1
            work%blist(i_max) = b1
            work%rlist(i_max) = area1

```

```

        work%elist(i_max) = error1
        work%level(i_max) = new_level
        work%alist(i_new) = a2
        work%blist(i_new) = b2
        work%rlist(i_new) = area2
        work%elist(i_new) = error2
        work%level(i_new) = new_level
    end if
    work%size = work%size + 1
    if (new_level > work%maximum_level) &
        work%maximum_level = new_level
    call work%sort ()
end subroutine int_workspace_update

```

<Numeric utils: workspace: TBP>+≡

```

procedure :: sort => int_workspace_sort

```

<Numeric utils: sub interfaces>+≡

```

module subroutine int_workspace_sort (work)
    class(int_workspace_t), intent(inout) :: work
end subroutine int_workspace_sort

```

<Numeric utils: procedures>+≡

```

module subroutine int_workspace_sort (work)
    class(int_workspace_t), intent(inout) :: work
    integer :: last, limit, i, k, top, i_nrmax, i_maxerr
    real(default) :: errmax, errmin
    last = work%size
    limit = work%limit
    i_nrmax = work%nrmax
    i_maxerr = work%order(i_nrmax)
    ! Check whether the list contains more than two error estimates
    if (last < 3) then
        work%order(1) = 1
        work%order(2) = 2
        work%i = i_maxerr
        return
    end if
    errmax = work%elist(i_maxerr)
    ! This part of the routine is only executed if, due to a difficult
    ! integrand, subdivision increased the error estimate. In the normal
    ! case the insert procedure should start after the nrmax-th largest
    ! error estimate.
    DESCEND_NRMAX: do while (i_nrmax > 1)
        if (errmax > work%elist(work%order(i_nrmax - 1))) then
            work%order(i_nrmax) = work%order(i_nrmax - 1)
            i_nrmax = i_nrmax - 1
        else
            exit DESCEND_NRMAX
        end if
    end do DESCEND_NRMAX
    ! Compute the number of elements in the list to be maintained in
    ! descending order. This number depends on the number of
    ! subdivisions still allowed.
    if (last < (limit/2 + 2)) then

```



```

        top = last
    else
        top = limit - last + 1
    end if
    ! Insert errmax by traversing the list top-down, starting
    ! comparison from the element elist(order(i_nrmax+1)).
    i = i_nrmax + 1
    ! The order of the tests in the following line is important to
    ! prevent a segmentation fault
    ASCEND_TOP: do while (i < top)
        if (errmax < work%elist(work%order(i))) then
            work%order(i-1) = work%order(i)
            i = i + 1
        else
            exit ASCEND_TOP
        end if
    end do ASCEND_TOP
    work%order(i-1) = i_maxerr
    ! Insert errmin by traversing the list bottom-up
    errmin = work%elist(last)
    k = top - 1
    DESCEND_K: do while (k > i-2)
        if (errmin >= work%elist(work%order(k))) then
            work%order(k+1) = work%order(k)
            k = k - 1
        else
            exit DESCEND_K
        end if
    end do DESCEND_K
    work%order(k+1) = last
    ! Set i_max and e_max
    i_maxerr = work%order(i_nrmax)
    work%i = i_maxerr
    work%nrmax = i_nrmax
end subroutine int_workspace_sort

```

<Numeric utils: public>≡
 public :: assert

<Numeric utils: sub interfaces>+≡
 module subroutine assert (unit, ok, description, exit_on_fail)
 integer, intent(in) :: unit
 logical, intent(in) :: ok
 character(*), intent(in), optional :: description
 logical, intent(in), optional :: exit_on_fail
 end subroutine assert

<Numeric utils: procedures>+≡
 module subroutine assert (unit, ok, description, exit_on_fail)
 integer, intent(in) :: unit
 logical, intent(in) :: ok
 character(*), intent(in), optional :: description
 logical, intent(in), optional :: exit_on_fail
 logical :: ef
 ef = .false.; if (present (exit_on_fail)) ef = exit_on_fail

```

    if (.not. ok) then
        if (present(description)) then
            write (unit, "(A)") "* FAIL: " // description
        else
            write (unit, "(A)") "* FAIL: Assertion error"
        end if
        if (ef) stop 1
    end if
end subroutine assert

```

Compare numbers and output error message if not equal.

<Numeric utils: public>+≡

```

public:: assert_equal
interface assert_equal
    module procedure assert_equal_integer, assert_equal_integers, &
        assert_equal_real, assert_equal_reals, &
        assert_equal_complex, assert_equal_complexs
end interface

```

<Numeric utils: sub interfaces>+≡

```

module subroutine assert_equal_integer (unit, lhs, rhs, description, exit_on_fail)
    integer, intent(in) :: unit
    integer, intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_integer

```

<Numeric utils: procedures>+≡

```

module subroutine assert_equal_integer (unit, lhs, rhs, description, exit_on_fail)
    integer, intent(in) :: unit
    integer, intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    logical, intent(in), optional :: exit_on_fail
    type(string_t) :: desc
    logical :: ok
    ok = lhs == rhs
    desc = ""; if (present (description)) desc = var_str(description) // ": "
    call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)
end subroutine assert_equal_integer

```

<Numeric utils: sub interfaces>+≡

```

module subroutine assert_equal_integers (unit, lhs, rhs, description, exit_on_fail)
    integer, intent(in) :: unit
    integer, dimension(:), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_integers

```

<Numeric utils: procedures>+≡

```

module subroutine assert_equal_integers (unit, lhs, rhs, description, exit_on_fail)
    integer, intent(in) :: unit
    integer, dimension(:), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description

```

```

logical, intent(in), optional :: exit_on_fail
type(string_t) :: desc
logical :: ok
ok = all(lhs == rhs)
desc = ''; if (present (description)) desc = var_str(description) // ": "
call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)
end subroutine assert_equal_integers

```

(Numeric utils: sub interfaces)+≡

```

module subroutine assert_equal_real (unit, lhs, rhs, description, &
                                   abs_smallness, rel_smallness, exit_on_fail)

  integer, intent(in) :: unit
  real(default), intent(in) :: lhs, rhs
  character(*), intent(in), optional :: description
  real(default), intent(in), optional :: abs_smallness, rel_smallness
  logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_real

```

(Numeric utils: procedures)+≡

```

module subroutine assert_equal_real (unit, lhs, rhs, description, &
                                   abs_smallness, rel_smallness, exit_on_fail)

  integer, intent(in) :: unit
  real(default), intent(in) :: lhs, rhs
  character(*), intent(in), optional :: description
  real(default), intent(in), optional :: abs_smallness, rel_smallness
  logical, intent(in), optional :: exit_on_fail
  type(string_t) :: desc
  logical :: ok
  ok = nearly_equal (lhs, rhs, abs_smallness, rel_smallness)
  desc = ''; if (present (description)) desc = var_str(description) // ": "
  call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)
end subroutine assert_equal_real

```

(Numeric utils: sub interfaces)+≡

```

module subroutine assert_equal_reals (unit, lhs, rhs, description, &
                                    abs_smallness, rel_smallness, exit_on_fail)

  integer, intent(in) :: unit
  real(default), dimension(:), intent(in) :: lhs, rhs
  character(*), intent(in), optional :: description
  real(default), intent(in), optional :: abs_smallness, rel_smallness
  logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_reals

```

(Numeric utils: procedures)+≡

```

module subroutine assert_equal_reals (unit, lhs, rhs, description, &
                                    abs_smallness, rel_smallness, exit_on_fail)

  integer, intent(in) :: unit
  real(default), dimension(:), intent(in) :: lhs, rhs
  character(*), intent(in), optional :: description
  real(default), intent(in), optional :: abs_smallness, rel_smallness
  logical, intent(in), optional :: exit_on_fail
  type(string_t) :: desc
  logical :: ok
  ok = all(nearly_equal (lhs, rhs, abs_smallness, rel_smallness))

```

```

desc = ""; if (present (description)) desc = var_str(description) // ": "
call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)
end subroutine assert_equal_reals

```

<Numeric utils: sub interfaces>+≡

```

module subroutine assert_equal_complex (unit, lhs, rhs, description, &
                                     abs_smallness, rel_smallness, exit_on_fail)
    integer, intent(in) :: unit
    complex(default), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_complex

```

<Numeric utils: procedures>+≡

```

module subroutine assert_equal_complex (unit, lhs, rhs, description, &
                                     abs_smallness, rel_smallness, exit_on_fail)
    integer, intent(in) :: unit
    complex(default), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: exit_on_fail
    type(string_t) :: desc
    logical :: ok
    ok = nearly_equal (real(lhs), real(rhs), abs_smallness, rel_smallness) &
        .and. nearly_equal (aimag(lhs), aimag(rhs), abs_smallness, rel_smallness)
    desc = ""; if (present (description)) desc = var_str(description) // ": "
    call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)
end subroutine assert_equal_complex

```

<Numeric utils: sub interfaces>+≡

```

module subroutine assert_equal_complexs (unit, lhs, rhs, description, &
                                     abs_smallness, rel_smallness, exit_on_fail)
    integer, intent(in) :: unit
    complex(default), dimension(:), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: exit_on_fail
end subroutine assert_equal_complexs

```

<Numeric utils: procedures>+≡

```

module subroutine assert_equal_complexs (unit, lhs, rhs, description, &
                                     abs_smallness, rel_smallness, exit_on_fail)
    integer, intent(in) :: unit
    complex(default), dimension(:), intent(in) :: lhs, rhs
    character(*), intent(in), optional :: description
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: exit_on_fail
    type(string_t) :: desc
    logical :: ok
    ok = all (nearly_equal (real(lhs), real(rhs), abs_smallness, rel_smallness)) &
        .and. all (nearly_equal (aimag(lhs), aimag(rhs), abs_smallness, rel_smallness))
    desc = ""; if (present (description)) desc = var_str(description) // ": "
    call assert (unit, ok, char(desc // str (lhs) // " /= " // str (rhs)), exit_on_fail)

```

```
end subroutine assert_equal_complexs
```

Note that this poor man's check will be disabled if someone compiles with `-ffast-math` or similar optimizations.

```
<Numeric utils: procedures>+≡
  elemental function ieee_is_nan (x) result (yorn)
    logical :: yorn
    real(default), intent(in) :: x
    yorn = (x /= x)
  end function ieee_is_nan
```

This is still not perfect but should work in most cases. Usually one wants to compare to a relative epsilon `rel_smallness`, except for numbers close to zero defined by `abs_smallness`. Both might need adaption to specific use cases but have reasonable defaults.

```
<Numeric utils: public>+≡
  public :: nearly_equal
```

```
<Numeric utils: interfaces>≡
  interface nearly_equal
    module procedure nearly_equal_real
    module procedure nearly_equal_complex
  end interface nearly_equal
```

```
<Numeric utils: sub interfaces>+≡
  elemental module function nearly_equal_real &
    (a, b, abs_smallness, rel_smallness) result (r)
    logical :: r
    real(default), intent(in) :: a, b
    real(default), intent(in), optional :: abs_smallness, rel_smallness
  end function nearly_equal_real
```

```
<Numeric utils: procedures>+≡
  elemental module function nearly_equal_real &
    (a, b, abs_smallness, rel_smallness) result (r)
    logical :: r
    real(default), intent(in) :: a, b
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    real(default) :: abs_a, abs_b, diff, abs_small, rel_small
    abs_a = abs (a)
    abs_b = abs (b)
    diff = abs (a - b)
    ! shortcut, handles infinities and nans
    if (a == b) then
      r = .true.
      return
    else if (ieee_is_nan (a) .or. ieee_is_nan (b) .or. ieee_is_nan (diff)) then
      r = .false.
      return
    end if
    abs_small = tiny_13; if (present (abs_smallness)) abs_small = abs_smallness
    rel_small = tiny_10; if (present (rel_smallness)) rel_small = rel_smallness
    if (abs_a < abs_small .and. abs_b < abs_small) then
```

```

        r = diff < abs_small
    else
        r = diff / max (abs_a, abs_b) < rel_small
    end if
end function nearly_equal_real

```

<Numeric utils: sub interfaces>+≡

```

    elemental module function nearly_equal_complex &
        (a, b, abs_smallness, rel_smallness) result (r)
        logical :: r
        complex(default), intent(in) :: a, b
        real(default), intent(in), optional :: abs_smallness, rel_smallness
    end function nearly_equal_complex

```

<Numeric utils: procedures>+≡

```

    elemental module function nearly_equal_complex &
        (a, b, abs_smallness, rel_smallness) result (r)
        logical :: r
        complex(default), intent(in) :: a, b
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        r = nearly_equal_real (real (a), real (b), abs_smallness, rel_smallness) .and. &
            nearly_equal_real (aimag (a), aimag(b), abs_smallness, rel_smallness)
    end function nearly_equal_complex

```

Often we will need to check whether floats vanish:

<Numeric utils: public>+≡

```

    public:: vanishes
    interface vanishes
        module procedure vanishes_real, vanishes_complex
    end interface

```

<Numeric utils: sub interfaces>+≡

```

    elemental module function vanishes_real &
        (x, abs_smallness, rel_smallness) result (r)
        logical :: r
        real(default), intent(in) :: x
        real(default), intent(in), optional :: abs_smallness, rel_smallness
    end function vanishes_real
    elemental module function vanishes_complex &
        (x, abs_smallness, rel_smallness) result (r)
        logical :: r
        complex(default), intent(in) :: x
        real(default), intent(in), optional :: abs_smallness, rel_smallness
    end function vanishes_complex

```

<Numeric utils: procedures>+≡

```

    elemental module function vanishes_real &
        (x, abs_smallness, rel_smallness) result (r)
        logical :: r
        real(default), intent(in) :: x
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        r = nearly_equal (x, zero, abs_smallness, rel_smallness)
    end function vanishes_real

    elemental module function vanishes_complex &

```

```

        (x, abs_smallness, rel_smallness) result (r)
    logical :: r
    complex(default), intent(in) :: x
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    r = vanishes_real (abs (x), abs_smallness, rel_smallness)
end function vanishes_complex

```

<Numeric utils: public>+≡

```
public :: expanded_amp2
```

<Numeric utils: sub interfaces>+≡

```

    pure module function expanded_amp2 (amp_tree, amp_blob) result (amp2)
        real(default) :: amp2
        complex(default), dimension(:), intent(in) :: amp_tree, amp_blob
    end function expanded_amp2

```

<Numeric utils: procedures>+≡

```

    pure module function expanded_amp2 (amp_tree, amp_blob) result (amp2)
        real(default) :: amp2
        complex(default), dimension(:), intent(in) :: amp_tree, amp_blob
        amp2 = sum (amp_tree * conjg (amp_tree) + &
                    amp_tree * conjg (amp_blob) + &
                    amp_blob * conjg (amp_tree))
    end function expanded_amp2

```

<Numeric utils: public>+≡

```
public :: abs2
```

<Numeric utils: sub interfaces>+≡

```

    elemental module function abs2 (c) result (c2)
        real(default) :: c2
        complex(default), intent(in) :: c
    end function abs2

```

<Numeric utils: procedures>+≡

```

    elemental module function abs2 (c) result (c2)
        real(default) :: c2
        complex(default), intent(in) :: c
        c2 = real (c * conjg(c))
    end function abs2

```

Remove element with index from array

<Numeric utils: public>+≡

```

    public:: remove_array_element
    interface remove_array_element
        module procedure remove_array_element_logical
    end interface

```

<Numeric utils: sub interfaces>+≡

```

    module function remove_array_element_logical &
        (array, index) result (array_reduced)
        logical, intent(in), dimension(:) :: array
        integer, intent(in) :: index
        logical, dimension(:), allocatable :: array_reduced
    end function remove_array_element_logical

```

```

<Numeric utils: procedures>+≡
module function remove_array_element_logical &
    (array, index) result (array_reduced)
    logical, intent(in), dimension(:) :: array
    integer, intent(in) :: index
    logical, dimension(:), allocatable :: array_reduced
    integer :: i
    allocate (array_reduced(0))
    do i = 1, size (array)
        if (i /= index) then
            array_reduced = [array_reduced, [array(i)]]
        end if
    end do
end function remove_array_element_logical

```

Remove all duplicates from an array of signed integers and returns an unordered array of remaining elements. This method does not really fit into this module. It could be part of a larger module which deals with array manipulations.

```

<Numeric utils: public>+≡
public :: remove_duplicates_from_int_array

<Numeric utils: sub interfaces>+≡
module function remove_duplicates_from_int_array &
    (array) result (array_unique)
    integer, intent(in), dimension(:) :: array
    integer, dimension(:), allocatable :: array_unique
end function remove_duplicates_from_int_array

```

```

<Numeric utils: procedures>+≡
module function remove_duplicates_from_int_array &
    (array) result (array_unique)
    integer, intent(in), dimension(:) :: array
    integer, dimension(:), allocatable :: array_unique
    integer :: i
    allocate (array_unique(0))
    do i = 1, size (array)
        if (any (array_unique == array(i))) cycle
        array_unique = [array_unique, [array(i)]]
    end do
end function remove_duplicates_from_int_array

```

```

<Numeric utils: public>+≡
public :: extend_integer_array

```

```

<Numeric utils: sub interfaces>+≡
module subroutine extend_integer_array (list, incr, initial_value)
    integer, intent(inout), dimension(:), allocatable :: list
    integer, intent(in) :: incr
    integer, intent(in), optional :: initial_value
end subroutine extend_integer_array

```

```

<Numeric utils: procedures>+≡
module subroutine extend_integer_array (list, incr, initial_value)
    integer, intent(inout), dimension(:), allocatable :: list
    integer, intent(in) :: incr

```



```

integer, intent(in), optional :: initial_value
integer, dimension(:), allocatable :: list_store
integer :: n, ini
ini = 0; if (present (initial_value)) ini = initial_value
n = size (list)
allocate (list_store (n))
list_store = list
deallocate (list)
allocate (list (n+incr))
list(1:n) = list_store
list(1+n : n+incr) = ini
deallocate (list_store)
end subroutine extend_integer_array

```

<Numeric utils: public>+≡

```
public :: crop_integer_array
```

<Numeric utils: sub interfaces>+≡

```

module subroutine crop_integer_array (list, i_crop)
  integer, intent(inout), dimension(:), allocatable :: list
  integer, intent(in) :: i_crop
end subroutine crop_integer_array

```

<Numeric utils: procedures>+≡

```

module subroutine crop_integer_array (list, i_crop)
  integer, intent(inout), dimension(:), allocatable :: list
  integer, intent(in) :: i_crop
  integer, dimension(:), allocatable :: list_store
  allocate (list_store (i_crop))
  list_store = list(1:i_crop)
  deallocate (list)
  allocate (list (i_crop))
  list = list_store
  deallocate (list_store)
end subroutine crop_integer_array

```

We also need an evaluation of $\log x$ which is stable near $x = 1$.

<Numeric utils: public>+≡

```
public :: log_prec
```

<Numeric utils: sub interfaces>+≡

```

module function log_prec (x, xb) result (lx)
  real(default), intent(in) :: x, xb
  real(default) :: lx
end function log_prec

```

<Numeric utils: procedures>+≡

```

module function log_prec (x, xb) result (lx)
  real(default), intent(in) :: x, xb
  real(default) :: a1, a2, a3, lx
  a1 = xb
  a2 = a1 * xb / two
  a3 = a2 * xb * two / three
  if (abs (a3) < epsilon (a3)) then
    lx = - a1 - a2 - a3
  end if
end function log_prec

```

```

        else
            lx = log (x)
        end if
    end function log_prec

<Numeric utils: public>+≡
    public :: split_array

<Numeric utils: interfaces>+≡
    interface split_array
        module procedure split_integer_array
        module procedure split_real_array
    end interface

<Numeric utils: sub interfaces>+≡
    module subroutine split_integer_array (list1, list2)
        integer, intent(inout), dimension(:), allocatable :: list1, list2
        integer, dimension(:), allocatable :: list_store
    end subroutine split_integer_array
    module subroutine split_real_array (list1, list2)
        real(default), intent(inout), dimension(:), allocatable :: list1, list2
        real(default), dimension(:), allocatable :: list_store
    end subroutine split_real_array

<Numeric utils: procedures>+≡
    module subroutine split_integer_array (list1, list2)
        integer, intent(inout), dimension(:), allocatable :: list1, list2
        integer, dimension(:), allocatable :: list_store
        allocate (list_store (size (list1) - size (list2)))
        list2 = list1(:size (list2))
        list_store = list1 (size (list2) + 1:)
        deallocate (list1)
        allocate (list1 (size (list_store)))
        list1 = list_store
        deallocate (list_store)
    end subroutine split_integer_array

    module subroutine split_real_array (list1, list2)
        real(default), intent(inout), dimension(:), allocatable :: list1, list2
        real(default), dimension(:), allocatable :: list_store
        allocate (list_store (size (list1) - size (list2)))
        list2 = list1(:size (list2))
        list_store = list1 (size (list2) + 1:)
        deallocate (list1)
        allocate (list1 (size (list_store)))
        list1 = list_store
        deallocate (list_store)
    end subroutine split_real_array

```

3.6.1 Integration routines

Gauss integration using the 41-point Gauss-Kronrod rule.

```

<Numeric utils: interfaces>+≡

```

```

abstract interface
  function g_func (x) result (f)
    import default
    real(default), intent(in) :: x
    real(default) :: f
  end function g_func
end interface

<Numeric utils: public>+≡
  public :: d1mach

<Numeric utils: sub interfaces>+≡
  module function d1mach (i) result (d1)
    integer, intent(in) :: i
    real(default) :: d1
  end function d1mach

<Numeric utils: procedures>+≡
  module function d1mach (i) result (d1)
    integer, intent(in) :: i
    real(default) :: b, x
    real(default) :: d1
    !***begin prologue d1mach
    !***purpose return floating point machine dependent constants.
    !***library slatec
    !***category r1
    !***type single precision (d1mach-s, d1mach-d)
    !***keywords machine constants
    !***author fox, p. a., (bell labs)
    !           hall, a. d., (bell labs)
    !           schryer, n. l., (bell labs)
    !***description
    !
    ! d1mach can be used to obtain machine-dependent parameters for the
    ! local machine environment. it is a function subprogram with one
    ! (input) argument, and can be referenced as follows:
    !
    !       a = d1mach(i)
    !
    ! where i=1,...,5. the (output) value of a above is determined by
    ! the (input) value of i. the results for various values of i are
    ! discussed below.
    !
    ! d1mach(1) = b**(emin-1), the smallest positive magnitude.
    ! d1mach(2) = b**emax*(1 - b**(-t)), the largest magnitude.
    ! d1mach(3) = b**(-t), the smallest relative spacing.
    ! d1mach(4) = b**(1-t), the largest relative spacing.
    ! d1mach(5) = log10(b)
    !
    ! assume single precision numbers are represented in the t-digit,
    ! base-b form
    !
    !       sign (b**e)*( (x(1)/b) + ... + (x(t)/b**t) )
    !
    ! where 0 .le. x(i) .lt. b for i=1,...,t, 0 .lt. x(1), and
    ! emin .le. e .le. emax.

```

```

!
!   the values of b, t, emin and emax are provided in ilmach as
!   follows:
!   ilmach(10) = b, the base.
!   ilmach(11) = t, the number of base-b digits.
!   ilmach(12) = emin, the smallest exponent e.
!   ilmach(13) = emax, the largest exponent e.
!
!
!***references   p. a. fox, a. d. hall and n. l. schryer, framework for
!                  a portable library, acm transactions on mathematical
!                  software 4, 2 (june 1978), pp. 177-188.
!***routines called  xmsgsr
!***revision history  (yymmdd)
!   790101  date written
!   960329  modified for fortran 90 (be after suggestions by ehg)
!***end prologue  dlmach
!
x = 1.0_default
b = radix(x)
select case (i)
case (1)
  d1 = b**(minexponent(x)-1) ! the smallest positive magnitude.
case (2)
  d1 = huge(X)               ! the largest magnitude.
case (3)
  d1 = b**(-digits(x))       ! the smallest relative spacing.
case (4)
  d1 = b**(1-digits(x))      ! the largest relative spacing.
case (5)
  d1 = log10(b)
case default
  d1 = b**(minexponent(x)-1)
end select
end function dlmach

```

<Numeric utils: public>+≡
 public :: dqk41

<Numeric utils: sub interfaces>+≡
 module subroutine dqk41 (f, a, b, result, abserr, resabs, resasc)
 procedure(g_func) :: f
 real(default), intent(in) :: a, b
 real(default), intent(out) :: result, abserr, resabs, resasc
end subroutine dqk41

<Numeric utils: procedures>+≡
 module subroutine dqk41 (f, a, b, result, abserr, resabs, resasc)
 !***begin prologue dqk41
 !***date written 800101 (yymmdd)
 !***revision date 830518 (yymmdd)
 !***category no. h2a1a2
 !***keywords 41-point gauss-kronrod rules
 !***author piessens,robert,appl. math. & progr. div. - k.u.leuven
 !c de doncker,elise,appl. math. & progr. div. - k.u.leuven

```

!c***purpose  to compute i = integral of f over (a,b), with error
!c              estimate
!c              j = integral of abs(f) over (a,b)
!c***description
!c
!c      integration rules
!c      standard fortran subroutine
!c      double precision version
!c
!c      parameters
!c      on entry
!c      f      - double precision
!c              function subprogram defining the integrand
!c              function f(x). the actual name for f needs to be
!c              declared e x t e r n a l in the calling program.
!c
!c      a      - double precision
!c              lower limit of integration
!c
!c      b      - double precision
!c              upper limit of integration
!c
!c      on return
!c      result - double precision
!c              approximation to the integral i
!c              result is computed by applying the 41-point
!c              gauss-kronrod rule (resk) obtained by optimal
!c              addition of abscissae to the 20-point gauss
!c              rule (resg).
!c
!c      abserr - double precision
!c              estimate of the modulus of the absolute error,
!c              which should not exceed abs(i-result)
!c
!c      resabs - double precision
!c              approximation to the integral j
!c
!c      resasc - double precision
!c              approximation to the integral of abs(f-i/(b-a))
!c              over (a,b)
!c
!c***references  (none)
!c***routines called  dlmach
!c***end prologue  dqk41
procedure(g_func) :: f
real(default), intent(in) :: a, b
real(default), intent(out) :: result, abserr, resabs, resasc
real(default) :: absc, centr, dhlgh, dmax1, dmin1, &
    epmach, fc, fsum, fval1, fval2, hlgth, &
    resg, resk, reskh, uflow
real(default), dimension(20) :: fv1, fv2
real(default), dimension(21) :: xgk, wgk
real(default), dimension(10) :: wg
integer :: j, jtw, jtwm1

```

```

!      the abscissae and weights are given for the interval (-1,1).
!      because of symmetry only the positive abscissae and their
!      corresponding weights are given.
!
!      xgk    - abscissae of the 41-point gauss-kronrod rule
!               xgk(2), xgk(4), ... abscissae of the 20-point
!               gauss rule
!               xgk(1), xgk(3), ... abscissae which are optimally
!               added to the 20-point gauss rule
!
!      wgk    - weights of the 41-point gauss-kronrod rule
!
!      wg      - weights of the 20-point gauss rule
!
!
! gauss quadrature weights and kronrod quadrature abscissae and weights
! as evaluated with 80 decimal digit arithmetic by l. w. fullerton,
! bell labs, nov. 1981.
!
data wg ( 1) / 0.017614007139152118311861962351853_default /
data wg ( 2) / 0.040601429800386941331039952274932_default /
data wg ( 3) / 0.062672048334109063569506535187042_default /
data wg ( 4) / 0.083276741576704748724758143222046_default /
data wg ( 5) / 0.101930119817240435036750135480350_default /
data wg ( 6) / 0.118194531961518417312377377711382_default /
data wg ( 7) / 0.131688638449176626898494499748163_default /
data wg ( 8) / 0.142096109318382051329298325067165_default /
data wg ( 9) / 0.149172986472603746787828737001969_default /
data wg (10) / 0.152753387130725850698084331955098_default /

data xgk ( 1) / 0.998859031588277663838315576545863_default /
data xgk ( 2) / 0.993128599185094924786122388471320_default /
data xgk ( 3) / 0.981507877450250259193342994720217_default /
data xgk ( 4) / 0.963971927277913791267666131197277_default /
data xgk ( 5) / 0.940822633831754753519982722212443_default /
data xgk ( 6) / 0.912234428251325905867752441203298_default /
data xgk ( 7) / 0.878276811252281976077442995113078_default /
data xgk ( 8) / 0.839116971822218823394529061701521_default /
data xgk ( 9) / 0.795041428837551198350638833272788_default /
data xgk (10) / 0.746331906460150792614305070355642_default /
data xgk (11) / 0.693237656334751384805490711845932_default /
data xgk (12) / 0.636053680726515025452836696226286_default /
data xgk (13) / 0.575140446819710315342946036586425_default /
data xgk (14) / 0.510867001950827098004364050955251_default /
data xgk (15) / 0.443593175238725103199992213492640_default /
data xgk (16) / 0.373706088715419560672548177024927_default /
data xgk (17) / 0.30162786811491300432055356858592_default /
data xgk (18) / 0.227785851141645078080496195368575_default /
data xgk (19) / 0.152605465240922675505220241022678_default /
data xgk (20) / 0.076526521133497333754640409398838_default /
data xgk (21) / 0.000000000000000000000000000000000_default /

data wgk ( 1) / 0.003073583718520531501218293246031_default /
data wgk ( 2) / 0.008600269855642942198661787950102_default /

```

```

data wgk ( 3) / 0.014626169256971252983787960308868_default /
data wgk ( 4) / 0.020388373461266523598010231432755_default /
data wgk ( 5) / 0.025882133604951158834505067096153_default /
data wgk ( 6) / 0.031287306777032798958543119323801_default /
data wgk ( 7) / 0.036600169758200798030557240707211_default /
data wgk ( 8) / 0.041668873327973686263788305936895_default /
data wgk ( 9) / 0.046434821867497674720231880926108_default /
data wgk (10) / 0.050944573923728691932707670050345_default /
data wgk (11) / 0.055195105348285994744832372419777_default /
data wgk (12) / 0.059111400880639572374967220648594_default /
data wgk (13) / 0.062653237554781168025870122174255_default /
data wgk (14) / 0.065834597133618422111563556969398_default /
data wgk (15) / 0.068648672928521619345623411885368_default /
data wgk (16) / 0.071054423553444068305790361723210_default /
data wgk (17) / 0.073030690332786667495189417658913_default /
data wgk (18) / 0.074582875400499188986581418362488_default /
data wgk (19) / 0.075704497684556674659542775376617_default /
data wgk (20) / 0.076377867672080736705502835038061_default /
data wgk (21) / 0.076600711917999656445049901530102_default /
!
!
!      list of major variables
!      -----
!
!      centr - mid point of the interval
!      hlgth - half-length of the interval
!      absc  - abscissa
!      fval* - function value
!      resg  - result of the 20-point gauss formula
!      resk  - result of the 41-point kronrod formula
!      reskh - approximation to mean value of f over (a,b), i.e.
!              to i/(b-a)
!
!      machine dependent constants
!      -----
!
!      epmach is the largest relative spacing.
!      uflow is the smallest positive magnitude.
!
!***first executable statement  dqk41
epmach = dlmach(4)
uflow = dlmach(1)

centr = 0.5d+00*(a+b)
hlgth = 0.5d+00*(b-a)
dhlgh = abs(hlgth)
!
! compute the 41-point gauss-kronrod approximation to
! the integral, and estimate the absolute error.
!
resg = 0.0d+00
fc = f(centr)
resk = wgk(21)*fc
resabs = abs(resk)

```

```

do j = 1, 10
  jtw = j*2
  absc = hlgth*xgk(jtw)
  fval1 = f(centr-absc)
  fval2 = f(centr+absc)
  fv1(jtw) = fval1
  fv2(jtw) = fval2
  fsum = fval1+fval2
  resg = resg+wg(j)*fsum
  resk = resk+wgk(jtw)*fsum
  resabs = resabs+wgk(jtw)*(abs(fval1)+abs(fval2))
end do
do j = 1,10
  jtwm1 = j*2-1
  absc = hlgth*xgk(jtwm1)
  fval1 = f(centr-absc)
  fval2 = f(centr+absc)
  fv1(jtwm1) = fval1
  fv2(jtwm1) = fval2
  fsum = fval1+fval2
  resk = resk+wgk(jtwm1)*fsum
  resabs = resabs+wgk(jtwm1)*(abs(fval1)+abs(fval2))
end do
reskh = resk*0.5d+00
resasc = wgk(21)*abs(fc-reskh)
do j = 1, 20
  resasc = resasc+wgk(j)*(abs(fv1(j)-reskh)+abs(fv2(j)-reskh))
end do
result = resk*hlgth
resabs = resabs*dhlgth
resasc = resasc*dhlgth
abserr = abs((resk-resg)*hlgth)
if (resasc.ne.0.0d+00.and.abserr.ne.0.0d+00) &
  abserr = resasc*dmin1(0.1d+01,(0.2d+03*abserr/resasc)**1.5d+00)
if (resabs.gt.uflow/(0.5d+02*epmach)) abserr = dmax1 &
  ((epmach*0.5d+02)*resabs,abserr)
end subroutine dqk41

```

<Numeric utils: public>+≡

public :: dqk61

<Numeric utils: sub interfaces>+≡

```

module subroutine dqk61 (f, a, b, result, abserr, resabs, resasc)
  procedure(g_func) :: f
  real(default), intent(in) :: a, b
  real(default), intent(out) :: result, abserr, resabs, resasc
end subroutine dqk61

```

<Numeric utils: procedures>+≡

```

module subroutine dqk61 (f, a, b, result, abserr, resabs, resasc)
!c***begin prologue dqk61
!c***purpose to compute i = integral of f over (a,b) with error
!c estimate
!c j = integral of abs(f) over (a,b)
!c***library slatec (quadpack)

```



```

!c***category  h2a1a2
!c***type      double precision (qk61-s, dqk61-d)
!c***keywords  61-point gauss-kronrod rules, quadpack, quadrature
!c***author    piessens, robert
!c              applied mathematics and programming division
!c              k. u. leuven
!c              de doncker, elise
!c              applied mathematics and programming division
!c              k. u. leuven
!c***description
!c
!c      integration rule
!c      standard fortran subroutine
!c      double precision version
!c
!c      parameters
!c      on entry
!c      f      - double precision
!c              function subprogram defining the integrand
!c              function f(x). the actual name for f needs to be
!c              declared e x t e r n a l in the calling program.
!c
!c      a      - double precision
!c              lower limit of integration
!c
!c      b      - double precision
!c              upper limit of integration
!c
!c      on return
!c      result - double precision
!c              approximation to the integral i
!c              result is computed by applying the 61-point
!c              kronrod rule (resk) obtained by optimal addition of
!c              abscissae to the 30-point gauss rule (resg).
!c
!c      abserr - double precision
!c              estimate of the modulus of the absolute error,
!c              which should equal or exceed abs(i-result)
!c
!c      resabs - double precision
!c              approximation to the integral j
!c
!c      resasc - double precision
!c              approximation to the integral of abs(f-i/(b-a))
!c
!c***references  (none)
!c***routines called  dlmach
!c***revision history  (yymmdd)
!c  800101  date written
!c  890531  changed all specific intrinsics to generic.  (wrb)
!c  890531  revision date from version 3.2
!c  891214  prologue converted to version 4.0 format.  (bab)
!c***end prologue  dqk61

```

```

!c
procedure(g_func) :: f
real(default), intent(in) :: a, b
real(default), intent(out) :: result, abserr, resabs, resasc
real(default) :: absc, centr, dhlgh, &
    epmach, fc, fsum, fval1, fval2, hlgth, &
    resg, resk, reskh, uflow
real(default), dimension(30) :: fv1, fv2
real(default), dimension(31) :: xgk, wgk
real(default), dimension(15) :: wg
integer :: j, jtw, jtwm1
!
!           the abscissae and weights are given for the
!           interval (-1,1). because of symmetry only the positive
!           abscissae and their corresponding weights are given.
!
!           xgk  - abscissae of the 61-point kronrod rule
!                  xgk(2), xgk(4) ... abscissae of the 30-point
!                  gauss rule
!                  xgk(1), xgk(3) ... optimally added abscissae
!                  to the 30-point gauss rule
!
!           wgk  - weights of the 61-point kronrod rule
!
!           wg   - weights of the 30-point gauss rule
!
!
! gauss quadrature weights and kronrod quadrature abscissae and weights
! as evaluated with 80 decimal digit arithmetic by l. w. fullerton,
! bell labs, nov. 1981.
!
data wg ( 1) / 0.007968192496166605615465883474674_default /
data wg ( 2) / 0.018466468311090959142302131912047_default /
data wg ( 3) / 0.028784707883323369349719179611292_default /
data wg ( 4) / 0.038799192569627049596801936446348_default /
data wg ( 5) / 0.048402672830594052902938140422808_default /
data wg ( 6) / 0.057493156217619066481721689402056_default /
data wg ( 7) / 0.065974229882180495128128515115962_default /
data wg ( 8) / 0.073755974737705206268243850022191_default /
data wg ( 9) / 0.080755895229420215354694938460530_default /
data wg (10) / 0.086899787201082979802387530715126_default /
data wg (11) / 0.092122522237786128717632707087619_default /
data wg (12) / 0.096368737174644259639468626351810_default /
data wg (13) / 0.099593420586795267062780282103569_default /
data wg (14) / 0.101762389748405504596428952168554_default /
data wg (15) / 0.102852652893558840341285636705415_default /

data xgk ( 1) / 0.999484410050490637571325895705811_default /
data xgk ( 2) / 0.996893484074649540271630050918695_default /
data xgk ( 3) / 0.991630996870404594858628366109486_default /
data xgk ( 4) / 0.983668123279747209970032581605663_default /
data xgk ( 5) / 0.973116322501126268374693868423707_default /
data xgk ( 6) / 0.960021864968307512216871025581798_default /
data xgk ( 7) / 0.944374444748559979415831324037439_default /

```

```

data xgk ( 8) / 0.926200047429274325879324277080474_default /
data xgk ( 9) / 0.905573307699907798546522558925958_default /
data xgk (10) / 0.882560535792052681543116462530226_default /
data xgk (11) / 0.857205233546061098958658510658944_default /
data xgk (12) / 0.829565762382768397442898119732502_default /
data xgk (13) / 0.799727835821839083013668942322683_default /
data xgk (14) / 0.767777432104826194917977340974503_default /
data xgk (15) / 0.733790062453226804726171131369528_default /
data xgk (16) / 0.697850494793315796932292388026640_default /
data xgk (17) / 0.660061064126626961370053668149271_default /
data xgk (18) / 0.620526182989242861140477556431189_default /
data xgk (19) / 0.579345235826361691756024932172540_default /
data xgk (20) / 0.536624148142019899264169793311073_default /
data xgk (21) / 0.492480467861778574993693061207709_default /
data xgk (22) / 0.447033769538089176780609900322854_default /
data xgk (23) / 0.400401254830394392535476211542661_default /
data xgk (24) / 0.352704725530878113471037207089374_default /
data xgk (25) / 0.304073202273625077372677107199257_default /
data xgk (26) / 0.254636926167889846439805129817805_default /
data xgk (27) / 0.204525116682309891438957671002025_default /
data xgk (28) / 0.153869913608583546963794672743256_default /
data xgk (29) / 0.102806937966737030147096751318001_default /
data xgk (30) / 0.051471842555317695833025213166723_default /
data xgk (31) / 0.0000000000000000000000000000000000_default /

data wgk ( 1) / 0.001389013698677007624551591226760_default /
data wgk ( 2) / 0.003890461127099884051267201844516_default /
data wgk ( 3) / 0.006630703915931292173319826369750_default /
data wgk ( 4) / 0.009273279659517763428441146892024_default /
data wgk ( 5) / 0.011823015253496341742232898853251_default /
data wgk ( 6) / 0.014369729507045804812451432443580_default /
data wgk ( 7) / 0.016920889189053272627572289420322_default /
data wgk ( 8) / 0.019414141193942381173408951050128_default /
data wgk ( 9) / 0.021828035821609192297167485738339_default /
data wgk (10) / 0.024191162078080601365686370725232_default /
data wgk (11) / 0.026509954882333101610601709335075_default /
data wgk (12) / 0.028754048765041292843978785354334_default /
data wgk (13) / 0.030907257562387762472884252943092_default /
data wgk (14) / 0.032981447057483726031814191016854_default /
data wgk (15) / 0.034979338028060024137499670731468_default /
data wgk (16) / 0.036882364651821229223911065617136_default /
data wgk (17) / 0.038678945624727592950348651532281_default /
data wgk (18) / 0.040374538951535959111995279752468_default /
data wgk (19) / 0.041969810215164246147147541285970_default /
data wgk (20) / 0.043452539701356069316831728117073_default /
data wgk (21) / 0.044814800133162663192355551616723_default /
data wgk (22) / 0.046059238271006988116271735559374_default /
data wgk (23) / 0.047185546569299153945261478181099_default /
data wgk (24) / 0.048185861757087129140779492298305_default /
data wgk (25) / 0.049055434555029778887528165367238_default /
data wgk (26) / 0.049795683427074206357811569379942_default /
data wgk (27) / 0.050405921402782346840893085653585_default /
data wgk (28) / 0.050881795898749606492297473049805_default /
data wgk (29) / 0.051221547849258772170656282604944_default /

```

```

data wgk ( 30) / 0.051426128537459025933862879215781_default /
data wgk ( 31) / 0.051494729429451567558340433647099_default /
!
!           list of major variables
!           -----
!
!           centr - mid point of the interval
!           hlgth - half-length of the interval
!           absc  - abscissa
!           fval* - function value
!           resg  - result of the 30-point gauss rule
!           resk  - result of the 61-point kronrod rule
!           reskh - approximation to the mean value of f
!                   over (a,b), i.e. to  $i/(b-a)$ 
!
!           machine dependent constants
!           -----
!
!           epmach is the largest relative spacing.
!           uflow is the smallest positive magnitude.
!
!***first executable statement  dqk61
epmach = dimach(4)
uflow = dimach(1)

centr = 0.5d+00*(b+a)
hlgth = 0.5d+00*(b-a)
dhlgth = abs(hlgth)
!
! compute the 61-point kronrod approximation to the
! integral, and estimate the absolute error.
!
resg = 0.0d+00
fc = f(centr)
resk = wgk(31)*fc
resabs = abs(resk)
do j = 1, 15
    jtw = j*2
    absc = hlgth*xgk(jtw)
    fval1 = f(centr-absc)
    fval2 = f(centr+absc)
    fv1(jtw) = fval1
    fv2(jtw) = fval2
    fsum = fval1+fval2
    resg = resg+wg(j)*fsum
    resk = resk+wgk(jtw)*fsum
    resabs = resabs+wgk(jtw)*(abs(fval1)+abs(fval2))
end do
do j = 1, 15
    jtwm1 = j*2-1
    absc = hlgth*xgk(jtwm1)
    fval1 = f(centr-absc)
    fval2 = f(centr+absc)
    fv1(jtwm1) = fval1

```

```

        fv2(jtwm1) = fval2
        fsum = fval1+fval2
        resk = resk+wgk(jtwm1)*fsum
        resabs = resabs+wgk(jtwm1)*(abs(fval1)+abs(fval2))
    end do
    reskh = resk*0.5d+00
    resasc = wgk(31)*abs(fc-reskh)
    do j = 1, 30
        RESASC = RESASC+WGK(J)*(ABS(FV1(J)-RESKH)+ABS(FV2(J)-RESKH))
    end do
    result = resk*hlgh
    resabs = resabs*dhlgh
    resasc = resasc*dhlgh
    abserr = abs((resk-resg)*hlgh)
    if (resasc.ne.0.0d+00.and.abserr.ne.0.0d+00) &
        abserr = resasc*min(0.1d+01,(0.2d+03*abserr/resasc)**1.5d+00)
    if (resabs.gt.uflow/(0.5d+02*epmach)) abserr = max &
        ((epmach*0.5d+02)*resabs,abserr)
end subroutine dqk61

```

<Numeric utils: parameters>≡

```
integer, parameter, public :: GAUSS_KRONROD_41 = 41, GAUSS_KRONROD_61 = 61
```

<Numeric utils: public>+≡

```
public :: gauss_kronrod
```

<Numeric utils: sub interfaces>+≡

```

module subroutine gauss_kronrod &
    (type, f, a, b, limit, result, abserr, epsabs, epsrel)
    integer, intent(in) :: type
    procedure(g_func) :: f
    real(default), intent(in) :: a, b
    real(default), intent(in) :: epsabs, epsrel
    real(default), intent(out) :: result, abserr
    integer, intent(in) :: limit
end subroutine gauss_kronrod

```

<Numeric utils: procedures>+≡

```

module subroutine gauss_kronrod &
    (type, f, a, b, limit, result, abserr, epsabs, epsrel)
    integer, intent(in) :: type
    procedure(g_func) :: f
    real(default), intent(in) :: a, b
    real(default), intent(in) :: epsabs, epsrel
    real(default), intent(out) :: result, abserr
    integer, intent(in) :: limit
    real(default) :: area, errsum
    real(default) :: tolerance_g, round_off
    real(default) :: result0, abserr0, resabs0, resasc0
    type(int_workspace_t) :: work
    real(default) :: a1, b1, a2, b2, a_i, b_i, r_i, e_i
    real(default) :: area1, area2, area12, error1, error2, error12
    real(default) :: resasc1, resasc2, resabs1, resabs2, delta
    integer :: i, iteration
    integer :: roundoff_type1, roundoff_type2

```

```

!!! epsilon(dbl)
real(default), parameter :: dbl_prec = 2.2204460492503131e-16_default
!!! tiny(dbl)
real(default), parameter :: dbl_min = 2.2250738585072014e-308_default
iteration = 0
if (epsabs <= 0) then
    if (epsrel < 50 * dbl_prec .or. epsrel < 0.5e-28_default) then
        error stop ("Gauss_Kronrod: tolerance cannot be achieved with given " &
            // "epsabs and epsrel")
    end if
end if
call work%init (a, b, limit)
! Perform the first integration
select case (type)
case (GAUSS_KRONROD_61)
    call dqk61 (f, a, b, result0, abserr0, resabs0, resasc0)
case default
    call dqk41 (f, a, b, result0, abserr0, resabs0, resasc0)
end select
call work%set_initial (result0, abserr0)
! Test on accuracy
tolerance_g = max (epsabs, epsrel * abs(result0))
round_off = 50 * dbl_prec * resabs0
if (abserr0 <= round_off .and. abserr0 > tolerance_g) then
    result = result0
    abserr = abserr0
    error stop ("Gauss_Kronrod: cannot reach tolerance because of roundoff " &
        // "error on first attempt")
else if ((abserr0 <= tolerance_g .and. abserr0 /= resasc0) .or. &
    abserr0 == 0.0_default) then
    result = result0
    abserr = abserr0
    return
else if (limit == 1) then
    result = result0
    abserr = abserr0
    error stop ("Gauss_Kronrod: a maximum of one iteration was insufficient")
end if
area = result0
errsum = abserr0
roundoff_type1 = 0
roundoff_type2 = 0
ITERATION_LOOP: do iteration = 1, limit
    a_i = work%alist(work%i)
    b_i = work%blist(work%i)
    r_i = work%rlist(work%i)
    e_i = work%elist(work%i)
    a1 = a_i
    b1 = 0.5_default * (a_i + b_i)
    a2 = b1
    b2 = b_i
    select case (type)
    case (GAUSS_KRONROD_61)
        call dqk61 (f, a1, b1, area1, error1, resabs1, resasc1)

```

```

        call dqk61 (f, a2, b2, area2, error2, resabs2, resasc2)
    case default
        call dqk41 (f, a1, b1, area1, error1, resabs1, resasc1)
        call dqk41 (f, a2, b2, area2, error2, resabs2, resasc2)
    end select
    area12 = area1 + area2
    error12 = error1 + error2
    errsum = errsum + error12 - e_i
    area = area + area12 - r_i
    if (resasc1 /= error1 .and. resasc2 /= error2) then
        delta = r_i - area12
        if (abs(delta) <= 1.0e-5_default * abs (area12) .and. &
            error12 >= 0.99_default * e_i) then
            roundoff_type1 = roundoff_type1 + 1
        end if
        if (iteration >= 10 .and. error12 > e_i) then
            roundoff_type2 = roundoff_type2 + 1
        end if
    end if
    tolerance_g = max (epsabs, epsrel * abs(area))
    if (errsum > tolerance_g) then
        if (roundoff_type1 >= 6 .or. roundoff_type2 >= 20) &
            error stop ("Gauss_Kronrod: roundoff error prevents tolerance " &
                // "from being achieved")
        ! Set error flag in the case of bad integrand behavior at a
        ! point of the integration range
        if (subinterval_too_small (a1, a2, b2)) &
            error stop ("Gauss_Kronrod: bad integrand behavior found in " &
                // "integration interval")
    end if
    call work%update (a1, b1, area1, error1, a2, b2, area2, error2)
    if (errsum <= tolerance_g) exit ITERATION_LOOP
end do ITERATION_LOOP
result = sum (work%rlist (1:work%size))
abserr = errsum
if (errsum > tolerance_g) &
    error stop ("Gauss_Kronrod: could not integrate function")
contains
function subinterval_too_small (a_1, a_2, b_2) result (flag)
    real(default), intent(in) :: a_1, a_2, b_2
    logical :: flag
    real(default) :: tmp
    tmp = (1._default + 100._default * dbl_prec) * (abs(a_2) + &
        1000._default * dbl_min)
    flag = abs(a_1) <= tmp .and. abs(b_2) <= tmp
end function subinterval_too_small
end subroutine gauss_kronrod

```

3.6.2 Suppression of numerical noise

<Numeric utils: public>+≡
 public :: pacify

```

<Numeric utils: interfaces>+≡
  interface pacify
    module procedure pacify_real_default
    module procedure pacify_complex_default
  end interface pacify

<Numeric utils: sub interfaces>+≡
  elemental module subroutine pacify_real_default (x, tolerance)
    real(default), intent(inout) :: x
    real(default), intent(in) :: tolerance
  end subroutine pacify_real_default

  elemental module subroutine pacify_complex_default (x, tolerance)
    complex(default), intent(inout) :: x
    real(default), intent(in) :: tolerance
  end subroutine pacify_complex_default

<Numeric utils: procedures>+≡
  elemental module subroutine pacify_real_default (x, tolerance)
    real(default), intent(inout) :: x
    real(default), intent(in) :: tolerance
    if (abs (x) < tolerance) x = 0._default
  end subroutine pacify_real_default

  elemental module subroutine pacify_complex_default (x, tolerance)
    complex(default), intent(inout) :: x
    real(default), intent(in) :: tolerance
    if (abs (real (x)) < tolerance) &
      x = cmplx (0._default, aimag (x), kind=default)
    if (abs (aimag (x)) < tolerance) &
      x = cmplx (real (x), 0._default, kind=default)
  end subroutine pacify_complex_default

<numeric_utils_ut.f90>≡
  <File header>

  module numeric_utils_ut
    use unit_tests
    use numeric_utils_uti

    <Standard module head>

    <Numeric utils: public test>

    contains

    <Numeric utils: test driver>

  end module numeric_utils_ut

<numeric_utils_uti.f90>≡
  <File header>

  module numeric_utils_uti

```



```

    <Use kinds>
        use constants, only: one, PI
        use numeric_utils

    <Standard module head>

    <Numeric utils: test declarations>

contains

    <Numeric utils: tests>

end module numeric_utils_uti
<Numeric utils: public test>≡
    public :: numeric_utils_test
<Numeric utils: test driver>≡
    subroutine numeric_utils_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        <Numeric utils: execute tests>
    end subroutine numeric_utils_test

```

Provide testing for routines in the numeric_utils module.

```

<Numeric utils: execute tests>≡
    call test (numeric_utils_1, "numeric_utils_1", &
        "check interface and implementation", &
        u, results)
<Numeric utils: test declarations>≡
    public :: numeric_utils_1
<Numeric utils: tests>≡
    subroutine numeric_utils_1 (u)
        integer, intent(in) :: u
        real(default) :: int, intabs, err, errabs
        real(default) :: a, b, c
        a = 0._default
        b = 1._default
        c = Pi

        write (u, "(A)") "* Test output: Numeric utils"
        write (u, "(A)") "* Purpose: test numeric routines"
        write (u, "(A)")

        write (u, "(A)") "* 41-point Gauss-Kronrod integration"
        write (u, "(A)")

        call dqk41 (f_x, a, b, int, intabs, err, errabs)
        write (u, "(1x,A,F9.6)") " Integral (x,[0,1])      = ", &
            int
        call dqk41 (f_x2, a, b, int, intabs, err, errabs)
        write (u, "(1x,A,F9.6)") " Integral (x**2,[0,1])    = ", &
            int
    end subroutine

```

```

call dqk41 (sinx, a, c, int, intabs, err, errabs)
write (u, "(1x,A,F9.6)") " Integral (sin(x),[0,Pi]) = ", &
    int

contains

function f_x (x) result (f)
    real(default), intent(in) :: x
    real(default) :: f
    f = x
end function f_x
function f_x2 (x) result (f)
    real(default), intent(in) :: x
    real(default) :: f
    f = x**2
end function f_x2
function sinx (x) result (f)
    real(default), intent(in) :: x
    real(default) :: f
    f = sin(x)
end function sinx
end subroutine numeric_utils_1

<Numeric utils: execute tests>+≡
call test (numeric_utils_2, "numeric_utils_2", &
    "check adaptive integration", &
    u, results)

<Numeric utils: test declarations>+≡
public :: numeric_utils_2

<Numeric utils: tests>+≡
subroutine numeric_utils_2 (u)
    integer, intent(in) :: u
    real(default) :: result, abserr
    real(default), parameter :: epsabs = 0.001_default, &
        epsrel = 0.001_default
    real(default), parameter :: a = 0._default, b = 1._default, &
        z = 0.1_default
    integer, parameter :: limit = 10000

    write (u, "(A)") "* Test output: Numeric utils"
    write (u, "(A)") "* Purpose: test adaptive Gauss-Kronrod 41"
    write (u, "(A)")

    write (u, "(A)") "* 41-point Gauss-Kronrod integration"
    write (u, "(A)")

    call gauss_kronrod (GAUSS_KRONROD_41, f1_x, a, b, limit, result, &
        abserr, epsabs, epsrel)
    write (u, "(1x,A,F9.6)") " Integral (f1_x,[0,1]) = ", &
        result
    call gauss_kronrod (GAUSS_KRONROD_41, f2_x, a, b, limit, result, &
        abserr, epsabs, epsrel)
    write (u, "(1x,A,F9.6)") " Integral (f2_x,[0,1]) = ", &

```

```

        result

contains

    function f1_x (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
        f = log(one - z/(one + (-one + z)*x))
    end function f1_x
    function f2_x (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
        f = log(one - z/(z + x))
    end function f2_x
end subroutine numeric_utils_2

```

3.7 Binary Tree

```

<binary_tree.f90>≡
<File header>
module binary_tree

<Standard module head>

<Binary trees: public>

<Binary trees: types>

    interface
<Binary trees: sub interfaces>
    end interface

contains

<Binary trees: module procedures>

end module binary_tree

<binary_tree_sub.f90>≡
<File header>

submodule (binary_tree) binary_tree_s

    use io_units

    implicit none

contains

<Binary trees: procedures>

end submodule binary_tree_s

```

```

<Binary trees: public>≡
    public :: binary_tree_iterator_t

<Binary trees: types>≡
    type :: binary_tree_iterator_t
           integer, dimension(:), allocatable :: key
           integer :: current
           !! current \in {1, N}.
    contains
        <Binary trees: iterator: TBP>
    end type binary_tree_iterator_t

<Binary trees: types>+≡
    type :: binary_tree_node_t
           integer :: height = 0
           type(binary_tree_node_t), pointer :: left => null ()
           type(binary_tree_node_t), pointer :: right => null ()
           !!
           integer :: key = 0
           class(*), pointer :: obj => null ()
    contains
        <Binary trees: node: TBP>
    end type binary_tree_node_t

<Binary trees: public>+≡
    public :: binary_tree_t

<Binary trees: types>+≡
    type :: binary_tree_t
           integer :: n_elements = 0
           type(binary_tree_node_t), pointer :: root => null ()
    contains
        <Binary trees: tree: TBP>
    end type binary_tree_t

<Binary trees: iterator: TBP>≡
    procedure :: init => binary_tree_iterator_init

<Binary trees: sub interfaces>≡
    module subroutine binary_tree_iterator_init (iterator, btree)
        class(binary_tree_iterator_t), intent(inout) :: iterator
        type(binary_tree_t), target :: btree
    end subroutine binary_tree_iterator_init

<Binary trees: procedures>≡
    !! We store all keys of the binary tree in an index array.
    !! Flatten the tree  $O(\log n)$ , each access is then  $O(1)$ .
    !! However, accessing the corresponding object costs one  $O(\log n)$ .
    module subroutine binary_tree_iterator_init (iterator, btree)
        class(binary_tree_iterator_t), intent(inout) :: iterator
        type(binary_tree_t), target :: btree
        type(binary_tree_node_t), pointer :: node
        integer :: idx

```

```

        iterator%current = 1
        allocate (iterator%key(btree%get_n_elements ()), source = 0)
        if (.not. btree%get_n_elements () > 0) return
        idx = 1; call fill_key (idx, iterator%key, btree%root)
contains
    recursive subroutine fill_key (idx, key, node)
        integer, intent(inout) :: idx
        integer, dimension(:), intent(inout) :: key
        type(binary_tree_node_t), pointer :: node
        if (associated (node%left)) &
            call fill_key (idx, key, node%left)
        key(idx) = node%key
        idx = idx + 1
        if (associated (node%right)) &
            call fill_key (idx, key, node%right)
    end subroutine fill_key
end subroutine binary_tree_iterator_init

<Binary trees: iterator: TBP>+≡
    procedure :: is_iterable => binary_tree_iterator_is_iterable

<Binary trees: sub interfaces>+≡
    module function binary_tree_iterator_is_iterable (iterator) result (flag)
        class(binary_tree_iterator_t), intent(in) :: iterator
        logical :: flag
    end function binary_tree_iterator_is_iterable

<Binary trees: procedures>+≡
    module function binary_tree_iterator_is_iterable (iterator) result (flag)
        class(binary_tree_iterator_t), intent(in) :: iterator
        logical :: flag
        flag = iterator%current <= size (iterator%key)
    end function binary_tree_iterator_is_iterable

<Binary trees: iterator: TBP>+≡
    procedure :: next => binary_tree_iterator_next

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_iterator_next (iterator, key)
        class(binary_tree_iterator_t), intent(inout) :: iterator
        integer, intent(out) :: key
    end subroutine binary_tree_iterator_next

<Binary trees: procedures>+≡
    module subroutine binary_tree_iterator_next (iterator, key)
        class(binary_tree_iterator_t), intent(inout) :: iterator
        integer, intent(out) :: key
        if (.not. iterator%is_iterable ()) then
            key = 0
        else
            key = iterator%key(iterator%current)
            iterator%current = iterator%current + 1
        end if
    end subroutine binary_tree_iterator_next

```

```

<Binary trees: node: TBP>≡
    procedure :: init => binary_tree_node_init

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_node_init (btree_node, key, obj)
        class(binary_tree_node_t), intent(inout) :: btree_node
        integer, intent(in) :: key
        class(*), pointer :: obj
    end subroutine binary_tree_node_init

<Binary trees: procedures>+≡
    module subroutine binary_tree_node_init (btree_node, key, obj)
        class(binary_tree_node_t), intent(inout) :: btree_node
        integer, intent(in) :: key
        class(*), pointer :: obj
        btree_node%height = 1
        btree_node%left => null ()
        btree_node%right => null ()
        btree_node%key = key
        btree_node%obj => obj
    end subroutine binary_tree_node_init

<Binary trees: node: TBP>+≡
    procedure :: write => binary_tree_node_write

<Binary trees: sub interfaces>+≡
    recursive module subroutine binary_tree_node_write &
        (btree_node, unit, level, mode)
        class(binary_tree_node_t), intent(in) :: btree_node
        integer, intent(in) :: unit
        integer, intent(in) :: level
        character(len=*), intent(in) :: mode
    end subroutine binary_tree_node_write

<Binary trees: procedures>+≡
    recursive module subroutine binary_tree_node_write &
        (btree_node, unit, level, mode)
        class(binary_tree_node_t), intent(in) :: btree_node
        integer, intent(in) :: unit
        integer, intent(in) :: level
        character(len=*), intent(in) :: mode
        character(len=24) :: fmt
        if (level > 0) then
            write (fmt, "(A,I3,A)") "(", 3 * level, "X,A,1X,I3,1X,I3,A)"
        else
            fmt = "(A,1X,I3,1X,I3,1X)"
        end if
        write (unit, fmt) mode, btree_node%key, btree_node%height
        ! write (unit, fmt) btree_node%key, btree_node%get_balance ()
        if (associated (btree_node%right)) &
            call btree_node%right%write (unit, level = level + 1, mode = ">")
        if (associated (btree_node%left)) &
            call btree_node%left%write (unit, level = level + 1, mode = "<")
    end subroutine binary_tree_node_write

```

```

<Binary trees: node: TBP>+≡
    procedure :: get_balance => binary_tree_node_get_balance

<Binary trees: sub interfaces>+≡
    module function binary_tree_node_get_balance (btree_node) result (balance)
        class(binary_tree_node_t), intent(in) :: btree_node
        integer :: balance
    end function binary_tree_node_get_balance

<Binary trees: procedures>+≡
    module function binary_tree_node_get_balance (btree_node) result (balance)
        class(binary_tree_node_t), intent(in) :: btree_node
        integer :: balance
        integer :: leftHeight, rightHeight
        leftHeight = 0
        rightHeight = 0
        if (associated (btree_node%left)) leftHeight = btree_node%left%height
        if (associated (btree_node%right)) rightHeight = btree_node%right%height
        balance = leftHeight - rightHeight
    end function binary_tree_node_get_balance

<Binary trees: node: TBP>+≡
    procedure :: increment_height => binary_tree_node_increment_height

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_node_increment_height (btree_node)
        class(binary_tree_node_t), intent(inout) :: btree_node
    end subroutine binary_tree_node_increment_height

<Binary trees: procedures>+≡
    module subroutine binary_tree_node_increment_height (btree_node)
        class(binary_tree_node_t), intent(inout) :: btree_node
        integer :: leftHeight, rightHeight
        leftHeight = 0
        rightHeight = 0
        if (associated (btree_node%left)) leftHeight = btree_node%left%height
        if (associated (btree_node%right)) rightHeight = btree_node%right%height
        btree_node%height = max (leftHeight, rightHeight) + 1
    end subroutine binary_tree_node_increment_height

<Binary trees: node: TBP>+≡
    final :: binary_tree_node_final

<Binary trees: sub interfaces>+≡
    !!! !!! NAG 7 compiler bug with finalizers and unlimited polymorphism
    !!! module subroutine binary_tree_node_final (btree_node)
    !!!     type(binary_tree_node_t), intent(inout) :: btree_node
    !!! end subroutine binary_tree_node_final

<Binary trees: module procedures>≡
    recursive subroutine binary_tree_node_final (btree_node)
        type(binary_tree_node_t), intent(inout) :: btree_node
        if (associated (btree_node%left)) deallocate (btree_node%left)
        if (associated (btree_node%right)) deallocate (btree_node%right)
        deallocate (btree_node%obj)
    end subroutine binary_tree_node_final

```

```

<Binary trees: tree: TBP>≡
    procedure :: write => binary_tree_write

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_write (btree, unit)
        class(binary_tree_t), intent(in) :: btree
        integer, intent(in), optional :: unit
    end subroutine binary_tree_write

<Binary trees: procedures>+≡
    module subroutine binary_tree_write (btree, unit)
        class(binary_tree_t), intent(in) :: btree
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit(unit=unit)
        write (u, "(A,I3)") "Number of elements", btree%n_elements
        if (associated (btree%root)) then
            call btree%root%write (u, level = 0, mode = "*")
        else
            write (u, "(A)") "Binary tree is empty."
        end if
    end subroutine binary_tree_write

<Binary trees: tree: TBP>+≡
    final :: binary_tree_final

<Binary trees: sub interfaces>+≡
    !!! !!! NAG 7 compiler bug with finalizers and unlimited polymorphism
    !!! module subroutine binary_tree_final (btree)
    !!!     type(binary_tree_t), intent(inout) :: btree
    !!! end subroutine binary_tree_final

<Binary trees: module procedures>+≡
    subroutine binary_tree_final (btree)
        type(binary_tree_t), intent(inout) :: btree
        btree%n_elements = 0
        if (associated (btree%root)) then
            deallocate (btree%root)
        end if
    end subroutine binary_tree_final

<Binary trees: tree: TBP>+≡
    procedure :: clear => binary_tree_clear

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_clear (btree)
        class(binary_tree_t), intent(inout) :: btree
    end subroutine binary_tree_clear

<Binary trees: procedures>+≡
    module subroutine binary_tree_clear (btree)
        class(binary_tree_t), intent(inout) :: btree
        call binary_tree_final (btree)
    end subroutine binary_tree_clear

```



```

<Binary trees: tree: TBP>+≡
    procedure :: get_n_elements => binary_tree_get_n_elements

<Binary trees: sub interfaces>+≡
    module function binary_tree_get_n_elements (btree) result (n)
        class(binary_tree_t), intent(in) :: btree
        integer :: n
    end function binary_tree_get_n_elements

<Binary trees: procedures>+≡
    module function binary_tree_get_n_elements (btree) result (n)
        class(binary_tree_t), intent(in) :: btree
        integer :: n
        n = btree%n_elements
    end function binary_tree_get_n_elements

<Binary trees: tree: TBP>+≡
    procedure :: insert => binary_tree_insert

<Binary trees: sub interfaces>+≡
    module subroutine binary_tree_insert (btree, key, obj)
        class(binary_tree_t), intent(inout) :: btree
        integer, intent(in) :: key
        class(*), pointer, intent(in) :: obj
    end subroutine binary_tree_insert

<Binary trees: procedures>+≡
    module subroutine binary_tree_insert (btree, key, obj)
        class(binary_tree_t), intent(inout) :: btree
        integer, intent(in) :: key
        class(*), pointer, intent(in) :: obj
        type(binary_tree_node_t), pointer :: node
        allocate (node)
        call node%init (key, obj)
        btree%n_elements = btree%n_elements + 1
        if (.not. associated (btree%root)) then
            btree%root => node
        else
            call btree%insert_node (btree%root, node)
        end if
    end subroutine binary_tree_insert

<Binary trees: tree: TBP>+≡
    procedure, private :: insert_node => binary_tree_insert_node

<Binary trees: sub interfaces>+≡
    recursive module subroutine binary_tree_insert_node (btree, parent, node)
        class(binary_tree_t), intent(in) :: btree
        type(binary_tree_node_t), intent(inout), pointer :: parent
        type(binary_tree_node_t), intent(in), pointer :: node
    end subroutine binary_tree_insert_node

<Binary trees: procedures>+≡
    recursive module subroutine binary_tree_insert_node (btree, parent, node)
        class(binary_tree_t), intent(in) :: btree
        type(binary_tree_node_t), intent(inout), pointer :: parent

```

```

type(binary_tree_node_t), intent(in), pointer :: node
!! Choose left or right, if associated descend recursively into subtree,
!! else insert node.
if (node%key > parent%key) then
    if (associated (parent%right)) then
        call btree%insert_node (parent%right, node)
    else
        parent%right => node
    end if
else if (node%key < parent%key) then
    if (associated (parent%left)) then
        call btree%insert_node (parent%left, node)
    else
        parent%left => node
    end if
else
    write (*, "(A,1X,I0)") "Error: MUST not insert duplicate key", node%key
    stop 1
end if
call parent%increment_height ()
call btree%balance (parent, node%key)
end subroutine binary_tree_insert_node

```

(Binary trees: tree: TBP)+≡

```

procedure, private :: balance => binary_tree_balance

```

(Binary trees: sub interfaces)+≡

```

module subroutine binary_tree_balance (btree, subtree, key)
    class(binary_tree_t), intent(in) :: btree
    type(binary_tree_node_t), intent(inout), pointer :: subtree
    integer, intent(in) :: key
end subroutine binary_tree_balance

```

(Binary trees: procedures)+≡

```

!! Subtree: root of subtree (which is unbalance, refer to A in diagrams.)
module subroutine binary_tree_balance (btree, subtree, key)
    class(binary_tree_t), intent(in) :: btree
    type(binary_tree_node_t), intent(inout), pointer :: subtree
    integer, intent(in) :: key
    type(binary_tree_node_t), pointer :: node, newNode
    integer :: balance
    balance = subtree%get_balance ()
    node => subtree
    newNode => null ()
    !! balance := h_left - h_right.
    !! Proof: balance > 0 => too many elements on the left side of the subtree.
    !! Proof: balance < 0 => too many elements on the right side of the subtree.
    if (balance > 1) then
        !! => left-side of subtree
        !!      A3(2)      B2(1)
        !!      /        /  \
        !!    B2(1)    C1(0) A1(0)
        !!      /
        !!    C1(0)
        !!

```

```

!!      A3(3)          A1(2)          C2(1)
!!      /              /              /  \
!!  B1(1) LEFT      C2(1)      RIGHT B1(0) A3(0)
!!      \              /
!!      C2(0)        B1(0)
if (subtree%left%key > key) then !! rotate right
  call btree%rotate_right (node, newNode)
else !! subtree%left%key < key, rotate left, then right.
  call btree%rotate_left (node%left, newNode)
  node%left => newNode
  call btree%rotate_right (node, newNode)
end if
else if (balance < -1) then
  !! => right-side of subtree
  !!      A0(2)          B1(1)
  !!      \              /  \
  !!      B1(1)        A1(0) C3(0)
  !!      \
  !!      C3(0)*
  !!
  !!      A1(2)          A1(2)          C2(1)
  !!      \              \              /  \
  !!      B3(1) RIGHT    C2(1)      LEFT A1(0) B3(0)
  !!      /              \
  !!      C2(0)          B3(0)
  if (subtree%right%key < key) then !! rotate left
    call btree%rotate_left (node, newNode)
  else !! subtree%right%key > key, rotate right, then left.
    call btree%rotate_right (node%right, newNode)
    node%right => newNode
    call btree%rotate_left (node, newNode)
  end if
end if
if (associated (newNode)) subtree => newNode
end subroutine binary_tree_balance

```

<Binary trees: tree: TBP>+≡

```

procedure :: search => binary_tree_search

```

<Binary trees: sub interfaces>+≡

```

module subroutine binary_tree_search (btree, key, obj)
  class(binary_tree_t), intent(in) :: btree
  integer, intent(in) :: key
  class(*), pointer, intent(out) :: obj
end subroutine binary_tree_search

```

<Binary trees: procedures>+≡

```

module subroutine binary_tree_search (btree, key, obj)
  class(binary_tree_t), intent(in) :: btree
  integer, intent(in) :: key
  class(*), pointer, intent(out) :: obj
  type(binary_tree_node_t), pointer :: current
  current => btree%root
  obj => null ()
  if (.not. associated (current)) return

```

```

do while (current%key /= key)
  if (current%key > key) then
    current => current%left
  else
    current => current%right
  end if
  if (.not. associated (current)) then
    !! Key not found.
    exit
  end if
end do
if (associated (current)) obj => current%obj
end subroutine binary_tree_search

```

<Binary trees: tree: TBP>+≡

```

procedure :: has_key => binary_tree_has_key

```

<Binary trees: sub interfaces>+≡

```

module function binary_tree_has_key (btree, key) result (flag)
  class(binary_tree_t), intent(in) :: btree
  integer, intent(in) :: key
  logical :: flag
end function binary_tree_has_key

```

<Binary trees: procedures>+≡

```

module function binary_tree_has_key (btree, key) result (flag)
  class(binary_tree_t), intent(in) :: btree
  integer, intent(in) :: key
  logical :: flag
  type(binary_tree_node_t), pointer :: current
  current => btree%root
  flag = .false.
  if (.not. associated (current)) return
  do while (current%key /= key)
    if (current%key > key) then
      current => current%left
    else
      current => current%right
    end if
    if (.not. associated (current)) then
      !! Key not found.
      return
    end if
  end do
  flag = .true.
end function binary_tree_has_key

```

<Binary trees: tree: TBP>+≡

```

procedure, private :: rotate_right => binary_tree_rotate_right

```

<Binary trees: sub interfaces>+≡

```

module subroutine binary_tree_rotate_right (btree, root, new_root)
  class(binary_tree_t), intent(in) :: btree
  type(binary_tree_node_t), pointer, intent(inout) :: root
  type(binary_tree_node_t), pointer, intent(out) :: new_root

```

```

end subroutine binary_tree_rotate_right

<Binary trees: procedures>+≡
!!      A      Move B to A.
!!      / \
!!      B   E   1. Split B from A%left.
!!      / \     2. Temporarily pointer to D.
!!      C   D     3. Replace pointer to D by pointer to A - E.
!!                  4. Set temporary pointer to D to A%left.
!!
!! 1.+2. B      T => D      A
!!      /          \
!!      C            E
!!
!! 3.      B      T => D
!!      / \
!!      C   A
!!          \
!!          E
!!
!! 4.      B
!!      / \
!!      C   A
!!          / \
!!          D   E
!!
!! \param[inout] root Root/parent root (A).
!! \param[out] new_root New root/parent root (B).
module subroutine binary_tree_rotate_right (btree, root, new_root)
  class(binary_tree_t), intent(in) :: btree
  type(binary_tree_node_t), pointer, intent(inout) :: root
  type(binary_tree_node_t), pointer, intent(out) :: new_root
  type(binary_tree_node_t), pointer :: tmp
  new_root => root%left
  tmp => new_root%right
  new_root%right => root
  root%left => tmp
  call root%increment_height ()
  call new_root%increment_height ()
end subroutine binary_tree_rotate_right

<Binary trees: tree: TBP>+≡
  procedure, private :: rotate_left => binary_tree_rotate_left

<Binary trees: sub interfaces>+≡
  module subroutine binary_tree_rotate_left (btree, root, new_root)
    class(binary_tree_t), intent(in) :: btree
    type(binary_tree_node_t), pointer, intent(inout) :: root
    type(binary_tree_node_t), pointer, intent(out) :: new_root
  end subroutine binary_tree_rotate_left

<Binary trees: procedures>+≡
!!      A      Move B to A.
!!      / \
!!      E   B   1. Split B from A%left.

```

```

!!      / \  2. Temporarily pointer to C.
!!      C  D  3. Replace pointer to C by pointer to A - E.
!!           4. Set temporary pointer to C to A%right.
!!
!! 1.+2. B      T => C    A
!!      \      /
!!      D      E
!!
!! 3.      B      T => C
!!      / \
!!      A  D
!!      /
!!      E
!!
!! 4.      B
!!      / \
!!      A  D
!!      / \
!!      E  C
module subroutine binary_tree_rotate_left (btree, root, new_root)
  class(binary_tree_t), intent(in) :: btree
  type(binary_tree_node_t), pointer, intent(inout) :: root
  type(binary_tree_node_t), pointer, intent(out) :: new_root
  type(binary_tree_node_t), pointer :: tmp
  new_root => root%right
  tmp => new_root%left
  new_root%left => root
  root%right => tmp
  call root%increment_height ()
  call new_root%increment_height ()
end subroutine binary_tree_rotate_left

```

3.7.1 Unit tests

```

<binary_tree_ut.f90>≡
<File header>

module binary_tree_ut
  use unit_tests
  use binary_tree_util

  <Standard module head>

  <Binary tree: public test>

  contains

  <Binary tree: test driver>

end module binary_tree_ut

<binary_tree_util.f90>≡
<File header>

```

```

module binary_tree_util

    use binary_tree

    <Standard module head>

    type :: btree_obj_t
        integer :: i = 0
    end type btree_obj_t

    <Binary tree: test declarations>

    contains

    <Binary tree: tests>

end module binary_tree_util

<Binary tree: public test>≡
    public :: binary_tree_test

<Binary tree: test driver>≡
    subroutine binary_tree_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        <Binary tree: execute tests>
    end subroutine binary_tree_test

```

Provide testing for interface stability and correct implementation for the binary tree and its iterator.

```

<Binary tree: execute tests>≡
    call test (binary_tree_1, "binary_tree_1", &
        "check interface and implementation", &
        u, results)

<Binary tree: test declarations>≡
    public :: binary_tree_1

<Binary tree: tests>≡
    subroutine binary_tree_1 (u)
        integer, intent(in) :: u
        integer, dimension(10) :: ndx = [1, 2, 5, 7, 19, 23, 97, -1, -6, 0]
        class(*), pointer :: obj
        type(binary_tree_t) :: btree
        type(binary_tree_iterator_t) :: iterator
        integer :: i, key
        write (u, "(A)") "* Test output: Binary tree"
        write (u, "(A)") "* Purpose: test interface and implementation of binary tree " // &
            "and its iterator using polymorph objects."
        write (u, "(A)")

        write (u, "(A)") "* Insert fixed number of objects into tree..."
        do i = 1, size (ndx)
            call allocate_obj (i, obj)
            call btree%insert (ndx(i), obj)
        end do
    end subroutine binary_tree_1

```

```

end do

write (u, "(A)") "* Search for all added objects in tree..."
do i = size (ndx), 1, -1
    write (u, "(A,1X,I3,1X,L1)") "- Has key", ndx(i), btree%has_key (ndx(i))
    call btree%search (ndx(i), obj)
    select type (obj)
    type is (btree_obj_t)
        write (u, "(2(A,1X,I3,1X))") "- NDX", ndx(i), "OBJ", obj%i
    end select
end do

write (u, "(A)") "* Output binary tree in preorder..."
call btree%write (u)

write (u, "(A)") "* Clear binary tree..."
call btree%clear ()
call btree%write (u)

write (u, "(A)") "* Insert fixed number of object into tree (reversed order)..."
do i = size (ndx), 1, -1
    call allocate_obj (i, obj)
    call btree%insert (ndx(i), obj)
end do

write (u, "(A)") "* Iterate over binary tree..."
call iterator%init (btree)
do while (iterator%is_iterable ())
    call iterator%next (key)
    call btree%search (key, obj)
    select type (obj)
    type is (btree_obj_t)
        write (u, "(2(A,1X,I3,1X))") "- KEY", key, "OBJ", obj%i
    end select
end do

write (u, "(A)") "* Search for a non-existing key..."
write (u, "(A,1X,I3,1X,L1)") "- Has key", 123, btree%has_key (123)
call btree%search (123, obj)
write (u, "(A,1X,L1)") "- Object found", associated (obj)

!! Do not test against a duplicate entry as the it will forcibly stop the program.
contains
subroutine allocate_obj (num, obj)
    integer, intent(in) :: num
    class(*), pointer, intent(out) :: obj
    allocate (btree_obj_t :: obj)
    select type (obj)
    type is (btree_obj_t)
        obj%i = num
    end select
end subroutine allocate_obj
end subroutine binary_tree_1

```


3.8 Array List

```
<array_list.f90>≡
  <File header>

  module array_list
    <Use kinds>

    <Standard module head>

    <Array list: public>

    <Array list: parameters>

    <Array list: types>

    interface
      <Array list: sub interfaces>
    end interface

  end module array_list

<array_list_sub.f90>≡
  <File header>

  submodule (array_list) array_list_s

    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT
    use io_units

    implicit none

    contains

    <Array list: procedures>

  end submodule array_list_s

<Array list: parameters>≡
  integer, parameter :: ARRAY_LIST_START_SIZE = 10
  real(default), parameter :: ARRAY_LIST_GROW_FACTOR = 1.5_default, &
    ARRAY_LIST_SHRINK_THRESHOLD = 0.3_default

<Array list: public>≡
  public :: array_list_t

<Array list: types>≡
  type :: array_list_t
    private
    integer, dimension(:), allocatable :: array
    !! Track the index to *current* item, to be stored.
    !! Must fulfill: 0 <= count <= size.
    integer :: count = 0
    !! size \in N.
```

```

        integer :: size = 0
contains
    <Array list: array list: TBP>
end type array_list_t

<Array list: array list: TBP>≡
    procedure :: write => array_list_write

<Array list: sub interfaces>≡
    module subroutine array_list_write (list, unit)
        class(array_list_t), intent(in) :: list
        integer, intent(in), optional :: unit
    end subroutine array_list_write

<Array list: procedures>≡
    module subroutine array_list_write (list, unit)
        class(array_list_t), intent(in) :: list
        integer, intent(in), optional :: unit
        integer :: u
        u = ERROR_UNIT; if (present (unit)) u = unit
        write (u, "(A,2(1X,I3))") "COUNT / SIZE", list%count, list%size
        write (u, "(999(1X,I4))") list%array
    end subroutine array_list_write

<Array list: array list: TBP>+≡
    procedure :: init => array_list_init

<Array list: sub interfaces>+≡
    module subroutine array_list_init (list)
        class(array_list_t), intent(out) :: list
    end subroutine array_list_init

<Array list: procedures>+≡
    module subroutine array_list_init (list)
        class(array_list_t), intent(out) :: list
        allocate (list%array(ARRAY_LIST_START_SIZE), source = 0)
        list%count = 0
        list%size = ARRAY_LIST_START_SIZE
    end subroutine array_list_init

<Array list: array list: TBP>+≡
    procedure :: get => array_list_get

<Array list: sub interfaces>+≡
    elemental module function array_list_get (list, index) result (data)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        integer :: data
    end function array_list_get

<Array list: procedures>+≡
    elemental module function array_list_get (list, index) result (data)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        integer :: data
        if (list%is_index (index)) then

```

```

        data = list%array(index)
    else
        data = 0
    end if
end function array_list_get

<Array list: array list: TBP>+≡
    procedure :: get_count => array_list_get_count

<Array list: sub interfaces>+≡
    pure module function array_list_get_count (list) result (count)
        class(array_list_t), intent(in) :: list
        integer :: count
    end function array_list_get_count

<Array list: procedures>+≡
    pure module function array_list_get_count (list) result (count)
        class(array_list_t), intent(in) :: list
        integer :: count
        count = list%count
    end function array_list_get_count

<Array list: array list: TBP>+≡
    procedure :: get_size => array_list_get_size

<Array list: sub interfaces>+≡
    pure module function array_list_get_size (list) result (size)
        class(array_list_t), intent(in) :: list
        integer :: size
    end function array_list_get_size

<Array list: procedures>+≡
    pure module function array_list_get_size (list) result (size)
        class(array_list_t), intent(in) :: list
        integer :: size
        size = list%size
    end function array_list_get_size

<Array list: array list: TBP>+≡
    procedure :: is_full => array_list_is_full

<Array list: sub interfaces>+≡
    pure module function array_list_is_full (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
    end function array_list_is_full

<Array list: procedures>+≡
    pure module function array_list_is_full (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
        flag = list%count >= list%size
    end function array_list_is_full

```

```

<Array list: array list: TBP>+≡
    procedure :: is_empty => array_list_is_empty
<Array list: sub interfaces>+≡
    pure module function array_list_is_empty (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
    end function array_list_is_empty
<Array list: procedures>+≡
    pure module function array_list_is_empty (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
        flag = .not. list%count > 0
    end function array_list_is_empty

<Array list: array list: TBP>+≡
    procedure :: is_index => array_list_is_index
<Array list: sub interfaces>+≡
    pure module function array_list_is_index (list, index) result (flag)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        logical :: flag
    end function array_list_is_index
<Array list: procedures>+≡
    pure module function array_list_is_index (list, index) result (flag)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        logical :: flag
        flag = 0 < index .and. index <= list%count
    end function array_list_is_index

<Array list: array list: TBP>+≡
    procedure :: clear => array_list_clear
<Array list: sub interfaces>+≡
    module subroutine array_list_clear (list)
        class(array_list_t), intent(inout) :: list
    end subroutine array_list_clear
<Array list: procedures>+≡
    module subroutine array_list_clear (list)
        class(array_list_t), intent(inout) :: list
        list%array = 0
        list%count = 0
        call list%shrink_size ()
    end subroutine array_list_clear

<Array list: array list: TBP>+≡
    procedure :: add => array_list_add
<Array list: sub interfaces>+≡
    module subroutine array_list_add (list, data)
        class(array_list_t), intent(inout) :: list
        integer, intent(in) :: data
    end subroutine array_list_add

```

```

<Array list: procedures>+≡
module subroutine array_list_add (list, data)
  class(array_list_t), intent(inout) :: list
  integer, intent(in) :: data
  list%count = list%count + 1
  if (list%is_full ()) then
    call list%grow_size ()
  end if
  list%array(list%count) = data
end subroutine array_list_add

<Array list: array list: TBP>+≡
  procedure :: grow_size => array_list_grow_size

<Array list: sub interfaces>+≡
  module subroutine array_list_grow_size (list)
    class(array_list_t), intent(inout) :: list
  end subroutine array_list_grow_size

<Array list: procedures>+≡
module subroutine array_list_grow_size (list)
  class(array_list_t), intent(inout) :: list
  integer, dimension(:), allocatable :: array
  integer :: new_size
  if (.not. list%is_full ()) return
  new_size = int (list%size * ARRAY_LIST_GROW_FACTOR)
  allocate (array(new_size), source = 0)
  array(:list%size) = list%array
  call move_alloc (array, list%array)
  list%size = size (list%array)
end subroutine array_list_grow_size

<Array list: array list: TBP>+≡
  procedure :: shrink_size => array_list_shrink_size

<Array list: sub interfaces>+≡
  module subroutine array_list_shrink_size (list)
    class(array_list_t), intent(inout) :: list
    integer, dimension(:), allocatable :: array
  end subroutine array_list_shrink_size

<Array list: procedures>+≡
module subroutine array_list_shrink_size (list)
  class(array_list_t), intent(inout) :: list
  integer, dimension(:), allocatable :: array
  integer :: new_size
  !! Apply shrink threshold on count.
  ! if (.not. list%count > 0) return
  new_size = max (list%count, ARRAY_LIST_START_SIZE)
  allocate (array(new_size), source = 0)
  !! \note We have to circumvent the allocate-on-assignment,
  !! hence, we explicitly set the array boundaries.
  array(:list%count) = list%array(:list%count)
  call move_alloc (array, list%array)
  list%size = new_size

```

```

end subroutine array_list_shrink_size

<Array list: array list: TBP>+≡
  procedure :: reverse_order => array_list_reverse_order

<Array list: sub interfaces>+≡
  module subroutine array_list_reverse_order (list)
    class(array_list_t), intent(inout) :: list
  end subroutine array_list_reverse_order

<Array list: procedures>+≡
  module subroutine array_list_reverse_order (list)
    class(array_list_t), intent(inout) :: list
    list%array(:list%count) = list%array(list%count:1:-1)
  end subroutine array_list_reverse_order

<Array list: array list: TBP>+≡
  procedure :: sort => array_list_sort

<Array list: sub interfaces>+≡
  pure module subroutine array_list_sort (list)
    class(array_list_t), intent(inout) :: list
  end subroutine array_list_sort

<Array list: procedures>+≡
  pure module subroutine array_list_sort (list)
    class(array_list_t), intent(inout) :: list
    if (list%is_empty ()) return
    call quick_sort (list%array(:list%count))
  contains
    pure recursive subroutine quick_sort (array)
      integer, dimension(:), intent(inout) :: array
      integer :: pivot, tmp
      integer :: first, last
      integer i, j
      first = 1
      last = size(array)
      pivot = array(int ((first+last) / 2.))
      i = first
      j = last
      do
        do while (array(i) < pivot)
          i = i + 1
        end do
        do while (pivot < array(j))
          j = j - 1
        end do
        if (i >= j) exit
        tmp = array(i)
        array(i) = array(j)
        array(j) = tmp
        i = i + 1
        j = j - 1
      end do
      if (first < i - 1) call quick_sort(array(first:i - 1))

```

```

        if (j + 1 < last) call quick_sort(array(j + 1:last))
    end subroutine quick_sort
end subroutine array_list_sort

<Array list: array list: TBP>+≡
    procedure :: is_element => array_list_is_element

<Array list: sub interfaces>+≡
    pure module function array_list_is_element (list, data) result (flag)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: data
        logical :: flag
    end function array_list_is_element

<Array list: procedures>+≡
    pure module function array_list_is_element (list, data) result (flag)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: data
        logical :: flag
        if (list%is_empty ()) then
            flag = .false.
        else
            flag = any (data == list%array)
        end if
    end function array_list_is_element

<Array list: array list: TBP>+≡
    procedure :: find => array_list_find

<Array list: sub interfaces>+≡
    module function array_list_find (list, data) result (index)
        class(array_list_t), intent(inout) :: list
        integer, intent(in) :: data
        integer :: index
    end function array_list_find

<Array list: procedures>+≡
    module function array_list_find (list, data) result (index)
        class(array_list_t), intent(inout) :: list
        integer, intent(in) :: data
        integer :: index
        if (list%is_empty () &
            .or. .not. list%is_element (data)) then
            index = 0
            return
        end if
        call list%sort () !! INTENT(INOUT)
        index = binary_search_leftmost (list%array(:list%count), data)
contains
    pure function binary_search_leftmost (array, data) result (index)
        integer, dimension(:), intent(in) :: array
        integer, intent(in) :: data
        integer :: index
        integer :: left, right
        left = 1

```

```

right = size (array)
do while (left < right)
  index = floor ((left + right) / 2.)
  if (array(index) < data) then
    left = index + 1
  else
    right = index
  end if
end do
index = left
end function binary_search_leftmost
end function array_list_find

```

<Array list: array list: TBP>+≡

```

procedure :: add_at => array_list_add_at

```

<Array list: sub interfaces>+≡

```

module subroutine array_list_add_at (list, index, data)
  class(array_list_t), intent(inout) :: list
  integer, intent(in) :: index
  integer, intent(in) :: data
end subroutine array_list_add_at

```

<Array list: procedures>+≡

```

module subroutine array_list_add_at (list, index, data)
  class(array_list_t), intent(inout) :: list
  integer, intent(in) :: index
  integer, intent(in) :: data
  if (.not. list%is_index (index)) return
  if (list%is_full ()) then
    call list%grow_size ()
  end if
  list%array(index + 1:list%count + 1) = list%array(index:list%count)
  list%array(index) = data
  list%count = list%count + 1
end subroutine array_list_add_at

```

<Array list: array list: TBP>+≡

```

procedure :: remove => array_list_remove

```

<Array list: sub interfaces>+≡

```

module function array_list_remove (list) result (data)
  class(array_list_t), intent(inout) :: list
  integer :: data
end function array_list_remove

```

<Array list: procedures>+≡

```

module function array_list_remove (list) result (data)
  class(array_list_t), intent(inout) :: list
  integer :: data
  if (list%is_empty ()) then
    data = 0
    return
  end if
  data = list%get (list%count)

```



```

        list%array(list%count) = 0
        list%count = list%count - 1
    end function array_list_remove

    <Array list: array list: TBP>+≡
        procedure :: remove_at => array_list_remove_at

    <Array list: sub interfaces>+≡
        module function array_list_remove_at (list, index) result (data)
            class(array_list_t), intent(inout) :: list
            integer, intent(in) :: index
            integer :: data
        end function array_list_remove_at

    <Array list: procedures>+≡
        module function array_list_remove_at (list, index) result (data)
            class(array_list_t), intent(inout) :: list
            integer, intent(in) :: index
            integer :: data
            if (list%is_empty ()) then
                data = 0
                return
            end if
            data = list%get (index)
            list%array(index:list%count - 1) = list%array(index + 1:list%count)
            list%array(list%count) = 0
            list%count = list%count - 1
        end function array_list_remove_at

```

3.8.1 Unit tests

```

    <array_list_ut.f90>≡
    <File header>

    module array_list_ut
        use unit_tests
        use array_list_ut

    <Standard module head>

    <Array list: public test>

    contains

    <Array list: test driver>
    end module array_list_ut

    <array_list_util.f90>≡
    <File header>

    module array_list_util

        use array_list

```

```

    <Standard module head>

    <Array list: test declarations>

    contains

    <Array list: tests>

    end module array_list_util

    <Array list: public test>≡
    public :: array_list_test

    <Array list: test driver>≡
    subroutine array_list_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        <Array list: execute tests>
    end subroutine array_list_test

```

Provide testing for interface stability and correct implementation for the binary tree and its iterator.

```

    <Array list: execute tests>≡
    call test (array_list_1, "array_list_1", &
        "check interface and implementation", &
        u, results)

    <Array list: test declarations>≡
    public :: array_list_1

    <Array list: tests>≡
    subroutine array_list_1 (u)
        integer, intent(in) :: u
        type(array_list_t) :: list
        integer :: ndx, data

        write (u, "(A)") "* Test output: Array list"
        write (u, "(A)") "* Purpose: test interface and implementation of array list"
        write (u, "(A)")

        write (u, "(A)") "* Init array_list_t ..."
        call list%init ()
        write (u, "(A)") "* Test adding a single element..."
        call list%add (1)
        write (u, "(A)") "* Test removing a single element..."
        data = list%remove ()
        write (u, "(A)") "* Test growing (unnecessary, so just return)..."
        call list%grow_size ()
        write (u, "(A)") "* Test adding elements beyond initial capacity..."
        call test_grow_and_add (list)
        write (u, "(A)") "* Test adding at specific position..."
        call list%add_at (10, -1)
        write (u, "(A)") "* Test removing at specific position..."
        data = list%remove_at (11)
        write (u, "(A)") "* Test reverse ordering..."

```

```

call list%reverse_order ()
write (u, "(A)") "* Test sorting..."
call list%sort ()
write (u, "(A)") "* Test finding..."
ndx = list%find (1)
write (u, "(A)") "* Test shrinking..."
call list%shrink_size ()
write (u, "(A)") "* Test get procedures..."
call test_get_procedures (list)
write (u, "(A)") "* Test clearing list..."
call list%clear ()
write (u, "(A)") "* Test (more complicated) combinations:"
write (u, "(A)") "* Test growing (necessary) during adding..."
call test_grow_and_add (list)
write (u, "(A)") "* Test adding random data and sorting..."
call test_sort (list)
write (u, "(A)") "* Test finding (before sorted)..."
call test_find (list)
contains
  subroutine test_get_procedures (list)
    type(array_list_t), intent(in) :: list
    integer :: n
    logical :: flag
    n = list%get(1)
    n = list%get_size ()
    n = list%get_count ()
    flag = list%is_element (1)
  end subroutine test_get_procedures

  subroutine test_grow_and_add (list)
    type(array_list_t), intent(inout) :: list
    integer :: i
    do i = 1, 2 * list%get_size ()
      call list%add (i)
    end do
  end subroutine test_grow_and_add

  subroutine test_get (list)
    class(array_list_t), intent(inout) :: list
    integer :: i, data
    do i = list%get_count (), 1, -1
      data = list%get (i)
      if (data == 0) then
        write (u, "(A,1X,I3)") "INDEX EMPTY", i
      end if
    end do
  end subroutine test_get

  subroutine test_sort (list)
    class(array_list_t), intent(inout) :: list
    call list%add (6)
    call list%add (2)
    call list%add (9)
    call list%add (4)

```

```

        call list%add (8)
        call list%add (7)
        call list%sort ()
    end subroutine test_sort

    subroutine test_find (list)
        class(array_list_t), intent(inout) :: list
        write (u, "(A,1X,I3)") " 6 INDEX", list%find (6)
        write (u, "(A,1X,I3)") "-1 INDEX", list%find (-1)
        write (u, "(A,1X,I3)") " 3 INDEX", list%find (3)
        write (u, "(A,1X,I3)") "26 INDEX", list%find (26)
        call list%write (u)
    end subroutine test_find
end subroutine array_list_1

```

3.9 Queue

```

⟨queue.f90⟩≡
  ⟨File header⟩

  module queue

    ⟨Standard module head⟩

    ⟨Queue: public⟩

    ⟨Queue: parameters⟩

    ⟨Queue: types⟩

    interface
    ⟨Queue: sub interfaces⟩
    end interface

  end module queue

⟨queue_sub.f90⟩≡
  ⟨File header⟩

  submodule (queue) queue_s

    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT

    implicit none

    contains

    ⟨Queue: procedures⟩

  end submodule queue_s

```

```

<Queue: parameters>≡
    integer, parameter :: QUEUE_SIZE = 10, &
        QUEUE_START = 0, &
        QUEUE_END = QUEUE_SIZE

<Queue: public>≡
    public :: queue_t

<Queue: types>≡
    type :: queue_t
        private
        integer, dimension(QUEUE_SIZE) :: item
        integer :: front = 0
        integer :: rear = 0
    contains
        <Queue: queue: TBP>
    end type queue_t

<Queue: queue: TBP>≡
    procedure :: is_full => queue_is_full

<Queue: sub interfaces>≡
    elemental module function queue_is_full (queue) result (flag)
        class(queue_t), intent(in) :: queue
        logical :: flag
    end function queue_is_full

<Queue: procedures>≡
    elemental module function queue_is_full (queue) result (flag)
        class(queue_t), intent(in) :: queue
        logical :: flag
        flag = queue%front == 1 .and. queue%rear == QUEUE_END
    end function queue_is_full

<Queue: queue: TBP>+≡
    procedure :: is_empty => queue_is_empty

<Queue: sub interfaces>+≡
    elemental module function queue_is_empty (queue) result (flag)
        class(queue_t), intent(in) :: queue
        logical :: flag
    end function queue_is_empty

<Queue: procedures>+≡
    elemental module function queue_is_empty (queue) result (flag)
        class(queue_t), intent(in) :: queue
        logical :: flag
        flag = queue%front == QUEUE_START
    end function queue_is_empty

<Queue: queue: TBP>+≡
    procedure :: enqueue => queue_enqueue

```

```

<Queue: sub interfaces>+≡
    module subroutine queue_enqueue (queue, item)
        class(queue_t), intent(inout) :: queue
        integer, intent(in) :: item
    end subroutine queue_enqueue

<Queue: procedures>+≡
    module subroutine queue_enqueue (queue, item)
        class(queue_t), intent(inout) :: queue
        integer, intent(in) :: item
        if (queue%is_full ()) then
            !! Do something.
        else
            if (queue%front == QUEUE_START) queue%front = 1
            queue%rear = queue%rear + 1
            queue%item(queue%rear) = item
        end if
    end subroutine queue_enqueue

<Queue: queue: TBP>+≡
    procedure :: dequeue => queue_dequeue

<Queue: sub interfaces>+≡
    module function queue_dequeue (queue) result (item)
        class(queue_t), intent(inout) :: queue
        integer :: item
    end function queue_dequeue

<Queue: procedures>+≡
    module function queue_dequeue (queue) result (item)
        class(queue_t), intent(inout) :: queue
        integer :: item
        if (queue%is_empty ()) then
            item = 0
        else
            item = queue%item(queue%front)
            if (queue%front >= queue%rear) then
                queue%front = QUEUE_START
                queue%rear = QUEUE_START
                !! Q has only one element,
                !! so we reset the queue after deleting it.
            else
                queue%front = queue%front + 1
            end if
        end if
    end function queue_dequeue

<Queue: queue: TBP>+≡
    procedure :: peek => queue_peek

<Queue: sub interfaces>+≡
    module function queue_peek (queue) result (item)
        class(queue_t), intent(in) :: queue
        integer :: item
    end function queue_peek

```

```

<Queue: procedures>+≡
  module function queue_peek (queue) result (item)
    class(queue_t), intent(in) :: queue
    integer :: item
    if (queue%is_empty ()) then
      item = 0
    else
      item = queue%item(queue%front)
    end if
  end function queue_peek

<Queue: queue: TBP>+≡
  procedure :: write => queue_write

<Queue: sub interfaces>+≡
  module subroutine queue_write (queue, unit)
    class(queue_t), intent(in) :: queue
    integer, intent(in), optional :: unit
  end subroutine queue_write

<Queue: procedures>+≡
  module subroutine queue_write (queue, unit)
    class(queue_t), intent(in) :: queue
    integer, intent(in), optional :: unit
    integer :: u, i
    u = ERROR_UNIT; if (present (unit)) u = unit
    if (queue%is_empty ()) then
      write (u, *) "Empty Queue."
    else
      write (u, *) "Front ->", queue%front
      write (u, *) "Items ->"
      do i = 1, queue%rear
        write (u, *) queue%item(i)
      end do
      write (u, *) "Rear ->", queue%rear
    end if
  end subroutine queue_write

```

3.10 Iterator

```

<iterator.f90>≡
  <File header>
  module iterator

  <Standard module head>

  <Iterator: public>

  <Iterator: types>

  interface
  <Iterator: sub interfaces>

```

```

        end interface

    end module iterator

<iterator_sub.f90>≡
    <File header>

    submodule (iterator) iterator_s

        use, intrinsic :: iso_fortran_env, only: ERROR_UNIT

        implicit none

        contains

        <Iterator: procedures>

    end submodule iterator_s

<Iterator: public>≡
    public :: iterator_t

<Iterator: types>≡
    !! Forward
    type :: iterator_t
        integer :: current = 0
        integer :: begin = 0
        integer :: end = 0
        integer :: step = 1
        contains
        <Iterator: iterator: TBP>
    end type iterator_t

<Iterator: iterator: TBP>≡
    procedure :: write => iterator_write

<Iterator: sub interfaces>≡
    module subroutine iterator_write (iter, unit)
        class(iterator_t), intent(in) :: iter
        integer, intent(in), optional :: unit
    end subroutine iterator_write

<Iterator: procedures>≡
    module subroutine iterator_write (iter, unit)
        class(iterator_t), intent(in) :: iter
        integer, intent(in), optional :: unit
        integer :: u
        u = ERROR_UNIT; if (present (unit)) u = unit
        write (u, "(3(A,1X,I3,1X))") "CURRENT", iter%current, &
            "BEGIN", iter%begin, "END", iter%end
        flush (u)
    end subroutine iterator_write

```



```

<Iterator: iterator: TBP>+≡
    procedure :: init => iterator_init

<Iterator: sub interfaces>+≡
    module subroutine iterator_init (iter, begin, end, step)
        class(iterator_t), intent(inout) :: iter
        integer, intent(in) :: begin
        integer, intent(in) :: end
        integer, intent(in), optional :: step
    end subroutine iterator_init

<Iterator: procedures>+≡
    !! Proof: step > 0, begin < end.
    !! Proof: step < 0, begin > end.
    !! Proof: step /= 0.
    module subroutine iterator_init (iter, begin, end, step)
        class(iterator_t), intent(inout) :: iter
        integer, intent(in) :: begin
        integer, intent(in) :: end
        integer, intent(in), optional :: step
        iter%begin = begin
        iter%end = end
        iter%step = 1; if (present (step)) iter%step = step
        if (abs (iter%step) > 0) then
            iter%current = iter%begin
        else
            write (ERROR_UNIT, "(A)") "ERROR: Step size MUST be unequal to zero."
            stop 1
        end if
    end subroutine iterator_init

<Iterator: iterator: TBP>+≡
    procedure :: at_begin => iterator_at_begin

<Iterator: sub interfaces>+≡
    pure module function iterator_at_begin (iter) result (flag)
        class(iterator_t), intent(in) :: iter
        logical :: flag
    end function iterator_at_begin

<Iterator: procedures>+≡
    pure module function iterator_at_begin (iter) result (flag)
        class(iterator_t), intent(in) :: iter
        logical :: flag
        flag = iter%current == iter%begin
    end function iterator_at_begin

<Iterator: iterator: TBP>+≡
    procedure :: at_end => iterator_at_end

<Iterator: sub interfaces>+≡
    pure module function iterator_at_end (iter) result (flag)
        class(iterator_t), intent(in) :: iter
        logical :: flag
    end function iterator_at_end

```

```

<Iterator: procedures>+≡
  pure module function iterator_at_end (iter) result (flag)
    class(iterator_t), intent(in) :: iter
    logical :: flag
    flag = iter%current == iter%end
  end function iterator_at_end

<Iterator: iterator: TBP>+≡
  procedure :: is_iterable => iterator_is_iterable

<Iterator: sub interfaces>+≡
  pure module function iterator_is_iterable (iter) result (flag)
    class(iterator_t), intent(in) :: iter
    logical :: flag
  end function iterator_is_iterable

<Iterator: procedures>+≡
  !! Proof: begin < current < end
  pure module function iterator_is_iterable (iter) result (flag)
    class(iterator_t), intent(in) :: iter
    logical :: flag
    if (iter%step > 0) then
      flag = iter%current <= iter%end
    else if (iter%step < 0) then
      flag = iter%current >= iter%end
    else
      flag = .false.
    end if
  end function iterator_is_iterable

<Iterator: iterator: TBP>+≡
  procedure :: next_step => iterator_next_step

<Iterator: sub interfaces>+≡
  module subroutine iterator_next_step (iter)
    class(iterator_t), intent(inout) :: iter
  end subroutine iterator_next_step

<Iterator: procedures>+≡
  module subroutine iterator_next_step (iter)
    class(iterator_t), intent(inout) :: iter
    if (.not. iter%is_iterable ()) return
    iter%current = iter%current + iter%step
  end subroutine iterator_next_step

<Iterator: iterator: TBP>+≡
  procedure :: next => iterator_next

<Iterator: sub interfaces>+≡
  module function iterator_next (iter) result (ndx)
    class(iterator_t), intent(inout) :: iter
    integer :: ndx
  end function iterator_next

```

```

<Iterator: procedures>+≡
    !! Proof: begin <= current <= end.
    !! However, after applying the step, this does not need to be true..
    module function iterator_next (iter) result (ndx)
        class(iterator_t), intent(inout) :: iter
        integer :: ndx
        if (.not. iter%is_iterable ()) then
            ndx = 0
            return
        end if
        ndx = iter%current
        iter%current = iter%current + iter%step
    end function iterator_next

<Iterator: iterator: TBP>+≡
    procedure :: get_current => iterator_get_current

<Iterator: sub interfaces>+≡
    pure module function iterator_get_current (iter) result (ndx)
        class(iterator_t), intent(in) :: iter
        integer :: ndx
    end function iterator_get_current

<Iterator: procedures>+≡
    pure module function iterator_get_current (iter) result (ndx)
        class(iterator_t), intent(in) :: iter
        integer :: ndx
        if (.not. iter%is_iterable ()) then
            ndx = 0
            return
        end if
        ndx = iter%current
    end function iterator_get_current

```

3.10.1 Unit tests

```

<iterator_ut.f90>≡
    <File header>

    module iterator_ut
        use unit_tests
        use iterator_util

    <Standard module head>

    <Iterator: public test>

    contains

    <Iterator: test driver>
    end module iterator_ut

```

```

<iterator_util.f90>≡
  <File header>

  module iterator_util

    use iterator

    <Standard module head>

    <Iterator: test declarations>

    contains

    <Iterator: tests>

  end module iterator_util

<Iterator: public test>≡
  public :: iterator_test

<Iterator: test driver>≡
  subroutine iterator_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Iterator: execute tests>
  end subroutine iterator_test

```

Provide testing for interface stability and correct implementation for the forward integer iterator.

```

<Iterator: execute tests>≡
  call test (iterator_1, "iterator_1", &
    "check interface and implementation", &
    u, results)

<Iterator: test declarations>≡
  public :: iterator_1

<Iterator: tests>≡
  subroutine iterator_1 (u)
    integer, intent(in) :: u
    type(iterator_t) :: iter

    write (u, "(A)") "* Test output: iterator_1"
    write (u, "(A)") "* Purpose: test interface and implementation of the forward integer iterator"
    write (u, "(A)")

    call iter%init (1, 10)
    call iter%write (u)
    do while (iter%is_iterable ())
      write (u, "(A,1X,I3)") "NDX", iter%next ()
    end do

    call iter%init (10, 1, -1)
    call iter%write (u)
    do while (iter%is_iterable ())
      write (u, "(A,1X,I3)") "NDX", iter%next ()
    end do
  end subroutine iterator_1

```

```

end do
write (u, "(A,1X,I3)") "INVALID NDX", iter%next ()

call iter%init (1, 10)
call iter%write (u)
do while (iter%is_iterable ())
    call iter%next_step ()
    write (u, "(A)") "STEP."
end do
end subroutine iterator_1

```

Chapter 4

Testing

This part contains tools for automatic testing.

unit_tests A handler that executes test procedures and compares and collects results.

4.1 Unit tests

We provide functionality for automated unit tests. Each test is required to produce output which is compared against a reference file. If the two are identical, we signal success. Otherwise, we signal failure and write the output to a file.

```
<unit_tests.f90>≡  
  <File header>
```

```
  module unit_tests
```

```
    <Use strings>
```

```
    <Standard module head>
```

```
    <Tests: public>
```

No internal dependencies

Figure 4.1: Module dependencies in `src/testing`.

```

    <Tests: types>

    <Tests: interfaces>

    interface
    <Tests: sub interfaces>
    end interface

    end module unit_tests

    <unit_tests_sub.f90>≡
    <File header>

    submodule (unit_tests) unit_tests_s

        use io_units

        implicit none

    <Tests: parameters>

    contains

    <Tests: procedures>

    end submodule unit_tests_s

```

4.1.1 Parameters

Building blocks of file names. The directory names and suffixes are hard-coded here, and they must reflect actual Makefile targets where applicable.

```

<Tests: parameters>≡
    character(*), parameter :: ref_prefix = "ref-output/"
    character(*), parameter :: ref = ".ref"

    character(*), parameter :: err_prefix = "err-output/"
    character(*), parameter :: err = ".out"

```

4.1.2 Type for storing test results

We store the results of the individual unit tests in a linked list. Here is the entry:

```

<Tests: public>≡
    public :: test_results_t

<Tests: types>≡
    type :: test_result_t
        logical :: success = .false.
        type(string_t) :: name
        type(string_t) :: description

```

```

        type(test_result_t), pointer :: next => null ()
    end type test_result_t

```

```

type :: test_results_t
    private
        type(test_result_t), pointer :: first => null ()
        type(test_result_t), pointer :: last => null ()
        integer :: n_success = 0
        integer :: n_failure = 0
    contains
        <Tests: test results: TBP>
    end type test_results_t

```

Add a test result.

<Tests: test results: TBP>≡

```

    procedure :: add => test_results_add

```

<Tests: sub interfaces>≡

```

    module subroutine test_results_add (list, name, description, success)
        class(test_results_t), intent(inout) :: list
        character(len=*), intent(in) :: name
        character(len=*), intent(in) :: description
        logical, intent(in) :: success
    end subroutine test_results_add

```

<Tests: procedures>≡

```

    module subroutine test_results_add (list, name, description, success)
        class(test_results_t), intent(inout) :: list
        character(len=*), intent(in) :: name
        character(len=*), intent(in) :: description
        logical, intent(in) :: success
        type(test_result_t), pointer :: result
        allocate (result)
        result%success = success
        result%name = name
        result%description = description
        if (associated (list%first)) then
            list%last%next => result
        else
            list%first => result
        end if
        list%last => result
        if (success) then
            list%n_success = list%n_success + 1
        else
            list%n_failure = list%n_failure + 1
        end if
    end subroutine test_results_add

```

Display the current state.

<Tests: test results: TBP>+≡

```

    procedure, private :: write => test_results_write

```


<Tests: sub interfaces>+≡

```

module subroutine test_results_write (list, u)
  class(test_results_t), intent(in) :: list
  integer, intent(in) :: u
end subroutine test_results_write

```

<Tests: procedures>+≡

```

module subroutine test_results_write (list, u)
  class(test_results_t), intent(in) :: list
  integer, intent(in) :: u
  type(test_result_t), pointer :: result
  write (u, "(A)")  "*** Test Summary ***"
  if (list%n_success > 0) then
    write (u, "(2x,A)") "Success:"
    result => list%first
    do while (associated (result))
      if (result%success) write (u, "(4x,A,': ',A)") &
        char (result%name), char (result%description)
      result => result%next
    end do
  end if
  if (list%n_failure > 0) then
    write (u, "(2x,A)") "Failure:"
    result => list%first
    do while (associated (result))
      if (.not. result%success) write (u, "(4x,A,': ',A)") &
        char (result%name), char (result%description)
      result => result%next
    end do
  end if
  write (u, "(A,I0)") "Total   = ", list%n_success + list%n_failure
  write (u, "(A,I0)") "Success = ", list%n_success
  write (u, "(A,I0)") "Failure = ", list%n_failure
  write (u, "(A)")  "*** End of test Summary ***"
end subroutine test_results_write

```

Return true if all tests were successful (or no test).

<Tests: test results: TBP>+≡

```

procedure, private :: report => test_results_report

```

<Tests: sub interfaces>+≡

```

module subroutine test_results_report (list, success)
  class(test_results_t), intent(in) :: list
  logical, intent(out) :: success
end subroutine test_results_report

```

<Tests: procedures>+≡

```

module subroutine test_results_report (list, success)
  class(test_results_t), intent(in) :: list
  logical, intent(out) :: success
  success = list%n_failure == 0
end subroutine test_results_report

```

Return the number of successful/failed/total tests..

<Tests: test results: TBP>+≡

```

    procedure :: get_n_pass => test_results_get_n_pass
    procedure :: get_n_fail => test_results_get_n_fail
    procedure :: get_n_total => test_results_get_n_total

    <Tests: sub interfaces>+≡
        module function test_results_get_n_pass (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
        end function test_results_get_n_pass
        module function test_results_get_n_fail (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
        end function test_results_get_n_fail
        module function test_results_get_n_total (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
        end function test_results_get_n_total

    <Tests: procedures>+≡
        module function test_results_get_n_pass (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
            n = list%n_success
        end function test_results_get_n_pass

        module function test_results_get_n_fail (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
            n = list%n_failure
        end function test_results_get_n_fail

        module function test_results_get_n_total (list) result (n)
            class(test_results_t), intent(in) :: list
            integer :: n
            n = list%n_success + list%n_failure
        end function test_results_get_n_total

```

Delete the list.

```

    <Tests: test results: TBP>+≡
        procedure, private :: final => test_results_final

    <Tests: sub interfaces>+≡
        module subroutine test_results_final (list)
            class(test_results_t), intent(inout) :: list
        end subroutine test_results_final

    <Tests: procedures>+≡
        module subroutine test_results_final (list)
            class(test_results_t), intent(inout) :: list
            type(test_result_t), pointer :: result
            do while (associated (list%first))
                result => list%first
                list%first => result%next
                deallocate (result)
            end do
            list%last => null ()

```

```

    list%n_success = 0
    list%n_failure = 0
end subroutine test_results_final

```

4.1.3 Wrapup

This will write results, report status, and finalize. This is the only method which we need to access from outside.

```

<Tests: test results: TBP>+≡
    procedure :: wrapup => test_results_wrapup

<Tests: sub interfaces>+≡
    module subroutine test_results_wrapup (list, u, success)
        class(test_results_t), intent(inout) :: list
        integer, intent(in) :: u
        logical, intent(out), optional :: success
    end subroutine test_results_wrapup

<Tests: procedures>+≡
    module subroutine test_results_wrapup (list, u, success)
        class(test_results_t), intent(inout) :: list
        integer, intent(in) :: u
        logical, intent(out), optional :: success
        call list%write (u)
        if (present (success)) call list%report (success)
        call list%final ()
    end subroutine test_results_wrapup

```

4.1.4 Tool for Unit Tests

This procedure takes a test routine as an argument. It runs the test, output directed to a temporary file. Then, it compares the file against a reference file.

The test routine must take the output unit as argument. We export this abstract interface, so the test drivers can reference it for declaring the actual test routines.

```

<Tests: public>+≡
    public :: unit_test

<Tests: interfaces>≡
    abstract interface
        subroutine unit_test (u)
            integer, intent(in) :: u
        end subroutine unit_test
    end interface

```

The test routine can print to screen and, optionally, to a logging unit. This driver runs the test given as an argument, directing its output to a scratch file which is then checked against a ref file. Only if it differs, it is copied to an err file.

NB: We call `fatal_force_crash` to produce a deliberate crash with back-trace on any fatal error, if the runtime system does allow it. This is not normal behavior, but should be useful if something goes wrong.

```

<Tests: public>+≡
    public :: test

<Tests: sub interfaces>+≡
    module subroutine test (test_proc, name, description, u_log, results)
        procedure(unit_test) :: test_proc
        character(*), intent(in) :: name
        character(*), intent(in) :: description
        integer, intent(in) :: u_log
        type(test_results_t), intent(inout) :: results
    end subroutine test

<Tests: procedures>+≡
    module subroutine test (test_proc, name, description, u_log, results)
        procedure(unit_test) :: test_proc
        character(*), intent(in) :: name
        character(*), intent(in) :: description
        integer, intent(in) :: u_log
        type(test_results_t), intent(inout) :: results
        integer :: u_test
        logical :: success

        call start_test (u_log, name)

        u_test = free_unit ()
        open (unit = u_test, status="scratch", action="readwrite")
        call fatal_force_crash ()
        call test_proc (u_test)
        rewind (u_test)

        call compare_test_results (u_test, u_log, name, success)
        call results%add (name, description, success)
        close (u_test)

    end subroutine test

```

Startup message. We expose this, as well as the comparison routine, for re-use in external test programs.

```

<Tests: public>+≡
    public :: start_test

<Tests: sub interfaces>+≡
    module subroutine start_test (u_log, name)
        integer, intent(in) :: u_log
        character(*), intent(in) :: name
    end subroutine start_test

<Tests: procedures>+≡
    module subroutine start_test (u_log, name)
        integer, intent(in) :: u_log
        character(*), intent(in) :: name

```

```

        write (*, "(A)", advance="no") "Running test: " // name
        write (u_log, "(A)") "Test: " // name

    end subroutine start_test

```

Do the actual comparison, given an open I/O unit `u_test`. In case of failure, copy the test results to an error file.

```

<Tests: public>+≡
    public :: compare_test_results

<Tests: sub interfaces>+≡
    module subroutine compare_test_results (u_test, u_log, name, success)
        integer, intent(in) :: u_test
        integer, intent(in) :: u_log
        character(*), intent(in) :: name
        logical, intent(out) :: success
    end subroutine compare_test_results

<Tests: procedures>+≡
    module subroutine compare_test_results (u_test, u_log, name, success)
        integer, intent(in) :: u_test
        integer, intent(in) :: u_log
        character(*), intent(in) :: name
        logical, intent(out) :: success

        integer :: u_ref, u_err
        logical :: exist
        character(256) :: buffer1, buffer2
        integer :: iostat1, iostat2

        inquire (file=ref_prefix//name//ref, exist=exist)
        if (exist) then
            open (newunit = u_ref, file=ref_prefix//name//ref, &
                status="old", action="read")
            COMPARE_FILES: do
                read (u_test, "(A)", iostat=iostat1) buffer1
                read (u_ref, "(A)", iostat=iostat2) buffer2
                if (iostat1 /= iostat2) then
                    success = .false.
                    exit COMPARE_FILES
                else if (iostat1 < 0) then
                    success = .true.
                    exit COMPARE_FILES
                else if (buffer1 /= buffer2) then
                    success = .false.
                    exit COMPARE_FILES
                end if
            end do COMPARE_FILES
            close (u_ref)
        else
            write (*, "(A)", advance="no") " ... no reference output available"
            write (u_log, "(A)") " No reference output available."
            success = .false.
        end if
        if (success) then

```

```

        write (*, "(A)") " ... success."
        write (u_log, "(A)") " Success."
    else
        write (*, "(A)") " ... failure. See: " // err_prefix//name//err
        write (u_log, "(A)") " Failure."
        rewind (u_test)
        open (newunit = u_err, file=err_prefix//name//err, &
              action="write", status="replace")
        WRITE_OUTPUT: do
            read (u_test, "(A)", end=1) buffer1
            write (u_err, "(A)") trim (buffer1)
        end do WRITE_OUTPUT
1      close (u_err)
    end if

end subroutine compare_test_results

```

Chapter 5

System: Interfaces and Handlers

Here, we collect modules that deal with the “system”: operating-system interfaces, error handlers and diagnostics.

system_defs Constants relevant for the modules in this set.

diagnostics Error and diagnostic message handling. Any messages and errors issued by WHIZARD functions are handled by the subroutines in this module, if possible.

os_interface Execute system calls, build and link external object files and libraries.

cputime Timer data type and methods, for measuring performance.

5.1 Constants

The parameters here are used in various parts of the program, starting from the modules in the current chapter. Some of them may be modified if the need

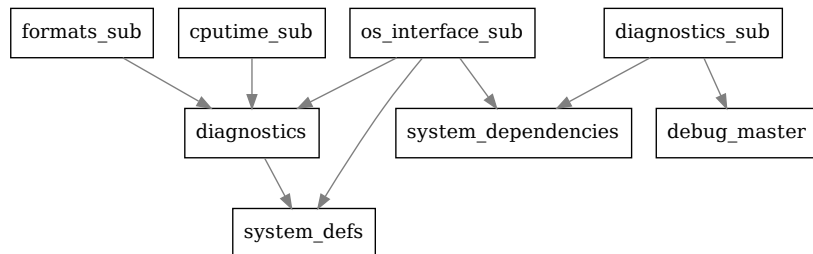


Figure 5.1: Module dependencies in `src/system`.

arises.

```
<system_defs.f90>≡  
  <File header>  
  
  module system_defs  
  
    use, intrinsic :: iso_fortran_env, only: iostat_end, iostat_eor !NODEP!  
  
    <Standard module head>  
  
    <System defs: public parameters>  
  
  end module system_defs
```

5.1.1 Version

The version string is used for checking files. Note that the string length MUST NOT be changed, because reading binary files relies on it.

```
<System defs: public parameters>≡  
  integer, parameter, public :: VERSION_STRLEN = 255  
  character(len=VERSION_STRLEN), parameter, public :: &  
    & VERSION_STRING = "WHIZARD version <Version> (<Date>)"
```

5.1.2 Text Buffer

There is a hard limit on the line length which we should export. This buffer size is used both by the message handler, the lexer, and some further modules.

```
<System defs: public parameters>+≡  
  integer, parameter, public :: BUFFER_SIZE = 1000
```

5.1.3 IOSTAT Codes

Defined in `iso_fortran_env`, but we would like to use shorthands.

```
<System defs: public parameters>+≡  
  integer, parameter, public :: EOF = iostat_end, EOR = iostat_eor
```

5.1.4 Character Codes

Single-character constants.

```
<System defs: public parameters>+≡  
  character, parameter, public :: BLANK = ' '  
  character, parameter, public :: TAB = achar(9)  
  character, parameter, public :: CR = achar(13)  
  character, parameter, public :: LF = achar(10)  
  character, parameter, public :: BACKSLASH = achar(92)
```


Character strings that indicate character classes.

```
<System defs: public parameters>+≡
    character(*), parameter, public :: WHITESPACE_CHARS = BLANK// TAB // CR // LF
    character(*), parameter, public :: LCLETTERS = "abcdefghijklmnopqrstuvwxyz"
    character(*), parameter, public :: UCLETTERS = "ABCDEFGHIJKLMNOPQRSTUVWXYZ"
    character(*), parameter, public :: DIGIT_CHARS = "0123456789"
```

5.2 C wrapper for sigaction

This implements calls to `sigaction` and the appropriate signal handlers in C. The functionality is needed for the `diagnostics` module.

```
<signal_interface.c>≡
/*
<File header>
*/
#include <signal.h>
#include <stdlib.h>

extern int wo_sigint;
extern int wo_sigterm;
extern int wo_sigxcpu;
extern int wo_sigxfsz;

static void wo_handler_sigint (int sig) {
    wo_sigint = sig;
}

static void wo_handler_sigterm (int sig) {
    wo_sigterm = sig;
}

static void wo_handler_sigxcpu (int sig) {
    wo_sigxcpu = sig;
}

static void wo_handler_sigxfsz (int sig) {
    wo_sigxfsz = sig;
}

int wo_mask_sigint () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = wo_handler_sigint;
    return sigaction(SIGINT, &sa, NULL);
}

int wo_mask_sigterm () {
    struct sigaction sa;
```

```

    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = wo_handler_sigterm;
    return sigaction(SIGTERM, &sa, NULL);
}

int wo_mask_sigxcpu () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = wo_handler_sigxcpu;
    return sigaction(SIGXCPU, &sa, NULL);
}

int wo_mask_sigxfsz () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = wo_handler_sigxfsz;
    return sigaction(SIGXFSZ, &sa, NULL);
}

int wo_release_sigint () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = SIG_DFL;
    return sigaction(SIGINT, &sa, NULL);
}

int wo_release_sigterm () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = SIG_DFL;
    return sigaction(SIGTERM, &sa, NULL);
}

int wo_release_sigxcpu () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;

```

```

    sa.sa_handler = SIG_DFL;
    return sigaction(SIGXCPU, &sa, NULL);
}

int wo_release_sigxfsz () {
    struct sigaction sa;
    sigset_t blocks;
    sigfillset (&blocks);
    sa.sa_flags = 0;
    sa.sa_mask = blocks;
    sa.sa_handler = SIG_DFL;
    return sigaction(SIGXFSZ, &sa, NULL);
}

```

5.3 C wrapper for printf

The `printf` family of functions is implemented in C with an undefined number of arguments. This is not supported by the `bind(C)` interface. We therefore write wrappers for the versions of `sprintf` that we will actually use.

This is used by the `formats` module.

```

⟨sprintf_interface.c⟩≡
/*
  ⟨File header⟩
*/
#include <stdio.h>

int sprintf_none(char* str, const char* format) {
    return sprintf(str, format);
}

int sprintf_int(char* str, const char* format, int val) {
    return sprintf(str, format, val);
}

int sprintf_double(char* str, const char* format, double val) {
    return sprintf(str, format, val);
}

int sprintf_str(char* str, const char* format, const char* val) {
    return sprintf(str, format, val);
}

⟨sprintf interfaces⟩≡
interface
    function sprintf_none (str, fmt) result (stat) bind(C)
        use iso_c_binding !NODEP!
        integer(c_int) :: stat
        character(c_char), dimension(*), intent(inout) :: str
        character(c_char), dimension(*), intent(in) :: fmt
    end function sprintf_none
end interface

```

```

interface
  function sprintf_int (str, fmt, val) result (stat) bind(C)
    use iso_c_binding !NODEP!
    integer(c_int) :: stat
    character(c_char), dimension(*), intent(inout) :: str
    character(c_char), dimension(*), intent(in) :: fmt
    integer(c_int), value :: val
  end function sprintf_int
end interface

interface
  function sprintf_double (str, fmt, val) result (stat) bind(C)
    use iso_c_binding !NODEP!
    integer(c_int) :: stat
    character(c_char), dimension(*), intent(inout) :: str
    character(c_char), dimension(*), intent(in) :: fmt
    real(c_double), value :: val
  end function sprintf_double
end interface

interface
  function sprintf_str(str, fmt, val) result (stat) bind(C)
    use iso_c_binding !NODEP!
    integer(c_int) :: stat
    character(c_char), dimension(*), intent(inout) :: str
    character(c_char), dimension(*), intent(in) :: fmt
    character(c_char), dimension(*), intent(in) :: val
  end function sprintf_str
end interface

```

5.4 Error, Message and Signal Handling

We are not so ambitious as to do proper exception handling in WHIZARD, but at least it may be useful to have a common interface for diagnostics: Results, messages, warnings, and such. As module variables we keep a buffer where the current message may be written to and a level indicator which tells which messages should be written on screen and which ones should be skipped. Alternatively, a string may be directly supplied to the message routine: this overrides the buffer, avoiding the necessity of formatted I/O in trivial cases.

```

<diagnostics.f90>≡
  <File header>

  module diagnostics

    use, intrinsic :: iso_c_binding !NODEP!

    <Use kinds>
    <Use strings>

    use system_defs, only: BUFFER_SIZE, MAX_ERRORS

```

```

    <Standard module head>

    <Diagnostics: public>

    <Diagnostics: parameters>

    <Diagnostics: types>

    <Diagnostics: variables>

    <Diagnostics: interfaces>

    interface
    <Diagnostics: sub interfaces>
    end interface

end module diagnostics

    <Diagnostics: external procedures>

<diagnostics_sub.f90>≡
    <File header>

    submodule (diagnostics) diagnostics_s

        use, intrinsic :: iso_fortran_env, only: output_unit !NODEP!

        use system_dependencies
    <Use debug>
        use string_utils, only: str
        use io_units

        implicit none

    contains

    <Diagnostics: procedures>

end submodule diagnostics_s

```

Diagnostics levels:

```

<Diagnostics: public>≡
    public :: RESULT, DEBUG, DEBUG2

<Diagnostics: parameters>≡
    integer, parameter :: TERMINATE=-2, BUG=-1, FATAL=1, &
        ERROR=2, WARNING=3, MESSAGE=4, RESULT=5, &
        DEBUG=6, DEBUG2=7

```

Diagnostics areas:

```

<Diagnostics: public>+≡
    public :: d_area

<Diagnostics: interfaces>≡
    interface d_area

```

```

        module procedure d_area_of_string
        module procedure d_area_to_string
    end interface

    <Diagnostics: sub interfaces>≡
        module function d_area_of_string (string) result (i)
            integer :: i
            type(string_t), intent(in) :: string
        end function d_area_of_string

        elemental module function d_area_to_string (i) result (string)
            type(string_t) :: string
            integer, intent(in) :: i
        end function d_area_to_string

    <Diagnostics: procedures>≡
        module function d_area_of_string (string) result (i)
            integer :: i
            type(string_t), intent(in) :: string
            select case (char (string))
            case ("particles")
                i = D_PARTICLES
            case ("events")
                i = D_EVENTS
            case ("shower")
                i = D_SHOWER
            case ("model_features")
                i = D_MODEL_F
            case ("matching")
                i = D_MATCHING
            case ("transforms")
                i = D_TRANSFORMS
            case ("subtraction")
                i = D_SUBTRACTION
            case ("virtual")
                i = D_VIRTUAL
            case ("threshold")
                i = D_THRESHOLD
            case ("phasespace")
                i = D_PHASESPACE
            case ("mismatch")
                i = D_MISMATCH
            case ("me_methods")
                i = D_ME_METHODS
            case ("process_integration")
                i = D_PROCESS_INTEGRATION
            case ("tauola")
                i = D_TAUOLA
            case ("core")
                i = D_CORE
            case ("vamp2")
                i = D_VAMP2
            case ("mpi")
                i = D_MPI
            case ("qft")

```

```

        i = D_QFT
    case ("beams")
        i = D_BEAMS
    case ("real")
        i = D_REAL
    case ("flavor")
        i = D_FLAVOR
    case ("all")
        i = D_ALL
    case default
        print "(A)", "Possible values for -debug are:"
        do i = 0, D_LAST
            print "(A)", char (' ' // d_area_to_string(i))
        end do
        call msg_fatal ("Please use one of the listed areas")
    end select
end function d_area_of_string

elemental module function d_area_to_string (i) result (string)
    type(string_t) :: string
    integer, intent(in) :: i
    select case (i)
    case (D_PARTICLES)
        string = "particles"
    case (D_EVENTS)
        string = "events"
    case (D_SHOWER)
        string = "shower"
    case (D_MODEL_F)
        string = "model_features"
    case (D_MATCHING)
        string = "matching"
    case (D_TRANSFORMS)
        string = "transforms"
    case (D_SUBTRACTION)
        string = "subtraction"
    case (D_VIRTUAL)
        string = "virtual"
    case (D_THRESHOLD)
        string = "threshold"
    case (D_PHASESPACE)
        string = "phasespace"
    case (D_MISMATCH)
        string = "mismatch"
    case (D_ME_METHODS)
        string = "me_methods"
    case (D_PROCESS_INTEGRATION)
        string = "process_integration"
    case (D_TAUOLA)
        string = "tauola"
    case (D_CORE)
        string = "core"
    case (D_VAMP2)
        string = "vamp2"
    end select
end function d_area_to_string

```

```

case (D_MPI)
  string = "mpi"
case (D_QFT)
  string = "qft"
case (D_BEAMS)
  string = "beams"
case (D_REAL)
  string = "real"
case (D_FLAVOR)
  string = "flavor"
case (D_ALL)
  string = "all"
case default
  string = "undefined"
end select
end function d_area_to_string

```

<Diagnostics: public>+≡

```

public :: D_PARTICLES, D_EVENTS, D_SHOWER, D_MODEL_F, &
  D_MATCHING, D_TRANSFORMS, D_SUBTRACTION, D_VIRTUAL, D_THRESHOLD, &
  D_PHASESPACE, D_MISMATCH, D_ME_METHODS, D_PROCESS_INTEGRATION, &
  D_TAUOLA, D_CORE, D_VAMP2, D_MPI, D_QFT, D_BEAMS, D_REAL, D_FLAVOR

```

<Diagnostics: parameters>+≡

```

integer, parameter :: D_ALL=0, D_PARTICLES=1, D_EVENTS=2, &
  D_SHOWER=3, D_MODEL_F=4, &
  D_MATCHING=5, D_TRANSFORMS=6, &
  D_SUBTRACTION=7, D_VIRTUAL=8, D_THRESHOLD=9, D_PHASESPACE=10, &
  D_MISMATCH=11, D_ME_METHODS=12, D_PROCESS_INTEGRATION=13, &
  D_TAUOLA=14, D_CORE=15, D_VAMP2 = 16, D_MPI = 17, D_QFT = 18, &
  D_BEAMS=19, D_REAL=20, D_FLAVOR=21, D_LAST=21

```

<Diagnostics: public>+≡

```

public :: msg_level

```

<Diagnostics: variables>≡

```

integer, save, dimension(D_ALL:D_LAST) :: msg_level = RESULT

```

<Diagnostics: parameters>+≡

```

integer, parameter, public :: COL_UNDEFINED = -1
integer, parameter, public :: COL_GREY = 90, COL_PEACH = 91, COL_LIGHT_GREEN = 92, &
  COL_LIGHT_YELLOW = 93, COL_LIGHT_BLUE = 94, COL_PINK = 95, &
  COL_LIGHT_AQUA = 96, COL_PEARL_WHITE = 97, COL_BLACK = 30, &
  COL_RED = 31, COL_GREEN = 32, COL_YELLOW = 33, COL_BLUE = 34, &
  COL_PURPLE = 35, COL_AQUA = 36

```

<Diagnostics: public>+≡

```

public :: set_debug_levels

```

<Diagnostics: sub interfaces>+≡

```

module subroutine set_debug_levels (area_str)
  type(string_t), intent(in) :: area_str
end subroutine set_debug_levels

```



```

<Diagnostics: procedures>+≡
  module subroutine set_debug_levels (area_str)
    type(string_t), intent(in) :: area_str
    integer :: area
    if (.not. debug_on) call msg_fatal ("Debugging options &
      &can be used only if configured with -enable-fc-debug")
    area = d_area (area_str)
    if (area == D_ALL) then
      msg_level = DEBUG
    else
      msg_level(area) = DEBUG
    end if
  end subroutine set_debug_levels

<Diagnostics: public>+≡
  public :: set_debug2_levels

<Diagnostics: sub interfaces>+≡
  module subroutine set_debug2_levels (area_str)
    type(string_t), intent(in) :: area_str
  end subroutine set_debug2_levels

<Diagnostics: procedures>+≡
  module subroutine set_debug2_levels (area_str)
    type(string_t), intent(in) :: area_str
    integer :: area
    if (.not. debug_on) call msg_fatal ("Debugging options &
      &can be used only if configured with -enable-fc-debug")
    area = d_area (area_str)
    if (area == D_ALL) then
      msg_level = DEBUG2
    else
      msg_level(area) = DEBUG2
    end if
  end subroutine set_debug2_levels

<Diagnostics: types>≡
  type :: terminal_color_t
    integer :: color = COL_UNDEFINED
  contains
    <Diagnostics: terminal color: TBP>
  end type terminal_color_t

<Diagnostics: public>+≡
  public :: term_col

<Diagnostics: interfaces>+≡
  interface term_col
    module procedure term_col_int
    module procedure term_col_char
  end interface term_col

```

<Diagnostics: sub interfaces>+≡

```
module function term_col_int (col_int) result (color)
  type (terminal_color_t) :: color
  integer, intent(in) :: col_int
end function term_col_int

module function term_col_char (col_char) result (color)
  type (terminal_color_t) :: color
  character(len=*), intent(in) :: col_char
end function term_col_char
```

<Diagnostics: procedures>+≡

```
module function term_col_int (col_int) result (color)
  type (terminal_color_t) :: color
  integer, intent(in) :: col_int
  color%color = col_int
end function term_col_int

module function term_col_char (col_char) result (color)
  type (terminal_color_t) :: color
  character(len=*), intent(in) :: col_char
  type (string_t) :: buf
  select case (col_char)
  case ('Grey')
    color%color = COL_GREY
  case ('Peach')
    color%color = COL_PEACH
  case ('Light Green')
    color%color = COL_LIGHT_GREEN
  case ('Light Yellow')
    color%color = COL_LIGHT_YELLOW
  case ('Light Blue')
    color%color = COL_LIGHT_BLUE
  case ('Pink')
    color%color = COL_PINK
  case ('Light Aqua')
    color%color = COL_LIGHT_AQUA
  case ('Pearl White')
    color%color = COL_PEARL_WHITE
  case ('Black')
    color%color = COL_BLACK
  case ('Red')
    color%color = COL_RED
  case ('Green')
    color%color = COL_GREEN
  case ('Yellow')
    color%color = COL_YELLOW
  case ('Blue')
    color%color = COL_BLUE
  case ('Purple')
    color%color = COL_PURPLE
  case ('Aqua')
    color%color = COL_AQUA
  case default
    buf = var_str ('Color ') // var_str (col_char) // var_str (' is not defined')
```

```

        call msg_warning (char (buf))
        color%color = COL_UNDEFINED
    end select
end function term_col_char

```

Mask fatal errors so that are treated as normal errors. Useful for interactive mode.

```

<Diagnostics: public>+≡
    public :: mask_fatal_errors

<Diagnostics: variables>+≡
    logical, save :: mask_fatal_errors = .false.

```

How to handle bugs and unmasked fatal errors. Either execute a normal stop statement, or call the C `exit()` function, or try to cause a program crash by dereferencing a null pointer.

These procedures are appended to the `diagnostics` source code, but not as module procedures but as external procedures. This avoids a circular module dependency across source directories.

```

<Diagnostics: parameters>+≡
    integer, parameter, public :: TERM_STOP = 0, TERM_EXIT = 1, TERM_CRASH = 2

<Diagnostics: public>+≡
    public :: handle_fatal_errors

<Diagnostics: variables>+≡
    integer, save :: handle_fatal_errors = TERM_EXIT

<Diagnostics: external procedures>≡
    subroutine fatal_force_crash ()
        use diagnostics, only: handle_fatal_errors, TERM_CRASH !NODEP!
        implicit none
        handle_fatal_errors = TERM_CRASH
    end subroutine fatal_force_crash

    subroutine fatal_force_exit ()
        use diagnostics, only: handle_fatal_errors, TERM_EXIT !NODEP!
        implicit none
        handle_fatal_errors = TERM_EXIT
    end subroutine fatal_force_exit

    subroutine fatal_force_stop ()
        use diagnostics, only: handle_fatal_errors, TERM_STOP !NODEP!
        implicit none
        handle_fatal_errors = TERM_STOP
    end subroutine fatal_force_stop

```

Keep track of errors. This might be used for exception handling, later. The counter is incremented only for screen messages, to avoid double counting.

```

<Diagnostics: public>+≡
    public :: msg_count

<Diagnostics: variables>+≡
    integer, dimension(TERMINATE:WARNING), save :: msg_count = 0

```

Keep a list of all errors and warnings. Since we do not know the number of entries beforehand, we use a linked list.

```

(Diagnostics: types)+≡
  type :: string_list
    character(len=BUFFER_SIZE) :: string
    type(string_list), pointer :: next
  end type string_list
  type :: string_list_pointer
    type(string_list), pointer :: first, last
  end type string_list_pointer

```

```

(Diagnostics: variables)+≡
  type(string_list_pointer), dimension(TERMINATE:WARNING), save :: &
    & msg_list = string_list_pointer (null(), null())

```

Create a format string indicating color

Add the current message buffer contents to the internal list.

```

(Diagnostics: procedures)+≡
  subroutine msg_add (level)
    integer, intent(in) :: level
    type(string_list), pointer :: message
    select case (level)
    case (TERMINATE:WARNING)
      allocate (message)
      message%string = msg_buffer
      nullify (message%next)
      if (.not.associated (msg_list(level)%first)) &
        & msg_list(level)%first => message
      if (associated (msg_list(level)%last)) &
        & msg_list(level)%last%next => message
      msg_list(level)%last => message
      msg_count(level) = msg_count(level) + 1
    end select
  end subroutine msg_add

```

Initialization:

```

(Diagnostics: public)+≡
  public :: msg_list_clear

(Diagnostics: sub interfaces)+≡
  module subroutine msg_list_clear
  end subroutine msg_list_clear

(Diagnostics: procedures)+≡
  module subroutine msg_list_clear
    integer :: level
    type(string_list), pointer :: message
    do level = TERMINATE, WARNING
      do while (associated (msg_list(level)%first))
        message => msg_list(level)%first
        msg_list(level)%first => message%next
        deallocate (message)
      end do
      nullify (msg_list(level)%last)
    end do
  end module msg_list_clear

```

```

end do
msg_count = 0
end subroutine msg_list_clear

```

Display the summary of errors and warnings (no need to count fatals...)

```

<Diagnostics: public>+≡
public :: msg_summary

<Diagnostics: sub interfaces>+≡
module subroutine msg_summary (unit)
integer, intent(in), optional :: unit
end subroutine msg_summary

<Diagnostics: procedures>+≡
module subroutine msg_summary (unit)
integer, intent(in), optional :: unit
call expect_summary (unit)
1  format (A,1x,I2,1x,A,I2,1x,A)
if (msg_count(ERROR) > 0 .and. msg_count(WARNING) > 0) then
write (msg_buffer, 1) "There were", &
& msg_count(ERROR), "error(s) and ", &
& msg_count(WARNING), "warning(s). "
call msg_message (unit=unit)
else if (msg_count(ERROR) > 0) then
write (msg_buffer, 1) "There were", &
& msg_count(ERROR), "error(s) and no warnings."
call msg_message (unit=unit)
else if (msg_count(WARNING) > 0) then
write (msg_buffer, 1) "There were no errors and ", &
& msg_count(WARNING), "warning(s). "
call msg_message (unit=unit)
end if
end subroutine msg_summary

```

Print the list of all messages of a given level.

```

<Diagnostics: public>+≡
public :: msg_listing

<Diagnostics: sub interfaces>+≡
module subroutine msg_listing (level, unit, prefix)
integer, intent(in) :: level
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: prefix
end subroutine msg_listing

<Diagnostics: procedures>+≡
module subroutine msg_listing (level, unit, prefix)
integer, intent(in) :: level
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: prefix
type(string_list), pointer :: message
integer :: u
u = given_output_unit (unit); if (u < 0) return
if (present (unit)) u = unit
message => msg_list(level)%first

```

```

do while (associated (message))
  if (present (prefix)) then
    write (u, "(A)") prefix // trim (message%string)
  else
    write (u, "(A)") trim (message%string)
  end if
  message => message%next
end do
flush (u)
end subroutine msg_listing

```

The message buffer:

```

<Diagnostics: public>+≡
  public :: msg_buffer

<Diagnostics: variables>+≡
  character(len=BUFFER_SIZE), save :: msg_buffer = " "

```

After a message is issued, the buffer should be cleared:

```

<Diagnostics: procedures>+≡
  subroutine buffer_clear
    msg_buffer = " "
  end subroutine buffer_clear

<Diagnostics: public>+≡
  public :: create_col_string

<Diagnostics: sub interfaces>+≡
  module function create_col_string (color) result (col_string)
    type(string_t) :: col_string
    integer, intent(in) :: color
  end function create_col_string

<Diagnostics: procedures>+≡
  module function create_col_string (color) result (col_string)
    type(string_t) :: col_string
    integer, intent(in) :: color
    character(2) :: buf
    write (buf, '(I2)') color
    col_string = var_str ("[" // var_str (buf) // var_str ("m")
  end function create_col_string

```

The generic handler for messages. If the unit is omitted (or = 6), the message is written to standard output if the precedence is sufficiently high (as determined by the value of `msg_level`). If the string is omitted, the buffer is used. In any case, the buffer is cleared after printing. In accordance with FORTRAN custom, the first column in the output is left blank. For messages and warnings, an additional exclamation mark and a blank is prepended. Furthermore, each message is appended to the internal message list (without prepending anything).

```

<Diagnostics: procedures>+≡
  subroutine message_print (level, string, str_arr, unit, logfile, area, color)
    integer, intent(in) :: level
    character(len=*), intent(in), optional :: string
    type(string_t), dimension(:), intent(in), optional :: str_arr

```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: logfile
integer, intent(in), optional :: area
integer, intent(in), optional :: color
type(string_t) :: col_string, prep_string, aux_string, head_footer, app_string
integer :: lu, i, ar
logical :: severe, is_error
ar = D_ALL; if (present (area)) ar = area
severe = .false.
head_footer = "*****"
aux_string = ""
is_error = .false.
app_string = ""
select case (level)
case (TERMINATE)
    prep_string = ""
case (BUG)
    prep_string = "*** WHIZARD BUG: "
    aux_string = "*** "
    severe = .true.
    is_error = .true.
case (FATAL)
    prep_string = "*** FATAL ERROR: "
    aux_string = "*** "
    severe = .true.
    is_error = .true.
case (ERROR)
    prep_string = "*** ERROR: "
    aux_string = "*** "
    is_error = .true.
case (WARNING)
    prep_string = "Warning: "
case (MESSAGE)
    prep_string = "| "
case (DEBUG, DEBUG2)
    prep_string = "D: "
case default
    prep_string = ""
end select
if (present (color)) then
    if (color > COL_UNDEFINED) then
        col_string = create_col_string (color)
        prep_string = achar(27) // col_string // prep_string
        app_string = app_string // achar(27) // "[0m"
    end if
end if
if (present(string)) msg_buffer = string
lu = log_unit
if (present(unit)) then
    if (unit /= output_unit) then
        if (severe) write (unit, "(A)") char(head_footer)
        if (is_error) write (unit, "(A)") char(head_footer)
        write (unit, "(A,A,A)") char(prep_string), trim(msg_buffer), &
            char(app_string)
    end if
end if

```

```

        if (present (str_arr)) then
            do i = 1, size(str_arr)
                write (unit, "(A,A)") char(aux_string), char(trim(str_arr(i)))
            end do
        end if
        if (is_error) write (unit, "(A)") char(head_footer)
        if (severe) write (unit, "(A)") char(head_footer)
        flush (unit)
        lu = -1
    else if (level <= msg_level(ar)) then
        if (severe) print "(A)", char(head_footer)
        if (is_error) print "(A)", char(head_footer)
        print "(A,A,A)", char(prepare_string), trim(msg_buffer), &
            char(app_string)
        if (present (str_arr)) then
            do i = 1, size(str_arr)
                print "(A,A)", char(aux_string), char(trim(str_arr(i)))
            end do
        end if
        if (is_error) print "(A)", char(head_footer)
        if (severe) print "(A)", char(head_footer)
        flush (output_unit)
        if (unit == log_unit) lu = -1
    end if
    else if (level <= msg_level(ar)) then
        if (severe) print "(A)", char(head_footer)
        if (is_error) print "(A)", char(head_footer)
        print "(A,A,A)", char(prepare_string), trim(msg_buffer), &
            char(app_string)
        if (present (str_arr)) then
            do i = 1, size(str_arr)
                print "(A,A)", char(aux_string), char(trim(str_arr(i)))
            end do
        end if
        if (is_error) print "(A)", char(head_footer)
        if (severe) print "(A)", char(head_footer)
        flush (output_unit)
    end if
    if (present (logfile)) then
        if (.not. logfile) lu = -1
    end if
    if (logging .and. lu >= 0) then
        if (severe) write (lu, "(A)") char(head_footer)
        if (is_error) write (lu, "(A)") char(head_footer)
        write (lu, "(A,A,A)") char(prepare_string), trim(msg_buffer), &
            char(app_string)
        if (present (str_arr)) then
            do i = 1, size(str_arr)
                write (lu, "(A,A)") char(aux_string), char(trim(str_arr(i)))
            end do
        end if
        if (is_error) write (lu, "(A)") char(head_footer)
        if (severe) write (lu, "(A)") char(head_footer)
        flush (lu)
    end if

```



```

end if
call msg_add (level)
call buffer_clear
end subroutine message_print

```

The number of non-fatal errors that we allow before stopping the program. We might trade this later for an adjustable number.

```

<System defs: public parameters>+≡
integer, parameter, public :: MAX_ERRORS = 10

```

The specific handlers. In the case of fatal errors, bugs (failed assertions) and normal termination execution is stopped. For non-fatal errors a message is printed to standard output if no unit is given. Only if the number of MAX_ERRORS errors is reached, we abort the program. There are no further actions in the other cases, but this may change.

```

<Diagnostics: public>+≡
public :: msg_terminate
public :: msg_bug, msg_fatal, msg_error, msg_warning
public :: msg_message, msg_result

<Diagnostics: sub interfaces>+≡
module subroutine msg_terminate (string, unit, quit_code)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
integer, intent(in), optional :: quit_code
end subroutine msg_terminate

module subroutine msg_bug (string, arr, unit)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
end subroutine msg_bug

recursive module subroutine msg_fatal (string, arr, unit)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
end subroutine msg_fatal

module subroutine msg_error (string, arr, unit)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
end subroutine msg_error

module subroutine msg_warning (string, arr, unit, color)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
type(terminal_color_t), intent(in), optional :: color
end subroutine msg_warning

module subroutine msg_message (string, unit, arr, logfile, color)
integer, intent(in), optional :: unit

```

```

character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
logical, intent(in), optional :: logfile
type(terminal_color_t), intent(in), optional :: color
end subroutine msg_message

```

```

module subroutine msg_result (string, arr, unit, logfile, color)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
logical, intent(in), optional :: logfile
type(terminal_color_t), intent(in), optional :: color
end subroutine msg_result

```

(Diagnostics: procedures)+≡

```

module subroutine msg_terminate (string, unit, quit_code)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
integer, intent(in), optional :: quit_code
integer(c_int) :: return_code
call release_term_signals ()
if (present (quit_code)) then
return_code = quit_code
else
return_code = 0
end if
if (present (string)) &
call message_print (MESSAGE, string, unit=unit)
call msg_summary (unit)
if (return_code == 0 .and. expect_failures /= 0) then
return_code = 5
call message_print (MESSAGE, &
"WHIZARD run finished with 'expect' failure(s).", unit=unit)
else if (return_code == 7) then
call message_print (MESSAGE, &
"WHIZARD run finished with failed self-test.", unit=unit)
else
call message_print (MESSAGE, "WHIZARD run finished.", unit=unit)
end if
call message_print (0, &
"|=====|", unit=u
call logfile_final ()
call msg_list_clear ()
if (return_code /= 0) then
call exit (return_code)
else
!!! Should implement WHIZARD exit code (currently only via C)
call exit (0)
end if
end subroutine msg_terminate

module subroutine msg_bug (string, arr, unit)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr

```

```

logical, pointer :: crash_ptr
call message_print (BUG, string, arr, unit)
call msg_summary (unit)
select case (handle_fatal_errors)
case (TERM_EXIT)
    call message_print (TERMINATE, "WHIZARD run aborted.", unit=unit)
    call exit (-1_c_int)
case (TERM_CRASH)
    print *, "*** Intentional crash ***"
    crash_ptr => null ()
    print *, crash_ptr
end select
stop "WHIZARD run aborted."
end subroutine msg_bug

recursive module subroutine msg_fatal (string, arr, unit)
    integer, intent(in), optional :: unit
    character(len=*), intent(in), optional :: string
    type(string_t), dimension(:), intent(in), optional :: arr
    logical, pointer :: crash_ptr
    if (mask_fatal_errors) then
        call msg_error (string, arr, unit)
    else
        call message_print (FATAL, string, arr, unit)
        call msg_summary (unit)
        select case (handle_fatal_errors)
        case (TERM_EXIT)
            call message_print (TERMINATE, "WHIZARD run aborted.", unit=unit)
            call exit (1_c_int)
        case (TERM_CRASH)
            print *, "*** Intentional crash ***"
            crash_ptr => null ()
            print *, crash_ptr
        end select
        stop "WHIZARD run aborted."
    end if
end subroutine msg_fatal

module subroutine msg_error (string, arr, unit)
    integer, intent(in), optional :: unit
    character(len=*), intent(in), optional :: string
    type(string_t), dimension(:), intent(in), optional :: arr
    call message_print (ERROR, string, arr, unit)
    if (msg_count(ERROR) >= MAX_ERRORS) then
        mask_fatal_errors = .false.
        call msg_fatal (" Too many errors encountered.")
    else if (.not.present(unit) .and. .not.mask_fatal_errors) then
        call message_print (MESSAGE, " (WHIZARD run continues)")
    end if
end subroutine msg_error

module subroutine msg_warning (string, arr, unit, color)
    integer, intent(in), optional :: unit
    character(len=*), intent(in), optional :: string

```

```

type(string_t), dimension(:), intent(in), optional :: arr
type(terminal_color_t), intent(in), optional :: color
integer :: cl
cl = COL_UNDEFINED; if (present (color)) cl = color%color
call message_print (level = WARNING, string = string, &
    str_arr = arr, unit = unit, color = cl)
end subroutine msg_warning

module subroutine msg_message (string, unit, arr, logfile, color)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
logical, intent(in), optional :: logfile
type(terminal_color_t), intent(in), optional :: color
integer :: cl
cl = COL_UNDEFINED; if (present (color)) cl = color%color
call message_print (level = MESSAGE, &
    string = string, str_arr = arr, unit = unit, &
    logfile = logfile, color = cl)
end subroutine msg_message

module subroutine msg_result (string, arr, unit, logfile, color)
integer, intent(in), optional :: unit
character(len=*), intent(in), optional :: string
type(string_t), dimension(:), intent(in), optional :: arr
logical, intent(in), optional :: logfile
type(terminal_color_t), intent(in), optional :: color
integer :: cl
cl = COL_UNDEFINED; if (present (color)) cl = color%color
call message_print (level = RESULT, string = string, &
    str_arr = arr, unit = unit, logfile = logfile, color = cl)
end subroutine msg_result

```

Debugging aids. Print messages or values of various kinds. All versions ultimately call `msg_debug_none`, which in turn uses `message_print`.

Safeguard: force crash if a routine (i.e., a debugging routine below) is called while the master switch `debug_on` is unset. Such calls should always be hidden behind `if (debug_on)`, since they can significantly slow down the program.

```

<debug guard>≡
if (.not. debug_on) call msg_bug ("msg_debug called with debug_on=.false.")

```

The `debug_on` flag is provided by the `debug_master` module, and we can assume that it is a compile-time parameter.

```

<Diagnostics: public>+≡
public :: msg_debug

<Diagnostics: interfaces>+≡
interface msg_debug
module procedure msg_debug_none
module procedure msg_debug_logical
module procedure msg_debug_integer
module procedure msg_debug_real
module procedure msg_debug_complex
module procedure msg_debug_string

```

```

end interface

<Diagnostics: sub interfaces>+≡
  module subroutine msg_debug_none (area, string, color)
    integer, intent(in) :: area
    character(len=*), intent(in), optional :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_none

  module subroutine msg_debug_logical (area, string, value, color)
    logical, intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_logical

  module subroutine msg_debug_integer (area, string, value, color)
    integer, intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_integer

  module subroutine msg_debug_real (area, string, value, color)
    real(default), intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_real

  module subroutine msg_debug_complex (area, string, value, color)
    complex(default), intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_complex

  module subroutine msg_debug_string (area, string, value, color)
    type(string_t), intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug_string

<Diagnostics: procedures>+≡
  module subroutine msg_debug_none (area, string, color)
    integer, intent(in) :: area
    character(len=*), intent(in), optional :: string
    type(terminal_color_t), intent(in), optional :: color
    integer :: cl
    if (debug_active (area)) then
      cl = COL_BLUE; if (present (color)) cl = color%color
      call message_print (DEBUG, string, unit = output_unit, &
        area = area, logfile = .false., color = cl)
    else

```

```

        <debug guard>
    end if
end subroutine msg_debug_none

module subroutine msg_debug_logical (area, string, value, color)
    logical, intent(in) :: value
    <msg debug implementation>
end subroutine msg_debug_logical

module subroutine msg_debug_integer (area, string, value, color)
    integer, intent(in) :: value
    <msg debug implementation>
end subroutine msg_debug_integer

module subroutine msg_debug_real (area, string, value, color)
    real(default), intent(in) :: value
    <msg debug implementation>
end subroutine msg_debug_real

module subroutine msg_debug_complex (area, string, value, color)
    complex(default), intent(in) :: value
    <msg debug implementation>
end subroutine msg_debug_complex

module subroutine msg_debug_string (area, string, value, color)
    type(string_t), intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
    if (debug_active (area)) then
        call msg_debug_none (area, string // " = " // char (value), &
            color = color)
    else
        <debug guard>
    end if
end subroutine msg_debug_string

<msg debug implementation>≡
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
    character(len=64) :: buffer
    if (debug_active (area)) then
        write (buffer, *) value
        call msg_debug_none (area, string // " = " // trim (buffer), &
            color = color)
    else
        <debug guard>
    end if

<Diagnostics: public>+≡
    public :: msg_print_color

<Diagnostics: interfaces>+≡
    interface msg_print_color

```

```

        module procedure msg_print_color_none
        module procedure msg_print_color_logical
        module procedure msg_print_color_integer
        module procedure msg_print_color_real
    end interface
    <Diagnostics: sub interfaces>+≡
        module subroutine msg_print_color_none (string, color)
            character(len=*), intent(in) :: string
            !!!type(terminal_color_t), intent(in) :: color
            integer, intent(in) :: color
        end subroutine msg_print_color_none

        module subroutine msg_print_color_logical (string, value, color)
            character(len=*), intent(in) :: string
            logical, intent(in) :: value
            integer, intent(in) :: color
        end subroutine msg_print_color_logical

        module subroutine msg_print_color_integer (string, value, color)
            character(len=*), intent(in) :: string
            integer, intent(in) :: value
            integer, intent(in) :: color
        end subroutine msg_print_color_integer

        module subroutine msg_print_color_real (string, value, color)
            character(len=*), intent(in) :: string
            real(default), intent(in) :: value
            integer, intent(in) :: color
        end subroutine msg_print_color_real
    <Diagnostics: procedures>+≡
        module subroutine msg_print_color_none (string, color)
            character(len=*), intent(in) :: string
            !!!type(terminal_color_t), intent(in) :: color
            integer, intent(in) :: color
            call message_print (0, string, color = color)
        end subroutine msg_print_color_none

        module subroutine msg_print_color_logical (string, value, color)
            character(len=*), intent(in) :: string
            logical, intent(in) :: value
            integer, intent(in) :: color
            call msg_print_color_none (char (string // " = " // str (value)), &
                color = color)
        end subroutine msg_print_color_logical

        module subroutine msg_print_color_integer (string, value, color)
            character(len=*), intent(in) :: string
            integer, intent(in) :: value
            integer, intent(in) :: color
            call msg_print_color_none (char (string // " = " // str (value)), &
                color = color)
        end subroutine msg_print_color_integer

```

```

module subroutine msg_print_color_real (string, value, color)
  character(len=*), intent(in) :: string
  real(default), intent(in) :: value
  integer, intent(in) :: color
  call msg_print_color_none (char (string // " = " // str (value)), &
    color = color)
end subroutine msg_print_color_real

```

Secondary debugging aids which implement more fine-grained debugging. Again, there is a safeguard against calling anything while `debug_on=.false..`

```

<debug2 guard>≡
  if (.not. debug_on) call msg_bug ("msg_debug2 called with debug_on=.false.")

<Diagnostics: public>+≡
  public :: msg_debug2

<Diagnostics: interfaces>+≡
  interface msg_debug2
    module procedure msg_debug2_none
    module procedure msg_debug2_logical
    module procedure msg_debug2_integer
    module procedure msg_debug2_real
    module procedure msg_debug2_complex
    module procedure msg_debug2_string
  end interface

<Diagnostics: sub interfaces>+≡
  module subroutine msg_debug2_none (area, string, color)
    integer, intent(in) :: area
    character(len=*), intent(in), optional :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug2_none

  module subroutine msg_debug2_logical (area, string, value, color)
    logical, intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug2_logical

  module subroutine msg_debug2_integer (area, string, value, color)
    integer, intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug2_integer

  module subroutine msg_debug2_real (area, string, value, color)
    real(default), intent(in) :: value
    integer, intent(in) :: area
    character(len=*), intent(in) :: string
    type(terminal_color_t), intent(in), optional :: color
  end subroutine msg_debug2_real

  module subroutine msg_debug2_complex (area, string, value, color)

```



```

        complex(default), intent(in) :: value
        integer, intent(in) :: area
        character(len=*), intent(in) :: string
        type(terminal_color_t), intent(in), optional :: color
    end subroutine msg_debug2_complex

    module subroutine msg_debug2_string (area, string, value, color)
        type(string_t), intent(in) :: value
        integer, intent(in) :: area
        character(len=*), intent(in) :: string
        type(terminal_color_t), intent(in), optional :: color
    end subroutine msg_debug2_string

    <Diagnostics: procedures>+≡
    module subroutine msg_debug2_none (area, string, color)
        integer, intent(in) :: area
        character(len=*), intent(in), optional :: string
        type(terminal_color_t), intent(in), optional :: color
        integer :: c1
        if (debug2_active (area)) then
            c1 = COL_BLUE; if (present (color)) c1 = color%color
            call message_print (DEBUG2, string, unit = output_unit, &
                area = area, logfile = .false., color = c1)
        else
            <debug2 guard>
        end if
    end subroutine msg_debug2_none

    module subroutine msg_debug2_logical (area, string, value, color)
        logical, intent(in) :: value
        <msg debug2 implementation>
    end subroutine msg_debug2_logical

    module subroutine msg_debug2_integer (area, string, value, color)
        integer, intent(in) :: value
        <msg debug2 implementation>
    end subroutine msg_debug2_integer

    module subroutine msg_debug2_real (area, string, value, color)
        real(default), intent(in) :: value
        <msg debug2 implementation>
    end subroutine msg_debug2_real

    module subroutine msg_debug2_complex (area, string, value, color)
        complex(default), intent(in) :: value
        <msg debug2 implementation>
    end subroutine msg_debug2_complex

    module subroutine msg_debug2_string (area, string, value, color)
        type(string_t), intent(in) :: value
        integer, intent(in) :: area
        character(len=*), intent(in) :: string
        type(terminal_color_t), intent(in), optional :: color
        if (debug2_active (area)) then
            call msg_debug2_none (area, string // " = " // char (value), &

```

```

        color = color)
    else
        <debug2 guard>
    end if
end subroutine msg_debug2_string

<msg debug2 implementation>≡
integer, intent(in) :: area
character(len=*), intent(in) :: string
type(terminal_color_t), intent(in), optional :: color
character(len=64) :: buffer
if (debug2_active (area)) then
    write (buffer, *) value
    call msg_debug2_none (area, string // " = " // trim (buffer), &
        color = color)
else
    <debug2 guard>
end if

<Diagnostics: public>+≡
public :: debug_active

<Diagnostics: sub interfaces>+≡
    elemental module function debug_active (area) result (active)
        logical :: active
        integer, intent(in) :: area
    end function debug_active

<Diagnostics: procedures>+≡
    elemental module function debug_active (area) result (active)
        logical :: active
        integer, intent(in) :: area
        active = debug_on .and. msg_level(area) >= DEBUG
    end function debug_active

<Diagnostics: public>+≡
public :: debug2_active

<Diagnostics: sub interfaces>+≡
    elemental module function debug2_active (area) result (active)
        logical :: active
        integer, intent(in) :: area
    end function debug2_active

<Diagnostics: procedures>+≡
    elemental module function debug2_active (area) result (active)
        logical :: active
        integer, intent(in) :: area
        active = debug_on .and. msg_level(area) >= DEBUG2
    end function debug2_active

```

Show the progress of a loop in steps of 10 %. Could be generalized to other step sizes with an optional argument.

```

<Diagnostics: public>+≡
public :: msg_show_progress

```

```

<Diagnostics: sub interfaces>+≡
  module subroutine msg_show_progress (i_call, n_calls)
    integer, intent(in) :: i_call, n_calls
  end subroutine msg_show_progress

```

Interface to the standard `clib` exit function

Print the WHIZARD banner:

[illegible]


```

<Diagnostics: public>+≡
    public :: logfile_init

<Diagnostics: sub interfaces>+≡
    module subroutine logfile_init (filename)
        type(string_t), intent(in) :: filename
    end subroutine logfile_init

<Diagnostics: procedures>+≡
    module subroutine logfile_init (filename)
        type(string_t), intent(in) :: filename
        call msg_message ("Writing log to '" // char (filename) // "'")
        if (.not. logging) call msg_message ("(Logging turned off.)")
        log_unit = free_unit ()
        open (file = char (filename), unit = log_unit, &
            action = "write", status = "replace")
    end subroutine logfile_init

<Diagnostics: public>+≡
    public :: logfile_final

<Diagnostics: sub interfaces>+≡
    module subroutine logfile_final ()
    end subroutine logfile_final

<Diagnostics: procedures>+≡
    module subroutine logfile_final ()
        if (log_unit >= 0) then
            close (log_unit)
            log_unit = -1
        end if
    end subroutine logfile_final

```

This returns the valid logfile unit only if the default is write to screen, and if logfile is not set false.

```

<Diagnostics: public>+≡
    public :: logfile_unit

<Diagnostics: sub interfaces>+≡
    module function logfile_unit (unit, logfile)
        integer :: logfile_unit
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: logfile
    end function logfile_unit

<Diagnostics: procedures>+≡
    module function logfile_unit (unit, logfile)
        integer :: logfile_unit
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: logfile
        if (logging) then
            if (present (unit)) then
                if (unit == output_unit) then
                    logfile_unit = log_unit
                else
                    logfile_unit = -1
                end if
            end if
        end if
    end function logfile_unit

```

```

        end if
    else if (present (logfile)) then
        if (logfile) then
            logfile_unit = log_unit
        else
            logfile_unit = -1
        end if
    else
        logfile_unit = log_unit
    end if
else
    logfile_unit = -1
end if
end function logfile_unit

```

5.4.2 Checking values

The `expect` function does not just check a value for correctness (actually, it checks if a logical expression is true); it records its result here. If failures are present when the program terminates, the exit code is nonzero.

```

<Diagnostics: variables>+≡
    integer, save :: expect_total = 0
    integer, save :: expect_failures = 0

<Diagnostics: public>+≡
    public :: expect_record

<Diagnostics: sub interfaces>+≡
    module subroutine expect_record (success)
        logical, intent(in) :: success
    end subroutine expect_record

<Diagnostics: procedures>+≡
    module subroutine expect_record (success)
        logical, intent(in) :: success
        expect_total = expect_total + 1
        if (.not. success) expect_failures = expect_failures + 1
    end subroutine expect_record

<Diagnostics: public>+≡
    public :: expect_clear

<Diagnostics: sub interfaces>+≡
    module subroutine expect_clear ()
    end subroutine expect_clear

<Diagnostics: procedures>+≡
    module subroutine expect_clear ()
        expect_total = 0
        expect_failures = 0
    end subroutine expect_clear

<Diagnostics: public>+≡
    public :: expect_summary

```

<Diagnostics: sub interfaces>+≡

```
module subroutine expect_summary (unit, force)
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: force
end subroutine expect_summary
```

<Diagnostics: procedures>+≡

```
module subroutine expect_summary (unit, force)
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: force
  logical :: force_output
  force_output = .false.; if (present (force)) force_output = force
  if (expect_total /= 0 .or. force_output) then
    call msg_message ("Summary of value checks:", unit)
    write (msg_buffer, "(2x,A,1x,I0,1x,A,1x,A,1x,I0)") &
      "Failures:", expect_failures, "/", "Total:", expect_total
    call msg_message (unit=unit)
  end if
end subroutine expect_summary
```

Helpers for converting integers into strings with minimal length.

<Diagnostics: public>+≡

```
public :: int2string
public :: int2char
public :: int2fixed
```

<Diagnostics: sub interfaces>+≡

```
pure module function int2fixed (i) result (c)
  integer, intent(in) :: i
  character(200) :: c
end function int2fixed
```

```
pure module function int2string (i) result (s)
  integer, intent(in) :: i
  type (string_t) :: s
end function int2string
```

```
pure module function int2char (i) result (c)
  integer, intent(in) :: i
  character(len (trim (int2fixed (i)))) :: c
end function int2char
```

<Diagnostics: procedures>+≡

```
pure module function int2fixed (i) result (c)
  integer, intent(in) :: i
  character(200) :: c
  c = ""
  write (c, *) i
  c = adjustl (c)
end function int2fixed
```

```
pure module function int2string (i) result (s)
  integer, intent(in) :: i
  type (string_t) :: s
  s = trim (int2fixed (i))
```

```

end function int2string

pure module function int2char (i) result (c)
  integer, intent(in) :: i
  character(len(trim(int2fixed(i)))) :: c
  c = int2fixed(i)
end function int2char

```

Dito for reals.

```

<Diagnostics: public>+≡
  public :: real2string
  public :: real2char
  public :: real2fixed

<Diagnostics: interfaces>+≡
  interface real2string
    module procedure real2string_list, real2string_fmt
  end interface
  interface real2char
    module procedure real2char_list, real2char_fmt
  end interface

<Diagnostics: sub interfaces>+≡
  pure module function real2fixed (x, fmt) result (c)
    real(default), intent(in) :: x
    character(*), intent(in), optional :: fmt
    character(200) :: c
  end function real2fixed

  pure module function real2fixed_fmt (x, fmt) result (c)
    real(default), intent(in) :: x
    character(*), intent(in) :: fmt
    character(200) :: c
  end function real2fixed_fmt

  pure module function real2string_list (x) result (s)
    real(default), intent(in) :: x
    type(string_t) :: s
  end function real2string_list

  pure module function real2string_fmt (x, fmt) result (s)
    real(default), intent(in) :: x
    character(*), intent(in) :: fmt
    type(string_t) :: s
  end function real2string_fmt

  pure module function real2char_list (x) result (c)
    real(default), intent(in) :: x
    character(len_trim(real2fixed(x))) :: c
  end function real2char_list

  pure module function real2char_fmt (x, fmt) result (c)
    real(default), intent(in) :: x
    character(*), intent(in) :: fmt
    character(len_trim(real2fixed_fmt(x, fmt))) :: c

```



```

        end function real2char_fmt
<Diagnostics: procedures>+≡
    pure module function real2fixed (x, fmt) result (c)
        real(default), intent(in) :: x
        character(*), intent(in), optional :: fmt
        character(200) :: c
        c = ""
        write (c, *) x
        c = adjustl (c)
    end function real2fixed

    pure module function real2fixed_fmt (x, fmt) result (c)
        real(default), intent(in) :: x
        character(*), intent(in) :: fmt
        character(200) :: c
        c = ""
        write (c, fmt) x
        c = adjustl (c)
    end function real2fixed_fmt

    pure module function real2string_list (x) result (s)
        real(default), intent(in) :: x
        type(string_t) :: s
        s = trim (real2fixed (x))
    end function real2string_list

    pure module function real2string_fmt (x, fmt) result (s)
        real(default), intent(in) :: x
        character(*), intent(in) :: fmt
        type(string_t) :: s
        s = trim (real2fixed_fmt (x, fmt))
    end function real2string_fmt

    pure module function real2char_list (x) result (c)
        real(default), intent(in) :: x
        character(len_trim (real2fixed (x))) :: c
        c = real2fixed (x)
    end function real2char_list

    pure module function real2char_fmt (x, fmt) result (c)
        real(default), intent(in) :: x
        character(*), intent(in) :: fmt
        character(len_trim (real2fixed_fmt (x, fmt))) :: c
        c = real2fixed_fmt (x, fmt)
    end function real2char_fmt

```

Dito for complex values; we do not use the slightly ugly FORTRAN output form here but instead introduce our own. Ifort and Portland seem to have problems with this, therefore temporarily disable it.

```

<CCC Diagnostics: public>≡
    public :: cmplx2string
    public :: cmplx2char

```

```

<CCC Diagnostics: procedures>≡
  pure function cmplx2string (x) result (s)
    complex(default), intent(in) :: x
    type(string_t) :: s
    s = real2string (real (x, default))
    if (aimag (x) /= 0) s = s // " + " // real2string (aimag (x)) // " I"
  end function cmplx2string

  pure function cmplx2char (x) result (c)
    complex(default), intent(in) :: x
    character(len (char (cmplx2string (x)))) :: c
    c = char (cmplx2string (x))
  end function cmplx2char

```

5.4.3 Signal handling

Killing the program by external signals may leave the files written by it in an undefined state. This can be avoided by catching signals and deferring program termination. Instead of masking only critical sections, we choose to mask signals globally (done in the main program) and terminate the program at predefined checkpoints only. Checkpoints are after each command, within the sampling function (so the program can be terminated after each event), and after each iteration in the phase-space generation algorithm.

Signal handling is done via a C interface to the `sigaction` system call. When a signal is raised that has been masked by the handler, the corresponding variable is set to the value of the signal. The variables are visible from the C signal handler.

The signal `SIGINT` is for keyboard interrupt (ctrl-C), `SIGTERM` is for system interrupt, e.g., at shutdown. The `SIGXCPU` and `SIGXFSZ` signals may be issued by batch systems.

```

<Diagnostics: public>+≡
  public :: wo_sigint
  public :: wo_sigterm
  public :: wo_sigxcpu
  public :: wo_sigxfsz

<Diagnostics: variables>+≡
  integer(c_int), bind(C), volatile :: wo_sigint = 0
  integer(c_int), bind(C), volatile :: wo_sigterm = 0
  integer(c_int), bind(C), volatile :: wo_sigxcpu = 0
  integer(c_int), bind(C), volatile :: wo_sigxfsz = 0

```

Here are the interfaces to the C functions. The routine `mask_term_signals` forces termination signals to be delayed. `release_term_signals` restores normal behavior. However, the program can be terminated anytime by calling `terminate_now_if_signal` which inspects the signals and terminates the program if requested..

```

<Diagnostics: public>+≡
  public :: mask_term_signals

```

```

<Diagnostics: sub interfaces>+≡
    module subroutine mask_term_signals ()
    end subroutine mask_term_signals

<Diagnostics: procedures>+≡
    module subroutine mask_term_signals ()
        logical :: ok
        wo_sigint = 0
        ok = wo_mask_sigint () == 0
        if (.not. ok) call msg_error ("Masking SIGINT failed")
        wo_sigterm = 0
        ok = wo_mask_sigterm () == 0
        if (.not. ok) call msg_error ("Masking SIGTERM failed")
        wo_sigxcpu = 0
        ok = wo_mask_sigxcpu () == 0
        if (.not. ok) call msg_error ("Masking SIGXCPU failed")
        wo_sigxfsz = 0
        ok = wo_mask_sigxfsz () == 0
        if (.not. ok) call msg_error ("Masking SIGXFSZ failed")
    end subroutine mask_term_signals

<Diagnostics: interfaces>+≡
    interface
        integer(c_int) function wo_mask_sigint () bind(C)
        import
    end function wo_mask_sigint
    end interface
    interface
        integer(c_int) function wo_mask_sigterm () bind(C)
        import
    end function wo_mask_sigterm
    end interface
    interface
        integer(c_int) function wo_mask_sigxcpu () bind(C)
        import
    end function wo_mask_sigxcpu
    end interface
    interface
        integer(c_int) function wo_mask_sigxfsz () bind(C)
        import
    end function wo_mask_sigxfsz
    end interface

<Diagnostics: public>+≡
    public :: release_term_signals

<Diagnostics: sub interfaces>+≡
    module subroutine release_term_signals ()
    end subroutine release_term_signals

<Diagnostics: procedures>+≡
    module subroutine release_term_signals ()
        logical :: ok
        ok = wo_release_sigint () == 0
        if (.not. ok) call msg_error ("Releasing SIGINT failed")

```

```

    ok = wo_release_sigterm () == 0
    if (.not. ok) call msg_error ("Releasing SIGTERM failed")
    ok = wo_release_sigxcpu () == 0
    if (.not. ok) call msg_error ("Releasing SIGXCPU failed")
    ok = wo_release_sigxfsz () == 0
    if (.not. ok) call msg_error ("Releasing SIGXFSZ failed")
end subroutine release_term_signals

```

<Diagnostics: interfaces>+≡

```

interface
  integer(c_int) function wo_release_sigint () bind(C)
  import
end function wo_release_sigint
end interface
interface
  integer(c_int) function wo_release_sigterm () bind(C)
  import
end function wo_release_sigterm
end interface
interface
  integer(c_int) function wo_release_sigxcpu () bind(C)
  import
end function wo_release_sigxcpu
end interface
interface
  integer(c_int) function wo_release_sigxfsz () bind(C)
  import
end function wo_release_sigxfsz
end interface

```

<Diagnostics: public>+≡

```

public :: signal_is_pending

```

<Diagnostics: sub interfaces>+≡

```

module function signal_is_pending () result (flag)
  logical :: flag
end function signal_is_pending

```

<Diagnostics: procedures>+≡

```

module function signal_is_pending () result (flag)
  logical :: flag
  flag = &
    wo_sigint /= 0 .or. &
    wo_sigterm /= 0 .or. &
    wo_sigxcpu /= 0 .or. &
    wo_sigxfsz /= 0
end function signal_is_pending

```

<Diagnostics: public>+≡

```

public :: terminate_now_if_signal

```

<Diagnostics: sub interfaces>+≡

```

module subroutine terminate_now_if_signal ()
end subroutine terminate_now_if_signal

```

```

<Diagnostics: procedures>+≡
module subroutine terminate_now_if_signal ()
  if (wo_sigint /= 0) then
    call msg_terminate ("Signal SIGINT (keyboard interrupt) received.", &
      quit_code=int (wo_sigint))
  else if (wo_sigterm /= 0) then
    call msg_terminate ("Signal SIGTERM (termination signal) received.", &
      quit_code=int (wo_sigterm))
  else if (wo_sigxcpu /= 0) then
    call msg_terminate ("Signal SIGXCPU (CPU time limit exceeded) received.", &
      quit_code=int (wo_sigxcpu))
  else if (wo_sigxfsz /= 0) then
    call msg_terminate ("Signal SIGXFSZ (file size limit exceeded) received.", &
      quit_code=int (wo_sigxfsz))
  end if
end subroutine terminate_now_if_signal

<Diagnostics: public>+≡
public :: single_event

<Diagnostics: variables>+≡
logical :: single_event = .false.

<Diagnostics: public>+≡
public :: terminate_now_if_single_event

<Diagnostics: sub interfaces>+≡
module subroutine terminate_now_if_single_event ()
end subroutine terminate_now_if_single_event

<Diagnostics: procedures>+≡
module subroutine terminate_now_if_single_event ()
  integer, save :: n_calls = 0
  n_calls = n_calls + 1
  if (single_event .and. n_calls > 1) then
    call msg_terminate ("Stopping after one event", quit_code=0)
  end if
end subroutine terminate_now_if_single_event

```

5.5 Operating-system interface

For specific purposes, we need direct access to the OS (system calls). This is, of course, system dependent. The current version is valid for GNU/Linux; we expect to use a preprocessor for this module if different OSs are to be supported.

The current implementation lacks error handling.

```

<os_interface.f90>≡
<File header>

module os_interface

  use, intrinsic :: iso_c_binding !NODEP!

```

```

    <Use strings>

    <Standard module head>

    <OS interface: public>

    <OS interface: types>

    <OS interface: interfaces>

    interface
    <OS interface: sub interfaces>
    end interface

end module os_interface

<os_interface_sub.f90>≡
<File header>

submodule (os_interface) os_interface_s

    use system_defs, only: DLERROR_LEN, ENVVAR_LEN
    use io_units
    use diagnostics
    use system_dependencies

    <Use mpi f08>

    implicit none

contains

    <OS interface: procedures>

end submodule os_interface_s

```

5.5.1 Path variables

This is a transparent container for storing user-defined path variables.

```

<OS interface: public>≡
    public :: paths_t

<OS interface: types>≡
    type :: paths_t
        type(string_t) :: prefix
        type(string_t) :: exec_prefix
        type(string_t) :: bindir
        type(string_t) :: libdir
        type(string_t) :: includedir
        type(string_t) :: datarootdir
        type(string_t) :: localprefix
        type(string_t) :: libtool
        type(string_t) :: lhapdfdir

```

```

end type paths_t

<OS interface: public>+≡
public :: paths_init

<OS interface: sub interfaces>≡
module subroutine paths_init (paths)
  type(paths_t), intent(out) :: paths
end subroutine paths_init

<OS interface: procedures>≡
module subroutine paths_init (paths)
  type(paths_t), intent(out) :: paths
  paths%prefix = ""
  paths%exec_prefix = ""
  paths%bindir = ""
  paths%libdir = ""
  paths%includedir = ""
  paths%datarootdir = ""
  paths%localprefix = ""
  paths%libtool = ""
  paths%lhapdfdir = ""
end subroutine paths_init

```

5.5.2 System dependencies

We store all potentially system- and user/run-dependent data in a transparent container. This includes compiler/linker names and flags, file extensions, etc. There are actually two different possibilities for extensions of shared libraries, depending on whether the Fortran compiler or the system linker (usually the C compiler) has been used for linking. The default for the Fortran compiler on most systems is `.so`.

```

<OS interface: public>+≡
public :: os_data_t

<OS interface: types>+≡
type :: os_data_t
  logical :: use_libtool
  logical :: use_testfiles
  type(string_t) :: fc
  type(string_t) :: fcflags
  type(string_t) :: fcflags_pic
  type(string_t) :: fclibs
  type(string_t) :: fc_src_ext
  type(string_t) :: cc
  type(string_t) :: cflags
  type(string_t) :: cflags_pic
  type(string_t) :: cxx
  type(string_t) :: cxxflags
  type(string_t) :: cxxlibs
  type(string_t) :: obj_ext
  type(string_t) :: ld
  type(string_t) :: ldflags

```

```

type(string_t) :: ldflags_so
type(string_t) :: ldflags_static
type(string_t) :: ldflags_hepmc
type(string_t) :: ldflags_lcio
type(string_t) :: ldflags_hoppet
type(string_t) :: ldflags_looptools
type(string_t) :: shrlib_ext
type(string_t) :: fc_shrlib_ext
type(string_t) :: pack_cmd
type(string_t) :: unpack_cmd
type(string_t) :: pack_ext
type(string_t) :: makeflags
type(string_t) :: prefix
type(string_t) :: exec_prefix
type(string_t) :: bindir
type(string_t) :: libdir
type(string_t) :: includedir
type(string_t) :: datarootdir
type(string_t) :: whizard_omega_binpath
type(string_t) :: whizard_includes
type(string_t) :: whizard_ldflags
type(string_t) :: whizard_libtool
type(string_t) :: whizard_modelpath
type(string_t) :: whizard_modelpath_ufo
type(string_t) :: whizard_models_libpath
type(string_t) :: whizard_susypath
type(string_t) :: whizard_gmlpath
type(string_t) :: whizard_cutspath
type(string_t) :: whizard_texpath
type(string_t) :: whizard_sharepath
type(string_t) :: whizard_testdatapath
type(string_t) :: whizard_modelpath_local
type(string_t) :: whizard_models_libpath_local
type(string_t) :: whizard_omega_binpath_local
type(string_t) :: whizard_circe2path
type(string_t) :: whizard_beamsimpath
type(string_t) :: whizard_mulipath
type(string_t) :: pdf_built_in_datapath
logical :: event_analysis = .false.
logical :: event_analysis_ps = .false.
logical :: event_analysis_pdf = .false.
type(string_t) :: latex
type(string_t) :: mpost
type(string_t) :: gml
type(string_t) :: dvips
type(string_t) :: ps2pdf
type(string_t) :: gosampath
type(string_t) :: golemath
type(string_t) :: formath
type(string_t) :: qgrafath
type(string_t) :: ninjath
type(string_t) :: samuraipath
contains
<OS interface: os data: TBP>

```



```
end type os_data_t
```

Since all are allocatable strings, explicit initialization is necessary.

```
<System defs: public parameters>+≡
    integer, parameter, public :: ENVVAR_LEN = 1000

<OS interface: os data: TBP>≡
    procedure :: init => os_data_init

<OS interface: sub interfaces>+≡
    module subroutine os_data_init (os_data, paths)
        class(os_data_t), intent(out) :: os_data
        type(paths_t), intent(in), optional :: paths
    end subroutine os_data_init

<OS interface: procedures>+≡
    module subroutine os_data_init (os_data, paths)
        class(os_data_t), intent(out) :: os_data
        type(paths_t), intent(in), optional :: paths
        character(len=ENVVAR_LEN) :: home
        type(string_t) :: localprefix, local_includes
        os_data%use_libtool = .true.
        inquire (file = "TESTFLAG", exist = os_data%use_testfiles)
        call get_environment_variable ("HOME", home)
        if (present(paths)) then
            if (paths%localprefix == "") then
                localprefix = trim (home) // "/.whizard"
            else
                localprefix = paths%localprefix
            end if
        else
            localprefix = trim (home) // "/.whizard"
        end if
        local_includes = localprefix // "/lib/whizard/mod/models"
        os_data%whizard_modelpath_local = localprefix // "/share/whizard/models"
        os_data%whizard_models_libpath_local = localprefix // "/lib/whizard/models"
        os_data%whizard_omega_binpath_local = localprefix // "/bin"
        os_data%fc = DEFAULT_FC
        os_data%fcflags = DEFAULT_FCFLAGS
        os_data%fcflags_pic = DEFAULT_FCFLAGS_PIC
        os_data%fclibs = FCLIBS
        os_data%fc_src_ext = DEFAULT_FC_SRC_EXT
        os_data%cc = DEFAULT_CC
        os_data%cflags = DEFAULT_CFLAGS
        os_data%cflags_pic = DEFAULT_CFLAGS_PIC
        os_data%cxx = DEFAULT_CXX
        os_data%cxxflags = DEFAULT_CXXFLAGS
        os_data%cxxlibs = DEFAULT_CXXLIBS
        os_data%obj_ext = DEFAULT_OBJ_EXT
        os_data%ld = DEFAULT_LD
        os_data%ldflags = DEFAULT_LDFLAGS
        os_data%ldflags_so = DEFAULT_LDFLAGS_SO
        os_data%ldflags_static = DEFAULT_LDFLAGS_STATIC
        os_data%ldflags_hepmc = DEFAULT_LDFLAGS_HEPMC
        os_data%ldflags_lcio = DEFAULT_LDFLAGS_LCIO
```

```

os_data%ldflags_hoppet = DEFAULT_LDFLAGS_HOPPET
os_data%ldflags_looptools = DEFAULT_LDFLAGS_LOOPTOOLS
os_data%shrlib_ext      = DEFAULT_SHRLIB_EXT
os_data%fc_shrlib_ext   = DEFAULT_FC_SHRLIB_EXT
os_data%pack_cmd        = DEFAULT_PACK_CMD
os_data%unpack_cmd      = DEFAULT_UNPACK_CMD
os_data%pack_ext        = DEFAULT_PACK_EXT
os_data%makeflags       = DEFAULT_MAKEFLAGS
os_data%prefix          = PREFIX
os_data%exec_prefix     = EXEC_PREFIX
os_data%bindir          = BINDIR
os_data%libdir          = LIBDIR
os_data%includedir      = INCLUDEDIR
os_data%datarootdir     = DATAROOTDIR
if (present (paths)) then
  if (paths%prefix      /= "") os_data%prefix      = paths%prefix
  if (paths%exec_prefix /= "") os_data%exec_prefix = paths%exec_prefix
  if (paths%bindir      /= "") os_data%bindir      = paths%bindir
  if (paths%libdir      /= "") os_data%libdir      = paths%libdir
  if (paths%includedir /= "") os_data%includedir  = paths%includedir
  if (paths%datarootdir /= "") os_data%datarootdir = paths%datarootdir
end if
if (os_data%use_testfiles) then
  os_data%whizard_omega_binpath = WHIZARD_TEST_OMEGA_BINPATH
  os_data%whizard_includes      = WHIZARD_TEST_INCLUDES
  os_data%whizard_ldflags       = WHIZARD_TEST_LDFLAGS
  os_data%whizard_libtool       = WHIZARD_LIBTOOL_TEST
  os_data%whizard_modelpath     = WHIZARD_TEST_MODELPATH
  os_data%whizard_modelpath_ufo = WHIZARD_TEST_MODELPATH_UFO
  os_data%whizard_models_libpath = WHIZARD_TEST_MODELS_LIBPATH
  os_data%whizard_susypath      = WHIZARD_TEST_SUSYPATH
  os_data%whizard_gmlpath       = WHIZARD_TEST_GMLPATH
  os_data%whizard_cutspath      = WHIZARD_TEST_CUTSPATH
  os_data%whizard_texpath       = WHIZARD_TEST_TEXPATH
  os_data%whizard_sharepath     = WHIZARD_TEST_SHAREPATH
  os_data%whizard_testdatapath  = WHIZARD_TEST_TESTDATAPATH
  os_data%whizard_circe2path    = WHIZARD_TEST_CIRCE2PATH
  os_data%whizard_beamsimpath   = WHIZARD_TEST_BEAMSIMPATH
  os_data%whizard_mulipath      = WHIZARD_TEST_MULIPATH
  os_data%pdf_builtin_datapath  = PDF_BUILTIN_TEST_DATAPATH
else
  if (os_dir_exist (local_includes)) then
    os_data%whizard_includes = "-I" // local_includes // " " // &
    WHIZARD_INCLUDES
  else
    os_data%whizard_includes = WHIZARD_INCLUDES
  end if
  os_data%whizard_omega_binpath = WHIZARD_OMEGA_BINPATH
  os_data%whizard_ldflags       = WHIZARD_LDFLAGS
  os_data%whizard_libtool       = WHIZARD_LIBTOOL
  if (present (paths)) then
    if (paths%libtool /= "") os_data%whizard_libtool = paths%libtool
  end if
  os_data%whizard_modelpath     = WHIZARD_MODELPATH

```

```

os_data%whizard_modelpath_ufo = WHIZARD_MODELPATH_UFO
os_data%whizard_models_libpath = WHIZARD_MODELS_LIBPATH
os_data%whizard_susypath      = WHIZARD_SUSYPATH
os_data%whizard_gmlpath      = WHIZARD_GMLPATH
os_data%whizard_cutspath     = WHIZARD_CUTSPATH
os_data%whizard_texpath      = WHIZARD_TEXPATH
os_data%whizard_sharepath    = WHIZARD_SHAREPATH
os_data%whizard_testdatapath = WHIZARD_TESTDATAPATH
os_data%whizard_circe2path   = WHIZARD_CIRCE2PATH
os_data%whizard_beamsimpath  = WHIZARD_BEAMSIMPATH
os_data%whizard_mulipath     = WHIZARD_MULIPATH
os_data%pdf_builtin_datapath = PDF_BUILTIN_DATAPATH
end if
os_data%event_analysis      = EVENT_ANALYSIS      == "yes"
os_data%event_analysis_ps   = EVENT_ANALYSIS_PS   == "yes"
os_data%event_analysis_pdf  = EVENT_ANALYSIS_PDF  == "yes"
os_data%latex = PRG_LATEX // " " // OPT_LATEX
os_data%mpost = PRG_MPOST // " " // OPT_MPOST
if (os_data%use_testfiles) then
  os_data%gml = os_data%whizard_gmlpath // "/whizard-gml" // " " // &
    OPT_MPOST // " " // "-gmlmdir " // os_data%whizard_gmlpath
else
  os_data%gml = os_data%bindir // "/whizard-gml" // " " // OPT_MPOST &
    // " " // "-gmlmdir " // os_data%whizard_gmlpath
end if
os_data%dvips = PRG_DVIPS
os_data%ps2pdf = PRG_PS2PDF
call os_data_expand_paths (os_data)
os_data%gosampath = GOSAM_DIR
os_data%golempath = GOLEM_DIR
os_data%formpath = FORM_DIR
os_data%qgrafpath = QGRAF_DIR
os_data%ninjabath = NINJA_DIR
os_data%samuraipath = SAMURAI_DIR
end subroutine os_data_init

```

Replace occurrences of GNU path variables (such as `${prefix}`) by their values. Do this for all strings that could depend on them, and do the replacement in reverse order, since the path variables may be defined in terms of each other.

(OS interface: procedures)+≡

```

subroutine os_data_expand_paths (os_data)
  type(os_data_t), intent(inout) :: os_data
  integer, parameter :: N_VARIABLES = 6
  type(string_t), dimension(N_VARIABLES) :: variable, value
  variable(1) = "${prefix}";      value(1) = os_data%prefix
  variable(2) = "${exec_prefix}"; value(2) = os_data%exec_prefix
  variable(3) = "${bindir}";      value(3) = os_data%bindir
  variable(4) = "${libdir}";      value(4) = os_data%libdir
  variable(5) = "${includedir}";  value(5) = os_data%includedir
  variable(6) = "${datarootdir}"; value(6) = os_data%datarootdir
  call expand_paths (os_data%whizard_omega_binpath)
  call expand_paths (os_data%whizard_includes)
  call expand_paths (os_data%whizard_ldflags)

```

```

call expand_paths (os_data%whizard_libtool)
call expand_paths (os_data%whizard_modelpath)
call expand_paths (os_data%whizard_modelpath_ufo)
call expand_paths (os_data%whizard_models_libpath)
call expand_paths (os_data%whizard_susypath)
call expand_paths (os_data%whizard_gmlpath)
call expand_paths (os_data%whizard_cutspath)
call expand_paths (os_data%whizard_texpath)
call expand_paths (os_data%whizard_sharepath)
call expand_paths (os_data%whizard_testdatapath)
call expand_paths (os_data%whizard_circe2path)
call expand_paths (os_data%whizard_beamsimp)
call expand_paths (os_data%whizard_mulipath)
call expand_paths (os_data%whizard_models_libpath_local)
call expand_paths (os_data%whizard_modelpath_local)
call expand_paths (os_data%whizard_omega_binpath_local)
call expand_paths (os_data%pdf_builtin_datapath)
call expand_paths (os_data%latex)
call expand_paths (os_data%mpost)
call expand_paths (os_data%gml)
call expand_paths (os_data%dvips)
call expand_paths (os_data%ps2pdf)
contains
subroutine expand_paths (string)
  type(string_t), intent(inout) :: string
  integer :: i
  do i = N_VARIABLES, 1, -1
    string = replace (string, variable(i), value(i), every=.true.)
  end do
end subroutine expand_paths
end subroutine os_data_expand_paths

```

Write contents

```

<OS interface: os data: TBP>+≡
  procedure :: write => os_data_write

<OS interface: sub interfaces>+≡
  module subroutine os_data_write (os_data, unit)
    class(os_data_t), intent(in) :: os_data
    integer, intent(in), optional :: unit
  end subroutine os_data_write

<OS interface: procedures>+≡
  module subroutine os_data_write (os_data, unit)
    class(os_data_t), intent(in) :: os_data
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A)") "OS data:"
    write (u, *) "use_libtool    = ", os_data%use_libtool
    write (u, *) "use_testfiles = ", os_data%use_testfiles
    write (u, *) "fc           = ", char (os_data%fc)
    write (u, *) "fcflags      = ", char (os_data%fcflags)
    write (u, *) "fcflags_pic   = ", char (os_data%fcflags_pic)
    write (u, *) "fclibs       = ", char (os_data%fclibs)

```

```

write (u, *) "fc_src_ext      = ", char (os_data%fc_src_ext)
write (u, *) "cc              = ", char (os_data%cc)
write (u, *) "cflags          = ", char (os_data%cflags)
write (u, *) "cflags_pic      = ", char (os_data%cflags_pic)
write (u, *) "cxx            = ", char (os_data%cxx)
write (u, *) "cxxflags        = ", char (os_data%cxxflags)
write (u, *) "cxxlibs         = ", char (os_data%cxxlibs)
write (u, *) "obj_ext         = ", char (os_data%obj_ext)
write (u, *) "ld              = ", char (os_data%ld)
write (u, *) "ldflags         = ", char (os_data%ldflags)
write (u, *) "ldflags_so       = ", char (os_data%ldflags_so)
write (u, *) "ldflags_static = ", char (os_data%ldflags_static)
write (u, *) "ldflags_hepmc    = ", char (os_data%ldflags_hepmc)
write (u, *) "ldflags_lcio     = ", char (os_data%ldflags_lcio)
write (u, *) "ldflags_hoppet = ", char (os_data%ldflags_hoppet)
write (u, *) "ldflags_looptools = ", char (os_data%ldflags_looptools)
write (u, *) "shrlib_ext       = ", char (os_data%shrlib_ext)
write (u, *) "fc_shrlib_ext   = ", char (os_data%fc_shrlib_ext)
write (u, *) "makeflags       = ", char (os_data%makeflags)
write (u, *) "prefix          = ", char (os_data%prefix)
write (u, *) "exec_prefix      = ", char (os_data%exec_prefix)
write (u, *) "bindir          = ", char (os_data%bindir)
write (u, *) "libdir          = ", char (os_data%libdir)
write (u, *) "includedir       = ", char (os_data%includedir)
write (u, *) "datarootdir      = ", char (os_data%datarootdir)
write (u, *) "whizard_omega_binpath = ", &
    char (os_data%whizard_omega_binpath)
write (u, *) "whizard_includes    = ", char (os_data%whizard_includes)
write (u, *) "whizard_ldflags     = ", char (os_data%whizard_ldflags)
write (u, *) "whizard_libtool      = ", char (os_data%whizard_libtool)
write (u, *) "whizard_modelpath    = ", &
    char (os_data%whizard_modelpath)
write (u, *) "whizard_modelpath_ufo = ", &
    char (os_data%whizard_modelpath_ufo)
write (u, *) "whizard_models_libpath = ", &
    char (os_data%whizard_models_libpath)
write (u, *) "whizard_susypath      = ", char (os_data%whizard_susypath)
write (u, *) "whizard_gmlpath       = ", char (os_data%whizard_gmlpath)
write (u, *) "whizard_cutspath      = ", char (os_data%whizard_cutspath)
write (u, *) "whizard_texpath       = ", char (os_data%whizard_texpath)
write (u, *) "whizard_circe2path    = ", char (os_data%whizard_circe2path)
write (u, *) "whizard_beamsimpath   = ", char (os_data%whizard_beamsimpath)
write (u, *) "whizard_mulipath      = ", char (os_data%whizard_mulipath)
write (u, *) "whizard_sharepath    = ", &
    char (os_data%whizard_sharepath)
write (u, *) "whizard_testdatapath = ", &
    char (os_data%whizard_testdatapath)
write (u, *) "whizard_modelpath_local = ", &
    char (os_data%whizard_modelpath_local)
write (u, *) "whizard_models_libpath_local = ", &
    char (os_data%whizard_models_libpath_local)
write (u, *) "whizard_omega_binpath_local = ", &
    char (os_data%whizard_omega_binpath_local)
write (u, *) "event_analysis        = ", os_data%event_analysis

```

```

write (u, *) "event_analysis_ps = ", os_data%event_analysis_ps
write (u, *) "event_analysis_pdf = ", os_data%event_analysis_pdf
write (u, *) "latex = ", char (os_data%latex)
write (u, *) "mpost = ", char (os_data%mpost)
write (u, *) "gml = ", char (os_data%gml)
write (u, *) "dvips = ", char (os_data%dvips)
write (u, *) "ps2pdf = ", char (os_data%ps2pdf)
if (os_data%gosampath /= "") then
  write (u, *) "gosam = ", char (os_data%gosampath)
  write (u, *) "golem = ", char (os_data%golempath)
  write (u, *) "form = ", char (os_data%formpath)
  write (u, *) "qgraf = ", char (os_data%qgrafpath)
  write (u, *) "ninja = ", char (os_data%ninjapath)
  write (u, *) "samurai = ", char (os_data%samuraipath)
end if
end subroutine os_data_write

```

<OS interface: os data: TBP>+≡

```

procedure :: build_latex_file => os_data_build_latex_file

```

<OS interface: sub interfaces>+≡

```

module subroutine os_data_build_latex_file (os_data, filename, stat_out)
  class(os_data_t), intent(in) :: os_data
  type(string_t), intent(in) :: filename
  integer, intent(out), optional :: stat_out
end subroutine os_data_build_latex_file

```

<OS interface: procedures>+≡

```

module subroutine os_data_build_latex_file (os_data, filename, stat_out)
  class(os_data_t), intent(in) :: os_data
  type(string_t), intent(in) :: filename
  integer, intent(out), optional :: stat_out
  type(string_t) :: setenv_tex, pipe, pipe_dvi
  integer :: unit_dev, status
  status = -1
  if (os_data%event_analysis_ps) then
    !!! Check if our OS has a /dev/null
    unit_dev = free_unit ()
    open (file = "/dev/null", unit = unit_dev, &
         action = "write", iostat = status)
    close (unit_dev)
    if (status /= 0) then
      pipe = ""
      pipe_dvi = ""
    else
      pipe = " > /dev/null"
      pipe_dvi = " 2>/dev/null 1>/dev/null"
    end if
  if (os_data%whizard_texpath /= "") then
    setenv_tex = "TEXINPUTS=" // &
      os_data%whizard_texpath // " :$TEXINPUTS "
  else
    setenv_tex = ""
  end if
  call os_system_call (setenv_tex // &

```

```

        os_data%latex // " " // filename // ".tex " // pipe, &
        verbose = .true., status = status)
    call os_system_call (os_data%dvips // " -o " // filename // &
        ".ps " // filename // ".dvi" // pipe_dvi, verbose = .true., &
        status = status)
    call os_system_call (os_data%ps2pdf // " " // filename // ".ps", &
        verbose = .true., status = status)
end if
if (present (stat_out)) stat_out = status
end subroutine os_data_build_latex_file

```

5.5.3 Dynamic linking

We define a type that holds the filehandle for a dynamically linked library (shared object), together with functions to open and close the library, and to access functions in this library.

```

<OS interface: public>+≡
    public :: dlaccess_t
<OS interface: types>+≡
    type :: dlaccess_t
        private
        type(string_t) :: filename
        type(c_ptr) :: handle = c_null_ptr
        logical :: is_open = .false.
        logical :: has_error = .false.
        type(string_t) :: error
    contains
    <OS interface: dlaccess: TBP>
end type dlaccess_t

```

Output. This is called by the output routine for the process library.

```

<OS interface: dlaccess: TBP>≡
    procedure :: write => dlaccess_write
<OS interface: sub interfaces>+≡
    module subroutine dlaccess_write (object, unit)
        class(dlaccess_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine dlaccess_write
<OS interface: procedures>+≡
    module subroutine dlaccess_write (object, unit)
        class(dlaccess_t), intent(in) :: object
        integer, intent(in) :: unit
        write (unit, "(1x,A)") "DL access info:"
        write (unit, "(3x,A,L1)") "is open   = ", object%is_open
        if (object%has_error) then
            write (unit, "(3x,A,A,A)") "error       = '", char (object%error), "'"
        else
            write (unit, "(3x,A)") "error       = [none]"
        end if
    end subroutine dlaccess_write

```

The interface to the library functions:

(OS interface: interfaces)≡

```

interface
  function dlopen (filename, flag) result (handle) bind(C)
  import
    character(c_char), dimension(*) :: filename
    integer(c_int), value :: flag
    type(c_ptr) :: handle
  end function dlopen
end interface

interface
  function dlclose (handle) result (status) bind(C)
  import
    type(c_ptr), value :: handle
    integer(c_int) :: status
  end function dlclose
end interface

interface
  function dlerror () result (str) bind(C)
  import
    type(c_ptr) :: str
  end function dlerror
end interface

interface
  function dlsym (handle, symbol) result (fp_ptr) bind(C)
  import
    type(c_ptr), value :: handle
    character(c_char), dimension(*) :: symbol
    type(c_funptr) :: fp_ptr
  end function dlsym
end interface

```

This reads an error string and transforms it into a `string_t` object, if an error has occurred. If not, set the error flag to false and return an empty string.

(System defs: public parameters)+≡

```

integer, parameter, public :: DLERROR_LEN = 160

```

(OS interface: procedures)+≡

```

subroutine read_dlerror (has_error, error)
  logical, intent(out) :: has_error
  type(string_t), intent(out) :: error
  type(c_ptr) :: err_cptr
  character(len=DLERROR_LEN, kind=c_char), pointer :: err_fptr
  integer :: str_end
  err_cptr = dlerror ()
  if (c_associated (err_cptr)) then
    call c_f_pointer (err_cptr, err_fptr)
    has_error = .true.
    str_end = scan (err_fptr, c_null_char)
    if (str_end > 0) then
      error = err_fptr(1:str_end-1)
    end if
  end if
end subroutine read_dlerror

```



```

        else
            error = err_fptr
        end if
    else
        has_error = .false.
        error = ""
    end if
end subroutine read_dlerror

```

This is the Fortran API. Init/final open and close the file, i.e., load and unload the library.

Note that a library can be opened more than once, and that for an ultimate close as many `dlclose` calls as `dlopen` calls are necessary. However, we assume that it is opened and closed only once.

```

<OS interface: public>+≡
    public :: dlaccess_init
    public :: dlaccess_final

<OS interface: dlaccess: TBP>+≡
    procedure :: init => dlaccess_init
    procedure :: final => dlaccess_final

<OS interface: sub interfaces>+≡
    module subroutine dlaccess_init (dlaccess, prefix, libname, os_data)
        class(dlaccess_t), intent(out) :: dlaccess
        type(string_t), intent(in) :: prefix, libname
        type(os_data_t), intent(in), optional :: os_data
    end subroutine dlaccess_init
    module subroutine dlaccess_final (dlaccess)
        class(dlaccess_t), intent(inout) :: dlaccess
    end subroutine dlaccess_final

<OS interface: procedures>+≡
    module subroutine dlaccess_init (dlaccess, prefix, libname, os_data)
        class(dlaccess_t), intent(out) :: dlaccess
        type(string_t), intent(in) :: prefix, libname
        type(os_data_t), intent(in), optional :: os_data
        type(string_t) :: filename
        logical :: exist
        dlaccess%filename = libname
        filename = prefix // "/" // libname
        inquire (file=char(filename), exist=exist)
        if (.not. exist) then
            filename = prefix // "/.libs/" // libname
            inquire (file=char(filename), exist=exist)
            if (.not. exist) then
                dlaccess%has_error = .true.
                dlaccess%error = "Library '" // filename // "' not found"
                return
            end if
        end if
    end if
    dlaccess%handle = dlopen (char (filename) // c_null_char, ior ( &
        RTLD_LAZY, RTLD_LOCAL))
    dlaccess%is_open = c_associated (dlaccess%handle)
    call read_dlerror (dlaccess%has_error, dlaccess%error)

```

```

end subroutine dlaccess_init

module subroutine dlaccess_final (dlaccess)
  class(dlaccess_t), intent(inout) :: dlaccess
  integer(c_int) :: status
  if (dlaccess%is_open) then
    status = dlclose (dlaccess%handle)
    dlaccess%is_open = .false.
    call read_dlerror (dlaccess%has_error, dlaccess%error)
  end if
end subroutine dlaccess_final

```

Return true if an error has occurred.

```

<OS interface: public>+≡
  public :: dlaccess_has_error

<OS interface: sub interfaces>+≡
  module function dlaccess_has_error (dlaccess) result (flag)
    logical :: flag
    type(dlaccess_t), intent(in) :: dlaccess
  end function dlaccess_has_error

<OS interface: procedures>+≡
  module function dlaccess_has_error (dlaccess) result (flag)
    logical :: flag
    type(dlaccess_t), intent(in) :: dlaccess
    flag = dlaccess%has_error
  end function dlaccess_has_error

```

Return the error string currently stored in the dlaccess object.

```

<OS interface: public>+≡
  public :: dlaccess_get_error

<OS interface: sub interfaces>+≡
  module function dlaccess_get_error (dlaccess) result (error)
    type(string_t) :: error
    type(dlaccess_t), intent(in) :: dlaccess
  end function dlaccess_get_error

<OS interface: procedures>+≡
  module function dlaccess_get_error (dlaccess) result (error)
    type(string_t) :: error
    type(dlaccess_t), intent(in) :: dlaccess
    error = dlaccess%error
  end function dlaccess_get_error

```

The symbol handler returns the C address of the function with the given string name. (It is a good idea to use `bind(C)` for all functions accessed by this, such that the name string is well-defined.) Call `c_f_procpointer` to cast this into a Fortran procedure pointer with an appropriate interface.

```

<OS interface: public>+≡
  public :: dlaccess_get_c_funptr

```

```

<OS interface: sub interfaces>+≡
    module function dlaccess_get_c_funptr (dlaccess, fname) result (fptr)
        type(c_funptr) :: fptr
        type(dlaccess_t), intent(inout) :: dlaccess
        type(string_t), intent(in) :: fname
    end function dlaccess_get_c_funptr

<OS interface: procedures>+≡
    module function dlaccess_get_c_funptr (dlaccess, fname) result (fptr)
        type(c_funptr) :: fptr
        type(dlaccess_t), intent(inout) :: dlaccess
        type(string_t), intent(in) :: fname
        fptr = dlsym (dlaccess%handle, char (fname) // c_null_char)
        call read_dlerror (dlaccess%has_error, dlaccess%error)
    end function dlaccess_get_c_funptr

```

5.5.4 Predicates

Return true if the library is loaded. In particular, this is false if loading was unsuccessful.

```

<OS interface: public>+≡
    public :: dlaccess_is_open

<OS interface: sub interfaces>+≡
    module function dlaccess_is_open (dlaccess) result (flag)
        logical :: flag
        type(dlaccess_t), intent(in) :: dlaccess
    end function dlaccess_is_open

<OS interface: procedures>+≡
    module function dlaccess_is_open (dlaccess) result (flag)
        logical :: flag
        type(dlaccess_t), intent(in) :: dlaccess
        flag = dlaccess%is_open
    end function dlaccess_is_open

```

5.5.5 Shell access

This is the standard system call for executing a shell command, such as invoking a compiler.

In F2008 there will be the equivalent built-in command `execute_command_line`.

```

<OS interface: public>+≡
    public :: os_system_call

<OS interface: sub interfaces>+≡
    module subroutine os_system_call (command_string, status, verbose)
        type(string_t), intent(in) :: command_string
        integer, intent(out), optional :: status
        logical, intent(in), optional :: verbose
    end subroutine os_system_call

```

```

<OS interface: procedures>+≡
module subroutine os_system_call (command_string, status, verbose)
  type(string_t), intent(in) :: command_string
  integer, intent(out), optional :: status
  logical, intent(in), optional :: verbose
  logical :: verb
  integer :: stat
  verb = .false.; if (present (verbose)) verb = verbose
  if (verb) &
    call msg_message ("command: " // char (command_string))
  stat = system (char (command_string) // c_null_char)
  if (present (status)) then
    status = stat
  else if (stat /= 0) then
    if (.not. verb) &
      call msg_message ("command: " // char (command_string))
    write (msg_buffer, "(A,I0)") "Return code = ", stat
    call msg_message ()
    call msg_fatal ("System command returned with nonzero status code")
  end if
end subroutine os_system_call

```

```

<OS interface: interfaces>+≡
interface
  function system (command) result (status) bind(C)
    import
    integer(c_int) :: status
    character(c_char), dimension(*) :: command
  end function system
end interface

```

5.5.6 Querying for a directory

This queries for the existence of a directory. There is no standard way to achieve this in FORTRAN, and if we were to call into libc, we would need access to C macros for evaluating the result, so we resort to calling `test` as a system call.

```

<OS interface: public>+≡
public :: os_dir_exist

<OS interface: sub interfaces>+≡
module function os_dir_exist (name) result (res)
  type(string_t), intent(in) :: name
  logical :: res
end function os_dir_exist

<OS interface: procedures>+≡
module function os_dir_exist (name) result (res)
  type(string_t), intent(in) :: name
  logical :: res
  integer :: status
  call os_system_call ('test -d "' // name // '"', status=status)
  res = status == 0
end function os_dir_exist

```

```

<OS interface: public>+≡
    public :: os_file_exist
<OS interface: sub interfaces>+≡
    module function os_file_exist (name) result (exist)
        type(string_t), intent(in) :: name
        logical :: exist
    end function os_file_exist
<OS interface: procedures>+≡
    module function os_file_exist (name) result (exist)
        type(string_t), intent(in) :: name
        logical :: exist
        inquire (file = char (name), exist=exist)
    end function os_file_exist

```

5.5.7 Pack/unpack

The argument to **pack** may be a file or a directory. The name of the packed file will get the **pack_ext** extension appended. The argument to **unpack** must be a file, with the extension already included in the file name.

```

<OS interface: public>+≡
    public :: os_pack_file
    public :: os_unpack_file
<OS interface: sub interfaces>+≡
    module subroutine os_pack_file (file, os_data, status)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
    end subroutine os_pack_file
    module subroutine os_unpack_file (file, os_data, status)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
    end subroutine os_unpack_file
<OS interface: procedures>+≡
    module subroutine os_pack_file (file, os_data, status)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
        type(string_t) :: command_string
        command_string = os_data%pack_cmd // " " &
            // file // os_data%pack_ext // " " // file
        call os_system_call (command_string, status)
    end subroutine os_pack_file

    module subroutine os_unpack_file (file, os_data, status)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
        type(string_t) :: command_string

```

```

        command_string = os_data%unpack_cmd // " " // file
        call os_system_call (command_string, status)
    end subroutine os_unpack_file

```

5.5.8 Fortran compiler and linker

Compile a single module for use in a shared library, but without linking.

```

<OS interface: public>+≡
    public :: os_compile_shared

<OS interface: sub interfaces>+≡
    module subroutine os_compile_shared (src, os_data, status)
        type(string_t), intent(in) :: src
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
    end subroutine os_compile_shared

<OS interface: procedures>+≡
    module subroutine os_compile_shared (src, os_data, status)
        type(string_t), intent(in) :: src
        type(os_data_t), intent(in) :: os_data
        integer, intent(out), optional :: status
        type(string_t) :: command_string
        if (os_data%use_libtool) then
            command_string = &
                os_data%whizard_libtool // " -mode=compile " // &
                os_data%fc // " " // &
                "-c " // &
                os_data%whizard_includes // " " // &
                os_data%fcflags // " " // &
                "' " // src // os_data%fc_src_ext // "' "
        else
            command_string = &
                os_data%fc // " " // &
                "-c " // &
                os_data%fcflags_pic // " " // &
                os_data%whizard_includes // " " // &
                os_data%fcflags // " " // &
                "' " // src // os_data%fc_src_ext // "' "
        end if
        call os_system_call (command_string, status)
    end subroutine os_compile_shared

```

Link an array of object files to build a shared object library. In the libtool case, we have to specify a `-rpath`, otherwise only a static library can be built. However, since the library is never installed, this `rpath` is irrelevant.

```

<OS interface: public>+≡
    public :: os_link_shared

<OS interface: sub interfaces>+≡
    module subroutine os_link_shared (objlist, lib, os_data, status)
        type(string_t), intent(in) :: objlist, lib
        type(os_data_t), intent(in) :: os_data

```

```

        integer, intent(out), optional :: status
    end subroutine os_link_shared

<OS interface: procedures>+≡
module subroutine os_link_shared (objlist, lib, os_data, status)
    type(string_t), intent(in) :: objlist, lib
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
    type(string_t) :: command_string
    if (os_data%use_libtool) then
        command_string = &
            os_data%whizard_libtool // " -mode=link " // &
            os_data%fc // " " // &
            "-module " // &
            "-rpath /usr/local/lib" // " " // &
            os_data%fcflags // " " // &
            os_data%whizard_ldflags // " " // &
            os_data%ldflags // " " // &
            "-o '" // lib // ".la' " // &
            objlist
    else
        command_string = &
            os_data%ld // " " // &
            os_data%ldflags_so // " " // &
            os_data%fcflags // " " // &
            os_data%whizard_ldflags // " " // &
            os_data%ldflags // " " // &
            "-o '" // lib // "." // os_data%fc_shrllib_ext // "' " // &
            objlist
    end if
    call os_system_call (command_string, status)
end subroutine os_link_shared

```

Link an array of object files / libraries to build a static executable.

```

<OS interface: public>+≡
    public :: os_link_static

<OS interface: sub interfaces>+≡
module subroutine os_link_static (objlist, exec_name, os_data, status)
    type(string_t), intent(in) :: objlist, exec_name
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
end subroutine os_link_static

<OS interface: procedures>+≡
module subroutine os_link_static (objlist, exec_name, os_data, status)
    type(string_t), intent(in) :: objlist, exec_name
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
    type(string_t) :: command_string
    if (os_data%use_libtool) then
        command_string = &
            os_data%whizard_libtool // " -mode=link " // &
            os_data%fc // " " // &
            "-static " // &

```

```

        os_data%fcflags // " " // &
        os_data%whizard_ldflags // " " // &
        os_data%ldflags // " " // &
        os_data%ldflags_static // " " // &
        "-o '" // exec_name // "' " // &
        objlist // " " // &
        os_data%ldflags_hepmc // " " // &
        os_data%ldflags_lcio // " " // &
        os_data%ldflags_hoppet // " " // &
        os_data%ldflags_looptools
    else
        command_string = &
        os_data%ld // " " // &
        os_data%ldflags_so // " " // &
        os_data%fcflags // " " // &
        os_data%whizard_ldflags // " " // &
        os_data%ldflags // " " // &
        os_data%ldflags_static // " " // &
        "-o '" // exec_name // "' " // &
        objlist // " " // &
        os_data%ldflags_hepmc // " " // &
        os_data%ldflags_lcio // " " // &
        os_data%ldflags_hoppet // " " // &
        os_data%ldflags_looptools
    end if
    call os_system_call (command_string, status)
end subroutine os_link_static

```

Determine the name of the shared library to link. If libtool is used, this is encoded in the .la file which resides in place of the library itself.

```

<OS interface: public>+≡
    public :: os_get_dlname

<OS interface: sub interfaces>+≡
    module function os_get_dlname (lib, os_data, ignore, silent) result (dlname)
        type(string_t) :: dlname
        type(string_t), intent(in) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: ignore, silent
    end function os_get_dlname

<OS interface: procedures>+≡
    module function os_get_dlname (lib, os_data, ignore, silent) result (dlname)
        type(string_t) :: dlname
        type(string_t), intent(in) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: ignore, silent
        type(string_t) :: filename
        type(string_t) :: buffer
        logical :: exist, required, quiet
        integer :: u
        u = free_unit ()
        if (present (ignore)) then
            required = .not. ignore
        else

```



```

        required = .true.
    end if
    if (present (silent)) then
        quiet = silent
    else
        quiet = .false.
    end if
    if (os_data%use_libtool) then
        filename = lib // ".la"
        inquire (file=char(filename), exist=exist)
        if (exist) then
            open (unit=u, file=char(filename), action="read", status="old")
            SCAN_LTFILE: do
                call get (u, buffer)
                if (extract (buffer, 1, 7) == "dlname=") then
                    dlname = extract (buffer, 9)
                    dlname = remove (dlname, len (dlname))
                    exit SCAN_LTFILE
                end if
            end do SCAN_LTFILE
            close (u)
        else if (required) then
            if (.not. quiet) call msg_fatal (" Library '" // char (lib) &
                // "': libtool archive not found")
            dlname = ""
        else
            if (.not. quiet) call msg_message ("[No compiled library '" &
                // char (lib) // "']")
            dlname = ""
        end if
    else
        dlname = lib // "." // os_data%fc_shrlib_ext
        inquire (file=char(dlname), exist=exist)
        if (.not. exist) then
            if (required) then
                if (.not. quiet) call msg_fatal (" Library '" // char (lib) &
                    // "' not found")
            else
                if (.not. quiet) call msg_message &
                    ("[No compiled process library '" // char (lib) // "']")
                dlname = ""
            end if
        end if
    end if
end function os_get_dlname

```

5.5.9 Controlling OpenMP

OpenMP is handled automatically by the library for the most part. Here is a convenience routine for setting the number of threads, with some diagnostics.

```

<OS interface: public>+≡
public :: openmp_set_num_threads_verbose

```

```

<OS interface: sub interfaces>+≡
    module subroutine openmp_set_num_threads_verbose (num_threads, openmp_logging)
        integer, intent(in) :: num_threads
        logical, intent(in), optional :: openmp_logging
    end subroutine openmp_set_num_threads_verbose

<OS interface: procedures>+≡
    module subroutine openmp_set_num_threads_verbose (num_threads, openmp_logging)
        integer, intent(in) :: num_threads
        integer :: n_threads
        logical, intent(in), optional :: openmp_logging
        logical :: logging
        if (present (openmp_logging)) then
            logging = openmp_logging
        else
            logging = .true.
        end if
        n_threads = num_threads
        if (openmp_is_active ()) then
            if (num_threads == 1) then
                if (logging) then
                    write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", num_threads, &
                        " thread"
                    call msg_message
                end if
                n_threads = num_threads
            else if (num_threads > 1) then
                if (logging) then
                    write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", num_threads, &
                        " threads"
                    call msg_message
                end if
                n_threads = num_threads
            else
                if (logging) then
                    write (msg_buffer, "(A,I0,A)") "OpenMP: " &
                        // "Illegal value of openmp_num_threads (", num_threads, &
                        ") ignored"
                    call msg_error
                end if
                n_threads = openmp_get_default_max_threads ()
                if (logging) then
                    write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", &
                        n_threads, " threads"
                    call msg_message
                end if
            end if
            if (n_threads > openmp_get_default_max_threads ()) then
                if (logging) then
                    write (msg_buffer, "(A,I0)") "OpenMP: " &
                        // "Number of threads is greater than library default of ", &
                        openmp_get_default_max_threads ()
                    call msg_warning
                end if
            end if
        end if
    end subroutine

```

```

        call openmp_set_num_threads (n_threads)
    else if (num_threads /= 1) then
        if (logging) then
            write (msg_buffer, "(A,I0,A)") "openmp_num_threads set to ", &
                num_threads, ", but OpenMP is not active: ignored"
            call msg_warning
        end if
    end if
end subroutine openmp_set_num_threads_verbose

```

5.5.10 Controlling MPI

The overall MPI handling has to be defined in a context specific way, but we can simplify things like logging or receiving `n_size` or `rank`.

```

<OS interface: public>+≡
    public :: mpi_set_logging
<OS interface: sub interfaces>+≡
    module subroutine mpi_set_logging (mpi_logging)
        logical, intent(in) :: mpi_logging
    end subroutine mpi_set_logging
<OS interface: procedures>+≡
    module subroutine mpi_set_logging (mpi_logging)
        logical, intent(in) :: mpi_logging
        integer :: n_size, rank
        call mpi_get_comm_id (n_size, rank)
        if (mpi_logging .and. n_size > 1) then
            write (msg_buffer, "(A,I0,A)") "MPI: Using ", n_size, " processes."
            call msg_message ()
            if (rank == 0) then
                call msg_message ("MPI: master worker")
            else
                write (msg_buffer, "(A,I0)") "MPI: slave worker #", rank
                call msg_message ()
            end if
        end if
    end subroutine mpi_set_logging

```

Receive communicator size and rank inside communicator. The subroutine is a stub, if not compiled with MPI.

```

<OS interface: public>+≡
    public :: mpi_get_comm_id
<OS interface: sub interfaces>+≡
    module subroutine mpi_get_comm_id (n_size, rank)
        integer, intent(out) :: n_size
        integer, intent(out) :: rank
    end subroutine mpi_get_comm_id
<OS interface: procedures>+≡
    module subroutine mpi_get_comm_id (n_size, rank)
        integer, intent(out) :: n_size
        integer, intent(out) :: rank
    end subroutine mpi_get_comm_id

```

```

        n_size = 1
        rank = 0
        <OS interface: mpi get comm id>
        end subroutine mpi_get_comm_id

<OS interface: mpi get comm id>≡

<MPI: OS interface: mpi get comm id>≡
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)

<OS interface: public>+≡
    public :: mpi_is_comm_master

<OS interface: sub interfaces>+≡
    module function mpi_is_comm_master () result (flag)
        logical :: flag
    end function mpi_is_comm_master

<OS interface: procedures>+≡
    module function mpi_is_comm_master () result (flag)
        integer :: n_size, rank
        logical :: flag
        call mpi_get_comm_id (n_size, rank)
        flag = (rank == 0)
    end function mpi_is_comm_master

```

5.5.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<os_interface_ut.f90>≡
    <File header>

    module os_interface_ut
        use unit_tests
        use os_interface_uti

    <Standard module head>

    <OS interface: public test>

    contains

    <OS interface: test driver>

    end module os_interface_ut

<os_interface_uti.f90>≡
    <File header>

    module os_interface_uti

        use, intrinsic :: iso_c_binding !NODEP!

```

```

    <Use strings>
    use io_units

    use os_interface

    <Standard module head>

    <OS interface: test declarations>

contains

    <OS interface: tests>

end module os_interface_util

```

API: driver for the unit tests below.

```

    <OS interface: public test>≡
    public :: os_interface_test

    <OS interface: test driver>≡
    subroutine os_interface_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <OS interface: execute tests>
    end subroutine os_interface_test

```

Write a Fortran source file, compile it to a shared library, load it, and execute the contained function.

```

    <OS interface: execute tests>≡
    call test (os_interface_1, "os_interface_1", &
        "check OS interface routines", &
        u, results)

    <OS interface: test declarations>≡
    public :: os_interface_1

    <OS interface: tests>≡
    subroutine os_interface_1 (u)
        integer, intent(in) :: u
        type(dlaccess_t) :: dlaccess
        type(string_t) :: fname, libname, ext
        type(os_data_t) :: os_data
        type(string_t) :: filename_src, filename_obj
        abstract interface
            function so_test_proc (i) result (j) bind(C)
                import c_int
                integer(c_int), intent(in) :: i
                integer(c_int) :: j
            end function so_test_proc
        end interface
        procedure(so_test_proc), pointer :: so_test => null ()
        type(c_funptr) :: c_funptr
        integer :: unit
        integer(c_int) :: i
        call os_data%init ()

```

```

fname = "so_test"
filename_src = fname // os_data%fc_src_ext
if (os_data%use_libtool) then
    ext = ".lo"
else
    ext = os_data%obj_ext
end if
filename_obj = fname // ext
libname = fname // '.' // os_data%fc_shrlib_ext

write (u, "(A)")  "* Test output: OS interface"
write (u, "(A)")  "* Purpose: check os_interface routines"
write (u, "(A)")

write (u, "(A)")  "* write source file 'so_test.f90'"
write (u, "(A)")
unit = free_unit ()
open (unit=unit, file=char(filename_src), action="write")
write (unit, "(A)") "function so_test (i) result (j) bind(C)"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " integer(c_int), intent(in) :: i"
write (unit, "(A)") " integer(c_int) :: j"
write (unit, "(A)") " j = 2 * i"
write (unit, "(A)") "end function so_test"
close (unit)
write (u, "(A)")  "* compile and link as 'so_test.so/dylib'"
write (u, "(A)")
call os_compile_shared (fname, os_data)
call os_link_shared (filename_obj, fname, os_data)
write (u, "(A)")  "* load library 'so_test.so/dylib'"
write (u, "(A)")
call dlaccess_init (dlaccess, var_str ("."), libname, os_data)
if (dlaccess_is_open (dlaccess)) then
    write (u, "(A)") " success"
else
    write (u, "(A)") " failure"
end if
write (u, "(A)")  "* load symbol 'so_test'"
write (u, "(A)")
c_fptr = dlaccess_get_c_funptr (dlaccess, fname)
if (c_associated (c_fptr)) then
    write (u, "(A)") " success"
else
    write (u, "(A)") " failure"
end if
call c_f_procpointer (c_fptr, so_test)
write (u, "(A)")  "* Execute function from 'so_test.so/dylib'"
i = 7
write (u, "(A,1x,I1)") " input = ", i
write (u, "(A,1x,I1)") " result = ", so_test(i)
if (so_test(i) / i .ne. 2) then
    write (u, "(A)")  "* Compiling and linking ISO C functions failed."
else
    write (u, "(A)")  "* Successful."

```

```

    end if
    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
    call dlaccess_final (dlaccess)
end subroutine os_interface_1

```

5.6 Interface for formatted I/O

For access to formatted printing (possibly input), we interface the C `printf` family of functions. There are two important issues here:

1. `printf` takes an arbitrary number of arguments, relying on the C stack. This is not interoperable. We interface it with C wrappers that output a single integer, real or string and restrict the allowed formats accordingly.
2. Restricting format strings is essential also for preventing format string attacks. Allowing arbitrary format string would create a real security hole in a Fortran program.
3. The string returned by `sprintf` must be allocated to the right size.

`<formats.f90>`≡
<File header>

```
module formats
```

```
    use, intrinsic :: iso_c_binding
```

<Use kinds>

<Use strings>

<Standard module head>

<Formats: public>

<Formats: parameters>

<Formats: types>

<Formats: interfaces>

```
    interface
```

<Formats: sub interfaces>

```
    end interface
```

```
end module formats
```

`<formats_sub.f90>`≡
<File header>

```
submodule (formats) formats_s
```

```
    use io_units
```

```

    use diagnostics

    implicit none

contains

  <Formats: procedures>

end submodule formats_s

```

5.6.1 Parsing a C format string

The C format string contains characters and format conversion specifications. The latter are initiated by a % sign. If the next letter is also a %, a percent sign is printed and no conversion is done. Otherwise, a conversion is done and applied to the next argument in the argument list. First comes an optional flag (#, 0, -, +, or space), an optional field width (decimal digits starting not with zero), an optional precision (period, then another decimal digit string), a length modifier (irrelevant for us, therefore not supported), and a conversion specifier: **d** or **i** for integer; **e**, **f**, **g** (also upper case) for double-precision real, **s** for a string.

We explicitly exclude all other conversion specifiers, and we check the specifiers against the actual arguments.

A type for passing arguments

This is a polymorphic type that can hold integer, real (double), and string arguments.

```

<Formats: parameters>≡
  integer, parameter, public :: ARGTYPE_NONE = 0
  integer, parameter, public :: ARGTYPE_LOG = 1
  integer, parameter, public :: ARGTYPE_INT = 2
  integer, parameter, public :: ARGTYPE_REAL = 3
  integer, parameter, public :: ARGTYPE_STR = 4

```

The integer and real entries are actually scalars, but we avoid relying on the allocatable-scalar feature and make them one-entry arrays. The character entry is a real array which is a copy of the string.

Logical values are mapped to strings (true or false), so this type parameter value is mostly unused.

```

<Formats: public>≡
  public :: sprintf_arg_t

<Formats: types>≡
  type :: sprintf_arg_t
  private
    integer :: type = ARGTYPE_NONE
    integer(c_int), dimension(:), allocatable :: ival
    real(c_double), dimension(:), allocatable :: rval
    character(c_char), dimension(:), allocatable :: sval
  end type sprintf_arg_t

```



```

<Formats: public>+≡
    public :: sprintf_arg_init

<Formats: interfaces>≡
    interface sprintf_arg_init
        module procedure sprintf_arg_init_log
        module procedure sprintf_arg_init_int
        module procedure sprintf_arg_init_real
        module procedure sprintf_arg_init_str
    end interface

<Formats: sub interfaces>≡
    module subroutine sprintf_arg_init_log (arg, lval)
        type(sprintf_arg_t), intent(out) :: arg
        logical, intent(in) :: lval
    end subroutine sprintf_arg_init_log
    module subroutine sprintf_arg_init_int (arg, ival)
        type(sprintf_arg_t), intent(out) :: arg
        integer, intent(in) :: ival
    end subroutine sprintf_arg_init_int
    module subroutine sprintf_arg_init_real (arg, rval)
        type(sprintf_arg_t), intent(out) :: arg
        real(default), intent(in) :: rval
    end subroutine sprintf_arg_init_real
    module subroutine sprintf_arg_init_str (arg, sval)
        type(sprintf_arg_t), intent(out) :: arg
        type(string_t), intent(in) :: sval
    end subroutine sprintf_arg_init_str

<Formats: procedures>≡
    module subroutine sprintf_arg_init_log (arg, lval)
        type(sprintf_arg_t), intent(out) :: arg
        logical, intent(in) :: lval
        arg%type = ARGTYPE_STR
        if (lval) then
            allocate (arg%sval (5))
            arg%sval = ['t', 'r', 'u', 'e', c_null_char]
        else
            allocate (arg%sval (6))
            arg%sval = ['f', 'a', 'l', 's', 'e', c_null_char]
        end if
    end subroutine sprintf_arg_init_log

    module subroutine sprintf_arg_init_int (arg, ival)
        type(sprintf_arg_t), intent(out) :: arg
        integer, intent(in) :: ival
        arg%type = ARGTYPE_INT
        allocate (arg%ival (1))
        arg%ival = ival
    end subroutine sprintf_arg_init_int

    module subroutine sprintf_arg_init_real (arg, rval)
        type(sprintf_arg_t), intent(out) :: arg
        real(default), intent(in) :: rval
        arg%type = ARGTYPE_REAL

```

```

        allocate (arg%rval (1))
        arg%rval = rval
    end subroutine sprintf_arg_init_real

module subroutine sprintf_arg_init_str (arg, sval)
    type(sprintf_arg_t), intent(out) :: arg
    type(string_t), intent(in) :: sval
    integer :: i
    arg%type = ARGTYPE_STR
    allocate (arg%sval (len (sval) + 1))
    do i = 1, len (sval)
        arg%sval(i) = extract (sval, i, i)
    end do
    arg%sval(len (sval) + 1) = c_null_char
end subroutine sprintf_arg_init_str

```

(Formats: procedures)+≡

```

subroutine sprintf_arg_write (arg, unit)
    type(sprintf_arg_t), intent(in) :: arg
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    select case (arg%type)
    case (ARGTYPE_NONE)
        write (u, *) "[none]"
    case (ARGTYPE_INT)
        write (u, "(1x,A,1x)", advance = "no") "[int]"
        write (u, *) arg%ival
    case (ARGTYPE_REAL)
        write (u, "(1x,A,1x)", advance = "no") "[real]"
        write (u, *) arg%rval
    case (ARGTYPE_STR)
        write (u, "(1x,A,1x,A)", advance = "no") "[string]", ''
        write (u, *) arg%rval, ''
    end select
end subroutine sprintf_arg_write

```

Return an upper bound for the length of the printed version; in case of strings the result is exact.

(Formats: procedures)+≡

```

elemental function sprintf_arg_get_length (arg) result (length)
    integer :: length
    type(sprintf_arg_t), intent(in) :: arg
    select case (arg%type)
    case (ARGTYPE_INT)
        length = log10 (real (huge (arg%ival(1)))) + 2
    case (ARGTYPE_REAL)
        length = log10 (real (radix (arg%rval(1))) ** digits (arg%rval(1))) + 8
    case (ARGTYPE_STR)
        length = size (arg%sval)
    case default
        length = 0
    end select

```

```
end function sprintf_arg_get_length
```

(Formats: procedures)+≡

```
subroutine sprintf_arg_apply_printf (arg, fmt, result, actual_length)
  type(sprintf_arg_t), intent(in) :: arg
  character(c_char), dimension(:), intent(in) :: fmt
  character(c_char), dimension(:), intent(inout) :: result
  integer, intent(out) :: actual_length
  integer(c_int) :: ival
  real(c_double) :: rval
  select case (arg%type)
  case (ARGTYPE_NONE)
    actual_length = sprintf_none (result, fmt)
  case (ARGTYPE_INT)
    ival = arg%ival(1)
    actual_length = sprintf_int (result, fmt, ival)
  case (ARGTYPE_REAL)
    rval = arg%rval(1)
    actual_length = sprintf_double (result, fmt, rval)
  case (ARGTYPE_STR)
    actual_length = sprintf_str (result, fmt, arg%sval)
  case default
    call msg_bug ("sprintf_arg_apply_printf called with illegal type")
  end select
  if (actual_length < 0) then
    write (msg_buffer, *) "Format: '", fmt, "'"
    call msg_message ()
    write (msg_buffer, *) "Output: '", result, "'"
    call msg_message ()
    call msg_error ("I/O error in sprintf call")
    actual_length = 0
  end if
end subroutine sprintf_arg_apply_printf
```

Container type for the output

There is a procedure which chops the format string into pieces that contain at most one conversion specifier. Pairing this with a `sprintf_arg` object, we get the actual input to the `sprintf` interface. The type below holds this input and can allocate the output string.

(Formats: types)+≡

```
type :: sprintf_interface_t
  private
  character(c_char), dimension(:), allocatable :: input_fmt
  type(sprintf_arg_t) :: arg
  character(c_char), dimension(:), allocatable :: output_str
  integer :: output_str_len = 0
end type sprintf_interface_t
```

(Formats: procedures)+≡

```
subroutine sprintf_interface_init (intf, fmt, arg)
```

```

type(sprintf_interface_t), intent(out) :: intf
type(string_t), intent(in) :: fmt
type(sprintf_arg_t), intent(in) :: arg
integer :: fmt_len, i
fmt_len = len (fmt)
allocate (intf%input_fmt (fmt_len + 1))
do i = 1, fmt_len
    intf%input_fmt(i) = extract (fmt, i, i)
end do
intf%input_fmt(fmt_len+1) = c_null_char
intf%arg = arg
allocate (intf%output_str (len (fmt) + sprintf_arg_get_length (arg) + 1))
end subroutine sprintf_interface_init

```

(Formats: procedures)+≡

```

subroutine sprintf_interface_write (intf, unit)
type(sprintf_interface_t), intent(in) :: intf
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
write (u, *) "Format string = ", "'", intf%input_fmt, "'"
write (u, "(1x,A,1x)", advance = "no") "Argument = "
call sprintf_arg_write (intf%arg, unit)
if (intf%output_str_len > 0) then
    write (u, *) "Result string = ", &
        "'", intf%output_str (1:intf%output_str_len), "'"
end if
end subroutine sprintf_interface_write

```

Return the output string:

(Formats: procedures)+≡

```

function sprintf_interface_get_result (intf) result (string)
type(string_t) :: string
type(sprintf_interface_t), intent(in) :: intf
character(kind = c_char, len = max (intf%output_str_len, 0)) :: buffer
integer :: i
if (intf%output_str_len > 0) then
    do i = 1, intf%output_str_len
        buffer(i:i) = intf%output_str(i)
    end do
    string = buffer(1:intf%output_str_len)
else
    string = ""
end if
end function sprintf_interface_get_result

```

(Formats: procedures)+≡

```

subroutine sprintf_interface_apply_sprintf (intf)
type(sprintf_interface_t), intent(inout) :: intf
call sprintf_arg_apply_sprintf &
    (intf%arg, intf%input_fmt, intf%output_str, intf%output_str_len)
end subroutine sprintf_interface_apply_sprintf

```

Import the interfaces defined in the previous section:

```

<Formats: interfaces> +=
  <sprintf interfaces>

```

Scan the format string

Chop it into pieces that contain one conversion specifier each. The zero-th piece contains the part before the first specifier. Check the specifiers and allow only the subset that we support. Also check for an exact match between conversion specifiers and input arguments. The result is an allocated array of `sprintf_interface` object; each one contains a piece of the format string and the corresponding argument.

```

<Formats: procedures> +=
  subroutine chop_and_check_format_string (fmt, arg, intf)
    type(string_t), intent(in) :: fmt
    type(sprintf_arg_t), dimension(:), intent(in) :: arg
    type(sprintf_interface_t), dimension(:), intent(out), allocatable :: intf
    integer :: n_args, i
    type(string_t), dimension(:), allocatable :: split_fmt
    type(string_t) :: word, buffer, separator
    integer :: pos, length, l
    logical :: ok
    type(sprintf_arg_t) :: arg_null
    ok = .true.
    length = 0
    n_args = size (arg)
    allocate (split_fmt (0:n_args))
    split_fmt = ""
    buffer = fmt
    SCAN_ARGS: do i = 1, n_args
      FIND_CONVERSION: do
        call split (buffer, word, "%", separator=separator)
        if (separator == "") then
          call msg_message ('"' // char (fmt) // '"')
          call msg_error ("C-formatting string: " &
            // "too few conversion specifiers in format string")
          ok = .false.; exit SCAN_ARGS
        end if
        split_fmt(i-1) = split_fmt(i-1) // word
        if (extract (buffer, 1, 1) /= "%") then
          split_fmt(i) = "%"
          exit FIND_CONVERSION
        else
          split_fmt(i-1) = split_fmt(i-1) // "%"
        end if
      end do FIND_CONVERSION
      pos = verify (buffer, "#0-+ ") ! Flag characters (zero or more)
      split_fmt(i) = split_fmt(i) // extract (buffer, 1, pos-1)
      buffer = remove (buffer, 1, pos-1)
      pos = verify (buffer, "123456890") ! Field width
      word = extract (buffer, 1, pos-1)
      if (len (word) /= 0) then

```

```

        call read_int_from_string (word, len (word), 1)
        length = length + 1
    end if
    split_fmt(i) = split_fmt(i) // word
    buffer = remove (buffer, 1, pos-1)
    if (extract (buffer, 1, 1) == ".") then
        buffer = remove (buffer, 1, 1)
        pos = verify (buffer, "1234567890")    ! Precision
        split_fmt(i) = split_fmt(i) // "." // extract (buffer, 1, pos-1)
        buffer = remove (buffer, 1, pos-1)
    end if
    ! Length modifier would come here, but is not allowed
    select case (char (extract (buffer, 1, 1))) ! conversion specifier
    case ("d", "i")
        if (arg(i)%type /= ARGTYPE_INT) then
            call msg_message (''' // char (fmt) // ''')
            call msg_error ("C-formatting string: " &
                // "argument type mismatch: integer value expected")
            ok = .false.; exit SCAN_ARGS
        end if
    case ("e", "E", "f", "F", "g", "G")
        if (arg(i)%type /= ARGTYPE_REAL) then
            call msg_message (''' // char (fmt) // ''')
            call msg_error ("C-formatting string: " &
                // "argument type mismatch: real value expected")
            ok = .false.; exit SCAN_ARGS
        end if
    case ("s")
        if (arg(i)%type /= ARGTYPE_STR) then
            call msg_message (''' // char (fmt) // ''')
            call msg_error ("C-formatting string: " &
                // "argument type mismatch: logical or string value expected")
            ok = .false.; exit SCAN_ARGS
        end if
    case default
        call msg_message (''' // char (fmt) // ''')
        call msg_error ("C-formatting string: " &
            // "illegal or incomprehensible conversion specifier")
        ok = .false.; exit SCAN_ARGS
    end select
    split_fmt(i) = split_fmt(i) // extract (buffer, 1, 1)
    buffer = remove (buffer, 1, 1)
end do SCAN_ARGS
if (ok) then
    FIND_EXTRA_CONVERSION: do
        call split (buffer, word, "%", separator=separator)
        split_fmt(n_args) = split_fmt(n_args) // word // separator
        if (separator == "") exit FIND_EXTRA_CONVERSION
        if (extract (buffer, 1, 1) == "%") then
            split_fmt(n_args) = split_fmt(n_args) // "%"
            buffer = remove (buffer, 1, 1)
        else
            call msg_message (''' // char (fmt) // ''')
            call msg_error ("C-formatting string: " &

```

```

        // "too many conversion specifiers in format string")
        ok = .false.; exit FIND_EXTRA_CONVERSION
    end if
    end do FIND_EXTRA_CONVERSION
    split_fmt(n_args) = split_fmt(n_args) // buffer
    allocate (intf (0:n_args))
    call sprintf_interface_init (intf(0), split_fmt(0), arg_null)
    do i = 1, n_args
        call sprintf_interface_init (intf(i), split_fmt(i), arg(i))
    end do
else
    allocate (intf (0))
end if
end if
contains
subroutine read_int_from_string (word, length, l)
    type(string_t), intent(in) :: word
    integer, intent(in) :: length
    integer, intent(out) :: l
    character(len=length) :: buffer
    buffer = word
    read (buffer, *) l
end subroutine read_int_from_string
end subroutine chop_and_check_format_string

```

5.6.2 API

```

<Formats: public>+≡
    public :: sprintf

<Formats: sub interfaces>+≡
    module function sprintf (fmt, arg) result (string)
        type(string_t) :: string
        type(string_t), intent(in) :: fmt
        type(sprintf_arg_t), dimension(:), intent(in) :: arg
    end function sprintf

<Formats: procedures>+≡
    module function sprintf (fmt, arg) result (string)
        type(string_t) :: string
        type(string_t), intent(in) :: fmt
        type(sprintf_arg_t), dimension(:), intent(in) :: arg
        type(sprintf_interface_t), dimension(:), allocatable :: intf
        integer :: i
        string = ""
        call chop_and_check_format_string (fmt, arg, intf)
        if (size (intf) > 0) then
            do i = 0, ubound (intf, 1)
                call sprintf_interface_apply_sprintf (intf(i))
                string = string // sprintf_interface_get_result (intf(i))
            end do
        end if
    end function sprintf

```

5.6.3 Unit tests

Test module, followed by the corresponding implementation module.

<formats_ut.f90>≡
<File header>

```
module formats_ut
  use unit_tests
  use formats_uti
```

<Standard module head>

<Formats: public test>

contains

<Formats: test driver>

```
end module formats_ut
```

<formats_uti.f90>≡
<File header>

```
module formats_uti
```

<Use kinds>

<Use strings>

```
  use formats
```

<Standard module head>

<Formats: test declarations>

<Formats: test types>

contains

<Formats: tests>

```
end module formats_uti
```

API: driver for the unit tests below.

<Formats: public test>≡
public :: format_test

<Formats: test driver>≡
subroutine format_test (u, results)
 integer, **intent**(in) :: u
 type(test_results_t), **intent**(inout) :: results
<Formats: execute tests>
end subroutine format_test

<Formats: execute tests>≡
call test (format_1, "format_1", &


```

        "check formatting routines", &
        u, results)

<Formats: test declarations>≡
    public :: format_1

<Formats: tests>≡
    subroutine format_1 (u)
        integer, intent(in) :: u
        write (u, "(A)")  "*** Test 1: a string ***"
        write (u, "(A)")
        call test_run (var_str("%s"), 1, [4], ['abcdefghij'], u)
        write (u, "(A)")  "*** Test 2: two integers ***"
        write (u, "(A)")
        call test_run (var_str("%d,%d"), 2, [2, 2], ['42', '13'], u)
        write (u, "(A)")  "*** Test 3: floating point number ***"
        write (u, "(A)")
        call test_run (var_str("%8.4f"), 1, [3], ['42567.12345'], u)
        write (u, "(A)")  "*** Test 4: general expression ***"
        call test_run (var_str("%g"), 1, [3], ['3.1415'], u)
        contains
        subroutine test_run (fmt, n_args, type, buffer, unit)
            type(string_t), intent(in) :: fmt
            integer, intent(in) :: n_args, unit
            logical :: lval
            integer :: ival
            real(default) :: rval
            integer :: i
            type(string_t) :: string
            type(sprintf_arg_t), dimension(:), allocatable :: arg
            integer, dimension(n_args), intent(in) :: type
            character(*), dimension(n_args), intent(in) :: buffer
            write (unit, "(A,A)")  "Format string :", char(fmt)
            write (unit, "(A,I1)") "Number of args:", n_args
            allocate (arg (n_args))
            do i = 1, n_args
                write (unit, "(A,I1)") "Argument (type ) = ", type(i)
                select case (type(i))
                case (ARGTYPE_LOG)
                    read (buffer(i), *) lval
                    call sprintf_arg_init (arg(i), lval)
                case (ARGTYPE_INT)
                    read (buffer(i), *) ival
                    call sprintf_arg_init (arg(i), ival)
                case (ARGTYPE_REAL)
                    read (buffer(i), *) rval
                    call sprintf_arg_init (arg(i), rval)
                case (ARGTYPE_STR)
                    call sprintf_arg_init (arg(i), var_str (trim (buffer(i))))
                end select
            end do
            string = sprintf (fmt, arg)
            write (unit, "(A,A,A)") "Result: '", char (string), "'"
            deallocate (arg)
        end subroutine test_run

```

```
end subroutine format_1
```

5.7 CPU timing

The time is stored in a simple derived type which just holds a floating-point number.

```
<cputime.f90>≡
  <File header>

  module cputime

    <Use kinds>
    <Use strings>

    <Standard module head>

    <CPU time: public>

    <CPU time: types>

    <CPU time: interfaces>

    interface
    <CPU time: sub interfaces>
    end interface

  end module cputime

<cputime_sub.f90>≡
  <File header>

  submodule (cputime) cputime_s

    use io_units
    use diagnostics

    implicit none

  contains

    <CPU time: procedures>

  end submodule cputime_s
```

The CPU time is a floating-point number with an arbitrary reference time. It is single precision (default real, not `real(default)`). It is measured in seconds.

```
<CPU time: public>≡
  public :: time_t

<CPU time: types>≡
  type :: time_t
    private
```

```

        logical :: known = .false.
        real :: value = 0
contains
    <CPU time: time: TBP>
end type time_t

<CPU time: time: TBP>≡
    procedure :: write => time_write

<CPU time: sub interfaces>≡
    module subroutine time_write (object, unit)
        class(time_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine time_write

<CPU time: procedures>≡
    module subroutine time_write (object, unit)
        class(time_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "Time in seconds ="
        if (object%known) then
            write (u, "(1x,ES10.3)") object%value
        else
            write (u, "(1x,A)") "[unknown]"
        end if
    end subroutine time_write

```

Set the current time

```

<CPU time: time: TBP>+≡
    procedure :: set_current => time_set_current

<CPU time: sub interfaces>+≡
    module subroutine time_set_current (time)
        class(time_t), intent(out) :: time
    end subroutine time_set_current

<CPU time: procedures>+≡
    module subroutine time_set_current (time)
        class(time_t), intent(out) :: time
        integer :: msec
        call system_clock (msec)
        time%value = real (msec) / 1000.
        time%known = time%value > 0
    end subroutine time_set_current

```

Assign to a real (default value. If the time is undefined, return zero.

```

<CPU time: public>+≡
    public :: assignment(=)

<CPU time: interfaces>≡
    interface assignment(=)
        module procedure real_assign_time
        module procedure real_default_assign_time
    end interface

```

```
end interface
```

<CPU time: sub interfaces>+≡

```
pure module subroutine real_assign_time (r, time)
  real, intent(out) :: r
  class(time_t), intent(in) :: time
end subroutine real_assign_time
pure module subroutine real_default_assign_time (r, time)
  real(default), intent(out) :: r
  class(time_t), intent(in) :: time
end subroutine real_default_assign_time
```

<CPU time: procedures>+≡

```
pure module subroutine real_assign_time (r, time)
  real, intent(out) :: r
  class(time_t), intent(in) :: time
  if (time%known) then
    r = time%value
  else
    r = 0
  end if
end subroutine real_assign_time

pure module subroutine real_default_assign_time (r, time)
  real(default), intent(out) :: r
  class(time_t), intent(in) :: time
  if (time%known) then
    r = time%value
  else
    r = 0
  end if
end subroutine real_default_assign_time
```

Assign an integer or (single precision) real value to the time object.

<CPU time: time: TBP>+≡

```
generic :: assignment(=) => time_assign_from_integer, time_assign_from_real
procedure, private :: time_assign_from_integer
procedure, private :: time_assign_from_real
```

<CPU time: sub interfaces>+≡

```
module subroutine time_assign_from_integer (time, ival)
  class(time_t), intent(out) :: time
  integer, intent(in) :: ival
end subroutine time_assign_from_integer
module subroutine time_assign_from_real (time, rval)
  class(time_t), intent(out) :: time
  real, intent(in) :: rval
end subroutine time_assign_from_real
```

<CPU time: procedures>+≡

```
module subroutine time_assign_from_integer (time, ival)
  class(time_t), intent(out) :: time
  integer, intent(in) :: ival
  time%value = ival
  time%known = .true.
```

```

end subroutine time_assign_from_integer

module subroutine time_assign_from_real (time, rval)
  class(time_t), intent(out) :: time
  real, intent(in) :: rval
  time%value = rval
  time%known = .true.
end subroutine time_assign_from_real

```

Add times and compute time differences. If any input value is undefined, the result is undefined.

```

<CPU time: time: TBP>+≡
  generic :: operator(-) => subtract_times
  generic :: operator(+) => add_times
  procedure, private :: subtract_times
  procedure, private :: add_times

<CPU time: sub interfaces>+≡
  pure module function subtract_times (t_end, t_begin) result (time)
    type(time_t) :: time
    class(time_t), intent(in) :: t_end, t_begin
  end function subtract_times
  pure module function add_times (t1, t2) result (time)
    type(time_t) :: time
    class(time_t), intent(in) :: t1, t2
  end function add_times

<CPU time: procedures>+≡
  pure module function subtract_times (t_end, t_begin) result (time)
    type(time_t) :: time
    class(time_t), intent(in) :: t_end, t_begin
    if (t_end%known .and. t_begin%known) then
      time%known = .true.
      time%value = t_end%value - t_begin%value
    end if
  end function subtract_times

  pure module function add_times (t1, t2) result (time)
    type(time_t) :: time
    class(time_t), intent(in) :: t1, t2
    if (t1%known .and. t2%known) then
      time%known = .true.
      time%value = t1%value + t2%value
    end if
  end function add_times

```

Check if a time is known, so we can use it:

```

<CPU time: time: TBP>+≡
  procedure :: is_known => time_is_known

<CPU time: sub interfaces>+≡
  module function time_is_known (time) result (flag)
    class(time_t), intent(in) :: time
    logical :: flag
  end function time_is_known

```

```

<CPU time: procedures>+≡
  module function time_is_known (time) result (flag)
    class(time_t), intent(in) :: time
    logical :: flag
    flag = time%known
  end function time_is_known

```

We define functions for converting the time into ss / mm:ss / hh:mm:ss / dd:mm:hh:ss.

```

<CPU time: time: TBP>+≡
  generic :: expand => time_expand_s, time_expand_ms, &
    time_expand_hms, time_expand_dhms
  procedure, private :: time_expand_s
  procedure, private :: time_expand_ms
  procedure, private :: time_expand_hms
  procedure, private :: time_expand_dhms

<CPU time: sub interfaces>+≡
  module subroutine time_expand_s (time, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: sec
  end subroutine time_expand_s
  module subroutine time_expand_ms (time, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: min, sec
  end subroutine time_expand_ms
  module subroutine time_expand_hms (time, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: hour, min, sec
  end subroutine time_expand_hms
  module subroutine time_expand_dhms (time, day, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: day, hour, min, sec
  end subroutine time_expand_dhms

<CPU time: procedures>+≡
  module subroutine time_expand_s (time, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: sec
    if (time%known) then
      sec = time%value
    else
      call msg_bug ("Time: attempt to expand undefined value")
    end if
  end subroutine time_expand_s

  module subroutine time_expand_ms (time, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: min, sec
    if (time%known) then
      if (time%value >= 0) then
        sec = mod (int (time%value), 60)
      else
        sec = - mod (int (- time%value), 60)
      end if
    end if
  end subroutine time_expand_ms

```

```

        min = time%value / 60
    else
        call msg_bug ("Time: attempt to expand undefined value")
    end if
end subroutine time_expand_ms

module subroutine time_expand_hms (time, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: hour, min, sec
    call time%expand (min, sec)
    hour = min / 60
    if (min >= 0) then
        min = mod (min, 60)
    else
        min = - mod (-min, 60)
    end if
end subroutine time_expand_hms

module subroutine time_expand_dhms (time, day, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: day, hour, min, sec
    call time%expand (hour, min, sec)
    day = hour / 24
    if (hour >= 0) then
        hour = mod (hour, 24)
    else
        hour = - mod (- hour, 24)
    end if
end subroutine time_expand_dhms

```

Use the above expansions to generate a time string.

```

<CPU time: time: TBP>+≡
    procedure :: to_string_s => time_to_string_s
    procedure :: to_string_ms => time_to_string_ms
    procedure :: to_string_hms => time_to_string_hms
    procedure :: to_string_dhms => time_to_string_dhms

<CPU time: sub interfaces>+≡
    module function time_to_string_s (time) result (str)
        class(time_t), intent(in) :: time
        type(string_t) :: str
    end function time_to_string_s
    module function time_to_string_ms (time, blank) result (str)
        class(time_t), intent(in) :: time
        logical, intent(in), optional :: blank
        type(string_t) :: str
    end function time_to_string_ms
    module function time_to_string_hms (time) result (str)
        class(time_t), intent(in) :: time
        type(string_t) :: str
    end function time_to_string_hms
    module function time_to_string_dhms (time) result (str)
        class(time_t), intent(in) :: time
        type(string_t) :: str
    end function time_to_string_dhms

```

```

end function time_to_string_dhms

<CPU time: procedures>+=
module function time_to_string_s (time) result (str)
  class(time_t), intent(in) :: time
  type(string_t) :: str
  character(256) :: buffer
  integer :: s
  call time%expand (s)
  write (buffer, "(I0,'s')") s
  str = trim (buffer)
end function time_to_string_s

module function time_to_string_ms (time, blank) result (str)
  class(time_t), intent(in) :: time
  logical, intent(in), optional :: blank
  type(string_t) :: str
  character(256) :: buffer
  integer :: s, m
  logical :: x_out
  x_out = .false.
  if (present (blank)) x_out = blank
  call time%expand (m, s)
  write (buffer, "(I0,'m:',I2.2,'s')") m, abs (s)
  str = trim (buffer)
  if (x_out) then
    str = replace (str, len(str)-1, "X")
  end if
end function time_to_string_ms

module function time_to_string_hms (time) result (str)
  class(time_t), intent(in) :: time
  type(string_t) :: str
  character(256) :: buffer
  integer :: s, m, h
  call time%expand (h, m, s)
  write (buffer, "(I0,'h:',I2.2,'m:',I2.2,'s')") h, abs (m), abs (s)
  str = trim (buffer)
end function time_to_string_hms

module function time_to_string_dhms (time) result (str)
  class(time_t), intent(in) :: time
  type(string_t) :: str
  character(256) :: buffer
  integer :: s, m, h, d
  call time%expand (d, h, m, s)
  write (buffer, "(I0,'d:',I2.2,'h:',I2.2,'m:',I2.2,'s')") &
    d, abs (h), abs (m), abs (s)
  str = trim (buffer)
end function time_to_string_dhms

```


5.7.1 Timer

A timer can measure real (wallclock) time differences. The base type corresponds to the result, i.e., time difference. The object contains two further times for start and stop time.

```

<CPU time: public>+≡
    public :: timer_t

<CPU time: types>+≡
    type, extends (time_t) :: timer_t
    private
        logical :: running = .false.
        type(time_t) :: t1, t2
    contains
        <CPU time: timer: TBP>
    end type timer_t

```

Output. If the timer is running, we indicate this, otherwise write just the result.

```

<CPU time: timer: TBP>≡
    procedure :: write => timer_write

<CPU time: sub interfaces>+≡
    module subroutine timer_write (object, unit)
        class(timer_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine timer_write

<CPU time: procedures>+≡
    module subroutine timer_write (object, unit)
        class(timer_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%running) then
            write (u, "(1x,A)") "Time in seconds = [running]"
        else
            call object%time_t%write (u)
        end if
    end subroutine timer_write

```

Start the timer: store the current time in the first entry and adapt the status. We forget any previous values.

```

<CPU time: timer: TBP>+≡
    procedure :: start => timer_start

<CPU time: sub interfaces>+≡
    module subroutine timer_start (timer)
        class(timer_t), intent(out) :: timer
    end subroutine timer_start

<CPU time: procedures>+≡
    module subroutine timer_start (timer)
        class(timer_t), intent(out) :: timer
        call timer%t1%set_current ()
        timer%running = .true.
    end subroutine timer_start

```

```
end subroutine timer_start
```

Restart the timer: simply adapt the status, keeping the start time.

```
<CPU time: timer: TBP>+≡
  procedure :: restart => timer_restart

<CPU time: sub interfaces>+≡
  module subroutine timer_restart (timer)
    class(timer_t), intent(inout) :: timer
  end subroutine timer_restart

<CPU time: procedures>+≡
  module subroutine timer_restart (timer)
    class(timer_t), intent(inout) :: timer
    if (timer%t1%known .and. .not. timer%running) then
      timer%running = .true.
    else
      call msg_bug ("Timer: restart attempt from wrong status")
    end if
  end subroutine timer_restart
```

Stop the timer: store the current time in the second entry, adapt the status, and compute the elapsed time.

```
<CPU time: timer: TBP>+≡
  procedure :: stop => timer_stop

<CPU time: sub interfaces>+≡
  module subroutine timer_stop (timer)
    class(timer_t), intent(inout) :: timer
  end subroutine timer_stop

<CPU time: procedures>+≡
  module subroutine timer_stop (timer)
    class(timer_t), intent(inout) :: timer
    call timer%t2%set_current ()
    timer%running = .false.
    call timer%evaluate ()
  end subroutine timer_stop
```

Manually set the time (for unit test)

```
<CPU time: timer: TBP>+≡
  procedure :: set_test_time1 => timer_set_test_time1
  procedure :: set_test_time2 => timer_set_test_time2

<CPU time: sub interfaces>+≡
  module subroutine timer_set_test_time1 (timer, t)
    class(timer_t), intent(inout) :: timer
    integer, intent(in) :: t
  end subroutine timer_set_test_time1
  module subroutine timer_set_test_time2 (timer, t)
    class(timer_t), intent(inout) :: timer
    integer, intent(in) :: t
  end subroutine timer_set_test_time2
```

```

⟨CPU time: procedures⟩+≡
  module subroutine timer_set_test_time1 (timer, t)
    class(timer_t), intent(inout) :: timer
    integer, intent(in) :: t
    timer%t1 = t
  end subroutine timer_set_test_time1

  module subroutine timer_set_test_time2 (timer, t)
    class(timer_t), intent(inout) :: timer
    integer, intent(in) :: t
    timer%t2 = t
  end subroutine timer_set_test_time2

```

This is separate, available for the unit test.

```

⟨CPU time: timer: TBP⟩+≡
  procedure :: evaluate => timer_evaluate

⟨CPU time: sub interfaces⟩+≡
  module subroutine timer_evaluate (timer)
    class(timer_t), intent(inout) :: timer
  end subroutine timer_evaluate

⟨CPU time: procedures⟩+≡
  module subroutine timer_evaluate (timer)
    class(timer_t), intent(inout) :: timer
    timer%time_t = timer%t2 - timer%t1
  end subroutine timer_evaluate

```

5.7.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨cputime_ut.f90⟩≡
  ⟨File header⟩

  module cputime_ut
    use unit_tests
    use cputime_util

    ⟨Standard module head⟩

    ⟨CPU time: public test⟩

    contains

    ⟨CPU time: test driver⟩

  end module cputime_ut

⟨cputime_util.f90⟩≡
  ⟨File header⟩

  module cputime_util

```

```

    <Use strings>

    use cputime

    <Standard module head>

    <CPU time: test declarations>

contains

    <CPU time: tests>

end module cputime_util
API: driver for the unit tests below.
<CPU time: public test>≡
    public :: cputime_test
<CPU time: test driver>≡
    subroutine cputime_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <CPU time: execute tests>
end subroutine cputime_test

```

Basic tests

Check basic functions of the time object. The part which we can't check is getting the actual time from the system clock, since the output will not be reproducible. However, we can check time formats and operations.

```

<CPU time: execute tests>≡
    call test (cputime_1, "cputime_1", &
        "time operations", &
        u, results)

<CPU time: test declarations>≡
    public :: cputime_1

<CPU time: tests>≡
    subroutine cputime_1 (u)
        integer, intent(in) :: u
        type(time_t) :: time, time1, time2
        real :: t
        integer :: d, h, m, s

        write (u, "(A)")  "* Test output: cputime_1"
        write (u, "(A)")  "* Purpose: check time operations"
        write (u, "(A)")

        write (u, "(A)")  "* Undefined time"
        write (u, *)

        call time%write (u)
    end subroutine cputime_1

```

```

write (u, *)
write (u, "(A)") "* Set time to zero"
write (u, *)

time = 0
call time%write (u)

write (u, *)
write (u, "(A)") "* Set time to 1.234 s"
write (u, *)

time = 1.234
call time%write (u)

t = time
write (u, "(1x,A,F6.3)") "Time as real =", t

write (u, *)
write (u, "(A)") "* Compute time difference"
write (u, *)

time1 = 5.33
time2 = 7.55
time = time2 - time1

call time1%write (u)
call time2%write (u)
call time%write (u)

write (u, *)
write (u, "(A)") "* Compute time sum"
write (u, *)

time = time2 + time1

call time1%write (u)
call time2%write (u)
call time%write (u)

write (u, *)
write (u, "(A)") "* Expand time"
write (u, *)

time1 = ((24 + 1) * 60 + 1) * 60 + 1
time2 = ((3 * 24 + 23) * 60 + 59) * 60 + 59

call time1%expand (s)
write (u, 1) "s =", s
call time1%expand (m,s)
write (u, 1) "ms =", m, s
call time1%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time1%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

```

```

call time2%expand (s)
write (u, 1) "s =", s
call time2%expand (m,s)
write (u, 1) "ms =", m, s
call time2%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time2%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

write (u, *)
write (u, "(A)") "* Expand negative time"
write (u, *)

time1 = - (((24 + 1) * 60 + 1) * 60 + 1)
time2 = - (((3 * 24 + 23) * 60 + 59) * 60 + 59)

call time1%expand (s)
write (u, 1) "s =", s
call time1%expand (m,s)
write (u, 1) "ms =", m, s
call time1%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time1%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

call time2%expand (s)
write (u, 1) "s =", s
call time2%expand (m,s)
write (u, 1) "ms =", m, s
call time2%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time2%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

1  format (1x,A,1x,4(I0,:',':'))

write (u, *)
write (u, "(A)") "* String from time"
write (u, *)

time1 = ((24 + 1) * 60 + 1) * 60 + 1
time2 = ((3 * 24 + 23) * 60 + 59) * 60 + 59

write (u, "(A)") char (time1%to_string_s ())
write (u, "(A)") char (time1%to_string_ms ())
write (u, "(A)") char (time1%to_string_hms ())
write (u, "(A)") char (time1%to_string_dhms ())

write (u, "(A)") char (time2%to_string_s ())
write (u, "(A)") char (time2%to_string_ms ())
write (u, "(A)") char (time2%to_string_hms ())
write (u, "(A)") char (time2%to_string_dhms ())

```

```

write (u, "(A)")
write (u, "(A)")  "* Blanking out the last second entry"
write (u, "(A)")

write (u, "(A)")  char (time1%to_string_ms ())
write (u, "(A)")  char (time1%to_string_ms (.true.))

write (u, *)
write (u, "(A)")  "* String from negative time"
write (u, *)

time1 = -(((24 + 1) * 60 + 1) * 60 + 1)
time2 = -(((3 * 24 + 23) * 60 + 59) * 60 + 59)

write (u, "(A)")  char (time1%to_string_s ())
write (u, "(A)")  char (time1%to_string_ms ())
write (u, "(A)")  char (time1%to_string_hms ())
write (u, "(A)")  char (time1%to_string_dhms ())

write (u, "(A)")  char (time2%to_string_s ())
write (u, "(A)")  char (time2%to_string_ms ())
write (u, "(A)")  char (time2%to_string_hms ())
write (u, "(A)")  char (time2%to_string_dhms ())

write (u, "(A)")
write (u, "(A)")  "* Test output end: cputime_1"

end subroutine cputime_1

```

Timer tests

Check a timer object.

```

<CPU time: execute tests>+≡
  call test (cputime_2, "cputime_2", &
    "timer", &
    u, results)

<CPU time: test declarations>+≡
  public :: cputime_2

<CPU time: tests>+≡
  subroutine cputime_2 (u)
    integer, intent(in) :: u
    type(timer_t) :: timer

    write (u, "(A)")  "* Test output: cputime_2"
    write (u, "(A)")  "* Purpose: check timer"
    write (u, "(A)")

    write (u, "(A)")  "* Undefined timer"
    write (u, *)

    call timer%write (u)

```

```

write (u, *)
write (u, "(A)") "* Start timer"
write (u, *)

call timer%start ()
call timer%write (u)

write (u, *)
write (u, "(A)") "* Stop timer (injecting fake timings)"
write (u, *)

call timer%stop ()
call timer%set_test_time1 (2)
call timer%set_test_time2 (5)
call timer%evaluate ()
call timer%write (u)

write (u, *)
write (u, "(A)") "* Restart timer"
write (u, *)

call timer%restart ()
call timer%write (u)

write (u, *)
write (u, "(A)") "* Stop timer again (injecting fake timing)"
write (u, *)

call timer%stop ()
call timer%set_test_time2 (10)
call timer%evaluate ()
call timer%write (u)

write (u, *)
write (u, "(A)") "* Test output end: cputime_2"

end subroutine cputime_2

```


Chapter 6

Combinatorics

These modules implement standard algorithms (sorting, hashing, etc.) that are not available in Fortran.

Fortran doesn't support generic programming, therefore the algorithms are implemented only for specific data types.

bytes Derived types for bytes and words.

hashes Types and tools for setting up hashtables.

md5 The MD5 algorithm for message digest.

permutations Permuting an array of integers.

sorting Sorting integer and real values.

grids d -dimensional grids can be saved to disk and used for interpolation, maximum finding, etc.

6.1 Bytes and such

In a few instances we will need the notion of a byte (8-bit) and a word (32 bit), even a 64-bit word. A block of 512 bit is also needed (for MD5).

We rely on integers up to 64 bit being supported by the processor. The main difference to standard integers is the interpretation as unsigned integers.

`<bytes.f90>` \equiv
<File header>

```
module bytes
```

```
    use kinds, only: i8, i32, i64
```

<Standard module head>

<Bytes: public>

<Bytes: types>

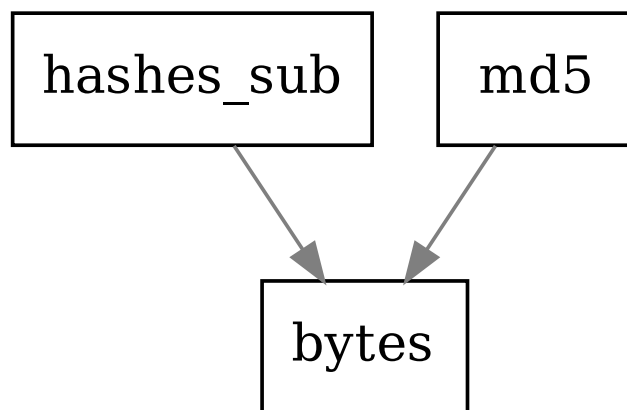


Figure 6.1: Module dependencies in `src/combinatorics`.

```

⟨Bytes: parameters⟩

⟨Bytes: interfaces⟩

  interface
⟨Bytes: sub interfaces⟩
  end interface

end module bytes
⟨bytes_sub.f90⟩≡
⟨File header⟩

submodule (bytes) bytes_s

  use io_units

  implicit none

contains

⟨Bytes: procedures⟩

end submodule bytes_s

```

6.1.1 8-bit words: bytes

This is essentially a wrapper around 8-bit integers. The wrapper emphasises their special interpretation as a sequence of bits. However, we interpret bytes as unsigned integers.

```
<Bytes: public>≡
    public :: byte_t

<Bytes: types>≡
    type :: byte_t
    private
        integer(i8) :: i
    end type byte_t

<Bytes: public>+≡
    public :: byte_zero

<Bytes: parameters>≡
    type(byte_t), parameter :: byte_zero = byte_t (0_i8)
```

Set a byte from 8-bit integer:

```
<Bytes: public>+≡
    public :: assignment(=)

<Bytes: interfaces>≡
    interface assignment(=)
        module procedure set_byte_from_i8
    end interface

<Bytes: sub interfaces>≡
    module subroutine set_byte_from_i8 (b, i)
        type(byte_t), intent(out) :: b
        integer(i8), intent(in) :: i
    end subroutine set_byte_from_i8

<Bytes: procedures>≡
    module subroutine set_byte_from_i8 (b, i)
        type(byte_t), intent(out) :: b
        integer(i8), intent(in) :: i
        b%i = i
    end subroutine set_byte_from_i8
```

Write a byte in one of two formats: either as a hexadecimal number (two digits, default) or as a decimal number (one to three digits). The decimal version is nontrivial because bytes are unsigned integers. Optionally append a newline.

```
<Bytes: public>+≡
    public :: byte_write

<Bytes: interfaces>+≡
    interface byte_write
        module procedure byte_write_unit, byte_write_string
    end interface
```

```

<Bytes: sub interfaces>+≡
    module subroutine byte_write_unit (b, unit, decimal, newline)
        type(byte_t), intent(in), optional :: b
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: decimal, newline
    end subroutine byte_write_unit

<Bytes: procedures>+≡
    module subroutine byte_write_unit (b, unit, decimal, newline)
        type(byte_t), intent(in), optional :: b
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: decimal, newline
        logical :: dc, nl
        type(word32_t) :: w
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        dc = .false.; if (present (decimal)) dc = decimal
        nl = .false.; if (present (newline)) nl = newline
        if (dc) then
            w = b
            write (u, '(I3)', advance='no') w%i
        else
            write (u, '(z2.2)', advance='no') b%i
        end if
        if (nl) write (u, *)
    end subroutine byte_write_unit

```

The string version is hex-only

```

<Bytes: sub interfaces>+≡
    module subroutine byte_write_string (b, s)
        type(byte_t), intent(in) :: b
        character(len=2), intent(inout) :: s
    end subroutine byte_write_string

<Bytes: procedures>+≡
    module subroutine byte_write_string (b, s)
        type(byte_t), intent(in) :: b
        character(len=2), intent(inout) :: s
        write (s, '(z2.2)') b%i
    end subroutine byte_write_string

```

6.1.2 32-bit words

This is not exactly a 32-bit integer. A word is to be filled with bytes, and it may be partially filled. The filling is done lowest-byte first, highest-byte last. We count the bits, so fill should be either 0, 8, 16, 24, or 32. In printing words, we correspondingly distinguish between printing zeros and printing blanks.

```

<Bytes: public>+≡
    public :: word32_t

<Bytes: types>+≡
    type :: word32_t
    private

```

```

        integer(i32) :: i
        integer :: fill = 0
    end type word32_t

```

Assignment: the word is filled by inserting a 32-bit integer

(Bytes: interfaces)+≡

```

    interface assignment(=)
        module procedure word32_set_from_i32
        module procedure word32_set_from_byte
    end interface

```

(Bytes: sub interfaces)+≡

```

    module subroutine word32_set_from_i32 (w, i)
        type(word32_t), intent(out) :: w
        integer(i32), intent(in) :: i
    end subroutine word32_set_from_i32

```

(Bytes: procedures)+≡

```

    module subroutine word32_set_from_i32 (w, i)
        type(word32_t), intent(out) :: w
        integer(i32), intent(in) :: i
        w%i = i
        w%fill = 32
    end subroutine word32_set_from_i32

```

Reverse assignment to a 32-bit integer. We do not check the fill status.

(Bytes: interfaces)+≡

```

    interface assignment(=)
        module procedure i32_from_word32
    end interface

```

(Bytes: sub interfaces)+≡

```

    module subroutine i32_from_word32 (i, w)
        integer(i32), intent(out) :: i
        type(word32_t), intent(in) :: w
    end subroutine i32_from_word32

```

(Bytes: procedures)+≡

```

    module subroutine i32_from_word32 (i, w)
        integer(i32), intent(out) :: i
        type(word32_t), intent(in) :: w
        i = w%i
    end subroutine i32_from_word32

```

Filling with a 8-bit integer is slightly tricky, because in this interpretation integers are unsigned.

(Bytes: sub interfaces)+≡

```

    module subroutine word32_set_from_byte (w, b)
        type(word32_t), intent(out) :: w
        type(byte_t), intent(in) :: b
    end subroutine word32_set_from_byte

```

```

<Bytes: procedures>+≡
module subroutine word32_set_from_byte (w, b)
  type(word32_t), intent(out) :: w
  type(byte_t), intent(in) :: b
  if (b%i >= 0_i8) then
    w%i = b%i
  else
    w%i = 2_i32*(huge(0_i8)+1_i32) + b%i
  end if
  w%fill = 32
end subroutine word32_set_from_byte

```

Check the fill status

```

<Bytes: public>+≡
public :: word32_empty, word32_filled, word32_fill

```

```

<Bytes: sub interfaces>+≡
module function word32_empty (w)
  type(word32_t), intent(in) :: w
  logical :: word32_empty
end function word32_empty
module function word32_filled (w)
  type(word32_t), intent(in) :: w
  logical :: word32_filled
end function word32_filled
module function word32_fill (w)
  type(word32_t), intent(in) :: w
  integer :: word32_fill
end function word32_fill

```

```

<Bytes: procedures>+≡
module function word32_empty (w)
  type(word32_t), intent(in) :: w
  logical :: word32_empty
  word32_empty = (w%fill == 0)
end function word32_empty

module function word32_filled (w)
  type(word32_t), intent(in) :: w
  logical :: word32_filled
  word32_filled = (w%fill == 32)
end function word32_filled

module function word32_fill (w)
  type(word32_t), intent(in) :: w
  integer :: word32_fill
  word32_fill = w%fill
end function word32_fill

```

Partial assignment: append a byte to a partially filled word. (Note: no assignment if the word is filled, so check this before if necessary.)

```

<Bytes: public>+≡
public :: word32_append_byte

```

```

<Bytes: sub interfaces>+≡
  module subroutine word32_append_byte (w, b)
    type(word32_t), intent(inout) :: w
    type(byte_t), intent(in) :: b
  end subroutine word32_append_byte

```

```

<Bytes: procedures>+≡
  module subroutine word32_append_byte (w, b)
    type(word32_t), intent(inout) :: w
    type(byte_t), intent(in) :: b
    type(word32_t) :: w1
    if (.not. word32_filled (w)) then
      w1 = b
      call mvbits (w1%i, 0, 8, w%i, w%fill)
      w%fill = w%fill + 8
    end if
  end subroutine word32_append_byte

```

Extract a byte from a word. The argument *i* is the position, which may be 0, 1, 2, or 3.

For the final assignment, we set the highest bit separately. Otherwise, we might trigger an overflow condition for a compiler with strict checking turned on.

```

<Bytes: public>+≡
  public :: byte_from_word32

```

```

<Bytes: sub interfaces>+≡
  module function byte_from_word32 (w, i) result (b)
    type(word32_t), intent(in) :: w
    integer, intent(in) :: i
    type(byte_t) :: b
  end function byte_from_word32

```

```

<Bytes: procedures>+≡
  module function byte_from_word32 (w, i) result (b)
    type(word32_t), intent(in) :: w
    integer, intent(in) :: i
    type(byte_t) :: b
    integer(i32) :: j
    j = 0
    if (i >= 0 .and. i*8 < w%fill) then
      call mvbits (w%i, i*8, 8, j, 0)
    end if
    b%i = int (ibclr (j, 7), kind=i8)
    if (btest (j, 7)) b%i = ibset (b%i, 7)
  end function byte_from_word32

```

Write a word to file or STDOUT. We understand words as unsigned integers, therefore we cannot use the built-in routine unchanged. However, we can make use of the existence of 64-bit integers and their output routine.

In hexadecimal format, the default version prints eight hex characters, highest-first. The `bytes` version prints four bytes (two-hex characters), lowest first, with

spaces in-between. The decimal bytes version is analogous. In the `bytes` version, missing bytes are printed as whitespace.

```

(Bytes: public) +=
    public :: word32_write

(Bytes: interfaces) +=
    interface word32_write
        module procedure word32_write_unit
    end interface

(Bytes: sub interfaces) +=
    module subroutine word32_write_unit (w, unit, bytes, decimal, newline)
        type(word32_t), intent(in) :: w
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: bytes, decimal, newline
    end subroutine word32_write_unit

(Bytes: procedures) +=
    module subroutine word32_write_unit (w, unit, bytes, decimal, newline)
        type(word32_t), intent(in) :: w
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: bytes, decimal, newline
        logical :: dc, by, nl
        type(word64_t) :: ww
        integer :: i, u
        u = given_output_unit (unit); if (u < 0) return
        by = .false.; if (present (bytes)) by = bytes
        dc = .false.; if (present (decimal)) dc = decimal
        nl = .false.; if (present (newline)) nl = newline
        if (by) then
            do i = 0, 3
                if (i>0) write (u, '(1x)', advance='no')
                if (8*i < w%fill) then
                    call byte_write (byte_from_word32 (w, i), unit, decimal=decimal)
                else if (dc) then
                    write (u, '(3x)', advance='no')
                else
                    write (u, '(2x)', advance='no')
                end if
            end do
        else if (dc) then
            ww = w
            write (u, '(I10)', advance='no') ww%i
        else
            select case (w%fill)
            case ( 0)
            case ( 8); write (6, '(1x,z8.2)', advance='no') ibits (w%i, 0, 8)
            case (16); write (6, '(1x,z8.4)', advance='no') ibits (w%i, 0,16)
            case (24); write (6, '(1x,z8.6)', advance='no') ibits (w%i, 0,24)
            case (32); write (6, '(1x,z8.8)', advance='no') ibits (w%i, 0,32)
            end select
        end if
        if (nl) write (u, *)
    end subroutine word32_write_unit

```


6.1.3 Operations on 32-bit words

Define the usual logical operations, as well as addition (mod 2^{32}). We assume that all operands are completely filled.

```
(Bytes: public)+≡
    public :: not, ior, ieor, iand, ishft, ishftc

(Bytes: interfaces)+≡
    interface not
        module procedure word_not
    end interface
    interface ior
        module procedure word_or
    end interface
    interface ieor
        module procedure word_eor
    end interface
    interface iand
        module procedure word_and
    end interface
    interface ishft
        module procedure word_shft
    end interface
    interface ishftc
        module procedure word_shftc
    end interface

(Bytes: sub interfaces)+≡
    module function word_not (w1) result (w2)
        type(word32_t), intent(in) :: w1
        type(word32_t) :: w2
    end function word_not
    module function word_or (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
    end function word_or
    module function word_eor (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
    end function word_eor
    module function word_and (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
    end function word_and
    module function word_shft (w1, s) result (w2)
        type(word32_t), intent(in) :: w1
        integer, intent(in) :: s
        type(word32_t) :: w2
    end function word_shft
    module function word_shftc (w1, s) result (w2)
        type(word32_t), intent(in) :: w1
        integer, intent(in) :: s
        type(word32_t) :: w2
    end function word_shftc
```

<Bytes: procedures>+≡

```
module function word_not (w1) result (w2)
  type(word32_t), intent(in) :: w1
  type(word32_t) :: w2
  w2 = not (w1%i)
end function word_not

module function word_or (w1, w2) result (w3)
  type(word32_t), intent(in) :: w1, w2
  type(word32_t) :: w3
  w3 = ior (w1%i, w2%i)
end function word_or

module function word_eor (w1, w2) result (w3)
  type(word32_t), intent(in) :: w1, w2
  type(word32_t) :: w3
  w3 = ieor (w1%i, w2%i)
end function word_eor

module function word_and (w1, w2) result (w3)
  type(word32_t), intent(in) :: w1, w2
  type(word32_t) :: w3
  w3 = iand (w1%i, w2%i)
end function word_and

module function word_shft (w1, s) result (w2)
  type(word32_t), intent(in) :: w1
  integer, intent(in) :: s
  type(word32_t) :: w2
  w2 = ishft (w1%i, s)
end function word_shft

module function word_shftc (w1, s) result (w2)
  type(word32_t), intent(in) :: w1
  integer, intent(in) :: s
  type(word32_t) :: w2
  w2 = ishftc (w1%i, s, 32)
end function word_shftc
```

Addition is defined mod 2^{32} , i.e., without overflow checking. This means that we have to work around a possible overflow check enforced by the compiler.

<Bytes: public>+≡

```
public :: operator(+)
```

<Bytes: interfaces>+≡

```
interface operator(+)
  module procedure word_add
  module procedure word_add_i8
  module procedure word_add_i32
end interface
```

<Bytes: sub interfaces>+≡

```
module function word_add (w1, w2) result (w3)
  type(word32_t), intent(in) :: w1, w2
```

```

        type(word32_t) :: w3
    end function word_add
    module function word_add_i8 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i8), intent(in) :: i
        type(word32_t) :: w3
    end function word_add_i8
    module function word_add_i32 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i32), intent(in) :: i
        type(word32_t) :: w3
    end function word_add_i32

```

(Bytes: procedures)+≡

```

    module function word_add (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (w2%i, 31), i64)
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31)) then
            if (btest (w1%i, 31) .eqv. btest (w2%i, 31)) w3 = ibset (w3%i, 31)
        else
            if (btest (w1%i, 31) .neqv. btest (w2%i, 31)) w3 = ibset (w3%i, 31)
        end if
    end function word_add

    module function word_add_i8 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i8), intent(in) :: i
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (i, 7), i64)
        if (btest (i, 7)) j = j + 128
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31) .neqv. btest (w1%i, 31)) w3 = ibset (w3%i, 31)
    end function word_add_i8

    module function word_add_i32 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i32), intent(in) :: i
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (i, 31), i64)
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31)) then
            if (btest (w1%i, 31) .eqv. btest (i, 31)) w3 = ibset (w3%i, 31)
        else
            if (btest (w1%i, 31) .neqv. btest (i, 31)) w3 = ibset (w3%i, 31)
        end if
    end function word_add_i32

```

6.1.4 64-bit words

These objects consist of two 32-bit words. They thus can hold integer numbers larger than 2^{32} (to be exact, 2^{31} since FORTRAN integers are signed). The order is low-word, high-word.

```
<Bytes: public>+≡  
    public :: word64_t
```

```
<Bytes: types>+≡  
    type :: word64_t  
    private  
        integer(i64) :: i  
    end type word64_t
```

Set a 64 bit word:

```
<Bytes: interfaces>+≡  
    interface assignment(=)  
        module procedure word64_set_from_i64  
        module procedure word64_set_from_word32  
    end interface
```

```
<Bytes: sub interfaces>+≡  
    module subroutine word64_set_from_i64 (ww, i)  
        type(word64_t), intent(out) :: ww  
        integer(i64), intent(in) :: i  
    end subroutine word64_set_from_i64
```

```
<Bytes: procedures>+≡  
    module subroutine word64_set_from_i64 (ww, i)  
        type(word64_t), intent(out) :: ww  
        integer(i64), intent(in) :: i  
        ww%i = i  
    end subroutine word64_set_from_i64
```

Filling with a 32-bit word:

```
<Bytes: sub interfaces>+≡  
    module subroutine word64_set_from_word32 (ww, w)  
        type(word64_t), intent(out) :: ww  
        type(word32_t), intent(in) :: w  
    end subroutine word64_set_from_word32
```

```
<Bytes: procedures>+≡  
    module subroutine word64_set_from_word32 (ww, w)  
        type(word64_t), intent(out) :: ww  
        type(word32_t), intent(in) :: w  
        if (w%i >= 0_i32) then  
            ww%i = w%i  
        else  
            ww%i = 2_i64*(huge(0_i32)+1_i64) + w%i  
        end if  
    end subroutine word64_set_from_word32
```

Extract a byte from a word. The argument *i* is the position, which may be between 0 and 7.

For the final assignment, we set the highest bit separately. Otherwise, we might trigger an overflow condition for a compiler with strict checking turned on.

```

<Bytes: public>+≡
    public :: byte_from_word64, word32_from_word64

<Bytes: sub interfaces>+≡
    module function byte_from_word64 (ww, i) result (b)
        type(word64_t), intent(in) :: ww
        integer, intent(in) :: i
        type(byte_t) :: b
    end function byte_from_word64

<Bytes: procedures>+≡
    module function byte_from_word64 (ww, i) result (b)
        type(word64_t), intent(in) :: ww
        integer, intent(in) :: i
        type(byte_t) :: b
        integer(i64) :: j
        j = 0
        if (i >= 0 .and. i*8 < 64) then
            call mvbits (ww%i, i*8, 8, j, 0)
        end if
        b%i = int (ibclr (j, 7), kind=i8)
        if (btest (j, 7)) b%i = ibset (b%i, 7)
    end function byte_from_word64

```

Extract a 32-bit word from a 64-bit word. The position is either 0 or 1.

```

<Bytes: sub interfaces>+≡
    module function word32_from_word64 (ww, i) result (w)
        type(word64_t), intent(in) :: ww
        integer, intent(in) :: i
        type(word32_t) :: w
    end function word32_from_word64

<Bytes: procedures>+≡
    module function word32_from_word64 (ww, i) result (w)
        type(word64_t), intent(in) :: ww
        integer, intent(in) :: i
        type(word32_t) :: w
        integer(i64) :: j
        j = 0
        select case (i)
            case (0); call mvbits (ww%i, 0, 32, j, 0)
            case (1); call mvbits (ww%i, 32, 32, j, 0)
        end select
        w = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31)) w = ibset (w%i, 31)
    end function word32_from_word64

```

Print a 64-bit word. Decimal version works up to 2^{63} . The `words` version uses the 'word32' printout, separated by two spaces. The low-word is printed first.

The `bytes` version also uses the 'word32' printout. This implies that the lowest byte is first. The default version prints a hexadecimal number without spaces, highest byte first.

```

<Bytes: public>+≡
    public :: word64_write

<Bytes: interfaces>+≡
    interface word64_write
        module procedure word64_write_unit
    end interface

<Bytes: sub interfaces>+≡
    module subroutine word64_write_unit (ww, unit, words, bytes, decimal, newline)
        type(word64_t), intent(in) :: ww
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: words, bytes, decimal, newline
    end subroutine word64_write_unit

<Bytes: procedures>+≡
    module subroutine word64_write_unit (ww, unit, words, bytes, decimal, newline)
        type(word64_t), intent(in) :: ww
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: words, bytes, decimal, newline
        logical :: wo, by, dc, nl
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        wo = .false.; if (present (words))    wo = words
        by = .false.; if (present (bytes))    by = bytes
        dc = .false.; if (present (decimal))  dc = decimal
        nl = .false.; if (present (newline))  nl = newline
        if (wo .or. by) then
            call word32_write_unit (word32_from_word64 (ww, 0), unit, by, dc)
            write (u, '(2x)', advance='no')
            call word32_write_unit (word32_from_word64 (ww, 1), unit, by, dc)
        else if (dc) then
            write (u, '(I19)', advance='no') ww%i
        else
            write (u, '(Z16)', advance='no') ww%i
        end if
        if (nl) write (u, *)
    end subroutine word64_write_unit

```

6.2 Hashtables

Hash tables, like lists, are not part of Fortran and must be defined on a per-case basis. In this section we define a module that contains a hash function.

Furthermore, for reference there is a complete framework of hashtable type definitions and access functions. This code is to be replicated where hash tables are used, mutatis mutandis.

```

<hashes.f90>≡
    <File header>

```

```

module hashes

    use kinds, only: i8, i32

    <Standard module head>

    <Hashes: public>

    interface
    <Hashes: sub interfaces>
    end interface

end module hashes

<hashes_sub.f90>≡
<File header>

submodule (hashes) hashes_s

    use bytes

    implicit none

contains

    <Hashes: procedures>

end submodule hashes_s

```

6.2.1 The hash function

This is the one-at-a-time hash function by Bob Jenkins (from Wikipedia), re-implemented in Fortran. The function works on an array of bytes (8-bit integers), as could be produced by, e.g., the `transfer` function, and returns a single 32-bit integer. For determining the position in a hashtable, one can pick the lower bits of the result as appropriate to the hashtable size (which should be a power of 2). Note that we are working on signed integers, so the interpretation of values differs from the C version. This should not matter in practice, however.

```

<Hashes: public>≡
    public :: hash

<Hashes: sub interfaces>≡
    module function hash (key) result (hashval)
        integer(i32) :: hashval
        integer(i8), dimension(:), intent(in) :: key
    end function hash

<Hashes: procedures>≡
    module function hash (key) result (hashval)
        integer(i32) :: hashval
        integer(i8), dimension(:), intent(in) :: key
        type(word32_t) :: w
        integer :: i

```

```

w = 0_i32
do i = 1, size (key)
    w = w + key(i)
    w = w + ishft (w, 10)
    w = ieor (w, ishft (w, -6))
end do
w = w + ishft (w, 3)
w = ieor (w, ishft (w, -11))
w = w + ishft (w, 15)
hashval = w
end function hash

```

6.2.2 The hash table

We define a generic hashtable type (that depends on the `hash_data_t` type) together with associated methods.

This is a template:

```

<Hashtables: types>≡
type :: hash_data_t
integer :: i
end type hash_data_t

```

Associated methods:

```

<Hashtables: procedures>≡
subroutine hash_data_final (data)
    type(hash_data_t), intent(inout) :: data
end subroutine hash_data_final

subroutine hash_data_write (data, unit)
    type(hash_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, *) data%i
end subroutine hash_data_write

```

Each hash entry stores the unmasked hash value, the key, and points to actual data if present. Note that this could be an allocatable scalar in principle, but making it a pointer avoids deep copy when expanding the hashtable.

```

<Hashtables: types>+≡
type :: hash_entry_t
integer(i32) :: hashval = 0
integer(i8), dimension(:), allocatable :: key
type(hash_data_t), pointer :: data => null ()
end type hash_entry_t

```

The hashtable object holds the actual table, the number of filled entries and the number of entries after which the size should be doubled. The mask is equal to

the table size minus one and thus coincides with the upper bound of the table index, which starts at zero.

```

<Hashtables: types>+≡
  type :: hashtable_t
    integer :: n_entries = 0
    real :: fill_ratio = 0
    integer :: n_entries_max = 0
    integer(i32) :: mask = 0
    type(hash_entry_t), dimension(:), allocatable :: entry
  end type hashtable_t

```

Initializer: The size has to be a power of two, the fill ratio is a real (machine-default!) number between 0 and 1.

```

<Hashtables: procedures>+≡
  subroutine hashtable_init (hashtable, size, fill_ratio)
    type(hashtable_t), intent(out) :: hashtable
    integer, intent(in) :: size
    real, intent(in) :: fill_ratio
    hashtable%fill_ratio = fill_ratio
    hashtable%n_entries_max = size * fill_ratio
    hashtable%mask = size - 1
    allocate (hashtable%entry (0:hashtable%mask))
  end subroutine hashtable_init

```

Finalizer: This calls a `hash_data_final` subroutine which must exist.

```

<Hashtables: procedures>+≡
  subroutine hashtable_final (hashtable)
    type(hashtable_t), intent(inout) :: hashtable
    integer :: i
    do i = 0, hashtable%mask
      if (associated (hashtable%entry(i)%data)) then
        call hash_data_final (hashtable%entry(i)%data)
        deallocate (hashtable%entry(i)%data)
      end if
    end do
    deallocate (hashtable%entry)
  end subroutine hashtable_final

```

Output. Here, we refer to a `hash_data_write` subroutine.

```

<Hashtables: procedures>+≡
  subroutine hashtable_write (hashtable, unit)
    type(hashtable_t), intent(in) :: hashtable
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    do i = 0, hashtable%mask
      if (associated (hashtable%entry(i)%data)) then
        write (u, *) i, "(hash =", hashtable%entry(i)%hashval, ")", &
          hashtable%entry(i)%key
        call hash_data_write (hashtable%entry(i)%data, unit)
      end if
    end do
  end subroutine hashtable_write

```

```
end subroutine hashtable_write
```

6.2.3 Hashtable insertion

Insert a single entry with the hash value as trial place. If the table is filled, first expand it.

```
(Hashtables: procedures)+≡
subroutine hashtable_insert (hashtable, key, data)
  type(hashtable_t), intent(inout) :: hashtable
  integer(i8), dimension(:), intent(in) :: key
  type(hash_data_t), intent(in), target :: data
  integer(i32) :: h
  if (hashtable%n_entries >= hashtable%n_entries_max) &
    call hashtable_expand (hashtable)
  h = hash (key)
  call hashtable_insert_rec (hashtable, h, h, key, data)
end subroutine hashtable_insert
```

We need this auxiliary routine for doubling the size of the hashtable. We rely on the fact that default assignment copies the data pointer, not the data themselves. The temporary array must not be finalized; it is deallocated automatically together with its allocatable components.

```
(Hashtables: procedures)+≡
subroutine hashtable_expand (hashtable)
  type(hashtable_t), intent(inout) :: hashtable
  type(hash_entry_t), dimension(:), allocatable :: table_tmp
  integer :: i, s
  allocate (table_tmp (0:hashtable%mask))
  table_tmp = hashtable%entry
  deallocate (hashtable%entry)
  s = 2 * size (table_tmp)
  hashtable%n_entries = 0
  hashtable%n_entries_max = s * hashtable%fill_ratio
  hashtable%mask = s - 1
  allocate (hashtable%entry (0:hashtable%mask))
  do i = 0, ubound (table_tmp, 1)
    if (associated (table_tmp(i)%data)) then
      call hashtable_insert_rec (hashtable, table_tmp(i)%hashval, &
        table_tmp(i)%hashval, table_tmp(i)%key, table_tmp(i)%data)
    end if
  end do
end subroutine hashtable_expand
```

Insert a single entry at a trial place *h*, reduced to the table size. Collision resolution is done simply by choosing the next element, recursively until the place is empty. For bookkeeping, we preserve the original hash value. For a good hash function, there should be no clustering.

Note that if the new key exactly matches an existing key, nothing is done.

```
(Hashtables: procedures)+≡
recursive subroutine hashtable_insert_rec (hashtable, h, hashval, key, data)
```

```

type(hashtable_t), intent(inout) :: hashtable
integer(i32), intent(in) :: h, hashval
integer(i8), dimension(:), intent(in) :: key
type(hash_data_t), intent(in), target :: data
integer(i32) :: i
i = iand (h, hashtable%mask)
if (associated (hashtable%entry(i)%data)) then
  if (size (hashtable%entry(i)%key) /= size (key)) then
    call hashtable_insert_rec (hashtable, h + 1, hashval, key, data)
  else if (any (hashtable%entry(i)%key /= key)) then
    call hashtable_insert_rec (hashtable, h + 1, hashval, key, data)
  end if
else
  hashtable%entry(i)%hashval = hashval
  allocate (hashtable%entry(i)%key (size (key)))
  hashtable%entry(i)%key = key
  hashtable%entry(i)%data => data
  hashtable%n_entries = hashtable%n_entries + 1
end if
end subroutine hashtable_insert_rec

```

6.2.4 Hashtable lookup

The lookup function has to parallel the insert function. If the place is filled, check if the key matches. Yes: return the pointer; no: increment the hash value and check again.

(Hashtables: procedures) +=

```

function hashtable_lookup (hashtable, key) result (ptr)
  type(hash_data_t), pointer :: ptr
  type(hashtable_t), intent(in) :: hashtable
  integer(i8), dimension(:), intent(in) :: key
  ptr => hashtable_lookup_rec (hashtable, hash (key), key)
end function hashtable_lookup

```

(Hashtables: procedures) +=

```

recursive function hashtable_lookup_rec (hashtable, h, key) result (ptr)
  type(hash_data_t), pointer :: ptr
  type(hashtable_t), intent(in) :: hashtable
  integer(i32), intent(in) :: h
  integer(i8), dimension(:), intent(in) :: key
  integer(i32) :: i
  i = iand (h, hashtable%mask)
  if (associated (hashtable%entry(i)%data)) then
    if (size (hashtable%entry(i)%key) == size (key)) then
      if (all (hashtable%entry(i)%key == key)) then
        ptr => hashtable%entry(i)%data
      else
        ptr => hashtable_lookup_rec (hashtable, h + 1, key)
      end if
    else
      ptr => hashtable_lookup_rec (hashtable, h + 1, key)
    end if
  end if
end function hashtable_lookup_rec

```

```

        else
            ptr => null ()
        end if
    end function hashtable_lookup_rec

<Hashtables: public>≡
    public :: hashtable_test

<Hashtables: procedures>+≡
    subroutine hashtable_test ()
        type(hash_data_t), pointer :: data
        type(hashtable_t) :: hashtable
        integer(i8) :: i
        call hashtable_init (hashtable, 16, 0.25)
        do i = 1, 10
            allocate (data)
            data%i = i*i
            call hashtable_insert (hashtable, [i, i+i], data)
        end do
        call hashtable_insert (hashtable, [2_i8, 4_i8], data)
        call hashtable_write (hashtable)
        data => hashtable_lookup (hashtable, [5_i8, 10_i8])
        if (associated (data)) then
            print *, "lookup:", data%i
        else
            print *, "lookup: -"
        end if
        data => hashtable_lookup (hashtable, [6_i8, 12_i8])
        if (associated (data)) then
            print *, "lookup:", data%i
        else
            print *, "lookup: -"
        end if
        data => hashtable_lookup (hashtable, [4_i8, 9_i8])
        if (associated (data)) then
            print *, "lookup:", data%i
        else
            print *, "lookup: -"
        end if
        call hashtable_final (hashtable)
    end subroutine hashtable_test

```

6.3 MD5 Checksums

Implementing MD5 checksums allows us to check input/file integrity on the basis of a well-known standard. The building blocks have been introduced in the `bytes` module.

```

<md5.f90>≡
    <File header>

```

```

    module md5

```

```

    use bytes

    <Standard module head>

    <MD5: public>

    <MD5: types>

    <MD5: interfaces>

    interface
    <MD5: sub interfaces>
    end interface

end module md5
<md5_sub.f90>≡
<File header>

submodule (md5) md5_s

    use kinds, only: i8, i32, i64
    use system_defs, only: BUFFER_SIZE
    use system_defs, only: LF, EOR, EOF
    use io_units
    use diagnostics

    implicit none

    <MD5: variables>

contains

    <MD5: procedures>

end submodule md5_s

```

6.3.1 Blocks

A block is a sequence of 16 words (64 bytes or 512 bits). We anticipate that blocks will be linked, so include a pointer to the next block. There is a fill status (word counter), as there is one for each word. The fill status is equal to the number of bytes that are in, so it may be between 0 and 64.

```

<MD5: types>≡
    type :: block_t
    private
    type(word32_t), dimension(0:15) :: w
    type(block_t), pointer :: next => null ()
    integer :: fill = 0
end type block_t

```

Check if a block is completely filled or empty:

```

<MD5: procedures>≡
function block_is_empty (b)
  type(block_t), intent(in) :: b
  logical :: block_is_empty
  block_is_empty = (b%fill == 0 .and. word32_empty (b%w(0)))
end function block_is_empty

function block_is_filled (b)
  type(block_t), intent(in) :: b
  logical :: block_is_filled
  block_is_filled = (b%fill == 64)
end function block_is_filled

```

Append a single byte to a block. Works only if the block is not yet filled.

```

<MD5: procedures>+≡
subroutine block_append_byte (bl, by)
  type(block_t), intent(inout) :: bl
  type(byte_t), intent(in) :: by
  if (.not. block_is_filled (bl)) then
    call word32_append_byte (bl%w(bl%fill/4), by)
    bl%fill = bl%fill + 1
  end if
end subroutine block_append_byte

```

The printing routine allows for printing as sequences of words or bytes, decimal or hex.

```

<MD5: interfaces>≡
interface block_write
  module procedure block_write_unit
end interface

<MD5: sub interfaces>≡
module subroutine block_write_unit (b, unit, bytes, decimal)
  type(block_t), intent(in) :: b
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: bytes, decimal
end subroutine block_write_unit

<MD5: procedures>+≡
module subroutine block_write_unit (b, unit, bytes, decimal)
  type(block_t), intent(in) :: b
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: bytes, decimal
  logical :: by, dc
  integer :: i, u
  u = given_output_unit (unit); if (u < 0) return
  by = .false.; if (present (bytes)) by = bytes
  dc = .false.; if (present (decimal)) dc = decimal
  do i = 0, b%fill/4 - 1
    call newline_or_blank (u, i, by, dc)
    call word32_write (b%w(i), unit, bytes, decimal)
  end do
  if (.not. block_is_filled (b)) then

```

```

        i = b%fill/4
        if (.not. word32_empty (b%w(i))) then
            call newline_or_blank (u, i, by, dc)
            call word32_write (b%w(i), unit, bytes, decimal)
        end if
    end if
    write (u, *)
contains
    subroutine newline_or_blank (u, i, bytes, decimal)
        integer, intent(in) :: u, i
        logical, intent(in) :: bytes, decimal
        if (decimal) then
            select case (i)
            case (0)
            case (2,4,6,8,10,12,14); write (u, *)
            case default
                write (u, '(2x)', advance='no')
            end select
        else if (bytes) then
            select case (i)
            case (0)
            case (4,8,12); write (u, *)
            case default
                write (u, '(2x)', advance='no')
            end select
        else
            if (i == 8) write (u, *)
        end if
    end subroutine newline_or_blank
end subroutine block_write_unit

```

6.3.2 Messages

A message (within this module) is a linked list of blocks.

(MD5: types)+≡

```

type :: message_t
private
type(block_t), pointer :: first => null ()
type(block_t), pointer :: last => null ()
integer :: n_blocks = 0
end type message_t

```

Clear the message list

(MD5: procedures)+≡

```

subroutine message_clear (m)
type(message_t), intent(inout) :: m
type(block_t), pointer :: b
nullify (m%last)
do
    b => m%first
    if (.not.(associated (b))) exit
    m%first => b%next
end do

```

```

        deallocate (b)
    end do
    m%n_blocks = 0
end subroutine message_clear

```

Append an empty block to the message list

```

<MD5: procedures>+≡
subroutine message_append_new_block (m)
    type(message_t), intent(inout) :: m
    if (associated (m%last)) then
        allocate (m%last%next)
        m%last => m%last%next
        m%n_blocks = m%n_blocks + 1
    else
        allocate (m%first)
        m%last => m%first
        m%n_blocks = 1
    end if
end subroutine message_append_new_block

```

Initialize: clear and allocate the first (empty) block.

```

<MD5: procedures>+≡
subroutine message_init (m)
    type(message_t), intent(inout) :: m
    call message_clear (m)
    call message_append_new_block (m)
end subroutine message_init

```

Append a single byte to a message. If necessary, allocate a new block. If the message is empty, initialize it.

```

<MD5: procedures>+≡
subroutine message_append_byte (m, b)
    type(message_t), intent(inout) :: m
    type(byte_t), intent(in) :: b
    if (.not. associated (m%last)) then
        call message_init (m)
    else if (block_is_filled (m%last)) then
        call message_append_new_block (m)
    end if
    call block_append_byte (m%last, b)
end subroutine message_append_byte

```

Append zero bytes until the current block is filled up to the required position. If we are already beyond that, append a new block and fill that one.

```

<MD5: procedures>+≡
subroutine message_pad_zero (m, i)
    type(message_t), intent(inout) :: m
    integer, intent(in) :: i
    type(block_t), pointer :: b
    integer :: j
    if (associated (m%last)) then
        b => m%last

```



```

        if (b%fill > i) then
            do j = b%fill + 1, 64 + i
                call message_append_byte (m, byte_zero)
            end do
        else
            do j = b%fill + 1, i
                call message_append_byte (m, byte_zero)
            end do
        end if
    end if
end subroutine message_pad_zero

```

This returns the number of bits within a message. We need a 64-bit word for the result since it may be more than 2^{31} . This is also required by the MD5 standard.

(MD5: procedures)+≡

```

function message_bits (m) result (length)
    type(message_t), intent(in) :: m
    type(word64_t) :: length
    type(block_t), pointer :: b
    integer(i64) :: n_blocks_filled, n_bytes_extra
    if (m%n_blocks > 0) then
        b => m%last
        if (block_is_filled (b)) then
            n_blocks_filled = m%n_blocks
            n_bytes_extra = 0
        else
            n_blocks_filled = m%n_blocks - 1
            n_bytes_extra = b%fill
        end if
        length = n_blocks_filled * 512 + n_bytes_extra * 8
    else
        length = 0_i64
    end if
end function message_bits

```

6.3.3 Message I/O

Append the contents of a string to a message. We first cast the character string into a 8-bit integer array and then append this byte by byte.

(MD5: procedures)+≡

```

subroutine message_append_string (m, s)
    type(message_t), intent(inout) :: m
    character(len=*), intent(in) :: s
    integer(i64) :: i, n_bytes
    integer(i8), dimension(:), allocatable :: buffer
    integer(i8), dimension(1) :: mold
    type(byte_t) :: b
    n_bytes = size (transfer (s, mold))
    allocate (buffer (n_bytes))
    buffer = transfer (s, mold)
    do i = 1, size (buffer)

```

```

        b = buffer(i)
        call message_append_byte (m, b)
    end do
    deallocate (buffer)
end subroutine message_append_string

```

Append the contents of a 32-bit integer to a message. We first cast the 32-bit integer into a 8-bit integer array and the append this byte by byte.

<MD5: procedures>+≡

```

subroutine message_append_i32 (m, x)
    type(message_t), intent(inout) :: m
    integer(i32), intent(in) :: x
    integer(i8), dimension(4) :: buffer
    type(byte_t) :: b
    integer :: i
    buffer = transfer (x, buffer, size(buffer))
    do i = 1, size (buffer)
        b = buffer(i)
        call message_append_byte (m, b)
    end do
end subroutine message_append_i32

```

Append one line from file to a message. Include the newline character.

<MD5: procedures>+≡

```

subroutine message_append_from_unit (m, u, iostat)
    type(message_t), intent(inout) :: m
    integer, intent(in) :: u
    integer, intent(out) :: iostat
    character(len=BUFFER_SIZE) :: buffer
    read (u, *, iostat=iostat) buffer
    call message_append_string (m, trim (buffer))
    call message_append_string (m, LF)
end subroutine message_append_from_unit

```

Fill a message from file. (Each line counts as a string.)

<MD5: procedures>+≡

```

subroutine message_read_from_file (m, f)
    type(message_t), intent(inout) :: m
    character(len=*), intent(in) :: f
    integer :: u, iostat
    u = free_unit ()
    open (file=f, unit=u, action='read')
    do
        call message_append_from_unit (m, u, iostat=iostat)
        if (iostat < 0) exit
    end do
    close (u)
end subroutine message_read_from_file

```

Write a message. After each block, insert an empty line.

<MD5: interfaces>+≡

```

interface message_write

```

```

        module procedure message_write_unit
    end interface
<MD5: sub interfaces>+≡
    module subroutine message_write_unit (m, unit, bytes, decimal)
        type(message_t), intent(in) :: m
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: bytes, decimal
    end subroutine message_write_unit
<MD5: procedures>+≡
    module subroutine message_write_unit (m, unit, bytes, decimal)
        type(message_t), intent(in) :: m
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: bytes, decimal
        type(block_t), pointer :: b
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        b => m%first
        if (associated (b)) then
            do
                call block_write_unit (b, unit, bytes, decimal)
                b => b%next
                if (.not. associated (b)) exit
                write (u, *)
            end do
        end if
    end subroutine message_write_unit

```

6.3.4 Auxiliary functions

These four functions on three words are defined in the MD5 standard:

```

<MD5: procedures>+≡
    function ff (x, y, z)
        type(word32_t), intent(in) :: x, y, z
        type(word32_t) :: ff
        ff = ior (iand (x, y), iand (not (x), z))
    end function ff

    function fg (x, y, z)
        type(word32_t), intent(in) :: x, y, z
        type(word32_t) :: fg
        fg = ior (iand (x, z), iand (y, not (z)))
    end function fg

    function fh (x, y, z)
        type(word32_t), intent(in) :: x, y, z
        type(word32_t) :: fh
        fh = ieor (ieor (x, y), z)
    end function fh

    function fi (x, y, z)
        type(word32_t), intent(in) :: x, y, z

```

```

        type(word32_t) :: fi
        fi = ieor (y, ior (x, not (z)))
    end function fi

```

6.3.5 Auxiliary stuff

This defines and initializes the table of transformation constants:

```

⟨MD5: variables⟩≡
    type(word32_t), dimension(64), save :: t
    logical, save :: table_initialized = .false.

⟨MD5: procedures⟩+≡
    subroutine table_init
        type(word64_t) :: ww
        integer :: i
        if (.not.table_initialized) then
            do i = 1, 64
                ww = int (4294967296d0 * abs (sin (i * 1d0)), kind=i64)
                t(i) = word32_from_word64 (ww, 0)
            end do
            table_initialized = .true.
        end if
    end subroutine table_init

```

This encodes the message digest (4 words) into a 32-character string.

```

⟨MD5: procedures⟩+≡
    function digest_string (aa) result (s)
        type(word32_t), dimension (0:3), intent(in) :: aa
        character(len=32) :: s
        integer :: i, j
        do i = 0, 3
            do j = 0, 3
                call byte_write (byte_from_word32 (aa(i), j), s(i*8+j*2+1:i*8+j*2+2))
            end do
        end do
    end function digest_string

```

6.3.6 MD5 algorithm

Pad the message with a byte x80 and then pad zeros up to a full block minus two words; in these words, insert the message length (before padding) as a 64-bit word, low-word first.

```

⟨MD5: procedures⟩+≡
    subroutine message_pad (m)
        type(message_t), intent(inout) :: m
        type(word64_t) :: length
        integer(i8), parameter :: ipad = -128 ! z'80'
        type(byte_t) :: b
        integer :: i
        length = message_bits (m)

```

```

b = ipad
call message_append_byte (m, b)
call message_pad_zero (m, 56)
do i = 0, 7
    call message_append_byte (m, byte_from_word64 (length, i))
end do
end subroutine message_pad

```

Apply a series of transformations onto a state a, b, c, d , where the transform function uses each word of the message together with the predefined words. Finally, encode the state as a 32-character string.

(MD5: procedures)+≡

```

subroutine message_digest (m, s)
    type(message_t), intent(in) :: m
    character(len=32), intent(out) :: s
    integer(i32), parameter :: ia = 1732584193 ! z'67452301'
    integer(i32), parameter :: ib = -271733879 ! z'efcdab89'
    integer(i32), parameter :: ic = -1732584194 ! z'98badcfe'
    integer(i32), parameter :: id = 271733878 ! z'10325476'
    type(word32_t) :: a, b, c, d
    type(word32_t) :: aa, bb, cc, dd
    type(word32_t), dimension(0:15) :: x
    type(block_t), pointer :: bl
    call table_init
    a = ia; b = ib; c = ic; d = id
    bl => m%first
    do
        if (.not.associated (bl)) exit
        x = bl%w
        aa = a; bb = b; cc = c; dd = d
        call transform (ff, a, b, c, d, 0, 7, 1)
        call transform (ff, d, a, b, c, 1, 12, 2)
        call transform (ff, c, d, a, b, 2, 17, 3)
        call transform (ff, b, c, d, a, 3, 22, 4)
        call transform (ff, a, b, c, d, 4, 7, 5)
        call transform (ff, d, a, b, c, 5, 12, 6)
        call transform (ff, c, d, a, b, 6, 17, 7)
        call transform (ff, b, c, d, a, 7, 22, 8)
        call transform (ff, a, b, c, d, 8, 7, 9)
        call transform (ff, d, a, b, c, 9, 12, 10)
        call transform (ff, c, d, a, b, 10, 17, 11)
        call transform (ff, b, c, d, a, 11, 22, 12)
        call transform (ff, a, b, c, d, 12, 7, 13)
        call transform (ff, d, a, b, c, 13, 12, 14)
        call transform (ff, c, d, a, b, 14, 17, 15)
        call transform (ff, b, c, d, a, 15, 22, 16)
        call transform (fg, a, b, c, d, 1, 5, 17)
        call transform (fg, d, a, b, c, 6, 9, 18)
        call transform (fg, c, d, a, b, 11, 14, 19)
        call transform (fg, b, c, d, a, 0, 20, 20)
        call transform (fg, a, b, c, d, 5, 5, 21)
        call transform (fg, d, a, b, c, 10, 9, 22)
        call transform (fg, c, d, a, b, 15, 14, 23)
    end do
end subroutine message_digest

```

```

call transform (fg, b, c, d, a, 4, 20, 24)
call transform (fg, a, b, c, d, 9, 5, 25)
call transform (fg, d, a, b, c, 14, 9, 26)
call transform (fg, c, d, a, b, 3, 14, 27)
call transform (fg, b, c, d, a, 8, 20, 28)
call transform (fg, a, b, c, d, 13, 5, 29)
call transform (fg, d, a, b, c, 2, 9, 30)
call transform (fg, c, d, a, b, 7, 14, 31)
call transform (fg, b, c, d, a, 12, 20, 32)
call transform (fh, a, b, c, d, 5, 4, 33)
call transform (fh, d, a, b, c, 8, 11, 34)
call transform (fh, c, d, a, b, 11, 16, 35)
call transform (fh, b, c, d, a, 14, 23, 36)
call transform (fh, a, b, c, d, 1, 4, 37)
call transform (fh, d, a, b, c, 4, 11, 38)
call transform (fh, c, d, a, b, 7, 16, 39)
call transform (fh, b, c, d, a, 10, 23, 40)
call transform (fh, a, b, c, d, 13, 4, 41)
call transform (fh, d, a, b, c, 0, 11, 42)
call transform (fh, c, d, a, b, 3, 16, 43)
call transform (fh, b, c, d, a, 6, 23, 44)
call transform (fh, a, b, c, d, 9, 4, 45)
call transform (fh, d, a, b, c, 12, 11, 46)
call transform (fh, c, d, a, b, 15, 16, 47)
call transform (fh, b, c, d, a, 2, 23, 48)
call transform (fi, a, b, c, d, 0, 6, 49)
call transform (fi, d, a, b, c, 7, 10, 50)
call transform (fi, c, d, a, b, 14, 15, 51)
call transform (fi, b, c, d, a, 5, 21, 52)
call transform (fi, a, b, c, d, 12, 6, 53)
call transform (fi, d, a, b, c, 3, 10, 54)
call transform (fi, c, d, a, b, 10, 15, 55)
call transform (fi, b, c, d, a, 1, 21, 56)
call transform (fi, a, b, c, d, 8, 6, 57)
call transform (fi, d, a, b, c, 15, 10, 58)
call transform (fi, c, d, a, b, 6, 15, 59)
call transform (fi, b, c, d, a, 13, 21, 60)
call transform (fi, a, b, c, d, 4, 6, 61)
call transform (fi, d, a, b, c, 11, 10, 62)
call transform (fi, c, d, a, b, 2, 15, 63)
call transform (fi, b, c, d, a, 9, 21, 64)
a = a + aa
b = b + bb
c = c + cc
d = d + dd
bl => bl%next
end do
s = digest_string ([a, b, c, d])
contains
<MD5: Internal subroutine transform>
end subroutine message_digest

```

And this is the actual transformation that depends on one of the previous functions, four words, and three integers. The implicit arguments are *x*, the word

from the message to digest, and *t*, the entry in the predefined table.

```

<MD5: Internal subroutine transform>≡
subroutine transform (f, a, b, c, d, k, s, i)
  interface
    function f (x, y, z)
      import word32_t
      type(word32_t), intent(in) :: x, y, z
      type(word32_t) :: f
    end function f
  end interface
  type(word32_t), intent(inout) :: a
  type(word32_t), intent(in) :: b, c, d
  integer, intent(in) :: k, s, i
  a = b + ishftc (a + f(b, c, d) + x(k) + t(i), s)
end subroutine transform

```

6.3.7 User interface

```

<MD5: public>≡
public :: md5sum

<MD5: interfaces>+≡
interface md5sum
  module procedure md5sum_from_string
  module procedure md5sum_from_unit
end interface

```

This function computes the MD5 sum of the input string and returns it as a 32-character string

```

<MD5: sub interfaces>+≡
module function md5sum_from_string (s) result (digest)
  character(len=*), intent(in) :: s
  character(len=32) :: digest
end function md5sum_from_string

<MD5: procedures>+≡
module function md5sum_from_string (s) result (digest)
  character(len=*), intent(in) :: s
  character(len=32) :: digest
  type(message_t) :: m
  call message_append_string (m, s)
  call message_pad (m)
  call message_digest (m, digest)
  call message_clear (m)
end function md5sum_from_string

```

This funct. reads from unit *u* (an unformatted sequence of integers) and computes the MD5 sum.

```

<MD5: sub interfaces>+≡
module function md5sum_from_unit (u) result (digest)
  integer, intent(in) :: u
  character(len=32) :: digest
end function md5sum_from_unit

```

```

<MD5: procedures>+≡
  module function md5sum_from_unit (u) result (digest)
    integer, intent(in) :: u
    character(len=32) :: digest
    type(message_t) :: m
    character :: char
    integer :: iostat
    READ_CHARS: do
      read (u, "(A)", advance="no", iostat=iostat) char
      select case (iostat)
        case (0)
          call message_append_string (m, char)
        case (EOR)
          call message_append_string (m, LF)
        case (EOF)
          exit READ_CHARS
        case default
          call msg_fatal &
            ("Computing MD5 sum: I/O error while reading from scratch file")
      end select
    end do READ_CHARS
    call message_pad (m)
    call message_digest (m, digest)
    call message_clear (m)
  end function md5sum_from_unit

```

6.3.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<md5_ut.f90>≡
  <File header>

  module md5_ut
    use unit_tests
    use md5_ut_i

    <Standard module head>

    <MD5: public test>

    contains

    <MD5: test driver>

  end module md5_ut

<md5_ut_i.f90>≡
  <File header>

  module md5_ut_i

    use diagnostics

```



```

write (u, "(A)")  "* Test output: MD5"
write (u, "(A)")  "* Purpose: test MD5 sums"
write (u, "(A)")

do i = 1, n
  write (u, "(A)") "MD5 test string = " // ' '// &
    trim (teststring(i)) // ' '
  s = md5sum (trim (teststring(i)))
  write (u, "(A)") "MD5 check sum   = " // trim (s)
  write (u, "(A)") "Ref check sum   = " // result(i)
  if (s == result(i)) then
    call msg_message ("=> ok", u)
  else
    call msg_message ("=> MD5 sum self-test failed", u)
  end if
end do
call msg_message ("=====
end subroutine md5_1

```

6.4 Permutations

Permute arrays of integers (of specific kind).

<permutations.f90>≡
<File header>

```
module permutations
```

```
  use kinds, only: TC
```

<Standard module head>

<Permutations: public>

<Permutations: types>

<Permutations: interfaces>

```
  interface
<Permutations: sub interfaces>
  end interface
```

```
end module permutations
```

<permutations_sub.f90>≡
<File header>

```
submodule (permutations) permutations_s
```

```
  implicit none
```

<Permutations: variables>

```
contains

<Permutations: procedures>

end submodule permutations_s
```

6.4.1 Permutations

A permutation is an array of integers. Each integer between one and `size` should occur exactly once.

```
<Permutations: public>≡
    public :: permutation_t

<Permutations: types>≡
    type :: permutation_t
    private
        integer, dimension(:), allocatable :: p
    end type permutation_t
```

Initialize with the identity permutation.

```
<Permutations: public>+≡
    public :: permutation_init
    public :: permutation_final

<Permutations: sub interfaces>≡
    elemental module subroutine permutation_init (p, size)
        type(permutation_t), intent(inout) :: p
        integer, intent(in) :: size
    end subroutine permutation_init
    elemental module subroutine permutation_final (p)
        type(permutation_t), intent(inout) :: p
    end subroutine permutation_final

<Permutations: procedures>≡
    elemental module subroutine permutation_init (p, size)
        type(permutation_t), intent(inout) :: p
        integer, intent(in) :: size
        integer :: i
        allocate (p%p (size))
        forall (i = 1:size)
            p%p(i) = i
        end forall
    end subroutine permutation_init

    elemental module subroutine permutation_final (p)
        type(permutation_t), intent(inout) :: p
        deallocate (p%p)
    end subroutine permutation_final
```

I/O:

```
<Permutations: public>+≡
    public :: permutation_write
```

```

<Permutations: sub interfaces>+≡
    module subroutine permutation_write (p, u)
        type(permutation_t), intent (in) :: p
        integer, intent(in) :: u
    end subroutine permutation_write

<Permutations: procedures>+≡
    module subroutine permutation_write (p, u)
        type(permutation_t), intent (in) :: p
        integer, intent(in) :: u
        integer :: i
        do i = 1, size (p%p)
            if (size (p%p) < 10) then
                write (u, "(1x,I1)", advance="no") p%p(i)
            else
                write (u, "(1x,I3)", advance="no") p%p(i)
            end if
        end do
        write (u, *)
    end subroutine permutation_write

```

Administration:

```

<Permutations: public>+≡
    public :: permutation_size

<Permutations: sub interfaces>+≡
    elemental module function permutation_size (perm) result (s)
        type(permutation_t), intent(in) :: perm
        integer :: s
    end function permutation_size

<Permutations: procedures>+≡
    elemental module function permutation_size (perm) result (s)
        type(permutation_t), intent(in) :: perm
        integer :: s
        s = size (perm%p)
    end function permutation_size

```

Extract an entry in a permutation.

```

<Permutations: public>+≡
    public :: permute

<Permutations: sub interfaces>+≡
    elemental module function permute (i, p) result (j)
        integer, intent(in) :: i
        type(permutation_t), intent(in) :: p
        integer :: j
    end function permute

<Permutations: procedures>+≡
    elemental module function permute (i, p) result (j)
        integer, intent(in) :: i
        type(permutation_t), intent(in) :: p
        integer :: j
        if (i > 0 .and. i <= size (p%p)) then

```

```

        j = p%p(i)
    else
        j = 0
    end if
end function permute

```

Check whether a permutation is valid: Each integer in the range occurs exactly once.

```

<Permutations: public>+≡
    public :: permutation_ok

<Permutations: sub interfaces>+≡
    elemental module function permutation_ok (perm) result (ok)
        type(permutation_t), intent(in) :: perm
        logical :: ok
    end function permutation_ok

<Permutations: procedures>+≡
    elemental module function permutation_ok (perm) result (ok)
        type(permutation_t), intent(in) :: perm
        logical :: ok
        integer :: i
        logical, dimension(:), allocatable :: set
        ok = .true.
        allocate (set (size (perm%p)))
        set = .false.
        do i = 1, size (perm%p)
            ok = (perm%p(i) > 0 .and. perm%p(i) <= size (perm%p))
            if (.not.ok) return
            set(perm%p(i)) = .true.
        end do
        ok = all (set)
    end function permutation_ok

```

Find the permutation that transforms the second array into the first one. We assume that this is possible and unique and all bounds are set correctly.

This cannot be elemental.

```

<Permutations: public>+≡
    public :: permutation_find

<Permutations: sub interfaces>+≡
    module subroutine permutation_find (perm, a1, a2)
        type(permutation_t), intent(inout) :: perm
        integer, dimension(:), intent(in) :: a1, a2
    end subroutine permutation_find

<Permutations: procedures>+≡
    module subroutine permutation_find (perm, a1, a2)
        type(permutation_t), intent(inout) :: perm
        integer, dimension(:), intent(in) :: a1, a2
        integer :: i, j
        if (allocated (perm%p)) deallocate (perm%p)
        allocate (perm%p (size (a1)))
        do i = 1, size (a1)
            do j = 1, size (a2)

```

```

        if (a1(i) == a2(j)) then
            perm%p(i) = j
            exit
        end if
        perm%p(i) = 0
    end do
end do
end subroutine permutation_find

```

Find all permutations that transform an array of integers into itself. The resulting permutation list is allocated with the correct length and filled.

The first step is to count the number of different entries in `code`. Next, we scan `code` again and assign a mask to each different entry, true for all identical entries. Finally, we recursively permute the identity for each possible mask.

The permutation is done as follows: A list of all permutations of the initial one with respect to the current mask is generated, then the permutations are generated in turn for each permutation in this list with the next mask. The result is always stored back into the main list, starting from the end of the current list.

```

<Permutations: public>+≡
    public :: permutation_array_make

<Permutations: sub interfaces>+≡
    module subroutine permutation_array_make (pa, code)
        type(permutation_t), dimension(:), allocatable, intent(out) :: pa
        integer, dimension(:), intent(in) :: code
    end subroutine permutation_array_make

<Permutations: procedures>+≡
    module subroutine permutation_array_make (pa, code)
        type(permutation_t), dimension(:), allocatable, intent(out) :: pa
        integer, dimension(:), intent(in) :: code
        logical, dimension(size(code)) :: mask
        logical, dimension(:,:), allocatable :: imask
        integer, dimension(:), allocatable :: n_i
        type(permutation_t) :: p_init
        type(permutation_t), dimension(:), allocatable :: p_tmp
        integer :: psize, i, j, k, n_different, n, nn_k
        psize = size (code)
        mask = .true.
        n_different = 0
        do i=1, psize
            if (mask(i)) then
                n_different = n_different + 1
                mask = mask .and. (code /= code(i))
            end if
        end do
        allocate (imask(psize, n_different), n_i(n_different))
        mask = .true.
        k = 0
        do i=1, psize
            if (mask(i)) then
                k = k + 1
                imask(:,k) = (code == code(i))
            end if
        end do
    end subroutine permutation_array_make

```

```

        n_i(k) = factorial (count(imask(:,k)))
        mask = mask .and. (code /= code(i))
    end if
end do
n = product (n_i)
allocate (pa (n))
call permutation_init (p_init, psize)
pa(1) = p_init
nn_k = 1
do k = 1, n_different
    allocate (p_tmp (n_i(k)))
    do i = nn_k, 1, -1
        call permutation_array_with_mask (p_tmp, imask(:,k), pa(i))
        do j = n_i(k), 1, -1
            pa((i-1)*n_i(k) + j) = p_tmp(j)
        end do
    end do
    deallocate (p_tmp)
    nn_k = nn_k * n_i(k)
end do
call permutation_final (p_init)
deallocate (imask, n_i)
end subroutine permutation_array_make

```

Make a list of permutations of the elements marked true in the `mask` array. The final permutation list must be allocated with the correct length ($n!$). The third argument is the initial permutation to start with, which must have the same length as the `mask` array (this is not checked).

(Permutations: procedures)+≡

```

subroutine permutation_array_with_mask (pa, mask, p_init)
    type(permutation_t), dimension(:), intent(inout) :: pa
    logical, dimension(:), intent(in) :: mask
    type(permutation_t), intent(in) :: p_init
    integer :: plen
    integer :: i, ii, j, fac_i, k, x
    integer, dimension(:), allocatable :: index
    plen = size (pa)
    allocate (index(count(mask)))
    ii = 0
    do i = 1, size (mask)
        if (mask(i)) then
            ii = ii + 1
            index(ii) = i
        end if
    end do
    pa = p_init
    ii = 0
    fac_i = 1
    do i = 1, size (mask)
        if (mask(i)) then
            ii = ii + 1
            fac_i = fac_i * ii
            x = permute (i, p_init)

```

```

        do j = 1, plen
            k = ii - mod (((j-1)*fac_i)/plen, ii)
            call insert (pa(j), x, k, ii, index)
        end do
    end if
end do
deallocate (index)
contains
subroutine insert (p, x, k, n, index)
    type(permutation_t), intent(inout) :: p
    integer, intent(in) :: x, k, n
    integer, dimension(:), intent(in) :: index
    integer :: i
    do i = n, k+1, -1
        p%p(index(i)) = p%p(index(i-1))
    end do
    p%p(index(k)) = x
end subroutine insert
end subroutine permutation_array_with_mask

```

The factorial function is needed for pre-determining the number of permutations that will be generated:

```

<Permutations: public>+≡
    public :: factorial

<Permutations: sub interfaces>+≡
    elemental module function factorial (n) result (f)
        integer, intent(in) :: n
        integer :: f
    end function factorial

<Permutations: procedures>+≡
    elemental module function factorial (n) result (f)
        integer, intent(in) :: n
        integer :: f
        integer :: i
        f = 1
        do i=2, abs(n)
            f = f*i
        end do
    end function factorial

```

6.4.2 Operations on binary codes

Binary codes are needed for phase-space trees. Since the permutation function uses permutations, and no other special type is involved, we put the functions here.

This is needed for phase space trees: permute bits in a tree binary code. If no permutation is given, leave as is. (We may want to access the permutation directly here if this is efficiency-critical.)

```

<Permutations: public>+≡
    public :: tc_permute

```



```

<Permutations: sub interfaces>+≡
  module function tc_permute (k, perm, mask_in) result (pk)
    integer(TC), intent(in) :: k, mask_in
    type(permutation_t), intent(in) :: perm
    integer(TC) :: pk
  end function tc_permute

```

```

<Permutations: procedures>+≡
  module function tc_permute (k, perm, mask_in) result (pk)
    integer(TC), intent(in) :: k, mask_in
    type(permutation_t), intent(in) :: perm
    integer(TC) :: pk
    integer :: i
    pk = iand (k, mask_in)
    do i = 1, size (perm%p)
      if (btest(k,i-1)) pk = ibset (pk, perm%p(i)-1)
    end do
  end function tc_permute

```

This routine returns the number of set bits in the tree code value **k**. Hence, it is the number of externals connected to the current line. If **mask** is present, the complement of the tree code is also considered, and the smaller number is returned. This gives the true distance from the external states, taking into account the initial particles. The complement number is increased by one, since for a scattering diagram the vertex with the sum of all final-state codes is still one point apart from the initial particles.

```

<Permutations: public>+≡
  public :: tc_decay_level

```

```

<Permutations: interfaces>≡
  interface tc_decay_level
    module procedure decay_level_simple
    module procedure decay_level_complement
  end interface

```

```

<Permutations: sub interfaces>+≡
  module function decay_level_complement (k, mask) result (l)
    integer(TC), intent(in) :: k, mask
    integer :: l
  end function decay_level_complement
  module function decay_level_simple (k) result(l)
    integer(TC), intent(in) :: k
    integer :: l
  end function decay_level_simple

```

```

<Permutations: procedures>+≡
  module function decay_level_complement (k, mask) result (l)
    integer(TC), intent(in) :: k, mask
    integer :: l
    l = min (decay_level_simple (k), &
      & decay_level_simple (ieor (k, mask)) + 1)
  end function decay_level_complement

  module function decay_level_simple (k) result(l)
    integer(TC), intent(in) :: k

```

```

integer :: l
integer :: i
l = 0
do i=0, bit_size(k)-1
  if (btest(k,i)) l = l+1
end do
end function decay_level_simple

```

6.5 Sorting

This small module provides functions for sorting integer or real arrays.

```

<sorting.f90>≡
  <File header>

  module sorting

    <Use kinds>

    <Standard module head>

    <Sorting: public>

    <Sorting: interfaces>

    interface
      <Sorting: sub interfaces>
    end interface

  end module sorting

<sorting_sub.f90>≡
  <File header>

  submodule (sorting) sorting_s

    use diagnostics

    implicit none

    contains

    <Sorting: procedures>

  end submodule sorting_s

```

6.5.1 Implementation

The `sort` function returns, for a given integer or real array, the array sorted by increasing value. The current implementation is *mergesort*, which has $O(n \ln n)$ behavior in all cases, and is stable for elements of equal value.

The `sort_abs` variant sorts by increasing absolute value, where for identical absolute value, the positive number comes first.

```

<Sorting: public>≡
  public :: sort
  public :: sort_abs

<Sorting: interfaces>≡
  interface sort
    module procedure sort_int
    module procedure sort_real
  end interface

  interface sort_abs
    module procedure sort_int_abs
  end interface

```

This variant of integer sort returns The body is identical, just the interface differs.

```

<Sorting: sub interfaces>≡
  module function sort_int (val_in) result (val)
    integer, dimension(:), intent(in) :: val_in
    integer, dimension(size(val_in)) :: val
  end function sort_int
  module function sort_real (val_in) result (val)
    real(default), dimension(:), intent(in) :: val_in
    real(default), dimension(size(val_in)) :: val
  end function sort_real
  module function sort_int_abs (val_in) result (val)
    integer, dimension(:), intent(in) :: val_in
    integer, dimension(size(val_in)) :: val
  end function sort_int_abs

<Sorting: procedures>≡
  module function sort_int (val_in) result (val)
    integer, dimension(:), intent(in) :: val_in
    integer, dimension(size(val_in)) :: val
  <Sorting: sort>
  end function sort_int

  module function sort_real (val_in) result (val)
    real(default), dimension(:), intent(in) :: val_in
    real(default), dimension(size(val_in)) :: val
  <Sorting: sort>
  end function sort_real

  module function sort_int_abs (val_in) result (val)
    integer, dimension(:), intent(in) :: val_in
    integer, dimension(size(val_in)) :: val
  <Sorting: sort abs>
  end function sort_int_abs

<Sorting: sort>≡
  val = val_in( order (val_in) )

```

```

<Sorting: sort abs>≡
  val = val_in( order_abs (val_in) )

```

The `order` function returns, for a given integer or real array, the array of indices of the elements sorted by increasing value.

```

<Sorting: public>+≡
  public :: order
  public :: order_abs

```

```

<Sorting: interfaces>+≡
  interface order
    module procedure order_int
    module procedure order_real
  end interface

  interface order_abs
    module procedure order_int_abs
  end interface

```

```

<Sorting: sub interfaces>+≡
  module function order_int (val) result (idx)
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  end function order_int
  module function order_real (val) result (idx)
    real(default), dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  end function order_real
  module function order_int_abs (val) result (idx)
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  end function order_int_abs

```

```

<Sorting: procedures>+≡
  module function order_int (val) result (idx)
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  <Sorting: order>
  end function order_int

  module function order_real (val) result (idx)
    real(default), dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  <Sorting: order>
  end function order_real

  module function order_int_abs (val) result (idx)
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
  <Sorting: order abs>
  end function order_int_abs

```

We start by individual elements, merge them to pairs, merge those to four-element subarrays, and so on. The last subarray can extend only up to the

original array bound, of course, and the second of the subarrays to merge should contain at least one element.

```

<Sorting: order>≡
  <Sorting: order1>
    call merge (idx(b1:e2), idx(b1:e1), idx(b2:e2), val)
  <Sorting: order2>

<Sorting: order abs>≡
  <Sorting: order1>
    call merge_abs (idx(b1:e2), idx(b1:e1), idx(b2:e2), val)
  <Sorting: order2>

<Sorting: order1>≡
  integer :: n, i, s, b1, b2, e1, e2
  n = size (idx)
  do i = 1, n
    idx(i) = i
  end do
  s = 1
  do while (s < n)
    do b1 = 1, n-s, 2*s
      b2 = b1 + s
      e1 = b2 - 1
      e2 = min (e1 + s, n)
    end do
    s = 2 * s
  end do

```

The merging step does the actual sorting. We take two sorted array sections and merge them to a sorted result array. We are working on the indices, and comparing is done by taking the associated `val` which is real or integer.

```

<Sorting: interfaces>+≡
  interface merge
    module procedure merge_int
    module procedure merge_real
  end interface

  interface merge_abs
    module procedure merge_int_abs
  end interface

<Sorting: sub interfaces>+≡
  module subroutine merge_int (res, src1, src2, val)
    integer, dimension(:), intent(out) :: res
    integer, dimension(:), intent(in) :: src1, src2
    integer, dimension(:), intent(in) :: val
  end subroutine merge_int
  module subroutine merge_real (res, src1, src2, val)
    integer, dimension(:), intent(out) :: res
    integer, dimension(:), intent(in) :: src1, src2
    real(default), dimension(:), intent(in) :: val
  end subroutine merge_real
  module subroutine merge_int_abs (res, src1, src2, val)

```

```

        integer, dimension(:), intent(out) :: res
        integer, dimension(:), intent(in) :: src1, src2
        integer, dimension(:), intent(in) :: val
    end subroutine merge_int_abs

    <Sorting: procedures>+≡
    module subroutine merge_int (res, src1, src2, val)
        integer, dimension(:), intent(out) :: res
        integer, dimension(:), intent(in) :: src1, src2
        integer, dimension(:), intent(in) :: val
        integer, dimension(size(res)) :: tmp
    <Sorting: merge>
    end subroutine merge_int

    module subroutine merge_real (res, src1, src2, val)
        integer, dimension(:), intent(out) :: res
        integer, dimension(:), intent(in) :: src1, src2
        real(default), dimension(:), intent(in) :: val
        integer, dimension(size(res)) :: tmp
    <Sorting: merge>
    end subroutine merge_real

    module subroutine merge_int_abs (res, src1, src2, val)
        integer, dimension(:), intent(out) :: res
        integer, dimension(:), intent(in) :: src1, src2
        integer, dimension(:), intent(in) :: val
        integer, dimension(size(res)) :: tmp
    <Sorting: merge abs>
    end subroutine merge_int_abs

```

```

    <Sorting: merge>≡
    <Sorting: merge1>
        if (val(src1(i1)) <= val(src2(i2))) then
    <Sorting: merge2>

```

We keep the elements if the absolute values are strictly ordered. If they are equal in magnitude, we keep them if the larger value comes first, or if they are equal.

```

    <Sorting: merge abs>≡
    <Sorting: merge1>
        if (abs (val(src1(i1))) < abs (val(src2(i2))) .or. &
            (abs (val(src1(i1))) == abs (val(src2(i2))) .and. &
            val(src1(i1)) >= val(src2(i2)))) then
    <Sorting: merge2>

    <Sorting: merge1>≡
        integer :: i1, i2, i
        i1 = 1
        i2 = 1
        do i = 1, size (tmp)
    <Sorting: merge2>≡
            tmp(i) = src1(i1); i1 = i1 + 1
            if (i1 > size (src1)) then
                tmp(i+1:) = src2(i2:)

```

```

        exit
    end if
else
    tmp(i) = src2(i2); i2 = i2 + 1
    if (i2 > size (src2)) then
        tmp(i+1:) = src1(i1:)
        exit
    end if
end if
end do
res = tmp

```

6.5.2 Unit tests

Test module, followed by the corresponding implementation module.

<sorting_ut.f90>≡
<File header>

```

module sorting_ut
  use unit_tests
  use sorting_uti

```

<Standard module head>

<Sorting: public test>

contains

<Sorting: test driver>

```

end module sorting_ut

```

<sorting_uti.f90>≡
<File header>

```

module sorting_uti

```

<Use kinds>

```

  use sorting

```

<Standard module head>

<Sorting: test declarations>

contains

<Sorting: tests>

```

end module sorting_uti

```

API: driver for the unit tests below.

<Sorting: public test>≡
 public :: sorting_test

```

<Sorting: test driver>≡
  subroutine sorting_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Sorting: execute tests>
  end subroutine sorting_test

```

This checks whether the sorting routine works correctly.

```

<Sorting: execute tests>≡
  call test (sorting_1, "sorting_1", &
    "check sorting routines", &
    u, results)

<Sorting: test declarations>≡
  public :: sorting_1

<Sorting: tests>≡
  subroutine sorting_1 (u)
    integer, intent(in) :: u
    integer, parameter :: NMAX = 10
    real(default), dimension(NMAX) :: rval
    integer, dimension(NMAX) :: ival
    real, dimension(NMAX,NMAX) :: harvest_r
    integer, dimension(NMAX,NMAX) :: harvest_i
    integer, dimension(NMAX,NMAX) :: harvest_a
    integer :: i, j
    harvest_r(:, 1) = [0.9976, 0., 0., 0., 0., 0., 0., 0., 0., 0.]
    harvest_r(:, 2) = [0.5668, 0.9659, 0., 0., 0., 0., 0., 0., 0., 0.]
    harvest_r(:, 3) = [0.7479, 0.3674, 0.4806, 0., 0., 0., 0., 0., 0., &
      0.]
    harvest_r(:, 4) = [0.0738, 0.0054, 0.3471, 0.3422, 0., 0., 0., 0., &
      0., 0.]
    harvest_r(:, 5) = [0.2180, 0.1332, 0.9005, 0.3868, 0.4455, 0., 0., &
      0., 0., 0.]
    harvest_r(:, 6) = [0.6619, 0.0161, 0.6509, 0.6464, 0.3230, &
      0.8557, 0., 0., 0., 0.]
    harvest_r(:, 7) = [0.4013, 0.2069, 0.9685, 0.5984, 0.6730, &
      0.4569, 0.3300, 0., 0., 0.]
    harvest_r(:, 8) = [0.1004, 0.7555, 0.6057, 0.7190, 0.8973, &
      0.6582, 0.1507, 0.6123, 0., 0.]
    harvest_r(:, 9) = [0.9787, 0.9991, 0.2568, 0.5509, 0.6590, &
      0.5540, 0.9778, 0.9019, 0.6579, 0.]
    harvest_r(:,10) = [0.7289, 0.4025, 0.9286, 0.1478, 0.6745, &
      0.7696, 0.3393, 0.1158, 0.6144, 0.8206]

    harvest_i(:, 1) = [18, 0, 0, 0, 0, 0, 0, 0, 0, 0]
    harvest_i(:, 2) = [14, 9, 0, 0, 0, 0, 0, 0, 0, 0]
    harvest_i(:, 3) = [ 7, 8,11, 0, 0, 0, 0, 0, 0, 0]
    harvest_i(:, 4) = [19,19,14,19, 0, 0, 0, 0, 0, 0]
    harvest_i(:, 5) = [ 1,14,15,18,14, 0, 0, 0, 0, 0]
    harvest_i(:, 6) = [16,11, 1, 9,11, 2, 0, 0, 0, 0]
    harvest_i(:, 7) = [11,10,17, 6,13,13,10, 0, 0, 0]
    harvest_i(:, 8) = [ 5, 1, 2,10, 7, 0,15,12, 0, 0]
    harvest_i(:, 9) = [15,19, 2, 6,11, 0, 2, 4, 2, 0]
    harvest_i(:,10) = [ 1, 4, 8, 4,11, 0, 8, 7,19,13]

```



```

harvest_a(:, 1) = [-6, 0, 0, 0, 0, 0, 0, 0, 0, 0]
harvest_a(:, 2) = [-8, -9, 0, 0, 0, 0, 0, 0, 0, 0]
harvest_a(:, 3) = [ 4, -3, 3, 0, 0, 0, 0, 0, 0, 0]
harvest_a(:, 4) = [-6, 6, 2, -2, 0, 0, 0, 0, 0, 0]
harvest_a(:, 5) = [ 1, -2, 0, -6, 8, 0, 0, 0, 0, 0]
harvest_a(:, 6) = [-2, -1, -8, -5, 8, -5, 0, 0, 0, 0]
harvest_a(:, 7) = [-9, 0, -6, 2, 5, 3, 2, 0, 0, 0]
harvest_a(:, 8) = [-5, -7, 6, 7, -3, 0, -7, 4, 0, 0]
harvest_a(:, 9) = [ 5, 0, -1, -7, 5, 2, 7, -3, 3, 0]
harvest_a(:,10) = [-9, 2, -6, 3, -9, 5, 5, 7, 5, -9]

write (u, "(A)")  "* Test output: Sorting"
write (u, "(A)")  "* Purpose: test sorting routines"
write (u, "(A)")

write (u, "(A)")  "* Sorting real values:"

do i = 1, NMAX
  write (u, "(A)")
  rval(:i) = harvest_r(:i,i)
  write (u, "(10(1x,F7.4))") rval(:i)
  rval(:i) = sort (rval(:i))
  write (u, "(10(1x,F7.4))") rval(:i)
  do j = i, 2, -1
    if (rval(j)-rval(j-1) < 0) &
      write (u, "(A)") "*** Sorting failure. ***"
  end do
end do

write (u, "(A)")
write (u, "(A)") "* Sorting integer values:"

do i = 1, NMAX
  write (u, "(A)")
  ival(:i) = harvest_i(:i,i)
  write (u, "(10(1x,I2))") ival(:i)
  ival(:i) = sort (ival(:i))
  write (u, "(10(1x,I2))") ival(:i)
  do j = i, 2, -1
    if (ival(j)-ival(j-1) < 0) &
      write (u, "(A)") "*** Sorting failure. ***"
  end do
end do

write (u, "(A)")
write (u, "(A)") "* Sorting integer values by absolute value:"

do i = 1, NMAX
  write (u, "(A)")
  ival(:i) = harvest_a(:i,i)
  write (u, "(10(1x,I2))") ival(:i)
  ival(:i) = sort_abs (ival(:i))

```

```

        write (u, "(10(1x,I2))") ival(:i)
        do j = i, 2, -1
            if (abs(ival(j))-abs(ival(j-1)) < 0 .or. &
                (abs(ival(j))==abs(ival(j-1))) .and. ival(j)>ival(j-1)) &
                write (u, "(A)")  "**** Sorting failure. ***"
        end do
    end do

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sorting_1"

end subroutine sorting_1

```

6.6 Grids

This is not really a combinatorics module but this directory is the closest I could find. Maybe this will be moved to a seperate directory or combined with related stuff.

```

<grids.f90>≡
  <File header>

  module grids

    <Use kinds>
    <Use mpi f08>

    <Standard module head>

    <Grids: public>

    <Grids: types>

    interface
    <Grids: sub interfaces>
    end interface

  end module grids

<grids_sub.f90>≡
  <File header>

  submodule (grids) grids_s

    use constants, only: zero, one, tiny_07
    use io_units
    use format_defs, only: FMT_16, FMT_12
    use diagnostics
    <Use mpi f08>

    implicit none

    <Grids: parameters>

```

```
contains

⟨Grids: procedures⟩

end submodule grids_s
```

Grids are used in many applications and a general implementation seems useful. The relevant properties implemented so far are

- Segments of the hypercube are represented by an integer array with size d corresponding to the dimension.
- There is a mapping from the indices to the location in the continuous memory block of values.
- Given a point in the hypercube, find the corresponding segment and the value of the grid therein.
- Update the grid sequentially to represent the maximum of a function over the unit hypercube.
- The grid can be saved to and recovered from disk.

The following might be implemented in the future

- Generate a random point in the hypercube by interpreting the grid as probability distribution.
This would most likely be solved by using projections and the `selector_t`, which would make a move of this module higher up in the dependency tree necessary.
- Update the grid sequentially to represent the *minimum* of a function over the unit hypercube.

```
⟨Grids: public⟩≡
  public :: grid_t

⟨Grids: types⟩≡
  type :: grid_t
  private
    real(default), dimension(:), allocatable :: values
    integer, dimension(:), allocatable :: points
  contains
    ⟨Grids: grid: TBP⟩
  end type grid_t
```

6.6.1 Initializer and finalizer

For initialization, we expect the number of points for each dimension as an array or the the number of dimensions as a scalar whereby the default number of points is used then for each dimension.

```
⟨Grids: grid: TBP⟩≡
```

```

generic :: init => init_base, init_simple
procedure :: init_base => grid_init_base
procedure :: init_simple => grid_init_simple

⟨Grids: sub interfaces⟩≡
  pure module subroutine grid_init_base (grid, points)
    class(grid_t), intent(inout) :: grid
    integer, dimension(:), intent(in) :: points
  end subroutine grid_init_base

⟨Grids: procedures⟩≡
  pure module subroutine grid_init_base (grid, points)
    class(grid_t), intent(inout) :: grid
    integer, dimension(:), intent(in) :: points
    allocate (grid%points (size (points)))
    allocate (grid%values (product (points)))
    grid%points = points
    grid%values = zero
  end subroutine grid_init_base

⟨Grids: sub interfaces⟩+≡
  pure module subroutine grid_init_simple (grid, dimensions)
    class(grid_t), intent(inout) :: grid
    integer, intent(in) :: dimensions
  end subroutine grid_init_simple

⟨Grids: procedures⟩+≡
  pure module subroutine grid_init_simple (grid, dimensions)
    class(grid_t), intent(inout) :: grid
    integer, intent(in) :: dimensions
    allocate (grid%points (dimensions))
    allocate (grid%values (DEFAULT_POINTS_PER_DIMENSION ** dimensions))
    grid%points = DEFAULT_POINTS_PER_DIMENSION
    grid%values = zero
  end subroutine grid_init_simple

```

Manual assignment (tests)

```

⟨Grids: grid: TBP⟩+≡
  procedure :: set_values => grid_set_values

⟨Grids: sub interfaces⟩+≡
  module subroutine grid_set_values (grid, values)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: values
  end subroutine grid_set_values

⟨Grids: procedures⟩+≡
  module subroutine grid_set_values (grid, values)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: values
    grid%values = values
  end subroutine grid_set_values

```

A reasonable default

```

⟨Grids: parameters⟩≡
  integer, parameter :: DEFAULT_POINTS_PER_DIMENSION = 100

```

Calling this is not mandatory, when an instance of `grid_t` goes out of scope as it will be done by Fortran automatically.

```

<Grids: grid: TBP>+≡
    procedure :: final => grid_final

<Grids: sub interfaces>+≡
    pure module subroutine grid_final (grid)
        class(grid_t), intent(inout) :: grid
    end subroutine grid_final

<Grids: procedures>+≡
    pure module subroutine grid_final (grid)
        class(grid_t), intent(inout) :: grid
        if (allocated (grid%values)) then
            deallocate (grid%values)
        end if
        if (allocated (grid%points)) then
            deallocate (grid%points)
        end if
    end subroutine grid_final

```

6.6.2 Segment finding and memory mapping

The `indices` array is expected to go from 1 to d whereby the entries for the different dims are from 1 to $n_{\text{points}}(\text{dim})$.

We get the value of the grid either from given `indices` or from a point `x` in the hypercube. In the latter case, we have to find the segment first.

```

<Grids: grid: TBP>+≡
    generic :: get_value => get_value_from_x, get_value_from_indices
    procedure :: get_value_from_x => grid_get_value_from_x
    procedure :: get_value_from_indices => grid_get_value_from_indices

<Grids: sub interfaces>+≡
    module function grid_get_value_from_indices (grid, indices)
        real(default) :: grid_get_value_from_indices
        class(grid_t), intent(in) :: grid
        integer, dimension(:), intent(in) :: indices
    end function grid_get_value_from_indices

<Grids: procedures>+≡
    module function grid_get_value_from_indices (grid, indices)
        real(default) :: grid_get_value_from_indices
        class(grid_t), intent(in) :: grid
        integer, dimension(:), intent(in) :: indices
        grid_get_value_from_indices = grid%values(grid%get_index(indices))
    end function grid_get_value_from_indices

<Grids: sub interfaces>+≡
    module function grid_get_value_from_x (grid, x)
        real(default) :: grid_get_value_from_x
        class(grid_t), intent(in) :: grid
        real(default), dimension(:), intent(in) :: x
    end function grid_get_value_from_x

```

```

⟨Grids: procedures⟩+≡
  module function grid_get_value_from_x (grid, x)
    real(default) :: grid_get_value_from_x
    class(grid_t), intent(in) :: grid
    real(default), dimension(:), intent(in) :: x
    grid_get_value_from_x = grid_get_value_from_indices &
      (grid, grid_get_segment (grid, x))
  end function grid_get_value_from_x

```

The segment is the part of the grid that contains the point x and is identified by a tuple of indices. This is just a brute force search, for fine grids one could also implement a binary search for $\mathcal{O}(\log N)$ behavior instead of $\mathcal{O}(N)$.

```

⟨Grids: grid: TBP⟩+≡
  procedure :: get_segment => grid_get_segment

⟨Grids: sub interfaces⟩+≡
  module function grid_get_segment (grid, x, unit) result (segment)
    class(grid_t), intent(in) :: grid
    real(default), dimension(:), intent(in) :: x
    integer, intent(in), optional :: unit
    integer, dimension(1:size (x)) :: segment
  end function grid_get_segment

⟨Grids: procedures⟩+≡
  module function grid_get_segment (grid, x, unit) result (segment)
    class(grid_t), intent(in) :: grid
    real(default), dimension(:), intent(in) :: x
    integer, intent(in), optional :: unit
    integer, dimension(1:size (x)) :: segment
    integer :: dim, i
    real(default) :: segment_width
    segment = 0
    do dim = 1, size (grid%points)
      segment_width = one / grid%points (dim)
      SEARCH: do i = 1, grid%points (dim)
        if (x (dim) <= i * segment_width + tiny_07) then
          segment (dim) = i
          exit SEARCH
        end if
      end do SEARCH
      if (segment (dim) == 0) then
        do i = 1, size(x)
          write (msg_buffer, "(A," // DEFAULT_OUTPUT_PRECISION // ")") &
            "x[i] = ", x(i)
          call msg_message ()
        end do
        call msg_error ("grid_get_segment: Did not find x in [0,1]^d", &
          unit=unit)
      end if
    end do
  end function grid_get_segment

```

This is a simple storage mapping function but more sophisticated ideas like

hashing could be implemented.

$$\begin{aligned} \text{index} = & \text{indices}(1) + \\ & \text{indices}(2) * \text{size}(1) + \\ & \text{indices}(3) * \text{size}(1) * \text{size}(2) + \dots \end{aligned} \quad (6.1)$$

```

<Grids: grid: TBP>+≡
  procedure :: get_index => grid_get_index

<Grids: sub interfaces>+≡
  pure module function grid_get_index (grid, indices) result (grid_index)
    integer :: grid_index
    class(grid_t), intent(in) :: grid
    integer, dimension(:), intent(in) :: indices
  end function grid_get_index

<Grids: procedures>+≡
  pure module function grid_get_index (grid, indices) result (grid_index)
    integer :: grid_index
    class(grid_t), intent(in) :: grid
    integer, dimension(:), intent(in) :: indices
    integer :: dim_innerloop, dim_outerloop, multiplier
    grid_index = 1
    do dim_outerloop = 1, size(indices)
      multiplier = 1
      do dim_innerloop = 1, dim_outerloop - 1
        multiplier = multiplier * grid%points (dim_innerloop)
      end do
      grid_index = grid_index + (indices(dim_outerloop) - 1) * multiplier
    end do
  end function grid_get_index

```

6.6.3 Grid manipulations

Given a point in the hypercube x and its value y , we update the grids, such that the stepwise function f defined by the grid is $f(x_i) \geq y_i \forall \{x_i, y_i\}$.

```

<Grids: grid: TBP>+≡
  procedure :: update_maxima => grid_update_maxima

<Grids: sub interfaces>+≡
  module subroutine grid_update_maxima (grid, x, y)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: x
    real(default), intent(in) :: y
  end subroutine grid_update_maxima

<Grids: procedures>+≡
  module subroutine grid_update_maxima (grid, x, y)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: x
    real(default), intent(in) :: y
    integer, dimension(1:size(x)) :: indices
    indices = grid%get_segment (x)
    if (grid%get_value (indices) < y) then

```

```

        grid%values (grid%get_index (indices)) = y
    end if
end subroutine grid_update_maxima

```

More general cases have to be thought through when they are needed. *This is inefficient and non-general.*

```

⟨Grids: grid: TBP⟩+≡
    procedure :: get_maximum_in_3d => grid_get_maximum_in_3d
⟨Grids: sub interfaces⟩+≡
    module function grid_get_maximum_in_3d (grid, projected_index) result (maximum)
        real(default) :: maximum
        class(grid_t), intent(in) :: grid
        integer, intent(in) :: projected_index
    end function grid_get_maximum_in_3d
⟨Grids: procedures⟩+≡
    module function grid_get_maximum_in_3d (grid, projected_index) result (maximum)
        real(default) :: maximum
        class(grid_t), intent(in) :: grid
        integer, intent(in) :: projected_index
        real(default) :: val
        integer :: i, j
        maximum = zero
        do i = 1, grid%points(1)
            do j = 1, grid%points(2)
                val = grid%get_value ([i, j, projected_index])
                if (val > maximum) then
                    maximum = val
                end if
            end do
        end do
    end function grid_get_maximum_in_3d

    end function grid_get_maximum_in_3d

⟨Grids: grid: TBP⟩+≡
    procedure :: is_non_zero_everywhere => grid_is_non_zero_everywhere
⟨Grids: sub interfaces⟩+≡
    pure module function grid_is_non_zero_everywhere (grid) result (yorn)
        logical :: yorn
        class(grid_t), intent(in) :: grid
    end function grid_is_non_zero_everywhere
⟨Grids: procedures⟩+≡
    pure module function grid_is_non_zero_everywhere (grid) result (yorn)
        logical :: yorn
        class(grid_t), intent(in) :: grid
        yorn = all (abs (grid%values) > zero)
    end function grid_is_non_zero_everywhere

```

Returns true if any value of the grid is non-zero. We need this to determine whether the grid has been filled during integration.

```

⟨Grids: grid: TBP⟩+≡
    procedure :: has_non_zero_entries => grid_has_non_zero_entries

```



```

<Grids: sub interfaces>+≡
  pure module function grid_has_non_zero_entries (grid) result (non_zero)
    logical :: non_zero
    class(grid_t), intent(in) :: grid
  end function grid_has_non_zero_entries

<Grids: procedures>+≡
  pure module function grid_has_non_zero_entries (grid) result (non_zero)
    logical :: non_zero
    class(grid_t), intent(in) :: grid
    non_zero = any (abs (grid%values) > zero)
  end function grid_has_non_zero_entries

```

MPI: We allow for several grids in a parallelized run to be combined with `MPI_reduce`. The operator has to be specified. We do not check on any specifications.

```

<MPI: Grids: grid: TBP>≡
  procedure :: mpi_reduce => grid_mpi_reduce

<MPI: Grids: sub interfaces>≡
  module subroutine grid_mpi_reduce (grid, operator)
    class(grid_t), intent(inout) :: grid
    type(MPI_op), intent(in) :: operator
  end subroutine grid_mpi_reduce

<MPI: Grids: procedures>≡
  module subroutine grid_mpi_reduce (grid, operator)
    class(grid_t), intent(inout) :: grid
    type(MPI_op), intent(in) :: operator
    real(default), dimension(size (grid%values)) :: root_values
    integer :: rank
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)
    call MPI_Reduce (grid%values, root_values, size (grid%values), &
      & MPI_DOUBLE_PRECISION, operator, 0, MPI_COMM_WORLD)
    if (rank == 0) then
      grid%values = root_values
    end if
  end subroutine grid_mpi_reduce

```

6.6.4 Input and Output to screen and disk

```

<Grids: grid: TBP>+≡
  procedure :: write => grid_write

<Grids: sub interfaces>+≡
  module subroutine grid_write (grid, unit)
    class(grid_t), intent(in) :: grid
    integer, intent(in), optional :: unit
  end subroutine grid_write

<Grids: procedures>+≡
  module subroutine grid_write (grid, unit)
    class(grid_t), intent(in) :: grid
    integer, intent(in), optional :: unit

```

```

integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(1X,A)") "Grid"
write (u, "(2X,A,2X)", advance='no') "Number of points per dimension:"
if (allocated (grid%points)) then
  do i = 1, size (grid%points)
    write (u, "(I12,1X)", advance='no') &
      grid%points (i)
  end do
end if
write (u, *)
write (u, "(2X,A)") "Values of the grid:"
if (allocated (grid%values)) then
  do i = 1, size (grid%values)
    write (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)") &
      grid%values (i)
  end do
end if
call grid%compute_and_write_mean_and_max (u)
end subroutine grid_write

```

<Grids: grid: TBP>+≡

```

procedure :: compute_and_write_mean_and_max => &
  grid_compute_and_write_mean_and_max

```

<Grids: sub interfaces>+≡

```

module subroutine grid_compute_and_write_mean_and_max (grid, unit)
  class(grid_t), intent(in) :: grid
  integer, intent(in), optional :: unit
end subroutine grid_compute_and_write_mean_and_max

```

<Grids: procedures>+≡

```

module subroutine grid_compute_and_write_mean_and_max (grid, unit)
  class(grid_t), intent(in) :: grid
  integer, intent(in), optional :: unit
  integer :: u, i, n_values
  real(default) :: mean, val, maximum
  u = given_output_unit (unit); if (u < 0) return
  mean = zero
  maximum = zero
  if (allocated (grid%values)) then
    n_values = size (grid%values)
    do i = 1, n_values
      val = grid%values (i)
      mean = mean + val / n_values
      if (val > maximum) then
        maximum = val
      end if
    end do
  end if
  write (msg_buffer, "(A," // FMT_12 // ")") &
    "Grid: Mean value of the grid: ", mean
  call msg_message ()
  write (msg_buffer, "(A," // FMT_12 // ")") &
    "Grid: Max value of the grid: ", maximum
  call msg_message ()

```

```

        if (maximum > zero) then
            write (msg_buffer, "(A," // FMT_12 // ")") &
                "Grid: Mean/Max value of the grid: ", mean / maximum
            call msg_message ()
        end if
    else
        call msg_warning ("Grid: Grid is not allocated!")
    end if
end subroutine grid_compute_and_write_mean_and_max

<Grids: grid: TBP>+≡
    procedure :: save_to_file => grid_save_to_file

<Grids: sub interfaces>+≡
    module subroutine grid_save_to_file (grid, file)
        class(grid_t), intent(in) :: grid
        character(len=*), intent(in) :: file
    end subroutine grid_save_to_file

<Grids: procedures>+≡
    module subroutine grid_save_to_file (grid, file)
        class(grid_t), intent(in) :: grid
        character(len=*), intent(in) :: file
        integer :: iostat, u, i
        u = free_unit ()
        open (file=file, unit=u, action='write')
        if (allocated (grid%points)) then
            write (u, "(I12)") size (grid%points)
            do i = 1, size (grid%points)
                write (u, "(I12,1X)", advance='no', iostat=iostat) &
                    grid%points (i)
            end do
        end if
        write (u, *)
        if (allocated (grid%values)) then
            do i = 1, size (grid%values)
                write (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)", &
                    advance='no', iostat=iostat) grid%values (i)
            end do
        end if
        if (iostat /= 0) then
            call msg_warning &
                ('grid_save_to_file: Could not save grid to file')
        end if
        close (u)
    end subroutine grid_save_to_file

<Grids: parameters>+≡
    character(len=*), parameter :: DEFAULT_OUTPUT_PRECISION = FMT_16

<Grids: public>+≡
    public :: verify_points_for_grid

```

```

<Grids: sub interfaces>+≡
    module function verify_points_for_grid (file, points) result (valid)
        logical :: valid
        character(len=*), intent(in) :: file
        integer, dimension(:), intent(in) :: points
    end function verify_points_for_grid

<Grids: procedures>+≡
    module function verify_points_for_grid (file, points) result (valid)
        logical :: valid
        character(len=*), intent(in) :: file
        integer, dimension(:), intent(in) :: points
        integer, dimension(:), allocatable :: points_from_file
        integer :: u
        call load_points_from_file (file, u, points_from_file)
        close (u)
        if (allocated (points_from_file)) then
            valid = all (points == points_from_file)
        else
            valid = .false.
        end if
    end function verify_points_for_grid

```

Returns the `unit` that has opened the input file and read the first two lines. The caller has to close it. Furthermore, we return `points` containing the number of points in each dimension.

```

<Grids: procedures>+≡
    subroutine load_points_from_file (file, unit, points)
        character(len=*), intent(in) :: file
        integer, intent(out) :: unit
        integer, dimension(:), allocatable :: points
        integer :: iostat, n_dimensions, i_dim
        unit = free_unit ()
        open (file=file, unit=unit, action='read', iostat=iostat)
        if (iostat /= 0) return
        read (unit, "(I12)", iostat=iostat) n_dimensions
        if (iostat /= 0) return
        allocate (points (n_dimensions))
        do i_dim = 1, size (points)
            read (unit, "(I12,1X)", advance='no', iostat=iostat) &
                points (i_dim)
        end do
        if (iostat /= 0) return
        read (unit, *)
        if (iostat /= 0) return
    end subroutine load_points_from_file

```

```

<Grids: grid: TBP>+≡
    procedure :: load_from_file => grid_load_from_file

```

```

<Grids: sub interfaces>+≡
    module subroutine grid_load_from_file (grid, file)
        class(grid_t), intent(out) :: grid
        character(len=*), intent(in) :: file
    end subroutine grid_load_from_file

```

```

        end subroutine grid_load_from_file
    <Grids: procedures>+≡
    module subroutine grid_load_from_file (grid, file)
        class(grid_t), intent(out) :: grid
        character(len=*), intent(in) :: file
        integer :: iostat, u, i
        integer, dimension(:), allocatable :: points
        call load_points_from_file (file, u, points)
        if (.not. allocated (points)) return
        call grid%init (points)
        do i = 1, size (grid%values)
            read (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)", advance='no', iostat=iostat) &
                grid%values (i)
        end do
        if (iostat /= 0) then
            call msg_warning ('grid_load_from_file: Could not load grid from file')
        end if
        close (u)
    end subroutine grid_load_from_file

```

6.6.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<grids_ut.f90>≡
    <File header>

    module grids_ut
        use unit_tests
        use grids_uti

    <Standard module head>

    <Grids: public test>

    contains

    <Grids: test driver>

    end module grids_ut
<grids_uti.f90>≡
    <File header>

    module grids_uti

    <Use kinds>
        use constants, only: zero, one, two, three, four, tiny_07
        use file_utils, only: delete_file
        use numeric_utils

        use grids

```

```

    <Standard module head>

    <Grids: test declarations>

contains

    <Grids: tests>

end module grids_util

API: driver for the unit tests below.
<Grids: public test>≡
    public :: grids_test
<Grids: test driver>≡
    subroutine grids_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Grids: execute tests>
end subroutine grids_test

```

Test Index Function

```

<Grids: execute tests>≡
    call test(grids_1, "grids_1", &
        "Test Index Function", u, results)
<Grids: test declarations>≡
    public :: grids_1
<Grids: tests>≡
    subroutine grids_1 (u)
        integer, intent(in) :: u
        type(grid_t) :: grid
        write (u, "(A)")  "* Test output: grids_1"
        write (u, "(A)")  "* Purpose: Test Index Function"
        write (u, "(A)")

        call grid%init ([3])
        call grid%write(u)
        call assert (u, grid%get_index([1]) == 1, "grid%get_index(1) == 1")
        call assert (u, grid%get_index([2]) == 2, "grid%get_index(2) == 2")
        call assert (u, grid%get_index([3]) == 3, "grid%get_index(3) == 3")
        call grid%final ()

        call grid%init ([3,3])
        call grid%write(u)
        call assert (u, grid%get_index([1,1]) == 1, "grid%get_index(1,1) == 1")
        call assert (u, grid%get_index([2,1]) == 2, "grid%get_index(2,1) == 2")
        call assert (u, grid%get_index([3,1]) == 3, "grid%get_index(3,1) == 3")
        call assert (u, grid%get_index([1,2]) == 4, "grid%get_index(1,2) == 4")
        call assert (u, grid%get_index([2,2]) == 5, "grid%get_index(2,2) == 5")
        call assert (u, grid%get_index([3,2]) == 6, "grid%get_index(3,2) == 6")
        call assert (u, grid%get_index([1,3]) == 7, "grid%get_index(1,3) == 7")
        call assert (u, grid%get_index([2,3]) == 8, "grid%get_index(2,3) == 8")
    end subroutine grids_1

```

```

call assert (u, grid%get_index([3,3]) == 9, "grid%get_index(3,3) == 9")
call grid%final ()

call grid%init ([3,3,2])
call grid%write(u)
call assert (u, grid%get_index([1,1,1]) == 1, "grid%get_index(1,1,1) == 1")
call assert (u, grid%get_index([2,1,2]) == 2+9, "grid%get_index(2,1,2) == 2+9")
call assert (u, grid%get_index([3,3,1]) == 9, "grid%get_index(3,3,1) == 3")
call assert (u, grid%get_index([3,1,2]) == 3+9, "grid%get_index(3,1,2) == 4+9")
call assert (u, grid%get_index([2,2,1]) == 5, "grid%get_index(2,2,1) == 5")
call assert (u, grid%get_index([3,2,2]) == 6+9, "grid%get_index(3,2,2) == 6+9")
call assert (u, grid%get_index([1,3,1]) == 7, "grid%get_index(1,3,1) == 7")
call assert (u, grid%get_index([2,3,2]) == 8+9, "grid%get_index(2,3,2) == 8+9")
call assert (u, grid%get_index([3,3,2]) == 9+9, "grid%get_index(3,3,2) == 9+9")
call grid%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: grids_1"
end subroutine grids_1

```

Saving and Loading

```

<Grids: execute tests>+≡
  call test(grids_2, "grids_2", &
    "Saving and Loading", u, results)

<Grids: test declarations>+≡
  public :: grids_2

<Grids: tests>+≡
  subroutine grids_2 (u)
    integer, intent(in) :: u
    type(grid_t) :: grid
    write (u, "(A)")  "* Test output: grids_2"
    write (u, "(A)")  "* Purpose: Saving and Loading"
    write (u, "(A)")

    call grid%init ([3])
    call grid%set_values ([one, two, three])
    call grid%save_to_file ('grids_2_test')
    call grid%final ()

    call assert (u, verify_points_for_grid('grids_2_test', [3]), &
      "verify_points_for_grid")
    call grid%load_from_file ('grids_2_test')
    call grid%write (u)
    call assert (u, nearly_equal (grid%get_value([1]), one), "grid%get_value(1) == 1")
    call assert (u, nearly_equal (grid%get_value([2]), two), "grid%get_value(2) == 2")
    call assert (u, nearly_equal (grid%get_value([3]), three), "grid%get_value(3) == 3")
    call grid%final ()

    call grid%init ([3,3])
    call grid%set_values ([one, two, three, four, zero, zero, zero, zero, zero])
    call grid%save_to_file ('grids_2_test')

```

```

call grid%final ()

call assert (u, verify_points_for_grid('grids_2_test', [3,3]), &
    "verify_points_for_grid")
call grid%load_from_file ('grids_2_test')
call grid%write (u)
call assert (u, nearly_equal (grid%get_value([1,1]), one),    "grid%get_value(1,1) == 1")
call assert (u, nearly_equal (grid%get_value([2,1]), two),    "grid%get_value(2,1) == 2")
call assert (u, nearly_equal (grid%get_value([3,1]), three),  "grid%get_value(3,1) == 3")
call assert (u, nearly_equal (grid%get_value([1,2]), four),   "grid%get_value(1,2) == 4")
call delete_file ('grids_2_test')

call grid%load_from_file ('grids_2_test')
call assert (u, .not. verify_points_for_grid('grids_2_test', [3,3]), &
    "verify_points_for_grid")
call grid%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: grids_2"
end subroutine grids_2

```

Get Segments

```

<Grids: execute tests>+≡
    call test(grids_3, "grids_3", &
        "Get Segments", u, results)

<Grids: test declarations>+≡
    public :: grids_3

<Grids: tests>+≡
    subroutine grids_3 (u)
        integer, intent(in) :: u
        type(grid_t) :: grid
        integer, dimension(2) :: fail
        write (u, "(A)")  "* Test output: grids_3"
        write (u, "(A)")  "* Purpose: Get Segments"
        write (u, "(A)")

        call grid%init ([3])
        call assert (u, all(grid%get_segment([0.00_default]) == [1]), &
            "all(grid%get_segment([0.00_default]) == [1])")
        call assert (u, all(grid%get_segment([0.32_default]) == [1]), &
            "all(grid%get_segment([0.32_default]) == [1])")
        call assert (u, all(grid%get_segment([0.52_default]) == [2]), &
            "all(grid%get_segment([0.52_default]) == [2])")
        call assert (u, all(grid%get_segment([1.00_default]) == [3]), &
            "all(grid%get_segment([1.00_default]) == [3])")
        call grid%final ()

        call grid%init ([3,3])
        call assert (u, all(grid%get_segment([0.00_default,0.00_default]) == [1,1]), &
            "all(grid%get_segment([0.00_default,0.00_default]) == [1,1])")
        call assert (u, all(grid%get_segment([0.32_default,0.32_default]) == [1,1]), &

```



```

        "all(grid%get_segment([0.32_default,0.32_default]) == [1,1])")
    call assert (u, all(grid%get_segment([0.52_default,0.52_default]) == [2,2]), &
        "all(grid%get_segment([0.52_default,0.52_default]) == [2,2])")
    call assert (u, all(grid%get_segment([1.00_default,1.00_default]) == [3,3]), &
        "all(grid%get_segment([1.00_default,1.00_default]) == [3,3])")
    write (u, "(A)")  "* A double error is expected"
    fail = grid%get_segment([1.10_default,1.10_default], u)
    call grid%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: grids_3"
end subroutine grids_3

```

Update Maxima

```

<Grids: execute tests>+≡
    call test(grids_4, "grids_4", &
        "Update Maxima", u, results)

<Grids: test declarations>+≡
    public :: grids_4

<Grids: tests>+≡
    subroutine grids_4 (u)
        integer, intent(in) :: u
        type(grid_t) :: grid
        write (u, "(A)")  "* Test output: grids_4"
        write (u, "(A)")  "* Purpose: Update Maxima"
        write (u, "(A)")

        call grid%init ([4,4])
        call grid%update_maxima ([0.1_default, 0.0_default], 0.3_default)
        call grid%update_maxima ([0.9_default, 0.95_default], 1.7_default)
        call grid%write (u)
        call assert_equal (u, grid%get_value([1,1]), 0.3_default, &
            "grid%get_value([1,1])")
        call assert_equal (u, grid%get_value([2,2]), 0.0_default, &
            "grid%get_value([2,2])")
        call assert_equal (u, grid%get_value([4,4]), 1.7_default, &
            "grid%get_value([4,4])")

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: grids_4"
    end subroutine grids_4

```

Finding and checking

```

<Grids: execute tests>+≡
    call test(grids_5, "grids_5", &
        "Finding and checking", u, results)

<Grids: test declarations>+≡
    public :: grids_5

```

```

<Grids: tests>+≡
subroutine grids_5 (u)
  integer, intent(in) :: u
  type(grid_t) :: grid
  real(default) :: first, second
  write (u, "(A)")  "* Test output: grids_5"
  write (u, "(A)")  "* Purpose: Finding and checking"
  write (u, "(A)")

  call grid%init ([2,2,2])
  first = one / two - tiny_07
  second = two / two - tiny_07
  call grid%update_maxima ([0.1_default, 0.0_default, first], 0.3_default)
  call grid%update_maxima ([0.9_default, 0.95_default, second], 1.7_default)
  call grid%write (u)
  call assert (u, .not. grid%is_non_zero_everywhere (), &
    ".not. grid%is_non_zero_everywhere (")
  call assert_equal (u, grid%get_maximum_in_3d (1), 0.3_default, &
    "grid%get_maximum_in_3d (1)")
  call assert_equal (u, grid%get_maximum_in_3d (2), 1.7_default, &
    "grid%get_maximum_in_3d (2)")

  call grid%update_maxima ([0.9_default, 0.95_default, first], 1.8_default)
  call grid%update_maxima ([0.1_default, 0.95_default, first], 1.5_default)
  call grid%update_maxima ([0.9_default, 0.15_default, first], 1.5_default)
  call grid%update_maxima ([0.1_default, 0.0_default, second], 0.2_default)
  call grid%update_maxima ([0.1_default, 0.9_default, second], 0.2_default)
  call grid%update_maxima ([0.9_default, 0.0_default, second], 0.2_default)
  call grid%write (u)
  call assert (u, grid%is_non_zero_everywhere (), &
    "grid%is_non_zero_everywhere (")
  call assert_equal (u, grid%get_maximum_in_3d (1), 1.8_default, &
    "grid%get_maximum_in_3d (1)")
  call assert_equal (u, grid%get_maximum_in_3d (2), 1.7_default, &
    "grid%get_maximum_in_3d (2)")

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: grids_5"
end subroutine grids_5

```

One could think of multiple implementations of a generic type.

```

<solver.f90>≡
<File header>

module solver

  <Use kinds>
  use constants, only: tiny_10

  <Standard module head>

  <Solver: public>

```

```

    <Solver: parameters>

    <Solver: types>

    <Solver: interfaces>

    interface
    <Solver: sub interfaces>
    end interface

    end module solver

    <solver_sub.f90>≡
    <File header>

    submodule (solver) solver_s

        use numeric_utils
        use diagnostics

        implicit none

    contains

    <Solver: procedures>

    end submodule solver_s

    <Solver: public>≡
    public :: solver_function_t

    <Solver: types>≡
    type, abstract :: solver_function_t
    contains
        procedure(solver_function_evaluate), deferred :: evaluate
    end type solver_function_t

    <Solver: interfaces>≡
    abstract interface
        function solver_function_evaluate (solver_f, x) result (f)
            import
            complex(default) :: f
            class(solver_function_t), intent(in) :: solver_f
            real(default), intent(in) :: x
        end function
    end interface

    <Solver: public>+≡
    public :: solve_secant

    <Solver: sub interfaces>≡
    module function solve_secant &
        (func, lower_start, upper_start, success, precision) result (x0)
        class(solver_function_t), intent(in) :: func

```

```

        real(default) :: x0
        real(default), intent(in) :: lower_start, upper_start
        real(default), intent(in), optional :: precision
        logical, intent(out) :: success
    end function solve_secant

<Solver: procedures>≡
    module function solve_secant &
        (func, lower_start, upper_start, success, precision) result (x0)
        class(solver_function_t), intent(in) :: func
        real(default) :: x0
        real(default), intent(in) :: lower_start, upper_start
        real(default), intent(in), optional :: precision
        logical, intent(out) :: success
        real(default) :: desired, x_curr, x_next, f_curr, f_next, x_new
        integer :: n_iter
        desired = DEFAULT_PRECISION; if (present(precision)) desired = precision
        x_curr = lower_start
        x_next = upper_start
        n_iter = 0
        success = .false.
        SEARCH: do
            n_iter = n_iter + 1
            f_curr = real( func%evaluate (x_curr) )
            f_next = real( func%evaluate (x_next) )
            <Exit if close to zero and handle exceptions>
            x_new = x_next - (x_next - x_curr) / (f_next - f_curr) * f_next
            x_curr = x_next
            x_next = x_new
        end do SEARCH
        if (x0 < lower_start .or. x0 > upper_start) then
            call msg_warning ("solve: The root of the function is not in boundaries")
            return
        end if
        success = .true.
    end function solve_secant

<Exit if close to zero and handle exceptions>≡
    if (abs (f_next) < desired) then
        x0 = x_next
        exit
    end if
    if (n_iter > MAX_TRIES) then
        call msg_warning ("solve: Couldn't find root of function")
        return
    end if
    if (vanishes (f_next - f_curr)) then
        x_next = x_next + (x_next - x_curr) / 10
        cycle
    end if

```

Implements the bisection root-finding method to find a root of `func` between `lower_start` and `upper_start` with tolerance `precision`.

<Solver: public>+≡

```

public :: solve_interval

(Solver: sub interfaces)+≡
  module function solve_interval &
    (func, lower_start, upper_start, success, precision) result (x0)
    class(solver_function_t), intent(in) :: func
    real(default) :: x0
    real(default), intent(in) :: lower_start, upper_start
    real(default), intent(in), optional :: precision
    logical, intent(out) :: success
  end function solve_interval

(Solver: procedures)+≡
  module function solve_interval &
    (func, lower_start, upper_start, success, precision) result (x0)
    class(solver_function_t), intent(in) :: func
    real(default) :: x0
    real(default), intent(in) :: lower_start, upper_start
    real(default), intent(in), optional :: precision
    logical, intent(out) :: success
    real(default) :: desired
    real(default) :: x_low, x_high, x_half
    real(default) :: f_low, f_high, f_half
    integer :: n_iter
    success = .false.
    desired = DEFAULT_PRECISION; if (present(precision)) desired = precision
    x0 = lower_start
    x_low = lower_start
    x_high = upper_start
    f_low = real( func%evaluate (x_low) )
    f_high = real( func%evaluate (x_high) )
    if (f_low * f_high > 0) return
    if (x_low > x_high) then
      call display_solver_status()
      call msg_fatal ("Interval solver: Upper bound must be &
        &greater than lower bound")
    end if
    n_iter = 0
    do n_iter = 1, MAX_TRIES
      x_half = (x_high + x_low)/2
      f_half = real( func%evaluate (x_half) )
      if (abs (f_half) <= desired) then
        x0 = x_half
        exit
      end if
      if (f_low * f_half > 0._default) then
        x_low = x_half
        f_low = f_half
      else
        x_high = x_half
        f_high = f_half
      end if
    end do
    if (x0 < lower_start .or. x0 > upper_start) then
      call msg_warning ("Interval solver: The root of the function&

```

```

                                & is out of boundaries")

    return
end if
success = .true.
contains
subroutine display_solver_status ()
    print *, '=====
    print *, 'Status of interval solver: '
    print *, 'initial values: ', lower_start, upper_start
    print *, 'iteration: ', n_iter
    print *, 'x_low: ', x_low, 'f_low: ', f_low
    print *, 'x_high: ', x_high, 'f_high: ', f_high
    print *, 'x_half: ', x_half, 'f_half: ', f_half
end subroutine display_solver_status
end function solve_interval

<Solver: public>+≡
public :: solve_qgaus

<Solver: sub interfaces>+≡
module function solve_qgaus (integrand, grid) result (integral)
    class(solver_function_t), intent(in) :: integrand
    complex(default) :: integral
    real(default), dimension(:), intent(in) :: grid
end function solve_qgaus

<Solver: procedures>+≡
module function solve_qgaus (integrand, grid) result (integral)
    class(solver_function_t), intent(in) :: integrand
    complex(default) :: integral
    real(default), dimension(:), intent(in) :: grid
    integer :: i, j
    real(default) :: xm, xr
    real(default), dimension(5) :: dx, &
        w = (/ 0.2955242247_default, 0.2692667193_default, &
            0.2190863625_default, 0.1494513491_default, 0.0666713443_default /), &
        x = (/ 0.1488743389_default, 0.4333953941_default, 0.6794095682_default, &
            0.8650633666_default, 0.9739065285_default /)
    integral = 0.0_default
    if ( size(grid) < 2 ) then
        call msg_warning ("solve_qgaus: size of integration grid smaller than 2.")
        return
    end if
    do i=1, size(grid)-1
        xm = 0.5_default * ( grid(i+1) + grid(i) )
        xr = 0.5_default * ( grid(i+1) - grid(i) )
        do j=1, 5
            dx(j) = xr * x(j)
            integral = integral + xr * w(j) * &
                ( integrand%evaluate (xm+dx(j)) + integrand%evaluate (xm-dx(j)) )
        end do
    end do
end function solve_qgaus

```

```

⟨Solver: parameters⟩≡
    real(default), parameter, public :: DEFAULT_PRECISION = tiny_10

⟨Solver: parameters⟩+≡
    integer, parameter :: MAX_TRIES = 10000

```

6.6.6 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨solver_ut.f90⟩≡
    ⟨File header⟩

    module solver_ut
        use unit_tests
        use solver_util

    ⟨Standard module head⟩

    ⟨Solver: public test⟩

    contains

    ⟨Solver: test driver⟩

    end module solver_ut

⟨solver_util.f90⟩≡
    ⟨File header⟩

    module solver_util

    ⟨Use kinds⟩
        use constants, only: zero, one, two
        use numeric_utils

        use solver

    ⟨Standard module head⟩

    ⟨Solver: test declarations⟩

    ⟨Solver: test types⟩

    contains

    ⟨Solver: tests⟩

    ⟨Solver: test auxiliary⟩

    end module solver_util

```

API: driver for the unit tests below.

```

⟨Solver: public test⟩≡
    public :: solver_test

```

```

<Solver: test driver>≡
  subroutine solver_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Solver: execute tests>
  end subroutine solver_test

```

Test functions

```

<Solver: test types>≡
  type, extends (solver_function_t) :: test_function_1_t
  contains
    procedure :: evaluate => test_func_1
  end type test_function_1_t

```

```

<Solver: test types>+≡
  type, extends (solver_function_t) :: test_function_2_t
  contains
    procedure :: evaluate => test_func_2
  end type test_function_2_t

```

```

<Solver: test types>+≡
  type, extends (solver_function_t) :: test_function_3_t
  contains
    procedure :: evaluate => test_func_3
  end type test_function_3_t

```

```

<Solver: test types>+≡
  type, extends (solver_function_t) :: test_function_4_t
  contains
    procedure :: evaluate => test_func_4
  end type test_function_4_t

```

```

<Solver: test auxiliary>≡
  function test_func_1 (solver_f, x) result (f)
    complex(default) :: f
    class(test_function_1_t), intent(in) :: solver_f
    real(default), intent(in) :: x
    f = x
  end function test_func_1

  function test_func_2 (solver_f, x) result (f)
    complex(default) :: f
    class(test_function_2_t), intent(in) :: solver_f
    real(default), intent(in) :: x
    f = x ** 2
  end function test_func_2

  function test_func_3 (solver_f, x) result (f)
    complex(default) :: f
    class(test_function_3_t), intent(in) :: solver_f

```



```

    real(default), intent(in) :: x
    f = x ** 3
end function test_func_3

function test_func_4 (solver_f, x) result (f)
    complex(default) :: f
    class(test_function_4_t), intent(in) :: solver_f
    real(default), intent(in) :: x
    real(default) :: s, cutoff
    s = 100.0_default
    cutoff = 1.01_default
    if (x < cutoff) then
        f = - (log (s) * log (log (s) / log(cutoff**2)) - log (s / cutoff**2)) - &
            log (one/two)
    else
        f = - (log (s) * log (log (s) / log(x**2)) - log (s / x**2)) - &
            log (one/two)
    end if
end function test_func_4

```

Solve trivial functions

```

<Solver: execute tests>≡
    call test(solver_1, "solver_1", &
        "Solve trivial functions", u, results)

<Solver: test declarations>≡
    public :: solver_1

<Solver: tests>≡
    subroutine solver_1 (u)
        integer, intent(in) :: u
        real(default) :: zero_position
        logical :: success
        type(test_function_1_t) :: test_func_1
        type(test_function_2_t) :: test_func_2
        type(test_function_3_t) :: test_func_3
        type(test_function_4_t) :: test_func_4
        write (u, "(A)")  "* Test output: solver_1"
        write (u, "(A)")  "* Purpose: Solve trivial functions"
        write (u, "(A)")

        zero_position = solve_interval (test_func_1, -one, one, success)
        call assert (u, success, "success")
        call assert_equal (u, zero_position, zero, "test_func_1: zero_position")

        zero_position = solve_interval (test_func_4, two, 10.0_default, success)
        call assert (u, success, "success")
        call assert_equal (u, zero_position, &
            3.5216674011865940283397224_default, &
            "test_func_4: zero_position", rel_smallness=1000*DEFAULT_PRECISION)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: solver_1"
    end subroutine solver_1

```

```
end subroutine solver_1
```

Chapter 7

Text handling

WHIZARD has to handle complex structures in input (and output) data. Doing this in a generic and transparent way requires a generic lexer and parser. The necessary modules are implemented here:

ifiles Implementation of line-oriented internal files in a more flexible way (linked lists of variable-length strings) than the Fortran builtin features.

lexers Read text and transform it into a token stream.

syntax_rules Define the rules for interpreting tokens, to be used by the WHIZARD parser.

parser Categorize tokens (keyword, string, number etc.) and use a set of syntax rules to transform the input into a parse tree.

xml Read and parse XML text, separate from the WHIZARD parser.

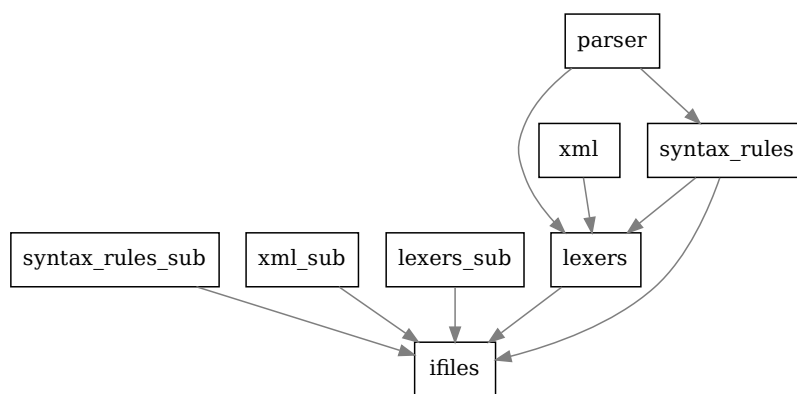


Figure 7.1: Module dependencies in `src/parsing`.

7.1 Internal files

The internal files introduced here (`ifile`) are a replacement for the built-in internal files, which are fixed-size arrays of fixed-length character strings. The `ifile` type is a doubly-linked list of variable-length character strings with line numbers.

```
<ifiles.f90>≡  
  <File header>  
  
  module ifiles  
  
    <Use strings>  
  
    <Standard module head>  
  
    <Ifiles: public>  
  
    <Ifiles: types>  
  
    <Ifiles: interfaces>  
  
    interface  
    <Ifiles: sub interfaces>  
    end interface  
  
  end module ifiles  
<ifiles_sub.f90>≡  
  <File header>  
  
  submodule (ifiles) ifiles_s  
  
    use system_defs, only: EOF  
    use io_units  
  
    implicit none  
  
  contains  
  
    <Ifiles: procedures>  
  
  end submodule ifiles_s
```

7.1.1 The line type

The line entry type is for internal use, it is the list entry to be collected in an `ifile` object.

```
<Ifiles: types>≡  
  type :: line_entry_t  
  private  
  type(line_entry_t), pointer :: previous => null ()  
  type(line_entry_t), pointer :: next => null ()
```

```

        type(string_t) :: string
        integer :: index
    end type line_entry_t

```

Create a new list entry, given a varying string as input. The line number and pointers are not set, these make sense only within an ifile.

```

<Ifiles: procedures>≡
    subroutine line_entry_create (line, string)
        type(line_entry_t), pointer :: line
        type(string_t), intent(in) :: string
        allocate (line)
        line%string = string
    end subroutine line_entry_create

```

Destroy a single list entry: Since the pointer components should not be deallocated explicitly, just deallocate the object itself.

```

<Ifiles: procedures>+≡
    subroutine line_entry_destroy (line)
        type(line_entry_t), pointer :: line
        deallocate (line)
    end subroutine line_entry_destroy

```

7.1.2 The ifile type

The internal file is a linked list of line entries.

```

<Ifiles: public>≡
    public :: ifile_t

<Ifiles: types>+≡
    type :: ifile_t
    private
        type(line_entry_t), pointer :: first => null ()
        type(line_entry_t), pointer :: last => null ()
        integer :: n_lines = 0
    contains
        <Ifiles: ifile: TBP>
    end type ifile_t

```

We need no explicit initializer, but a routine which recursively deallocates the contents may be appropriate. After this, existing line pointers may become undefined, so they should be nullified before the file is destroyed.

```

<Ifiles: public>+≡
    public :: ifile_clear

<Ifiles: sub interfaces>≡
    module subroutine ifile_clear (ifile)
        class(ifile_t), intent(inout) :: ifile
    end subroutine ifile_clear

```

```

<Ifiles: procedures>+=
  module subroutine ifile_clear (ifile)
    class(ifile_t), intent(inout) :: ifile
    type(line_entry_t), pointer :: current
    do while (associated (ifile%first))
      current => ifile%first
      ifile%first => current%next
      call line_entry_destroy (current)
    end do
    nullify (ifile%last)
    ifile%n_lines = 0
  end subroutine ifile_clear

```

The finalizer is just an alias for the above.

```

<Ifiles: public>+=
  public :: ifile_final

<Ifiles: ifile: TBP>=
  procedure :: final => ifile_clear

<Ifiles: interfaces>=
  interface ifile_final
    module procedure ifile_clear
  end interface

```

7.1.3 I/O on ifiles

Fill an ifile from an ordinary external file, i.e., I/O unit. If the ifile is not empty, the old contents will be destroyed. We can read a fixed-length character string, an ISO varying string, an ordinary internal file (character-string array), or from an external unit. In the latter case, lines are appended until EOF is reached. Finally, there is a variant which reads from another ifile, effectively copying it.

```

<Ifiles: public>+=
  public :: ifile_read

<Ifiles: interfaces>+=
  interface ifile_read
    module procedure ifile_read_from_string
    module procedure ifile_read_from_char
    module procedure ifile_read_from_unit
    module procedure ifile_read_from_char_array
    module procedure ifile_read_from_ifile
  end interface

<Ifiles: sub interfaces>+=
  module subroutine ifile_read_from_string (ifile, string)
    type(ifile_t), intent(inout) :: ifile
    type(string_t), intent(in) :: string
  end subroutine ifile_read_from_string
  module subroutine ifile_read_from_char (ifile, char)
    type(ifile_t), intent(inout) :: ifile
    character(*), intent(in) :: char
  end subroutine ifile_read_from_char
  module subroutine ifile_read_from_char_array (ifile, char)

```

```

        type(ifile_t), intent(inout) :: ifile
        character(*), dimension(:), intent(in) :: char
    end subroutine ifile_read_from_char_array
    module subroutine ifile_read_from_unit (ifile, unit, iostat)
        type(ifile_t), intent(inout) :: ifile
        integer, intent(in) :: unit
        integer, intent(out), optional :: iostat
    end subroutine ifile_read_from_unit
    module subroutine ifile_read_from_ifile (ifile, ifile_in)
        type(ifile_t), intent(inout) :: ifile
        type(ifile_t), intent(in) :: ifile_in
    end subroutine ifile_read_from_ifile
<Ifiles: procedures>+=
    module subroutine ifile_read_from_string (ifile, string)
        type(ifile_t), intent(inout) :: ifile
        type(string_t), intent(in) :: string
        call ifile_clear (ifile)
        call ifile_append (ifile, string)
    end subroutine ifile_read_from_string

    module subroutine ifile_read_from_char (ifile, char)
        type(ifile_t), intent(inout) :: ifile
        character(*), intent(in) :: char
        call ifile_clear (ifile)
        call ifile_append (ifile, char)
    end subroutine ifile_read_from_char

    module subroutine ifile_read_from_char_array (ifile, char)
        type(ifile_t), intent(inout) :: ifile
        character(*), dimension(:), intent(in) :: char
        call ifile_clear (ifile)
        call ifile_append (ifile, char)
    end subroutine ifile_read_from_char_array

    module subroutine ifile_read_from_unit (ifile, unit, iostat)
        type(ifile_t), intent(inout) :: ifile
        integer, intent(in) :: unit
        integer, intent(out), optional :: iostat
        call ifile_clear (ifile)
        call ifile_append (ifile, unit, iostat)
    end subroutine ifile_read_from_unit

    module subroutine ifile_read_from_ifile (ifile, ifile_in)
        type(ifile_t), intent(inout) :: ifile
        type(ifile_t), intent(in) :: ifile_in
        call ifile_clear (ifile)
        call ifile_append (ifile, ifile_in)
    end subroutine ifile_read_from_ifile

```

Append to an ifile. The same as reading, but without resetting the ifile. In addition, there is a routine for appending a whole ifile.

```

<Ifiles: public>+=
    public :: ifile_append

```



```

<Ifiles: ifile: TBP>+=
    generic :: append => &
        ifile_append_from_char
    procedure, private :: ifile_append_from_char

<Ifiles: interfaces>+=
    interface ifile_append
        module procedure ifile_append_from_string
        module procedure ifile_append_from_char
        module procedure ifile_append_from_unit
        module procedure ifile_append_from_char_array
        module procedure ifile_append_from_ifile
    end interface

<Ifiles: sub interfaces>+=
    module subroutine ifile_append_from_string (ifile, string)
        class(ifile_t), intent(inout) :: ifile
        type(string_t), intent(in) :: string
    end subroutine ifile_append_from_string
    module subroutine ifile_append_from_char (ifile, char)
        class(ifile_t), intent(inout) :: ifile
        character(*), intent(in) :: char
    end subroutine ifile_append_from_char
    module subroutine ifile_append_from_char_array (ifile, char)
        class(ifile_t), intent(inout) :: ifile
        character(*), dimension(:), intent(in) :: char
    end subroutine ifile_append_from_char_array
    module subroutine ifile_append_from_ifile (ifile, ifile_in)
        class(ifile_t), intent(inout) :: ifile
        type(ifile_t), intent(in) :: ifile_in
    end subroutine ifile_append_from_ifile
    module subroutine ifile_append_from_unit (ifile, unit, iostat)
        class(ifile_t), intent(inout) :: ifile
        integer, intent(in) :: unit
        integer, intent(out), optional :: iostat
    end subroutine ifile_append_from_unit

<Ifiles: procedures>+=
    module subroutine ifile_append_from_string (ifile, string)
        class(ifile_t), intent(inout) :: ifile
        type(string_t), intent(in) :: string
        type(line_entry_t), pointer :: current
        call line_entry_create (current, string)
        current%index = ifile%n_lines + 1
        if (associated (ifile%last)) then
            current%previous => ifile%last
            ifile%last%next => current
        else
            ifile%first => current
        end if
        ifile%last => current
        ifile%n_lines = current%index
    end subroutine ifile_append_from_string

    module subroutine ifile_append_from_char (ifile, char)
        class(ifile_t), intent(inout) :: ifile

```

```

character(*), intent(in) :: char
call ifile_append_from_string (ifile, var_str (trim (char)))
end subroutine ifile_append_from_char

module subroutine ifile_append_from_char_array (ifile, char)
class(ifile_t), intent(inout) :: ifile
character(*), dimension(:), intent(in) :: char
integer :: i
do i = 1, size (char)
    call ifile_append_from_string (ifile, var_str (trim (char(i))))
end do
end subroutine ifile_append_from_char_array

module subroutine ifile_append_from_unit (ifile, unit, iostat)
class(ifile_t), intent(inout) :: ifile
integer, intent(in) :: unit
integer, intent(out), optional :: iostat
type(string_t) :: buffer
integer :: ios
ios = 0
READ_LOOP: do
    call get (unit, buffer, iostat = ios)
    if (ios == EOF .or. ios > 0) exit READ_LOOP
    call ifile_append_from_string (ifile, buffer)
end do READ_LOOP
if (present (iostat)) then
    iostat = ios
else if (ios > 0) then
    call get (unit, buffer) ! trigger error again
end if
end subroutine ifile_append_from_unit

module subroutine ifile_append_from_ifile (ifile, ifile_in)
class(ifile_t), intent(inout) :: ifile
type(ifile_t), intent(in) :: ifile_in
type(line_entry_t), pointer :: current
current => ifile_in%first
do while (associated (current))
    call ifile_append_from_string (ifile, current%string)
    current => current%next
end do
end subroutine ifile_append_from_ifile

```

Write the ifile contents to an external unit

```

<Ifiles: public>+≡
    public :: ifile_write

<Ifiles: sub interfaces>+≡
    module subroutine ifile_write (ifile, unit, iostat)
        type(ifile_t), intent(in) :: ifile
        integer, intent(in), optional :: unit
        integer, intent(out), optional :: iostat
    end subroutine ifile_write

<Ifiles: procedures>+≡

```

```

module subroutine ifile_write (ifile, unit, iostat)
  type(ifile_t), intent(in) :: ifile
  integer, intent(in), optional :: unit
  integer, intent(out), optional :: iostat
  integer :: u
  type(line_entry_t), pointer :: current
  u = given_output_unit (unit); if (u < 0) return
  current => ifile%first
  do while (associated (current))
    call put_line (u, current%string, iostat)
    current => current%next
  end do
end subroutine ifile_write

```

Convert the ifile to an array of strings, which is allocated by this function:

<Ifiles: public>+≡

```
public :: ifile_to_string_array
```

<Ifiles: sub interfaces>+≡

```

module subroutine ifile_to_string_array (ifile, string)
  type(ifile_t), intent(in) :: ifile
  type(string_t), dimension(:), intent(inout), allocatable :: string
end subroutine ifile_to_string_array

```

<Ifiles: procedures>+≡

```

module subroutine ifile_to_string_array (ifile, string)
  type(ifile_t), intent(in) :: ifile
  type(string_t), dimension(:), intent(inout), allocatable :: string
  type(line_entry_t), pointer :: current
  integer :: i
  allocate (string (ifile_get_length (ifile)))
  current => ifile%first
  do i = 1, ifile_get_length (ifile)
    string(i) = current%string
    current => current%next
  end do
end subroutine ifile_to_string_array

```

7.1.4 Ifile tools

<Ifiles: public>+≡

```
public :: ifile_get_length
```

<Ifiles: sub interfaces>+≡

```

module function ifile_get_length (ifile) result (length)
  integer :: length
  type(ifile_t), intent(in) :: ifile
end function ifile_get_length

```

<Ifiles: procedures>+≡

```

module function ifile_get_length (ifile) result (length)
  integer :: length
  type(ifile_t), intent(in) :: ifile
  length = ifile%n_lines

```

```
end function ifile_get_length
```

7.1.5 Line pointers

Instead of the implicit pointer used in ordinary file access, we define explicit pointers, so there can be more than one at a time.

```
<Ifiles: public>+≡
    public :: line_p

<Ifiles: types>+≡
    type :: line_p
        private
            type(line_entry_t), pointer :: p => null ()
    end type line_p
```

Assign a file pointer to the first or last line in an ifile:

```
<Ifiles: public>+≡
    public :: line_init

<Ifiles: sub interfaces>+≡
    module subroutine line_init (line, ifile, back)
        type(line_p), intent(inout) :: line
        type(ifile_t), intent(in) :: ifile
        logical, intent(in), optional :: back
    end subroutine line_init

<Ifiles: procedures>+≡
    module subroutine line_init (line, ifile, back)
        type(line_p), intent(inout) :: line
        type(ifile_t), intent(in) :: ifile
        logical, intent(in), optional :: back
        if (present (back)) then
            if (back) then
                line%p => ifile%last
            else
                line%p => ifile%first
            end if
        else
            line%p => ifile%first
        end if
    end subroutine line_init
```

Remove the pointer association:

```
<Ifiles: public>+≡
    public :: line_final

<Ifiles: sub interfaces>+≡
    module subroutine line_final (line)
        type(line_p), intent(inout) :: line
    end subroutine line_final
```

```

<Ifiles: procedures>+≡
  module subroutine line_final (line)
    type(line_p), intent(inout) :: line
    nullify (line%p)
  end subroutine line_final

Go one step forward

<Ifiles: public>+≡
  public :: line_advance

<Ifiles: sub interfaces>+≡
  module subroutine line_advance (line)
    type(line_p), intent(inout) :: line
  end subroutine line_advance

<Ifiles: procedures>+≡
  module subroutine line_advance (line)
    type(line_p), intent(inout) :: line
    if (associated (line%p)) line%p => line%p%next
  end subroutine line_advance

Go one step backward

<Ifiles: public>+≡
  public :: line_backspace

<Ifiles: sub interfaces>+≡
  module subroutine line_backspace (line)
    type(line_p), intent(inout) :: line
  end subroutine line_backspace

<Ifiles: procedures>+≡
  module subroutine line_backspace (line)
    type(line_p), intent(inout) :: line
    if (associated (line%p)) line%p => line%p%previous
  end subroutine line_backspace

Check whether we are accessing a valid line

<Ifiles: public>+≡
  public :: line_is_associated

<Ifiles: sub interfaces>+≡
  module function line_is_associated (line) result (ok)
    logical :: ok
    type(line_p), intent(in) :: line
  end function line_is_associated

<Ifiles: procedures>+≡
  module function line_is_associated (line) result (ok)
    logical :: ok
    type(line_p), intent(in) :: line
    ok = associated (line%p)
  end function line_is_associated

```

7.1.6 Access lines via pointers

We do not need the ifile as an argument to these functions, because the `line` type will point to an existing ifile.

```
<Ifiles: public>+≡
    public :: line_get_string

<Ifiles: sub interfaces>+≡
    module function line_get_string (line) result (string)
        type(string_t) :: string
        type(line_p), intent(in) :: line
    end function line_get_string

<Ifiles: procedures>+≡
    module function line_get_string (line) result (string)
        type(string_t) :: string
        type(line_p), intent(in) :: line
        if (associated (line%p)) then
            string = line%p%string
        else
            string = ""
        end if
    end function line_get_string
```

Variant where the line pointer is advanced after reading.

```
<Ifiles: public>+≡
    public :: line_get_string_advance

<Ifiles: sub interfaces>+≡
    module function line_get_string_advance (line) result (string)
        type(string_t) :: string
        type(line_p), intent(inout) :: line
    end function line_get_string_advance

<Ifiles: procedures>+≡
    module function line_get_string_advance (line) result (string)
        type(string_t) :: string
        type(line_p), intent(inout) :: line
        if (associated (line%p)) then
            string = line%p%string
            call line_advance (line)
        else
            string = ""
        end if
    end function line_get_string_advance

<Ifiles: public>+≡
    public :: line_get_index

<Ifiles: sub interfaces>+≡
    module function line_get_index (line) result (index)
        integer :: index
        type(line_p), intent(in) :: line
    end function line_get_index
```

```

<Ifiles: procedures>+≡
  module function line_get_index (line) result (index)
    integer :: index
    type(line_p), intent(in) :: line
    if (associated (line%p)) then
      index = line%p%index
    else
      index = 0
    end if
  end function line_get_index

<Ifiles: public>+≡
  public :: line_get_length

<Ifiles: sub interfaces>+≡
  module function line_get_length (line) result (length)
    integer :: length
    type(line_p), intent(in) :: line
  end function line_get_length

<Ifiles: procedures>+≡
  module function line_get_length (line) result (length)
    integer :: length
    type(line_p), intent(in) :: line
    if (associated (line%p)) then
      length = len (line%p%string)
    else
      length = 0
    end if
  end function line_get_length

```

7.2 Lexer

The lexer purpose is to read from a line-separated character input stream (usually a file) and properly chop the stream into lexemes (tokens). [The parser will transform lexemes into meaningful tokens, to be stored in a parse tree, therefore we do not use the term 'token' here.] The input is read line-by-line, but interpreted free-form, except for quotes and the comment syntax. (Fortran 2003 would allow us to use a stream type for reading.)

In an object-oriented approach, we can dynamically create and destroy lexers, including the lexer setup.

The main lexer function is to return a lexeme according to the basic lexer rules (quotes, comments, whitespace, special classes). There is also a routine to write back a lexeme to the input stream (but only once).

For the rules, we separate the possible characters into classes. Whitespace usually consists of blank, tab, and line-feed, where any number of consecutive whitespace is equivalent to one. Quoted strings are enclosed by a pair of quote characters, possibly multiline. Comments are similar to quotes, but interpreted as whitespace. Numbers are identified (not distinguishing real and integer) but not interpreted. Other character classes make up identifiers.

```
<lexers.f90>≡
<File header>

module lexers

  <Use strings>
    use ifiles, only: ifile_t
    use ifiles, only: line_p

  <Standard module head>

  <Lexer: public>

  <Lexer: parameters>

  <Lexer: types>

  <Lexer: interfaces>

  interface
    <Lexer: sub interfaces>
      end interface

end module lexers

<lexers_sub.f90>≡
<File header>

submodule (lexers) lexers_s

  use io_units
  use string_utils
  use system_defs, only: EOF, EOR
  use system_defs, only: LF
```



```

    use system_defs, only: WHITESPACE_CHARS, LCLETTERS, UCLETTERS, DIGIT_CHARS
    use ifiles, only: line_get_string_advance
    use ifiles, only: line_is_associated, line_init, line_final
    use diagnostics

    implicit none

contains

<Lexer: procedures>

end submodule lexers_s

```

7.2.1 Input streams

For flexible input, we define a generic stream type that refers to either an external file, an external unit which is already open, a string, an `ifile` object (internal file, i.e., string list), or a line pointer to an `ifile` object. The stream type actually follows the idea of a formatted external file, which is line-oriented. Thus, the stream reader always returns a whole record (input line).

Note that only in the string version, the stream contents are stored inside the stream object. In the `ifile` version, the stream contains only the line pointer, while in the external-file case, the line pointer is implicitly created by the runtime library.

```

<Lexer: public>≡
    public :: stream_t

<Lexer: types>≡
    type :: stream_t
        type(string_t), pointer :: filename => null ()
        integer, pointer :: unit => null ()
        type(string_t), pointer :: string => null ()
        type(ifile_t), pointer :: ifile => null ()
        type(line_p), pointer :: line => null ()
        integer :: record = 0
        logical :: eof = .false.
    contains
        <Lexer: stream: TBP>
    end type stream_t

```

The initializers refer to the specific version. The stream should be undefined before calling this.

```

<Lexer: public>+≡
    public :: stream_init

<Lexer: stream: TBP>≡
    generic :: init => &
        stream_init_filename, &
        stream_init_unit, &
        stream_init_string, &
        stream_init_ifile, &
        stream_init_line

```

```

procedure, private :: stream_init_filename
procedure, private :: stream_init_unit
procedure, private :: stream_init_string
procedure, private :: stream_init_ifile
procedure, private :: stream_init_line

<Lexer: interfaces>≡
interface stream_init
  module procedure stream_init_filename
  module procedure stream_init_unit
  module procedure stream_init_string
  module procedure stream_init_ifile
  module procedure stream_init_line
end interface

<Lexer: sub interfaces>≡
module subroutine stream_init_filename (stream, filename)
  class(stream_t), intent(out) :: stream
  character(*), intent(in) :: filename
end subroutine stream_init_filename
module subroutine stream_init_unit (stream, unit)
  class(stream_t), intent(out) :: stream
  integer, intent(in) :: unit
end subroutine stream_init_unit
module subroutine stream_init_string (stream, string)
  class(stream_t), intent(out) :: stream
  type(string_t), intent(in) :: string
end subroutine stream_init_string
module subroutine stream_init_ifile (stream, ifile)
  class(stream_t), intent(out) :: stream
  type(ifile_t), intent(in) :: ifile
end subroutine stream_init_ifile
module subroutine stream_init_line (stream, line)
  class(stream_t), intent(out) :: stream
  type(line_p), intent(in) :: line
end subroutine stream_init_line

<Lexer: procedures>≡
module subroutine stream_init_filename (stream, filename)
  class(stream_t), intent(out) :: stream
  character(*), intent(in) :: filename
  integer :: unit
  unit = free_unit ()
  open (unit=unit, file=filename, status="old", action="read")
  call stream_init_unit (stream, unit)
  allocate (stream%filename)
  stream%filename = filename
end subroutine stream_init_filename

module subroutine stream_init_unit (stream, unit)
  class(stream_t), intent(out) :: stream
  integer, intent(in) :: unit
  allocate (stream%unit)
  stream%unit = unit
  stream%eof = .false.
end subroutine stream_init_unit

```

```

module subroutine stream_init_string (stream, string)
  class(stream_t), intent(out) :: stream
  type(string_t), intent(in) :: string
  allocate (stream%string)
  stream%string = string
end subroutine stream_init_string

module subroutine stream_init_ifile (stream, ifile)
  class(stream_t), intent(out) :: stream
  type(ifile_t), intent(in) :: ifile
  type(line_p) :: line
  call line_init (line, ifile)
  call stream_init_line (stream, line)
  allocate (stream%ifile)
  stream%ifile = ifile
end subroutine stream_init_ifile

module subroutine stream_init_line (stream, line)
  class(stream_t), intent(out) :: stream
  type(line_p), intent(in) :: line
  allocate (stream%line)
  stream%line = line
end subroutine stream_init_line

```

The finalizer restores the initial state. If an external file was opened, it is closed.

```

<Lexer: public>+≡
  public :: stream_final

<Lexer: stream: TBP>+≡
  procedure :: final => stream_final

<Lexer: sub interfaces>+≡
  module subroutine stream_final (stream)
    class(stream_t), intent(inout) :: stream
  end subroutine stream_final

<Lexer: procedures>+≡
  module subroutine stream_final (stream)
    class(stream_t), intent(inout) :: stream
    if (associated (stream%filename)) then
      close (stream%unit)
      deallocate (stream%unit)
      deallocate (stream%filename)
    else if (associated (stream%unit)) then
      deallocate (stream%unit)
    else if (associated (stream%string)) then
      deallocate (stream%string)
    else if (associated (stream%ifile)) then
      call line_final (stream%line)
      deallocate (stream%line)
      deallocate (stream%ifile)
    else if (associated (stream%line)) then
      call line_final (stream%line)
      deallocate (stream%line)
    end if
  end subroutine stream_final

```

```

        end if
    end subroutine stream_final

```

This returns the next record from the input stream. Depending on the stream type, the stream pointers are modified: Reading from external unit, the external file is advanced (implicitly). Reading from string, the string is replaced by an empty string. Reading from ifile, the line pointer is advanced. Note that the `iostat` argument is mandatory.

<Lexer: public>+≡

```

    public :: stream_get_record

```

<Lexer: sub interfaces>+≡

```

    module subroutine stream_get_record (stream, string, iostat)
        type(stream_t), intent(inout) :: stream
        type(string_t), intent(out) :: string
        integer, intent(out) :: iostat
    end subroutine stream_get_record

```

<Lexer: procedures>+≡

```

    module subroutine stream_get_record (stream, string, iostat)
        type(stream_t), intent(inout) :: stream
        type(string_t), intent(out) :: string
        integer, intent(out) :: iostat
        if (associated (stream%unit)) then
            if (stream%eof) then
                iostat = EOF
            else
                call get (stream%unit, string, iostat=iostat)
                if (iostat == EOR) then
                    iostat = 0
                    stream%record = stream%record + 1
                end if
                if (iostat == EOF) then
                    iostat = 0
                    stream%eof = .true.
                    if (len (string) /= 0) stream%record = stream%record + 1
                end if
            end if
        else if (associated (stream%string)) then
            if (len (stream%string) /= 0) then
                string = stream%string
                stream%string = ""
                iostat = 0
                stream%record = stream%record + 1
            else
                string = ""
                iostat = EOF
            end if
        else if (associated (stream%line)) then
            if (line_is_associated (stream%line)) then
                string = line_get_string_advance (stream%line)
                iostat = 0
                stream%record = stream%record + 1
            else

```

```

        string = ""
        iostat = EOF
    end if
else
    call msg_bug (" Attempt to read from uninitialized input stream")
end if
end subroutine stream_get_record

```

Return the current stream source as a message string.

```

<Lexer: public>+≡
    public :: stream_get_source_info_string

<Lexer: sub interfaces>+≡
    module function stream_get_source_info_string (stream) result (string)
        type(string_t) :: string
        type(stream_t), intent(in) :: stream
    end function stream_get_source_info_string

<Lexer: procedures>+≡
    module function stream_get_source_info_string (stream) result (string)
        type(string_t) :: string
        type(stream_t), intent(in) :: stream
        character(20) :: buffer
        if (associated (stream%filename)) then
            string = "File '" // stream%filename // "' (unit = "
            write (buffer, "(I0)") stream%unit
            string = string // trim (buffer) // ")"
        else if (associated (stream%unit)) then
            write (buffer, "(I0)") stream%unit
            string = "Unit " // trim (buffer)
        else if (associated (stream%string)) then
            string = "Input string"
        else if (associated (stream%ifile) .or. associated (stream%line)) then
            string = "Internal file"
        else
            string = ""
        end if
    end function stream_get_source_info_string

```

Return the index of the record just read as a message string.

```

<Lexer: public>+≡
    public :: stream_get_record_info_string

<Lexer: sub interfaces>+≡
    module function stream_get_record_info_string (stream) result (string)
        type(string_t) :: string
        type(stream_t), intent(in) :: stream
    end function stream_get_record_info_string

<Lexer: procedures>+≡
    module function stream_get_record_info_string (stream) result (string)
        type(string_t) :: string
        type(stream_t), intent(in) :: stream
        character(20) :: buffer
        string = stream_get_source_info_string (stream)

```

```

        if (string /= "") string = string // ", "
        write (buffer, "(I0)") stream%record
        string = string // "line " // trim (buffer)
    end function stream_get_record_info_string

```

7.2.2 Keyword list

The lexer should be capable of identifying a token as a known keyword. To this end, we store a list of keywords:

```

<Lexer: public>+≡
    public :: keyword_list_t

<Lexer: types>+≡
    type :: keyword_entry_t
        private
            type(string_t) :: string
            type(keyword_entry_t), pointer :: next => null ()
        end type keyword_entry_t

    type :: keyword_list_t
        private
            type(keyword_entry_t), pointer :: first => null ()
            type(keyword_entry_t), pointer :: last => null ()
        end type keyword_list_t

```

Add a new string to the keyword list, unless it is already there:

```

<Lexer: public>+≡
    public :: keyword_list_add

<Lexer: sub interfaces>+≡
    module subroutine keyword_list_add (keylist, string)
        type(keyword_list_t), intent(inout) :: keylist
        type(string_t), intent(in) :: string
    end subroutine keyword_list_add

<Lexer: procedures>+≡
    module subroutine keyword_list_add (keylist, string)
        type(keyword_list_t), intent(inout) :: keylist
        type(string_t), intent(in) :: string
        type(keyword_entry_t), pointer :: k_entry_new
        if (.not. keyword_list_contains (keylist, string)) then
            allocate (k_entry_new)
            k_entry_new%string = string
            if (associated (keylist%first)) then
                keylist%last%next => k_entry_new
            else
                keylist%first => k_entry_new
            end if
            keylist%last => k_entry_new
        end if
    end subroutine keyword_list_add

```

Return true if a string is a keyword.

```

<Lexer: public>+≡
    public :: keyword_list_contains

<Lexer: sub interfaces>+≡
    module function keyword_list_contains (keylist, string) result (found)
        type(keyword_list_t), intent(in) :: keylist
        type(string_t), intent(in) :: string
        logical :: found
    end function keyword_list_contains

<Lexer: procedures>+≡
    module function keyword_list_contains (keylist, string) result (found)
        type(keyword_list_t), intent(in) :: keylist
        type(string_t), intent(in) :: string
        logical :: found
        found = .false.
        call check_rec (keylist%first)
contains
        recursive subroutine check_rec (k_entry)
            type(keyword_entry_t), pointer :: k_entry
            if (associated (k_entry)) then
                if (k_entry%string /= string) then
                    call check_rec (k_entry%next)
                else
                    found = .true.
                end if
            end if
        end subroutine check_rec
    end function keyword_list_contains

```

Write the keyword list

```

<Lexer: public>+≡
    public :: keyword_list_write

<Lexer: interfaces>+≡
    interface keyword_list_write
        module procedure keyword_list_write_unit
    end interface

<Lexer: sub interfaces>+≡
    module subroutine keyword_list_write_unit (keylist, unit)
        type(keyword_list_t), intent(in) :: keylist
        integer, intent(in) :: unit
    end subroutine keyword_list_write_unit

<Lexer: procedures>+≡
    module subroutine keyword_list_write_unit (keylist, unit)
        type(keyword_list_t), intent(in) :: keylist
        integer, intent(in) :: unit
        write (unit, "(A)") "Keyword list:"
        if (associated (keylist%first)) then
            call keyword_write_rec (keylist%first)
            write (unit, *)
        else
            write (unit, "(1x,A)") "[empty]"
        end if
    end subroutine keyword_list_write_unit

```

```

        end if
contains
    recursive subroutine keyword_write_rec (k_entry)
        type(keyword_entry_t), intent(in), pointer :: k_entry
        if (associated (k_entry)) then
            write (unit, "(1x,A)", advance="no") char (k_entry%string)
            call keyword_write_rec (k_entry%next)
        end if
    end subroutine keyword_write_rec
end subroutine keyword_list_write_unit

```

Clear the keyword list

```

<Lexer: public>+≡
    public :: keyword_list_final
<Lexer: sub interfaces>+≡
    module subroutine keyword_list_final (keylist)
        type(keyword_list_t), intent(inout) :: keylist
    end subroutine keyword_list_final
<Lexer: procedures>+≡
    module subroutine keyword_list_final (keylist)
        type(keyword_list_t), intent(inout) :: keylist
        call keyword_destroy_rec (keylist%first)
        nullify (keylist%last)
contains
    recursive subroutine keyword_destroy_rec (k_entry)
        type(keyword_entry_t), pointer :: k_entry
        if (associated (k_entry)) then
            call keyword_destroy_rec (k_entry%next)
            deallocate (k_entry)
        end if
    end subroutine keyword_destroy_rec
end subroutine keyword_list_final

```

7.2.3 Lexeme templates

This type is handled like a rudimentary regular expression. It determines the lexer behavior when matching a string. The actual objects made from this type and the corresponding matching routines are listed below.

```

<Lexer: types>+≡
    type :: template_t
        !!! !!! Compiler bug in ifort 20/21/22: no structure constants for
        !!! !!! types with private components in submodules possible
        !!! private
        integer :: type
        character(256) :: charset1, charset2
        integer :: len1, len2
    end type template_t

```

These are the types that valid lexemes can have:

```

<Lexer: public>+≡
    public :: T_KEYWORD, T_IDENTIFIER, T_QUOTED, T_NUMERIC

```



```

<Lexer: parameters>+=
    integer, parameter :: T_KEYWORD = 1
    integer, parameter :: T_IDENTIFIER = 2, T_QUOTED = 3, T_NUMERIC = 4

```

These are special types:

```

<Lexer: parameters>+=
    integer, parameter :: EMPTY = 0, WHITESPACE = 10
    integer, parameter :: NO_MATCH = 11, IO_ERROR = 12, OVERFLOW = 13
    integer, parameter :: UNMATCHED_QUOTE = 14

```

In addition, we have EOF which is a negative integer, normally -1 . Printout for debugging:

```

<Lexer: procedures>+=
    subroutine lexeme_type_write (type, unit)
        integer, intent(in) :: type
        integer, intent(in) :: unit
        select case (type)
            case (EMPTY);      write(unit,"(A)",advance="no") " EMPTY      "
            case (WHITESPACE); write(unit,"(A)",advance="no") " WHITESPACE "
            case (T_IDENTIFIER);write(unit,"(A)",advance="no") " IDENTIFIER "
            case (T_QUOTED);   write(unit,"(A)",advance="no") " QUOTED   "
            case (T_NUMERIC);  write(unit,"(A)",advance="no") " NUMERIC   "
            case (IO_ERROR);   write(unit,"(A)",advance="no") " IO_ERROR  "
            case (OVERFLOW);   write(unit,"(A)",advance="no") " OVERFLOW  "
            case (UNMATCHED_QUOTE); write(unit,"(A)",advance="no") " UNMATCHEDQ "
            case (NO_MATCH);   write(unit,"(A)",advance="no") " NO_MATCH   "
            case (EOF);        write(unit,"(A)",advance="no") " EOF        "
            case default;      write(unit,"(A)",advance="no") " [illegal]  "
        end select
    end subroutine lexeme_type_write

    subroutine template_write (tt, unit)
        type(template_t), intent(in) :: tt
        integer, intent(in) :: unit
        call lexeme_type_write (tt%type, unit)
        write (unit, "(A)", advance="no") " '" // tt%charset1(1:tt%len1) // "' "
        write (unit, "(A)", advance="no") " '" // tt%charset2(1:tt%len2) // "' "
    end subroutine template_write

```

The matching functions all return the number of matched characters in the provided string. If this number is zero, the match has failed.

The `template` functions are declared `pure` because they appear in `forall` loops below.

A template for whitespace:

```

<Lexer: procedures>+=
    pure function template_whitespace (chars) result (tt)
        character(*), intent(in) :: chars
        type(template_t) :: tt
        tt = template_t (WHITESPACE, chars, "", len (chars), 0)
    end function template_whitespace

```

Just match the string against the character set.

```

<Lexer: procedures>+=

```

```

subroutine match_whitespace (tt, s, n)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  n = verify (s, tt%charset1(1:tt%len1)) - 1
  if (n < 0) n = len (s)
end subroutine match_whitespace

```

A template for normal identifiers. To match, a lexeme should have a first character in class `chars1` and an arbitrary number of further characters in class `chars2`. If the latter is empty, we are looking for a single-character lexeme.

<Lexer: procedures>+≡

```

pure function template_identifier (chars1, chars2) result (tt)
  character(*), intent(in) :: chars1, chars2
  type(template_t) :: tt
  tt = template_t (T_IDENTIFIER, chars1, chars2, len(chars1), len(chars2))
end function template_identifier

```

Here, the first letter must match, the others may or may not.

<Lexer: procedures>+≡

```

subroutine match_identifier (tt, s, n)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  if (verify (s(1:1), tt%charset1(1:tt%len1)) == 0) then
    n = verify (s(2:), tt%charset2(1:tt%len2))
    if (n == 0) n = len (s)
  else
    n = 0
  end if
end subroutine match_identifier

```

A template for quoted strings. The same template applies for comments. The first character set indicates the left quote (could be a sequence of several characters), the second one the matching right quote.

<Lexer: procedures>+≡

```

pure function template_quoted (chars1, chars2) result (tt)
  character(*), intent(in) :: chars1, chars2
  type(template_t) :: tt
  tt = template_t (T_QUOTED, chars1, chars2, len (chars1), len (chars2))
end function template_quoted

```

Here, the beginning of the string must exactly match the first character set, then we look for the second one. If found, return. If there is a first quote but no second one, return a negative number, indicating this error condition.

<Lexer: procedures>+≡

```

subroutine match_quoted (tt, s, n, range)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer, dimension(2), intent(out) :: range

```

```

character(tt%len1) :: ch1
character(tt%len2) :: ch2
integer :: i
ch1 = tt%charset1
if (s(1:tt%len1) == ch1) then
  ch2 = tt%charset2
  do i = tt%len1 + 1, len (s) - tt%len2 + 1
    if (s(i:i+tt%len2-1) == ch2) then
      n = i + tt%len2 - 1
      range(1) = tt%len1 + 1
      range(2) = i - 1
      return
    end if
  end do
  n = -1
  range = 0
else
  n = 0
  range = 0
end if
end subroutine match_quoted

```

A template for real numbers. The first character set is the set of allowed exponent letters. In accordance with the other functions we return the lexeme as a string but do not read it.

<Lexer: procedures>+≡

```

pure function template_numeric (chars) result (tt)
  character(*), intent(in) :: chars
  type(template_t) :: tt
  tt = template_t (T_NUMERIC, chars, "", len (chars), 0)
end function template_numeric

```

A numeric lexeme may be real or integer. We purposely do not allow for a preceding sign. If the number is followed by an exponent, this is included, otherwise the rest is ignored.

There is a possible pitfall with this behavior: while the string `1e3` will be interpreted as a single number, the analogous string `1a3` will be split into the number `1` and an identifier `a3`. There is no easy way around such an ambiguity. We should make sure that the syntax does not contain identifiers like `a3` or `e3`.

<Lexer: procedures>+≡

```

subroutine match_numeric (tt, s, n)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer :: i, n0
  character(10), parameter :: digits = "0123456789"
  character(2), parameter :: signs = "-+"
  n = verify (s, digits) - 1
  if (n < 0) then
    n = 0
    return
  else if (s(n+1:n+1) == ".") then

```

```

        i = verify (s(n+2:), digits) - 1
        if (i < 0) then
            n = len (s)
            return
        else if (i > 0 .or. n > 0) then
            n = n + 1 + i
        end if
    end if
    n0 = n
    if (n > 0) then
        if (verify (s(n+1:n+1), tt%charset1(1:tt%len1)) == 0) then
            n = n + 1
            if (verify (s(n+1:n+1), signs) == 0) n = n + 1
            i = verify (s(n+1:), digits) - 1
            if (i < 0) then
                n = len (s)
            else if (i == 0) then
                n = n0
            else
                n = n + i
            end if
        end if
    end if
end subroutine match_numeric

```

The generic matching routine. With Fortran 2003 we would define separate types and use a SELECT TYPE instead.

(Lexer: procedures)+≡

```

subroutine match_template (tt, s, n, range)
    type(template_t), intent(in) :: tt
    character(*), intent(in) :: s
    integer, intent(out) :: n
    integer, dimension(2), intent(out) :: range
    select case (tt%type)
    case (WHITESPACE)
        call match_whitespace (tt, s, n)
        range = 0
    case (T_IDENTIFIER)
        call match_identifier (tt, s, n)
        range(1) = 1
        range(2) = len_trim (s)
    case (T_QUOTED)
        call match_quoted (tt, s, n, range)
    case (T_NUMERIC)
        call match_numeric (tt, s, n)
        range(1) = 1
        range(2) = len_trim (s)
    case default
        call msg_bug ("Invalid lexeme template encountered")
    end select
end subroutine match_template

```

Match against an array of templates. Return the index of the first template

that matches together with the number of characters matched and the range of the relevant substring. If all fails, these numbers are zero.

(Lexer: procedures)+≡

```

subroutine match (tt, s, n, range, ii)
  type(template_t), dimension(:), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer, dimension(2), intent(out) :: range
  integer, intent(out) :: ii
  integer :: i
  do i = 1, size (tt)
    call match_template (tt(i), s, n, range)
    if (n /= 0) then
      ii = i
      return
    end if
  end do
  n = 0
  ii = 0
end subroutine match

```

7.2.4 The lexer setup

This object contains information about character classes. As said above, one class consists of quoting chars (matching left and right), another one of comment chars (similar), a class of whitespace, and several classes of characters that make up identifiers. When creating the lexer setup, the character classes are transformed into lexeme templates which are to be matched in a certain predefined order against the input stream.

BLANK should always be taken as whitespace, some things may depend on this. TAB is also fixed by convention, but may in principle be modified. Newline (DOS!) and linefeed are also defined as whitespace. The lexer setup, containing the list of lexeme templates. No defaults yet. The type with index zero will be assigned to the NO_MATCH lexeme.

The keyword list is not stored, just a pointer to it. We anticipate that the keyword list is part of the syntax table, and the lexer needs not alter it. Furthermore, the lexer is typically finished before the syntax table is.

(Lexer: parameters)+≡

```

integer, parameter :: CASE_KEEP = 0, CASE_UP = 1, CASE_DOWN = 2

```

(Lexer: types)+≡

```

type :: lexer_setup_t
  private
  type(template_t), dimension(:), allocatable :: tt
  integer, dimension(:), allocatable :: type
  integer :: keyword_case = CASE_KEEP
  type(keyword_list_t), pointer :: keyword_list => null ()
end type lexer_setup_t

```

Fill the lexer setup object. Some things are hardcoded here (whitespace, alphanumeric identifiers), some are free: comment chars (but these must be single, and comments must be terminated by line-feed), quote chars and matches (must be single), characters to be read as one-character lexeme, special classes (characters of one class that should be glued together as identifiers).

(Lexer: procedures)+≡

```

subroutine lexer_setup_init (setup, &
    comment_chars, quote_chars, quote_match, &
    single_chars, special_class, &
    keyword_list, upper_case_keywords)
type(lexer_setup_t), intent(inout) :: setup
character(*), intent(in) :: comment_chars
character(*), intent(in) :: quote_chars, quote_match
character(*), intent(in) :: single_chars
character(*), dimension(:), intent(in) :: special_class
type(keyword_list_t), pointer :: keyword_list
logical, intent(in), optional :: upper_case_keywords
integer :: n, i
if (present (upper_case_keywords)) then
    if (upper_case_keywords) then
        setup%keyword_case = CASE_UP
    else
        setup%keyword_case = CASE_DOWN
    end if
else
    setup%keyword_case = CASE_KEEP
end if
n = 1 + len (comment_chars) + len (quote_chars) + 1 &
    + len (single_chars) + size (special_class) + 1
allocate (setup%tt(n))
allocate (setup%type(0:n))
n = 0
setup%type(n) = NO_MATCH
n = n + 1
setup%tt(n) = template_whitespace (WHITESPACE_CHARS)
setup%type(n) = EMPTY
forall (i = 1:len(comment_chars))
    setup%tt(n+i) = template_quoted (comment_chars(i:i), LF)
    setup%type(n+i) = EMPTY
end forall
n = n + len (comment_chars)
forall (i = 1:len(quote_chars))
    setup%tt(n+i) = template_quoted (quote_chars(i:i), quote_match(i:i))
    setup%type(n+i) = T_QUOTED
end forall
n = n + len (quote_chars)
setup%tt(n+1) = template_numeric ("EeDd")
setup%type(n+1) = T_NUMERIC
n = n + 1
forall (i = 1:len (single_chars))
    setup%tt(n+i) = template_identifier (single_chars(i:i), "")
    setup%type(n+i) = T_IDENTIFIER
end forall

```

```

n = n + len (single_chars)
forall (i = 1:size (special_class))
    setup%tt(n+i) = template_identifier &
        (trim (special_class(i)), trim (special_class(i)))
    setup%type(n+i) = T_IDENTIFIER
end forall
n = n + size (special_class)
setup%tt(n+1) = template_identifier &
    (LCLETTERS//UCLETTERS, LCLETTERS//DIGIT_CHARS//"_"/UCLETTERS)
setup%type(n+1) = T_IDENTIFIER
n = n + 1
if (n /= size (setup%tt)) &
    call msg_bug ("Size mismatch in lexer setup")
setup%keyword_list => keyword_list
end subroutine lexer_setup_init

```

The destructor is needed only if the object is not itself part of an allocatable array

```

<Lexer: procedures>+≡
subroutine lexer_setup_final (setup)
    type(lexer_setup_t), intent(inout) :: setup
    deallocate (setup%tt, setup%type)
    setup%keyword_list => null ()
end subroutine lexer_setup_final

```

For debugging: Write the lexer setup

```

<Lexer: procedures>+≡
subroutine lexer_setup_write (setup, unit)
    type(lexer_setup_t), intent(in) :: setup
    integer, intent(in) :: unit
    integer :: i
    write (unit, "(A)") "Lexer setup:"
    if (allocated (setup%tt)) then
        do i = 1, size (setup%tt)
            call template_write (setup%tt(i), unit)
            write (unit, '(A)', advance = "no") " -> "
            call lexeme_type_write (setup%type(i), unit)
            write (unit, *)
        end do
    else
        write (unit, *) "[empty]"
    end if
    if (associated (setup%keyword_list)) then
        call keyword_list_write (setup%keyword_list, unit)
    end if
end subroutine lexer_setup_write

```

7.2.5 The lexeme type

An object of this type is returned by the lexer. Apart from the lexeme string, it gives information about the relevant substring (first and last character index)

and the lexeme type. Interpreting the string is up to the parser.

```

<Lexer: public>+≡
    public :: lexeme_t

<Lexer: types>+≡
    type :: lexeme_t
    private
        integer :: type = EMPTY
        type(string_t) :: s
        integer :: b = 0, e = 0
    end type lexeme_t

```

Debugging aid:

```

<Lexer: public>+≡
    public :: lexeme_write

<Lexer: sub interfaces>+≡
    module subroutine lexeme_write (t, unit)
        type(lexeme_t), intent(in) :: t
        integer, intent(in) :: unit
    end subroutine lexeme_write

<Lexer: procedures>+≡
    module subroutine lexeme_write (t, unit)
        type(lexeme_t), intent(in) :: t
        integer, intent(in) :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        select case (t%type)
        case (T_KEYWORD)
            write (u, *) "KEYWORD:      '" // char (t%s) // "'"
        case (T_IDENTIFIER)
            write (u, *) "IDENTIFIER: '" // char (t%s) // "'"
        case (T_QUOTED)
            write (u, *) "QUOTED:      '" // char (t%s) // "'"
        case (T_NUMERIC)
            write (u, *) "NUMERIC:      '" // char (t%s) // "'"
        case (UNMATCHED_QUOTE)
            write (u, *) "Unmatched quote: //" char (t%s)
        case (OVERFLOW); write (u, *) "Overflow: //" char (t%s)
        case (EMPTY);   write (u, *) "Empty lexeme"
        case (NO_MATCH); write (u, *) "No match"
        case (IO_ERROR); write (u, *) "IO error"
        case (EOF);     write (u, *) "EOF"
        case default
            write (u, *) "Error"
        end select
    end subroutine lexeme_write

```

Store string and type in a lexeme. The range determines the beginning and end of the relevant part of the string. Check for a keyword.

```

<Lexer: procedures>+≡
    subroutine lexeme_set (t, keyword_list, s, range, type, keyword_case)
        type(lexeme_t), intent(out) :: t

```



```

type(keyword_list_t), pointer :: keyword_list
type(string_t), intent(in) :: s
type(string_t) :: keyword
integer, dimension(2), intent(in) :: range
integer, intent(in) :: type
integer, intent(in), optional :: keyword_case
t%type = type
if (present (keyword_case)) then
  select case (keyword_case)
    case (CASE_KEEP);   keyword = s
    case (CASE_UP);     keyword = upper_case (s)
    case (CASE_DOWN);   keyword = lower_case (s)
  end select
else
  keyword = s
end if
if (type == T_IDENTIFIER) then
  if (associated (keyword_list)) then
    if (keyword_list_contains (keyword_list, keyword)) &
      t%type = T_KEYWORD
    end if
  end if
  select case (t%type)
    case (T_KEYWORD);   t%s = keyword
    case default;       t%s = s
  end select
  t%b = range(1)
  t%e = range(2)
end subroutine lexeme_set

subroutine lexeme_clear (t)
  type(lexeme_t), intent(out) :: t
  t%type = EMPTY
  t%s = ""
end subroutine lexeme_clear

```

Retrieve the lexeme string, the relevant part of it, and the type. The last function returns true if there is a break condition reached (error or EOF).

(Lexer: public)+≡

```

public :: lexeme_get_string
public :: lexeme_get_contents
public :: lexeme_get_delimiters
public :: lexeme_get_type

```

(Lexer: sub interfaces)+≡

```

module function lexeme_get_string (t) result (s)
  type(string_t) :: s
  type(lexeme_t), intent(in) :: t
end function lexeme_get_string
module function lexeme_get_contents (t) result (s)
  type(string_t) :: s
  type(lexeme_t), intent(in) :: t
end function lexeme_get_contents
module function lexeme_get_delimiters (t) result (del)

```

```

        type(string_t), dimension(2) :: del
        type(lexeme_t), intent(in) :: t
    end function lexeme_get_delimiters
    module function lexeme_get_type (t) result (type)
        integer :: type
        type(lexeme_t), intent(in) :: t
    end function lexeme_get_type
<Lexer: procedures>+≡
    module function lexeme_get_string (t) result (s)
        type(string_t) :: s
        type(lexeme_t), intent(in) :: t
        s = t%s
    end function lexeme_get_string

    module function lexeme_get_contents (t) result (s)
        type(string_t) :: s
        type(lexeme_t), intent(in) :: t
        s = extract (t%s, t%b, t%e)
    end function lexeme_get_contents

    module function lexeme_get_delimiters (t) result (del)
        type(string_t), dimension(2) :: del
        type(lexeme_t), intent(in) :: t
        del(1) = extract (t%s, finish = t%b-1)
        del(2) = extract (t%s, start = t%e+1)
    end function lexeme_get_delimiters

    module function lexeme_get_type (t) result (type)
        integer :: type
        type(lexeme_t), intent(in) :: t
        type = t%type
    end function lexeme_get_type

```

Check for a generic break condition (error/eof) and for eof in particular.

```

<Lexer: public>+≡
    public :: lexeme_is_break
    public :: lexeme_is_eof
<Lexer: sub interfaces>+≡
    module function lexeme_is_break (t) result (break)
        logical :: break
        type(lexeme_t), intent(in) :: t
    end function lexeme_is_break
    module function lexeme_is_eof (t) result (ok)
        logical :: ok
        type(lexeme_t), intent(in) :: t
    end function lexeme_is_eof
<Lexer: procedures>+≡
    module function lexeme_is_break (t) result (break)
        logical :: break
        type(lexeme_t), intent(in) :: t
        select case (t%type)
        case (EOF, IO_ERROR, OVERFLOW, NO_MATCH)

```

```

        break = .true.
    case default
        break = .false.
    end select
end function lexeme_is_break

module function lexeme_is_eof (t) result (ok)
    logical :: ok
    type.lexeme_t, intent(in) :: t
    ok = t%type == EOF
end function lexeme_is_eof

```

7.2.6 The lexer object

We store the current lexeme and the current line. The line buffer is set each time a new line is read from file. The working buffer has one character more, to hold any trailing blank. Pointers to line and column are for debugging, they will be used to make up readable error messages for the parser.

```

<Lexer: public>+≡
    public :: lexer_t

<Lexer: types>+≡
    type :: lexer_t
    private
    type(lexer_setup_t) :: setup
    type(stream_t), pointer :: stream => null ()
    type.lexeme_t :: lexeme
    type(string_t) :: previous_line2
    type(string_t) :: previous_line1
    type(string_t) :: current_line
    integer :: lines_read = 0
    integer :: current_column = 0
    integer :: previous_column = 0
    type(string_t) :: buffer
    type(lexer_t), pointer :: parent => null ()
contains
    <Lexer: lexer: TBP>
end type lexer_t

```

Create-setup wrapper

```

<Lexer: public>+≡
    public :: lexer_init

<Lexer: lexer: TBP>≡
    procedure :: init => lexer_init

<Lexer: sub interfaces>+≡
    module subroutine lexer_init (lexer, &
        comment_chars, quote_chars, quote_match, &
        single_chars, special_class, &
        keyword_list, upper_case_keywords, &
        parent)
        class(lexer_t), intent(inout) :: lexer
        character(*), intent(in) :: comment_chars
    end module

```

```

        character(*), intent(in) :: quote_chars, quote_match
        character(*), intent(in) :: single_chars
        character(*), dimension(:), intent(in) :: special_class
        type(keyword_list_t), pointer :: keyword_list
        logical, intent(in), optional :: upper_case_keywords
        type(lexer_t), target, intent(in), optional :: parent
    end subroutine lexer_init
<Lexer: procedures>+≡
    module subroutine lexer_init (lexer, &
        comment_chars, quote_chars, quote_match, &
        single_chars, special_class, &
        keyword_list, upper_case_keywords, &
        parent)
        class(lexer_t), intent(inout) :: lexer
        character(*), intent(in) :: comment_chars
        character(*), intent(in) :: quote_chars, quote_match
        character(*), intent(in) :: single_chars
        character(*), dimension(:), intent(in) :: special_class
        type(keyword_list_t), pointer :: keyword_list
        logical, intent(in), optional :: upper_case_keywords
        type(lexer_t), target, intent(in), optional :: parent
        call lexer_setup_init (lexer%setup, &
            comment_chars = comment_chars, &
            quote_chars = quote_chars, &
            quote_match = quote_match, &
            single_chars = single_chars, &
            special_class = special_class, &
            keyword_list = keyword_list, &
            upper_case_keywords = upper_case_keywords)
        if (present (parent)) lexer%parent => parent
        call lexer_clear (lexer)
    end subroutine lexer_init

```

Clear the lexer state, but not the setup. This should be done when the lexing starts, but it is not known whether the lexer was used before.

```

<Lexer: public>+≡
    public :: lexer_clear
<Lexer: lexer: TBP>+≡
    procedure :: clear => lexer_clear
<Lexer: sub interfaces>+≡
    module subroutine lexer_clear (lexer)
        class(lexer_t), intent(inout) :: lexer
    end subroutine lexer_clear
<Lexer: procedures>+≡
    module subroutine lexer_clear (lexer)
        class(lexer_t), intent(inout) :: lexer
        call lexeme_clear (lexer%lexeme)
        lexer%previous_line2 = ""
        lexer%previous_line1 = ""
        lexer%current_line = ""
        lexer%lines_read = 0
        lexer%current_column = 0
    end subroutine lexer_clear

```

```

lexer%previous_column = 0
lexer%buffer = ""
end subroutine lexer_clear

```

Reset lexer state and delete setup

```

<Lexer: public>+≡
public :: lexer_final

<Lexer: lexer: TBP>+≡
procedure :: final => lexer_final

<Lexer: sub interfaces>+≡
module subroutine lexer_final (lexer)
  class(lexer_t), intent(inout) :: lexer
end subroutine lexer_final

<Lexer: procedures>+≡
module subroutine lexer_final (lexer)
  class(lexer_t), intent(inout) :: lexer
  call lexer%clear ()
  call lexer_setup_final (lexer%setup)
end subroutine lexer_final

```

7.2.7 The lexer routine

For lexing we need to associate an input stream to the lexer.

```

<Lexer: public>+≡
public :: lexer_assign_stream

<Lexer: lexer: TBP>+≡
procedure :: assign_stream => lexer_assign_stream

<Lexer: sub interfaces>+≡
module subroutine lexer_assign_stream (lexer, stream)
  class(lexer_t), intent(inout) :: lexer
  type(stream_t), intent(in), target :: stream
end subroutine lexer_assign_stream

<Lexer: procedures>+≡
module subroutine lexer_assign_stream (lexer, stream)
  class(lexer_t), intent(inout) :: lexer
  type(stream_t), intent(in), target :: stream
  lexer%stream => stream
end subroutine lexer_assign_stream

```

The lexer. The lexer function takes the lexer and returns the currently stored lexeme. If there is none, it is read from buffer, matching against the lexeme templates in the lexer setup. Empty lexemes, i.e., comments and whitespace, are discarded and the buffer is read again until we have found a nonempty lexeme (which may also be EOF or an error condition).

The initial state of the lexer contains an empty lexeme, so reading from buffer is forced. The empty state is restored after returning the lexeme. A nonempty lexeme is present in the lexer only if `lex_back` has been executed before.

The workspace is the `lexer%buffer`, treated as a sort of input stream. We chop off lexemes from the beginning, adjusting the buffer to the left. Whenever the buffer is empty, or we are matching against an open quote which has not terminated, we read a new line and append it to the right. This may result in special conditions, which for simplicity are also returned as lexemes: I/O error, buffer overflow, end of file. If the latter happens during reading a quoted string, we return an unmatched-quote lexeme. Obviously, the special-condition lexemes have to be caught by the parser.

Note that reading further lines is only necessary when reading a quoted string. Otherwise, the line-feed that ends each line is interpreted as whitespace which terminates a preceding lexeme, so there are no other valid multiline lexemes.

To enable meaningful error messages, we also keep track of the line number of the last line read, and the beginning and the end of the current lexeme with respect to this line.

The lexer is implemented as a function that returns the next lexeme (i.e., token). It uses the `lexer` setup and modifies the buffers and pointers stored within the lexer, a side effect. The lexer reads from an input stream object, which also is modified by this reading, e.g., a line pointer is advanced.

```

(Lexer: public)+≡
    public :: lex

(Lexer: sub interfaces)+≡
    module subroutine lex (lexeme, lexer)
        type(lexeme_t), intent(out) :: lexeme
        type(lexer_t), intent(inout) :: lexer
    end subroutine lex

(Lexer: procedures)+≡
    module subroutine lex (lexeme, lexer)
        type(lexeme_t), intent(out) :: lexeme
        type(lexer_t), intent(inout) :: lexer
        integer :: iostat1, iostat2
        integer :: pos
        integer, dimension(2) :: range
        integer :: template_index, type
        if (.not. associated (lexer%stream)) &
            call msg_bug ("Lexer called without assigned stream")
        GET_LEXEME: do while (lexeme_get_type (lexer%lexeme) == EMPTY)
            if (len (lexer%buffer) /= 0) then
                iostat1 = 0
            else
                call lexer_read_line (lexer, iostat1)
            end if
            select case (iostat1)
            case (0)
                MATCH_BUFFER: do
                    call match (lexer%setup%tt, char (lexer%buffer), &
                                pos, range, template_index)
                    if (pos >= 0) then
                        type = lexer%setup%type(template_index)
                        exit MATCH_BUFFER
                    else

```

```

        pos = 0
        call lexer_read_line (lexer, iostat2)
        select case (iostat2)
        case (EOF); type = UNMATCHED_QUOTE; exit MATCH_BUFFER
        case (1);   type = IO_ERROR;         exit MATCH_BUFFER
        case (2);   type = OVERFLOW;         exit MATCH_BUFFER
        end select
    end if
end do MATCH_BUFFER
case (EOF); type = EOF
case (1);   type = IO_ERROR
case (2);   type = OVERFLOW
end select
call lexeme_set (lexer%lexeme, lexer%setup%keyword_list, &
    extract (lexer%buffer, finish=pos), range, type, &
    lexer%setup%keyword_case)
lexer%buffer = remove (lexer%buffer, finish=pos)
lexer%previous_column = lexer%current_column
lexer%current_column = lexer%current_column + pos
end do GET_LEXEME
lexeme = lexer%lexeme
call lexeme_clear (lexer%lexeme)
end subroutine lex

```

Read a line and append it to the input buffer. If the input buffer overflows, return `iostat=2`. Otherwise, `iostat=1` indicates an I/O error, and `iostat=-1` the EOF.

The input stream may either be an external unit or a `ifile` object. In the latter case, a line is read and the line pointer is advanced.

Note that inserting LF between input lines is the Unix convention. Since we are doing this explicitly when gluing lines together, we can pattern-match against LF without having to worry about the system.

<Lexer: procedures>+≡

```

subroutine lexer_read_line (lexer, iostat)
    type(lexer_t), intent(inout) :: lexer
    integer, intent(out) :: iostat
    type(string_t) :: current_line
    current_line = lexer%current_line
    call stream_get_record (lexer%stream, lexer%current_line, iostat)
    if (iostat == 0) then
        lexer%lines_read = lexer%lines_read + 1
        lexer%previous_line2 = lexer%previous_line1
        lexer%previous_line1 = current_line
        lexer%buffer = lexer%buffer // lexer%current_line // LF
        lexer%previous_column = 0
        lexer%current_column = 0
    end if
end subroutine lexer_read_line

```

Once in a while we have read one lexeme to many, which can be pushed back into the input stream. Do not do this more than once.

<Lexer: public>+≡

```

public :: lexer_put_back
<Lexer: sub interfaces>+≡
  module subroutine lexer_put_back (lexer, lexeme)
    type(lexer_t), intent(inout) :: lexer
    type(lexeme_t), intent(in) :: lexeme
  end subroutine lexer_put_back
<Lexer: procedures>+≡
  module subroutine lexer_put_back (lexer, lexeme)
    type(lexer_t), intent(inout) :: lexer
    type(lexeme_t), intent(in) :: lexeme
    if (lexeme_get_type (lexer%lexeme) == EMPTY) then
      lexer%lexeme = lexeme
    else
      call msg_bug (" Lexer: lex_back fails; probably called twice")
    end if
  end subroutine lexer_put_back

```

7.2.8 Diagnostics

For debugging: print just the setup

```

<Lexer: public>+≡
  public :: lexer_write_setup
<Lexer: sub interfaces>+≡
  module subroutine lexer_write_setup (lexer, unit)
    type(lexer_t), intent(in) :: lexer
    integer, intent(in), optional :: unit
  end subroutine lexer_write_setup
<Lexer: procedures>+≡
  module subroutine lexer_write_setup (lexer, unit)
    type(lexer_t), intent(in) :: lexer
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call lexer_setup_write (lexer%setup, u)
  end subroutine lexer_write_setup

```

This is useful for error printing: show the current line with index and a pointer to the current column within the line.

```

<Lexer: public>+≡
  public :: lexer_show_location
<Lexer: sub interfaces>+≡
  module subroutine lexer_show_location (lexer)
    type(lexer_t), intent(in) :: lexer
  end subroutine lexer_show_location
<Lexer: procedures>+≡
  module subroutine lexer_show_location (lexer)
    type(lexer_t), intent(in) :: lexer
    type(string_t) :: loc_str
    if (associated (lexer%parent)) then

```



```

        call lexer_show_source (lexer%parent)
        call msg_message ("[includes]")
    else
        call msg_message ()
    end if
    if (associated (lexer%stream)) then
        call msg_message &
            (char (stream_get_record_info_string (lexer%stream)) // ":")
    end if
    if (lexer%lines_read >= 4) call msg_result ("[...]")
    if (lexer%lines_read >= 3) call msg_result (char (lexer%previous_line2))
    if (lexer%lines_read >= 2) call msg_result (char (lexer%previous_line1))
    if (lexer%lines_read >= 1) then
        call msg_result (char (lexer%current_line))
        loc_str = repeat (" ", lexer%previous_column)
        loc_str = loc_str // "^"
        if (lexer%current_column > lexer%previous_column) then
            loc_str = loc_str &
                // repeat ("-", max (lexer%current_column &
                    - lexer%previous_column - 1, 0)) &
                // "^"
        end if
        call msg_result (char (loc_str))
    end if
end subroutine lexer_show_location

```

This just prints the current stream source.

<Lexer: procedures>+≡

```

recursive subroutine lexer_show_source (lexer)
    type(lexer_t), intent(in) :: lexer
    if (associated (lexer%parent)) then
        call lexer_show_source (lexer%parent)
        call msg_message ("[includes]")
    else
        call msg_message ()
    end if
    if (associated (lexer%stream)) then
        call msg_message &
            (char (stream_get_source_info_string (lexer%stream)) // ":")
    end if
end subroutine lexer_show_source

```

7.2.9 Unit tests

Test module, followed by the corresponding implementation module.

<lexers_ut.f90>≡

<File header>

```

module lexers_ut
    use unit_tests
    use lexers_uti

```

```

    <Standard module head>

    <Lexer: public test>

    contains

    <Lexer: test driver>

    end module lexers_ut
<lexers_uti.f90>≡
    <File header>

    module lexers_uti

    <Use strings>

        use lexers

    <Standard module head>

    <Lexer: test declarations>

    contains

    <Lexer: tests>

    end module lexers_uti
API: driver for the unit tests below.
<Lexer: public test>≡
    public :: lexer_test
<Lexer: test driver>≡
    subroutine lexer_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Lexer: execute tests>
    end subroutine lexer_test

```

Test the lexer by lexing and printing all lexemes from unit u, one per line, using preset conventions.

```

<Lexer: execute tests>≡
    call test (lexer_1, "lexer_1", &
        "check lexer", u, results)
<Lexer: test declarations>≡
    public :: lexer_1
<Lexer: tests>≡
    subroutine lexer_1 (u)
        integer, intent(in) :: u
        type(lexer_t), target :: lexer
        type(stream_t), target :: stream
        type(string_t) :: string
        type(lexeme_t) :: lexeme
    end subroutine

```

```

string = "abcdefghij"
call lexer_init (lexer, &
  comment_chars = "", &
  quote_chars = "<'\"", &
  quote_match = ">'\"", &
  single_chars = "?*+=,()", &
  special_class = ["."], &
  keyword_list = null ())
call stream_init (stream, string)
call lexer_assign_stream (lexer, stream)
do
  call lex (lexeme, lexer)
  call lexeme_write (lexeme, u)
  if (lexeme_is_break (lexeme)) exit
end do
call stream_final (stream)
call lexer_final (lexer)
end subroutine lexer_1

```

7.3 Syntax rules

This module provides tools to handle syntax rules in an abstract way.

```
<syntax_rules.f90>≡  
  <File header>  
  
  module syntax_rules  
  
    <Use strings>  
    use ifiles, only: ifile_t  
    use lexers  
  
    <Standard module head>  
  
    <Syntax: public>  
  
    <Syntax: parameters>  
  
    <Syntax: types>  
  
    <Syntax: interfaces>  
  
    interface  
    <Syntax: sub interfaces>  
    end interface  
  
  end module syntax_rules  
  
<syntax_rules_sub.f90>≡  
  <File header>  
  
  submodule (syntax_rules) syntax_rules_s  
  
    use system_defs, only: LCLETTERS, UCLETTERS, DIGIT_CHARS  
    use io_units  
    use diagnostics  
    use ifiles, only: ifile_get_length  
    use ifiles, only: line_p, line_init, line_get_string_advance, line_final  
  
    implicit none  
  
    <Syntax: sub parameters>  
  
    contains  
  
    <Syntax: procedures>  
  
  end submodule syntax_rules_s
```

7.3.1 Syntax rules

Syntax rules are used by the parser. They determine how to translate the stream of lexemes as returned by the lexer into the parse tree node. A rule may be

terminal, i.e., replace a matching lexeme into a terminal node. The node will contain the lexeme interpreted as a recognized token:

- a keyword: unquoted fixed character string;
- a real number, to be determined at runtime;
- an integer, to be determined at runtime;
- a boolean value, to be determined at runtime;
- a quoted token (e.g., string), to be determined at runtime;
- an identifier (unquoted string that is not a recognized keyword), to be determined at runtime.

It may be nonterminal, i.e., contain a sequence of child rules. These are matched consecutively (and recursively) against the input stream; the resulting node will be a branch node.

- the file, i.e., the input stream as a whole;
- a sequence of syntax elements, where the last syntax element may be optional, or optional repetitive;

Sequences carry a flag that tells whether the last child is optional or may be repeated an arbitrary number of times, corresponding to the regexp modifiers `?`, `*`, and `+`.

We also need an alternative rule; this will be replaced by the node generated by one of its children that matches; thus, it does not create a node of its own.

- an alternative of syntax elements.

We also define special types of sequences as convenience macros:

- a list: a sequence where the elements are separated by a separator keyword (e.g., commas), the separators are thrown away when parsing the list;
- a group: a sequence of three tokens, where the first and third ones are left and right delimiters, the delimiters are thrown away;
- an argument list: a delimited list, containing both delimiters and separators.

It would be great to have a polymorphic type for this purpose, but until Fortran 2003 is out we have to emulate this.

Here are the syntax element codes:

```
<Syntax: public>≡
public :: S_UNKNOWN
public :: S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, S_QUOTED
public :: S_IDENTIFIER, S_KEYWORD
public :: S_SEQUENCE, S_LIST, S_GROUP, S_ARGS
public :: S_ALTERNATIVE
public :: S_IGNORE
```

```

<Syntax: parameters>≡
integer, parameter :: &
    S_UNKNOWN = 0, &
    S_LOGICAL = 1, S_INTEGER = 2, S_REAL = 3, S_COMPLEX = 4, &
    S_QUOTED = 5, S_IDENTIFIER = 6, S_KEYWORD = 7, &
    S_SEQUENCE = 8, S_LIST = 9, S_GROUP = 10, S_ARGS = 11, &
    S_ALTERNATIVE = 12, &
    S_IGNORE = 99

```

We need arrays of rule pointers, therefore this construct.

```

<Syntax: types>≡
type :: rule_p
private
    type(syntax_rule_t), pointer :: p => null ()
end type rule_p

```

Return the association status of the rule pointer:

```

<Syntax: procedures>≡
elemental function rule_is_associated (rp) result (ok)
    logical :: ok
    type (rule_p), intent(in) :: rp
    ok = associated (rp%p)
end function rule_is_associated

```

The rule type is one of the types listed above, represented by an integer code. The keyword, for a non-keyword rule, is an identifier used for the printed syntax table. The array of children is needed for nonterminal rules. In that case, there is a modifier for the last element (blank, "?", "*", or "+"), mirrored in the flags `opt` and `rep`. Then, we have the character constants used as separators and delimiters for this rule. Finally, the `used` flag can be set to indicate that this rule is the child of another rule.

```

<Syntax: types>+≡
public :: syntax_rule_t

<Syntax: types>+≡
type :: syntax_rule_t
private
    integer :: type = S_UNKNOWN
    logical :: used = .false.
    type(string_t) :: keyword
    type(string_t) :: separator
    type(string_t), dimension(2) :: delimiter
    type(rule_p), dimension(:), allocatable :: child
    character(1) :: modifier = ""
    logical :: opt = .false., rep = .false.
contains
    <Syntax: syntax rule: TBP>
end type syntax_rule_t

```

Initializer: Set type and key for a rule, but do not (yet) allocate anything.
 Finalizer: not needed (no pointer components).

```

<Syntax: procedures>+≡

```

```

subroutine syntax_rule_init (rule, key, type)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in) :: key
  integer, intent(in) :: type
  rule%keyword = key
  rule%type = type
  select case (rule%type)
  case (S_GROUP)
    call syntax_rule_set_delimiter (rule)
  case (S_LIST)
    call syntax_rule_set_separator (rule)
  case (S_ARGS)
    call syntax_rule_set_delimiter (rule)
    call syntax_rule_set_separator (rule)
  end select
end subroutine syntax_rule_init

```

These characters will not be enclosed in quotes when writing syntax rules:

```

<Syntax: sub parameters>≡
  character(*), parameter :: &
    UNQUOTED = "(),|_"/LCLETTERS/UCLETTERS/DIGIT_CHARS

```

7.3.2 Accessing rules

This is the API for syntax rules:

```

<Syntax: public>+≡
  public :: syntax_rule_get_type

<Syntax: sub interfaces>≡
  module function syntax_rule_get_type (rule) result (type)
    integer :: type
    type(syntax_rule_t), intent(in) :: rule
  end function syntax_rule_get_type

<Syntax: procedures>+≡
  module function syntax_rule_get_type (rule) result (type)
    integer :: type
    type(syntax_rule_t), intent(in) :: rule
    type = rule%type
  end function syntax_rule_get_type

<Syntax: public>+≡
  public :: syntax_rule_get_key

<Syntax: sub interfaces>+≡
  module function syntax_rule_get_key (rule) result (key)
    class(syntax_rule_t), intent(in) :: rule
    type(string_t) :: key
  end function syntax_rule_get_key

<Syntax: syntax rule: TBP>≡
  procedure :: get_key => syntax_rule_get_key

```

```

<Syntax: procedures>+≡
module function syntax_rule_get_key (rule) result (key)
  class(syntax_rule_t), intent(in) :: rule
  type(string_t) :: key
  key = rule%keyword
end function syntax_rule_get_key

<Syntax: public>+≡
public :: syntax_rule_get_separator
public :: syntax_rule_get_delimiter

<Syntax: sub interfaces>+≡
module function syntax_rule_get_separator (rule) result (separator)
  type(string_t) :: separator
  type(syntax_rule_t), intent(in) :: rule
end function syntax_rule_get_separator
module function syntax_rule_get_delimiter (rule) result (delimiter)
  type(string_t), dimension(2) :: delimiter
  type(syntax_rule_t), intent(in) :: rule
end function syntax_rule_get_delimiter

<Syntax: procedures>+≡
module function syntax_rule_get_separator (rule) result (separator)
  type(string_t) :: separator
  type(syntax_rule_t), intent(in) :: rule
  separator = rule%separator
end function syntax_rule_get_separator

module function syntax_rule_get_delimiter (rule) result (delimiter)
  type(string_t), dimension(2) :: delimiter
  type(syntax_rule_t), intent(in) :: rule
  delimiter = rule%delimiter
end function syntax_rule_get_delimiter

```

Accessing child rules. If we use `syntax_rule_get_n_sub` for determining loop bounds, we do not need a check in the second routine.

```

<Syntax: public>+≡
public :: syntax_rule_get_n_sub
public :: syntax_rule_get_sub_ptr

<Syntax: sub interfaces>+≡
module function syntax_rule_get_sub_ptr (rule, i) result (sub)
  type(syntax_rule_t), pointer :: sub
  type(syntax_rule_t), intent(in), target :: rule
  integer, intent(in) :: i
end function syntax_rule_get_sub_ptr
module function syntax_rule_get_n_sub (rule) result (n)
  integer :: n
  type(syntax_rule_t), intent(in) :: rule
end function syntax_rule_get_n_sub

<Syntax: procedures>+≡
module function syntax_rule_get_n_sub (rule) result (n)
  integer :: n
  type(syntax_rule_t), intent(in) :: rule

```



```

        if (allocated (rule%child)) then
            n = size (rule%child)
        else
            n = 0
        end if
    end function syntax_rule_get_n_sub

    module function syntax_rule_get_sub_ptr (rule, i) result (sub)
        type(syntax_rule_t), pointer :: sub
        type(syntax_rule_t), intent(in), target :: rule
        integer, intent(in) :: i
        sub => rule%child(i)%p
    end function syntax_rule_get_sub_ptr

    subroutine syntax_rule_set_sub (rule, i, sub)
        type(syntax_rule_t), intent(inout) :: rule
        integer, intent(in) :: i
        type(syntax_rule_t), intent(in), target :: sub
        rule%child(i)%p => sub
    end subroutine syntax_rule_set_sub

```

Return the modifier flags:

<Syntax: public>+≡

```

    public :: syntax_rule_last_optional
    public :: syntax_rule_last_repetitive

```

<Syntax: sub interfaces>+≡

```

    module function syntax_rule_last_optional (rule) result (opt)
        logical :: opt
        type(syntax_rule_t), intent(in) :: rule
    end function syntax_rule_last_optional
    module function syntax_rule_last_repetitive (rule) result (rep)
        logical :: rep
        type(syntax_rule_t), intent(in) :: rule
    end function syntax_rule_last_repetitive

```

<Syntax: procedures>+≡

```

    module function syntax_rule_last_optional (rule) result (opt)
        logical :: opt
        type(syntax_rule_t), intent(in) :: rule
        opt = rule%opt
    end function syntax_rule_last_optional
    module function syntax_rule_last_repetitive (rule) result (rep)
        logical :: rep
        type(syntax_rule_t), intent(in) :: rule
        rep = rule%rep
    end function syntax_rule_last_repetitive

```

Return true if the rule is atomic, i.e., logical, real, keyword etc.

<Syntax: public>+≡

```

    public :: syntax_rule_is_atomic

```

<Syntax: sub interfaces>+≡

```

    module function syntax_rule_is_atomic (rule) result (atomic)

```

```

        logical :: atomic
        type(syntax_rule_t), intent(in) :: rule
    end function syntax_rule_is_atomic

<Syntax: procedures>+≡
module function syntax_rule_is_atomic (rule) result (atomic)
    logical :: atomic
    type(syntax_rule_t), intent(in) :: rule
    select case (rule%type)
    case (S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, S_IDENTIFIER, &
          S_KEYWORD, S_QUOTED)
        atomic = .true.
    case default
        atomic = .false.
    end select
end function syntax_rule_is_atomic

```

7.3.3 I/O

Write an account of the rule. Setting `short` true will suppress the node type. Setting `key_only` true will suppress the definition. Setting `advance` false will suppress the trailing newline.

```

<Syntax: public>+≡
    public :: syntax_rule_write

<Syntax: syntax rule: TBP>+≡
    procedure :: write => syntax_rule_write

<Syntax: sub interfaces>+≡
    module subroutine syntax_rule_write (rule, unit, short, key_only, advance)
        class(syntax_rule_t), intent(in) :: rule
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: short, key_only, advance
    end subroutine syntax_rule_write

<Syntax: procedures>+≡
    module subroutine syntax_rule_write (rule, unit, short, key_only, advance)
        class(syntax_rule_t), intent(in) :: rule
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: short, key_only, advance
        logical :: typ, def, adv
        integer :: u

        u = given_output_unit (unit); if (u < 0) return
        typ = .true.; if (present (short)) typ = .not. short
        def = .true.; if (present (key_only)) def = .not. key_only
        adv = .true.; if (present (advance)) adv = advance
        select case (rule%type)
        case (S_UNKNOWN); call write_atom ("???", typ)
        case (S_IGNORE); call write_atom ("IGNORE", typ)
        case (S_LOGICAL); call write_atom ("LOGICAL", typ)
        case (S_INTEGER); call write_atom ("INTEGER", typ)
        case (S_REAL); call write_atom ("REAL", typ)
        case (S_COMPLEX); call write_atom ("COMPLEX", typ)
        case (S_IDENTIFIER); call write_atom ("IDENTIFIER", typ)

```

```

case (S_KEYWORD);    call write_atom ("KEYWORD", typ)
case (S_QUOTED)
    call write_quotes (typ, def, &
        del = rule%delimiter)
case (S_SEQUENCE)
    call write_sequence ("SEQUENCE", typ, def, size (rule%child))
case (S_GROUP)
    call write_sequence ("GROUP", typ, def, size (rule%child), &
        del = rule%delimiter)
case (S_LIST)
    call write_sequence ("LIST", typ, def, size (rule%child), &
        sep = rule%separator)
case (S_ARGS)
    call write_sequence ("ARGUMENTS", typ, def, size (rule%child), &
        del = rule%delimiter, &
        sep = rule%separator)
case (S_ALTERNATIVE)
    call write_sequence ("ALTERNATIVE", typ, def, size (rule%child), &
        sep = var_str ("|"))
end select
if (adv) write (u, *)
contains
subroutine write_type (type)
    character(*), intent(in) :: type
    character(11) :: str
    str = type
    write (u, "(1x,A)", advance="no") str
end subroutine write_type
subroutine write_key
    write (u, "(1x,A)", advance="no") char (wkey (rule))
end subroutine write_key
subroutine write_atom (type, typ)
    character(*), intent(in) :: type
    logical, intent(in) :: typ
    if (typ) call write_type (type)
    call write_key
end subroutine write_atom
subroutine write_maybe_quoted (string)
    character(*), intent(in) :: string
    character, parameter :: q = '"'
    character, parameter :: qq = '\''
    if (verify (string, UNQUOTED) == 0) then
        write (u, "(1x,A)", advance = "no") trim (string)
    else if (verify (string, q) == 0) then
        write (u, "(1x,A)", advance = "no") qq // trim (string) // qq
    else
        write (u, "(1x,A)", advance = "no") q // trim (string) // q
    end if
end subroutine write_maybe_quoted
subroutine write_quotes (typ, def, del)
    logical, intent(in) :: typ, def
    type(string_t), dimension(2), intent(in) :: del
    if (typ) call write_type ("QUOTED")
    call write_key

```

```

        if (def) then
            write (u, "(1x,'=')", advance="no")
            call write_maybe_quoted (char (del(1)))
            write (u, "(1x,A)", advance="no") "..."
            call write_maybe_quoted (char (del(2)))
        end if
    end subroutine write_quotes
    subroutine write_sequence (type, typ, def, n, del, sep)
        character(*), intent(in) :: type
        logical, intent(in) :: typ, def
        integer, intent(in) :: n
        type(string_t), dimension(2), intent(in), optional :: del
        type(string_t), intent(in), optional :: sep
        integer :: i
        if (typ) call write_type (type)
        call write_key
        if (def) then
            write (u, "(1x,'=')", advance="no")
            if (present (del)) call write_maybe_quoted (char (del(1)))
            do i = 1, n
                if (i > 1 .and. present (sep)) &
                    call write_maybe_quoted (char (sep))
                write (u, "(1x,A)", advance="no") &
                    char (wkey (syntax_rule_get_sub_ptr(rule, i)))
                if (i == n) write (u, "(A)", advance="no") trim (rule%modifier)
            end do
            if (present (del)) call write_maybe_quoted (char (del(2)))
        end if
    end subroutine write_sequence
end subroutine syntax_rule_write

```

In the printed representation, the keyword strings are enclosed as `<...>`, unless they are bare keywords. Bare keywords are enclosed as `'...'` if they contain a character which is not a letter, digit, or underscore. If they contain a single-quote character, they are enclosed as `".."`. (A keyword must not contain both single- and double-quotes.)

<Syntax: procedures>+≡

```

function wkey (rule) result (string)
    type(string_t) :: string
    type(syntax_rule_t), intent(in) :: rule
    select case (rule%type)
    case (S_KEYWORD)
        if (verify (rule%keyword, UNQUOTED) == 0) then
            string = rule%keyword
        else if (scan (rule%keyword, "'") == 0) then
            string = "'" // rule%keyword // "'"
        else
            string = '""' // rule%keyword // '""'
        end if
    case default
        string = "<" // rule%keyword // ">"
    end select
end function wkey

```

7.3.4 Completing syntax rules

Set the separator and delimiter entries, using defaults:

```
<Syntax: procedures>+≡
subroutine syntax_rule_set_separator (rule, separator)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in), optional :: separator
  if (present (separator)) then
    rule%separator = separator
  else
    rule%separator = ","
  end if
end subroutine syntax_rule_set_separator

subroutine syntax_rule_set_delimiter (rule, delimiter)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), dimension(2), intent(in), optional :: delimiter
  if (present (delimiter)) then
    rule%delimiter = delimiter
  else
    rule%delimiter(1) = "("
    rule%delimiter(2) = ")"
  end if
end subroutine syntax_rule_set_delimiter
```

Set the modifier entry and corresponding flags:

```
<Syntax: procedures>+≡
function is_modifier (string) result (ok)
  logical :: ok
  type(string_t), intent(in) :: string
  select case (char (string))
    case (" ", "?", "*", "+"); ok = .true.
    case default; ok = .false.
  end select
end function is_modifier

subroutine syntax_rule_set_modifier (rule, modifier)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in) :: modifier
  rule%modifier = char (modifier)
  select case (rule%modifier)
    case (" ")
    case ("?"); rule%opt = .true.
    case ("*"); rule%opt = .true.; rule%rep = .true.
    case ("+"); rule%rep = .true.
    case default
      call msg_bug (" Syntax: sequence modifier '" // rule%modifier &
        // "' is not one of '+' '*' '?'")
  end select
end subroutine syntax_rule_set_modifier
```

Check a finalized rule for completeness

(Syntax: procedures)+≡

```

subroutine syntax_rule_check (rule)
  type(syntax_rule_t), intent(in) :: rule
  if (rule%keyword == "") call msg_bug ("Rule key not set")
  select case (rule%type)
  case (S_UNKNOWN); call bug (" Undefined rule")
  case (S_IGNORE, S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, &
        S_IDENTIFIER, S_KEYWORD)
  case (S_QUOTED)
    if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
      call bug (" Missing quote character(s)")
  case (S_SEQUENCE)
  case (S_GROUP)
    if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
      call bug (" Missing delimiter(s)")
  case (S_LIST)
    if (rule%separator == "") call bug (" Missing separator")
  case (S_ARGS)
    if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
      call bug (" Missing delimiter(s)")
    if (rule%separator == "") call bug (" Missing separator")
  case (S_ALTERNATIVE)
  case default
    call bug (" Undefined syntax code")
  end select
  select case (rule%type)
  case (S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)
    if (allocated (rule%child)) then
      if (.not.all (rule_is_associated (rule%child))) &
        call bug (" Child rules not all associated")
    else
      call bug (" Parent rule without children")
    end if
  case default
    if (allocated (rule%child)) call bug (" Non-parent rule with children")
  end select
contains
  subroutine bug (string)
    character(*), intent(in) :: string
    call msg_bug (" Syntax table: Rule " // char (rule%keyword) // ": " &
      // string)
  end subroutine bug
end subroutine syntax_rule_check

```

7.3.5 Syntax tables

A syntax table contains the tree of syntax rules and, for direct parser access, the list of valid keywords.

Types

The syntax contains an array of rules and a list of keywords. The array is actually used as a tree, where the top rule is the first array element, and the other rules are recursively pointed to by this first rule. (No rule should be used twice or be unused.) The keyword list is derived from the rule tree.

Objects of this type need the target attribute if they are associated with a lexer. The keyword list will be pointed to by this lexer.

```
<Syntax: public>+≡
    public :: syntax_t

<Syntax: types>+≡
    type :: syntax_t
    private
        type(syntax_rule_t), dimension(:), allocatable :: rule
        type(keyword_list_t) :: keyword_list
    end type syntax_t
```

Constructor/destructor

Initialize and finalize syntax tables

```
<Syntax: public>+≡
    public :: syntax_init
    public :: syntax_final
```

There are two ways to create a syntax: hard-coded from rules or dynamically from file.

```
<Syntax: interfaces>≡
    interface syntax_init
        module procedure syntax_init_from_ifile
    end interface
```

The syntax definition is read from an ifile object which contains the syntax definitions in textual form, one rule per line. This interface allows for determining the number of rules beforehand.

To parse the rule definitions, we make up a temporary lexer. Obviously, we cannot use a generic parser yet, so we have to hardcode the parsing process.

```
<Syntax: sub interfaces>+≡
    module subroutine syntax_init_from_ifile (syntax, ifile)
        type(syntax_t), intent(out), target :: syntax
        type(ifile_t), intent(in) :: ifile
    end subroutine syntax_init_from_ifile

<Syntax: procedures>+≡
    module subroutine syntax_init_from_ifile (syntax, ifile)
        type(syntax_t), intent(out), target :: syntax
        type(ifile_t), intent(in) :: ifile
        type(lexer_t) :: lexer
        type(line_p) :: line
        type(string_t) :: string
        integer :: n_token
        integer :: i
```

```

call lexer_init (lexer, &
  comment_chars = "", &
  quote_chars = "<'\"", &
  quote_match = ">'\"", &
  single_chars = "?*+|=,()", &
  special_class = ["."], &
  keyword_list = null ())
allocate (syntax%rule (ifile_get_length (ifile)))
call line_init (line, ifile)
do i = 1, size (syntax%rule)
  string = line_get_string_advance (line)
  call set_rule_type_and_key (syntax%rule(i), string, lexer)
end do
call line_init (line, ifile)
do i = 1, size (syntax%rule)
  string = line_get_string_advance (line)
  select case (syntax%rule(i)%type)
  case (S_QUOTED, S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)
    n_token = get_n_token (string, lexer)
    call set_rule_contents &
      (syntax%rule(i), syntax, n_token, string, lexer)
  end select
end do
call line_final (line)
call lexer_final (lexer)
call syntax_make_keyword_list (syntax)
if (.not. all (syntax%rule%used)) then
  do i = 1, size (syntax%rule)
    if (.not. syntax%rule(i)%used) then
      call syntax_rule_write (syntax%rule(i), 6)
    end if
  end do
  call msg_bug (" Syntax table: unused rules")
end if
end subroutine syntax_init_from_ifile

```

For a given rule defined in the input, the first task is to determine its type and key. With these, we can initialize the rule in the table, postponing the association of children.

(Syntax: procedures)+≡

```

subroutine set_rule_type_and_key (rule, string, lexer)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in) :: string
  type(lexer_t), intent(inout) :: lexer
  type(stream_t), target :: stream
  type(lexeme_t) :: lexeme
  type(string_t) :: key
  character(2) :: type
  call lexer_clear (lexer)
  call stream_init (stream, string)
  call lexer_assign_stream (lexer, stream)
  call lex (lexeme, lexer)
  type = lexeme_get_string (lexeme)

```



```

call lex (lexeme, lexer)
key = lexeme_get_contents (lexeme)
call stream_final (stream)
if (trim (key) /= "") then
  select case (type)
    case ("IG"); call syntax_rule_init (rule, key, S_IGNORE)
    case ("LO"); call syntax_rule_init (rule, key, S_LOGICAL)
    case ("IN"); call syntax_rule_init (rule, key, S_INTEGER)
    case ("RE"); call syntax_rule_init (rule, key, S_REAL)
    case ("CO"); call syntax_rule_init (rule, key, S_COMPLEX)
    case ("ID"); call syntax_rule_init (rule, key, S_IDENTIFIER)
    case ("KE"); call syntax_rule_init (rule, key, S_KEYWORD)
    case ("QU"); call syntax_rule_init (rule, key, S_QUOTED)
    case ("SE"); call syntax_rule_init (rule, key, S_SEQUENCE)
    case ("GR"); call syntax_rule_init (rule, key, S_GROUP)
    case ("LI"); call syntax_rule_init (rule, key, S_LIST)
    case ("AR"); call syntax_rule_init (rule, key, S_ARGS)
    case ("AL"); call syntax_rule_init (rule, key, S_ALTERNATIVE)
    case default
      call lexer_show_location (lexer)
      call msg_bug (" Syntax definition: unknown type '" // type // "'")
    end select
  else
    print *, char (string)
    call msg_bug (" Syntax definition: empty rule key")
  end if
end subroutine set_rule_type_and_key

```

This function returns the number of tokens in an input line.

<Syntax: procedures>+≡

```

function get_n_token (string, lexer) result (n)
  integer :: n
  type(string_t), intent(in) :: string
  type(lexer_t), intent(inout) :: lexer
  type(stream_t), target :: stream
  type(lexeme_t) :: lexeme
  integer :: i
  call lexer_clear (lexer)
  call stream_init (stream, string)
  call lexer_assign_stream (lexer, stream)
  i = 0
  do
    call lex (lexeme, lexer)
    if (lexeme_is_break (lexeme)) exit
    i = i + 1
  end do
  n = i
  call stream_final (stream)
end function get_n_token

```

Assign the pointer to the rule associated with a given key (assumes that the rule array is allocated)

<Syntax: public>+≡

```

public :: syntax_get_rule_ptr
<Syntax: sub interfaces>+≡
    module function syntax_get_rule_ptr (syntax, key) result (rule)
        type(syntax_rule_t), pointer :: rule
        type(syntax_t), intent(in), target :: syntax
        type(string_t), intent(in) :: key
    end function syntax_get_rule_ptr
<Syntax: procedures>+≡
    module function syntax_get_rule_ptr (syntax, key) result (rule)
        type(syntax_rule_t), pointer :: rule
        type(syntax_t), intent(in), target :: syntax
        type(string_t), intent(in) :: key
        integer :: i
        do i = 1, size (syntax%rule)
            if (syntax%rule(i)%keyword == key) then
                rule => syntax%rule(i)
                return
            end if
        end do
        call msg_bug (" Syntax table: Rule " // char (key) // " not found")
    end function syntax_get_rule_ptr

```

This subroutine extracts the rule contents for an input line. There are three tasks: (1) determine the number of children, depending on the rule type; (2) find and set the separator and delimiter strings, if required; (3) scan the child rules, find them in the syntax table and associate the parent rule with them.

```

<Syntax: procedures>+≡
    subroutine set_rule_contents (rule, syntax, n_token, string, lexer)
        type(syntax_rule_t), intent(inout) :: rule
        type(syntax_t), intent(in), target :: syntax
        integer, intent(in) :: n_token
        type(string_t), intent(in) :: string
        type(lexer_t), intent(inout) :: lexer
        type(stream_t), target :: stream
        type(lexeme_t), dimension(n_token) :: lexeme
        integer :: i, n_children
        call lexer_clear (lexer)
        call stream_init (stream, string)
        call lexer_assign_stream (lexer, stream)
        do i = 1, n_token
            call lex (lexeme(i), lexer)
        end do
        call stream_final (stream)
        n_children = get_n_children ()
        call set_delimiters
        if (n_children > 1) call set_separator
        if (n_children > 0) call set_children
    contains
        function get_n_children () result (n_children)
            integer :: n_children
            select case (rule%type)
            case (S_QUOTED)

```

```

        if (n_token /= 6) call broken_rule (rule)
        n_children = 0
    case (S_GROUP)
        if (n_token /= 6) call broken_rule (rule)
        n_children = 1
    case (S_SEQUENCE)
        if (is_modifier (lexeme_get_string (lexeme(n_token)))) then
            if (n_token <= 4) call broken_rule (rule)
            call syntax_rule_set_modifier &
                (rule, lexeme_get_string (lexeme(n_token)))
            n_children = n_token - 4
        else
            if (n_token <= 3) call broken_rule (rule)
            n_children = n_token - 3
        end if
    case (S_LIST)
        if (is_modifier (lexeme_get_string (lexeme(n_token)))) then
            if (n_token <= 4 .or. mod (n_token, 2) /= 1) &
                call broken_rule (rule)
            call syntax_rule_set_modifier &
                (rule, lexeme_get_string (lexeme(n_token)))
        else if (n_token <= 3 .or. mod (n_token, 2) /= 0) then
            call broken_rule (rule)
        end if
        n_children = (n_token - 2) / 2
    case (S_ARGS)
        if (is_modifier (lexeme_get_string (lexeme(n_token-1)))) then
            if (n_token <= 6 .or. mod (n_token, 2) /= 1) &
                call broken_rule (rule)
            call syntax_rule_set_modifier &
                (rule, lexeme_get_string (lexeme(n_token-1)))
        else if (n_token <= 5 .or. mod (n_token, 2) /= 0) then
            call broken_rule (rule)
        end if
        n_children = (n_token - 4) / 2
    case (S_ALTERNATIVE)
        if (n_token <= 3 .or. mod (n_token, 2) /= 0) call broken_rule (rule)
        n_children = (n_token - 2) / 2
    end select
end function get_n_children
subroutine set_delimiters
    type(string_t), dimension(2) :: delimiter
    select case (rule%type)
    case (S_QUOTED, S_GROUP, S_ARGS)
        delimiter(1) = lexeme_get_contents (lexeme(4))
        delimiter(2) = lexeme_get_contents (lexeme(n_token))
        call syntax_rule_set_delimiter (rule, delimiter)
    end select
end subroutine set_delimiters
subroutine set_separator
    type(string_t) :: separator
    select case (rule%type)
    case (S_LIST)
        separator = lexeme_get_contents (lexeme(5))

```

```

        call syntax_rule_set_separator (rule, separator)
    case (S_ARGS)
        separator = lexeme_get_contents (lexeme(6))
        call syntax_rule_set_separator (rule, separator)
    end select
end subroutine set_separator
subroutine set_children
    allocate (rule%child(n_children))
    select case (rule%type)
    case (S_GROUP)
        call syntax_rule_set_sub (rule, 1, syntax_get_rule_ptr (syntax, &
            lexeme_get_contents (lexeme(5))))
    case (S_SEQUENCE)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(i+3))))
        end do
    case (S_LIST, S_ALTERNATIVE)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(2*i+2))))
        end do
    case (S_ARGS)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(2*i+3))))
        end do
    end select
end subroutine set_children
subroutine broken_rule (rule)
    type(syntax_rule_t), intent(in) :: rule
    call lexer_show_location (lexer)
    call msg_bug (" Syntax definition: broken rule '" &
        // char (wkey (rule)) // "'")
end subroutine broken_rule
end subroutine set_rule_contents

```

This routine completes the syntax table object. We assume that the rule array is set up. We associate the top rule with the first entry in the rule array and build up the keyword list.

The keyword list includes delimiters and separators. Filling it can only be done after all rules are set. We scan the rule tree. For each keyword that we find, we try to add it to the keyword list; the pointer to the last element is carried along with the recursive scanning. Before appending a keyword, we check whether it is already in the list.

<Syntax: procedures>+≡

```

subroutine syntax_make_keyword_list (syntax)
    type(syntax_t), intent(inout), target :: syntax
    type(syntax_rule_t), pointer :: rule
    rule => syntax%rule(1)
    call rule_scan_rec (rule, syntax%keyword_list)
contains
    recursive subroutine rule_scan_rec (rule, keyword_list)

```

```

type(syntax_rule_t), pointer :: rule
type(keyword_list_t), intent(inout) :: keyword_list
integer :: i
if (rule%used) return
rule%used = .true.
select case (rule%type)
case (S_UNKNOWN)
  call msg_bug (" Syntax: rule tree contains undefined rule")
case (S_KEYWORD)
  call keyword_list_add (keyword_list, rule%keyword)
end select
select case (rule%type)
case (S_LIST, S_ARGS)
  call keyword_list_add (keyword_list, rule%separator)
end select
select case (rule%type)
case (S_GROUP, S_ARGS)
  call keyword_list_add (keyword_list, rule%delimiter(1))
  call keyword_list_add (keyword_list, rule%delimiter(2))
end select
select case (rule%type)
case (S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)
  if (.not. allocated (rule%child)) &
    call msg_bug (" Syntax: Non-terminal rule without children")
case default
  if (allocated (rule%child)) &
    call msg_bug (" Syntax: Terminal rule with children")
end select
if (allocated (rule%child)) then
  do i = 1, size (rule%child)
    call rule_scan_rec (rule%child(i)%p, keyword_list)
  end do
end if
end subroutine rule_scan_rec
end subroutine syntax_make_keyword_list

```

The finalizer deallocates the rule pointer array and deletes the keyword list.

```

<Syntax: sub interfaces>+≡
  module subroutine syntax_final (syntax)
    type(syntax_t), intent(inout) :: syntax
    end subroutine syntax_final

<Syntax: procedures>+≡
  module subroutine syntax_final (syntax)
    type(syntax_t), intent(inout) :: syntax
    if (allocated (syntax%rule)) deallocate (syntax%rule)
    call keyword_list_final (syntax%keyword_list)
  end subroutine syntax_final

```

7.3.6 Accessing the syntax table

Return a pointer to the top rule

```

<Syntax: public>+≡

```

```

    public :: syntax_get_top_rule_ptr
<Syntax: sub interfaces>+≡
    module function syntax_get_top_rule_ptr (syntax) result (rule)
        type(syntax_rule_t), pointer :: rule
        type(syntax_t), intent(in), target :: syntax
    end function syntax_get_top_rule_ptr
<Syntax: procedures>+≡
    module function syntax_get_top_rule_ptr (syntax) result (rule)
        type(syntax_rule_t), pointer :: rule
        type(syntax_t), intent(in), target :: syntax
        if (allocated (syntax%rule)) then
            rule => syntax%rule(1)
        else
            rule => null ()
        end if
    end function syntax_get_top_rule_ptr

```

Return a pointer to the keyword list

```

<Syntax: public>+≡
    public :: syntax_get_keyword_list_ptr
<Syntax: sub interfaces>+≡
    module function syntax_get_keyword_list_ptr (syntax) result (keyword_list)
        type(keyword_list_t), pointer :: keyword_list
        type(syntax_t), intent(in), target :: syntax
    end function syntax_get_keyword_list_ptr
<Syntax: procedures>+≡
    module function syntax_get_keyword_list_ptr (syntax) result (keyword_list)
        type(keyword_list_t), pointer :: keyword_list
        type(syntax_t), intent(in), target :: syntax
        keyword_list => syntax%keyword_list
    end function syntax_get_keyword_list_ptr

```

7.3.7 I/O

Write a readable representation of the syntax table

```

<Syntax: public>+≡
    public :: syntax_write
<Syntax: sub interfaces>+≡
    module subroutine syntax_write (syntax, unit)
        type(syntax_t), intent(in) :: syntax
        integer, intent(in), optional :: unit
    end subroutine syntax_write
<Syntax: procedures>+≡
    module subroutine syntax_write (syntax, unit)
        type(syntax_t), intent(in) :: syntax
        integer, intent(in), optional :: unit
        integer :: u
        integer :: i
        u = given_output_unit (unit); if (u < 0) return

```

```

write (u, "(A)") "Syntax table:"
if (allocated (syntax%rule)) then
  do i = 1, size (syntax%rule)
    call syntax_rule_write (syntax%rule(i), u)
  end do
else
  write (u, "(1x,A)") "[not allocated]"
end if
call keyword_list_write (syntax%keyword_list, u)
end subroutine syntax_write

```

7.4 The parser

On a small scale, the parser interprets the string tokens returned by the lexer; they are interpreted as numbers, keywords and such and stored as a typed object. On a large scale, a text is read, parsed, and a syntax rule set is applied such that the tokens are stored as a parse tree. Syntax errors are spotted in this process, so the resulting parse tree is syntactically correct by definition.

```
<parser.f90>≡
  <File header>

  module parser

    <Use kinds>
    <Use strings>
    use lexers
    use syntax_rules

    <Standard module head>

    <Parser: public>

    <Parser: types>

    <Parser: interfaces>

    interface
    <Parser: sub interfaces>
    end interface

  end module parser

<parser_sub.f90>≡
  <File header>

  submodule (parser) parser_s

    use io_units
    use diagnostics
    use md5
    use system_defs, only: DIGIT_CHARS
    use format_defs, only: FMT_19

    implicit none

  contains

    <Parser: procedures>

  end submodule parser_s
```


7.4.1 The token type

Tokens are elements of the parsed input that carry a value: logical, integer, real, quoted string, (unquoted) identifier, or known keyword. Note that non-keyword tokens also have an abstract key attached to them.

This is an obvious candidate for polymorphism.

(Parser: types)≡

```
type :: token_t
private
integer :: type = S_UNKNOWN
logical, pointer :: lval => null ()
integer, pointer :: ival => null ()
real(default), pointer :: rval => null ()
complex(default), pointer :: cval => null ()
type(string_t), pointer :: sval => null ()
type(string_t), pointer :: kval => null ()
type(string_t), dimension(:), pointer :: quote => null ()
end type token_t
```

Create a token from the lexeme returned by the lexer: Allocate storage and try to interpret the lexeme according to the type that is requested by the parser. For a keyword token, match the lexeme against the requested key. If successful, set the token type, value, and key. Otherwise, set the type to S_UNKNOWN.

(Parser: procedures)≡

```
subroutine token_init (token, lexeme, requested_type, key)
type(token_t), intent(out) :: token
type(lexeme_t), intent(in) :: lexeme
integer, intent(in) :: requested_type
type(string_t), intent(in) :: key
integer :: type
type = lexeme_get_type (lexeme)
token%type = S_UNKNOWN
select case (requested_type)
case (S_LOGICAL)
if (type == T_IDENTIFIER) call read_logical &
(char (lexeme_get_string (lexeme)))
case (S_INTEGER)
if (type == T_NUMERIC) call read_integer &
(char (lexeme_get_string (lexeme)))
case (S_REAL)
if (type == T_NUMERIC) call read_real &
(char (lexeme_get_string (lexeme)))
case (S_COMPLEX)
if (type == T_NUMERIC) call read_complex &
(char (lexeme_get_string (lexeme)))
case (S_IDENTIFIER)
if (type == T_IDENTIFIER) call read_identifier &
(lexeme_get_string (lexeme))
case (S_KEYWORD)
if (type == T_KEYWORD) call check_keyword &
(lexeme_get_string (lexeme), key)
case (S_QUOTED)
if (type == T_QUOTED) call read_quoted &
```

```

        (lexeme_get_contents (lexeme), lexeme_get_delimiters (lexeme))
case default
    print *, requested_type
    call msg_bug (" Invalid token type code requested by the parser")
end select
if (token%type /= S_UNKNOWN) then
    allocate (token%kval)
    token%kval = key
end if
contains
subroutine read_logical (s)
    character(*), intent(in) :: s
    select case (s)
    case ("t", "T", "true", "TRUE", "y", "Y", "yes", "YES")
        allocate (token%lval)
        token%lval = .true.
        token%type = S_LOGICAL
    case ("f", "F", "false", "FALSE", "n", "N", "no", "NO")
        allocate (token%lval)
        token%lval = .false.
        token%type = S_LOGICAL
    end select
end subroutine read_logical
subroutine read_integer (s)
    character(*), intent(in) :: s
    integer :: tmp, iostat
    if (verify (s, DIGIT_CHARS) == 0) then
        read (s, *, iostat=iostat) tmp
        if (iostat == 0) then
            allocate (token%ival)
            token%ival = tmp
            token%type = S_INTEGER
        end if
    end if
end subroutine read_integer
subroutine read_real (s)
    character(*), intent(in) :: s
    real(default) :: tmp
    integer :: iostat
    read (s, *, iostat=iostat) tmp
    if (iostat == 0) then
        allocate (token%rval)
        token%rval = tmp
        token%type = S_REAL
    end if
end subroutine read_real
subroutine read_complex (s)
    character(*), intent(in) :: s
    complex(default) :: tmp
    integer :: iostat
    read (s, *, iostat=iostat) tmp
    if (iostat == 0) then
        allocate (token%cval)
        token%cval = tmp
    end if
end subroutine read_complex

```

```

        token%type = S_COMPLEX
    end if
end subroutine read_complex
subroutine read_identifier (s)
    type(string_t), intent(in) :: s
    allocate (token%sval)
    token%sval = s
    token%type = S_IDENTIFIER
end subroutine read_identifier
subroutine check_keyword (s, key)
    type(string_t), intent(in) :: s
    type(string_t), intent(in) :: key
    if (key == s) token%type = S_KEYWORD
end subroutine check_keyword
subroutine read_quoted (s, del)
    type(string_t), intent(in) :: s
    type(string_t), dimension(2), intent(in) :: del
    allocate (token%sval, token%quote(2))
    token%sval = s
    token%quote(1) = del(1)
    token%quote(2) = del(2)
    token%type = S_QUOTED
end subroutine read_quoted
end subroutine token_init

```

Manually set a token to a keyword.

```

(Parser: procedures)+≡
subroutine token_init_key (token, key)
    type(token_t), intent(out) :: token
    type(string_t), intent(in) :: key
    token%type = S_KEYWORD
    allocate (token%kval)
    token%kval = key
end subroutine token_init_key

```

Reset a token to an empty state, freeing allocated memory, and deallocate the token itself.

```

(Parser: procedures)+≡
subroutine token_final (token)
    type(token_t), intent(inout) :: token
    token%type = S_UNKNOWN
    if (associated (token%lval)) deallocate (token%lval)
    if (associated (token%ival)) deallocate (token%ival)
    if (associated (token%rval)) deallocate (token%rval)
    if (associated (token%sval)) deallocate (token%sval)
    if (associated (token%kval)) deallocate (token%kval)
    if (associated (token%quote)) deallocate (token%quote)
end subroutine token_final

```

Check for empty=valid token:

```

(Parser: procedures)+≡
function token_is_valid (token) result (valid)

```

```

logical :: valid
type(token_t), intent(in) :: token
valid = token%type /= S_UNKNOWN
end function token_is_valid

```

Write the contents of a token.

```

(Parser: procedures)+≡
subroutine token_write (token, unit)
  type(token_t), intent(in) :: token
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  select case (token%type)
  case (S_LOGICAL)
    write (u, "(L1)") token%lval
  case (S_INTEGER)
    write (u, "(I0)") token%ival
  case (S_REAL)
    write (u, "(" // FMT_19 // ")") token%rval
  case (S_COMPLEX)
    write (u, "((''," // FMT_19 // "',''," // FMT_19 // "',''))" token%cval
  case (S_IDENTIFIER)
    write (u, "(A)") char (token%sval)
  case (S_KEYWORD)
    write (u, "(A,A)" '[keyword]' // char (token%kval)
  case (S_QUOTED)
    write (u, "(A)" &
      char (token%quote(1)) // char (token%sval) // char (token%quote(2))
  case default
    write (u, "(A)" '[empty]'
  end select
end subroutine token_write

```

Token assignment via deep copy. This is useful to avoid confusion when the token is transferred to some parse-tree node.

```

(Parser: interfaces)≡
interface assignment(=)
  module procedure token_assign
  module procedure token_assign_integer
  module procedure token_assign_real
  module procedure token_assign_complex
  module procedure token_assign_logical
  module procedure token_assign_string
end interface

```

We need to copy only the contents that are actually assigned, the other pointers remain disassociated.

```

(Parser: sub interfaces)≡
module subroutine token_assign (token, token_in)
  type(token_t), intent(out) :: token
  type(token_t), intent(in) :: token_in
end subroutine token_assign

```

```

(Parser: procedures)+≡
module subroutine token_assign (token, token_in)
  type(token_t), intent(out) :: token
  type(token_t), intent(in) :: token_in
  token%type = token_in%type
  select case (token%type)
  case (S_LOGICAL);    allocate (token%lval); token%lval = token_in%lval
  case (S_INTEGER);    allocate (token%ival); token%ival = token_in%ival
  case (S_REAL);       allocate (token%rval); token%rval = token_in%rval
  case (S_COMPLEX);    allocate (token%cval); token%cval = token_in%cval
  case (S_IDENTIFIER); allocate (token%sval); token%sval = token_in%sval
  case (S_QUOTED);     allocate (token%sval); token%sval = token_in%sval
                      allocate (token%quote(2)); token%quote = token_in%quote
  end select
  if (token%type /= S_UNKNOWN) then
    allocate (token%kval); token%kval = token_in%kval
  end if
end subroutine token_assign

```

We need to copy only the contents that are actually assigned, the other pointers remain disassociated.

```

(Parser: sub interfaces)+≡
module subroutine token_assign_integer (token, ival)
  type(token_t), intent(out) :: token
  integer, intent(in) :: ival
end subroutine token_assign_integer
module subroutine token_assign_real (token, rval)
  type(token_t), intent(out) :: token
  real(default), intent(in) :: rval
end subroutine token_assign_real
module subroutine token_assign_complex (token, cval)
  type(token_t), intent(out) :: token
  complex(default), intent(in) :: cval
end subroutine token_assign_complex
module subroutine token_assign_logical (token, lval)
  type(token_t), intent(out) :: token
  logical, intent(in) :: lval
end subroutine token_assign_logical
module subroutine token_assign_string (token, sval)
  type(token_t), intent(out) :: token
  type(string_t), intent(in) :: sval
end subroutine token_assign_string

```

```

(Parser: procedures)+≡
module subroutine token_assign_integer (token, ival)
  type(token_t), intent(out) :: token
  integer, intent(in) :: ival
  token%type = S_INTEGER
  allocate (token%ival)
  token%ival = ival
end subroutine token_assign_integer

module subroutine token_assign_real (token, rval)
  type(token_t), intent(out) :: token

```

```

    real(default), intent(in) :: rval
    token%type = S_REAL
    allocate (token%rval)
    token%rval = rval
end subroutine token_assign_real

module subroutine token_assign_complex (token, cval)
    type(token_t), intent(out) :: token
    complex(default), intent(in) :: cval
    token%type = S_COMPLEX
    allocate (token%cval)
    token%cval = cval
end subroutine token_assign_complex

module subroutine token_assign_logical (token, lval)
    type(token_t), intent(out) :: token
    logical, intent(in) :: lval
    token%type = S_LOGICAL
    allocate (token%lval)
    token%lval = lval
end subroutine token_assign_logical

module subroutine token_assign_string (token, sval)
    type(token_t), intent(out) :: token
    type(string_t), intent(in) :: sval
    token%type = S_QUOTED
    allocate (token%sval)
    token%sval = sval
    allocate (token%quote(2)); token%quote = ''
end subroutine token_assign_string

```

7.4.2 Retrieve token contents

These functions all do a trivial sanity check that should avoid crashes.

(Parser: procedures)+≡

```

function token_get_logical (token) result (lval)
    logical :: lval
    type(token_t), intent(in) :: token
    if (associated (token%lval)) then
        lval = token%lval
    else
        call token_mismatch (token, "logical")
    end if
end function token_get_logical

function token_get_integer (token) result (ival)
    integer :: ival
    type(token_t), intent(in) :: token
    if (associated (token%ival)) then
        ival = token%ival
    else
        call token_mismatch (token, "integer")
    end if
end function token_get_integer

```

```

    end if
end function token_get_integer

function token_get_real (token) result (rval)
    real(default) :: rval
    type(token_t), intent(in) :: token
    if (associated (token%rval)) then
        rval = token%rval
    else
        call token_mismatch (token, "real")
    end if
end function token_get_real

function token_get_cmplx (token) result (cval)
    complex(default) :: cval
    type(token_t), intent(in) :: token
    if (associated (token%cval)) then
        cval = token%cval
    else
        call token_mismatch (token, "complex")
    end if
end function token_get_cmplx

function token_get_string (token) result (sval)
    type(string_t) :: sval
    type(token_t), intent(in) :: token
    if (associated (token%sval)) then
        sval = token%sval
    else
        call token_mismatch (token, "string")
    end if
end function token_get_string

function token_get_key (token) result (kval)
    type(string_t) :: kval
    type(token_t), intent(in) :: token
    if (associated (token%kval)) then
        kval = token%kval
    else
        call token_mismatch (token, "keyword")
    end if
end function token_get_key

function token_get_quote (token) result (quote)
    type(string_t), dimension(2) :: quote
    type(token_t), intent(in) :: token
    if (associated (token%quote)) then
        quote = token%quote
    else
        call token_mismatch (token, "quote")
    end if
end function token_get_quote

```

(Parser: procedures)+≡

```

subroutine token_mismatch (token, type)
  type(token_t), intent(in) :: token
  character(*), intent(in) :: type
  write (6, "(A)", advance="no") "Token: "
  call token_write (token)
  call msg_bug (" Token type mismatch; value required as " // type)
end subroutine token_mismatch

```

7.4.3 The parse tree: nodes

The parser will generate a parse tree from the input stream. Each node in this parse tree points to the syntax rule that was applied. (Since syntax rules are stored in a pointer-type array within the syntax table, they qualify as targets.) A leaf node contains a token. A branch node has subnodes. The subnodes are stored as a list, so each node also has a `next` pointer.

```

(Parser: public)≡
  public :: parse_node_t

(Parser: types)+≡
  type :: parse_node_t
  private
    type(syntax_rule_t), pointer :: rule => null ()
    type(token_t) :: token
    integer :: n_sub = 0
    type(parse_node_t), pointer :: sub_first => null ()
    type(parse_node_t), pointer :: sub_last => null ()
    type(parse_node_t), pointer :: next => null ()
  contains
    (Parser: parse node: TBP)
  end type parse_node_t

```

Container for parse node pointers, useful for creating pointer arrays:

```

(Parser: public)+≡
  public :: parse_node_p

(Parser: types)+≡
  type :: parse_node_p
    type(parse_node_t), pointer :: ptr => null ()
  end type parse_node_p

```

Output. The first version writes a node together with its sub-node tree, organized by indentation.

```

(Parser: parse node: TBP)≡
  procedure :: write => parse_node_write_rec

(Parser: public)+≡
  public :: parse_node_write_rec

(Parser: sub interfaces)+≡
  recursive module subroutine parse_node_write_rec (node, unit, short, depth)
    class(parse_node_t), intent(in), target :: node
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: short

```



```

        integer, intent(in), optional :: depth
    end subroutine parse_node_write_rec

<Parser: procedures>+≡
recursive module subroutine parse_node_write_rec (node, unit, short, depth)
    class(parse_node_t), intent(in), target :: node
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: short
    integer, intent(in), optional :: depth
    integer :: u, d
    type(parse_node_t), pointer :: current
    u = given_output_unit (unit); if (u < 0) return
    d = 0; if (present (depth)) d = depth
    call parse_node_write (node, u, short=short)
    current => node%sub_first
    do while (associated (current))
        write (u, "(A)", advance = "no") repeat ("| ", d)
        call parse_node_write_rec (current, unit, short, d+1)
        current => current%next
    end do
end subroutine parse_node_write_rec

```

This does the actual output for a single node, without recursion.

```

<Parser: public>+≡
public :: parse_node_write

<Parser: sub interfaces>+≡
module subroutine parse_node_write (node, unit, short)
    class(parse_node_t), intent(in) :: node
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: short
end subroutine parse_node_write

<Parser: procedures>+≡
module subroutine parse_node_write (node, unit, short)
    class(parse_node_t), intent(in) :: node
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: short
    integer :: u
    type(parse_node_t), pointer :: current
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(' + ')", advance = "no")
    if (associated (node%rule)) then
        call syntax_rule_write (node%rule, u, &
            short=short, key_only=.true., advance=.false.)
    if (token_is_valid (node%token)) then
        write (u, "(' = ')", advance="no")
        call token_write (node%token, u)
    else if (associated (node%sub_first)) then
        write (u, "(' = ')", advance="no")
        current => node%sub_first
        do while (associated (current))
            call syntax_rule_write (current%rule, u, &
                short=.true., key_only=.true., advance=.false.)
            current => current%next
        end do
    end if
end subroutine parse_node_write

```

```

        end do
        write (u, *)
    else
        write (u, *)
    end if
else
    write (u, *) "[empty]"
end if
end subroutine parse_node_write

```

Finalize the token and recursively finalize and deallocate all sub-nodes.

```

<Parser: public>+≡
    public :: parse_node_final

<Parser: sub interfaces>+≡
    recursive module subroutine parse_node_final (node, recursive)
        type(parse_node_t), intent(inout) :: node
        logical, intent(in), optional :: recursive
    end subroutine parse_node_final

<Parser: procedures>+≡
    recursive module subroutine parse_node_final (node, recursive)
        type(parse_node_t), intent(inout) :: node
        type(parse_node_t), pointer :: current
        logical, intent(in), optional :: recursive
        logical :: rec
        rec = .true.; if (present (recursive)) rec = recursive
        call token_final (node%token)
        if (rec) then
            do while (associated (node%sub_first))
                current => node%sub_first
                node%sub_first => node%sub_first%next
                call parse_node_final (current)
                deallocate (current)
            end do
        end if
    end subroutine parse_node_final

```

7.4.4 Filling nodes

The constructors allocate and initialize the node. There are two possible initializers (in a later version, should correspond to different type extensions).

First, leaf (terminal) nodes. The token constructor does the actual work, looking at the requested type and key for the given rule and matching against the lexeme contents. If it fails, the token will keep the type `S_UNKNOWN` and remain empty. Otherwise, we have a valid node which contains the new token.

If the lexeme argument is absent, the token is left empty.

```

<Parser: procedures>+≡
    subroutine parse_node_create_leaf (node, rule, lexeme)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        type(lexeme_t), intent(in) :: lexeme
    end subroutine parse_node_create_leaf

```

```

allocate (node)
node%rule => rule
call token_init (node%token, lexeme, &
    syntax_rule_get_type (rule), syntax_rule_get_key (rule))
if (.not. token_is_valid (node%token)) deallocate (node)
end subroutine parse_node_create_leaf

```

This version allows us to manually create a leaf node that holds a keyword.

```

(Parser: public)+≡
    public :: parse_node_create_key

(Parser: sub interfaces)+≡
    module subroutine parse_node_create_key (node, rule)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
    end subroutine parse_node_create_key

(Parser: procedures)+≡
    module subroutine parse_node_create_key (node, rule)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
        node%rule => rule
        call token_init_key (node%token, syntax_rule_get_key (rule))
    end subroutine parse_node_create_key

```

This version allows us to manually create a leaf node that holds a fixed value. Only one of the optional values should be provided.

```

(Parser: public)+≡
    public :: parse_node_create_value

(Parser: sub interfaces)+≡
    module subroutine parse_node_create_value (node, rule, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
    end subroutine parse_node_create_value

(Parser: procedures)+≡
    module subroutine parse_node_create_value (node, rule, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
        node%rule => rule
        call parse_node_set_value (node, ival, rval, cval, sval, lval)
    end subroutine parse_node_create_value

```

Directly set the value without changing anything else.

```
<Parser: public>+≡
    public :: parse_node_set_value

<Parser: sub interfaces>+≡
    module subroutine parse_node_set_value (node, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(inout) :: node
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
    end subroutine parse_node_set_value

<Parser: procedures>+≡
    module subroutine parse_node_set_value (node, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(inout) :: node
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
        if (present (ival)) then
            node%token = ival
        else if (present (rval)) then
            node%token = rval
        else if (present (cval)) then
            node%token = cval
        else if (present (lval)) then
            node%token = lval
        else if (present (sval)) then
            node%token = sval
        end if
    end subroutine parse_node_set_value
```

Second, branch nodes. We first assign the rule:

```
<Parser: public>+≡
    public :: parse_node_create_branch

<Parser: sub interfaces>+≡
    module subroutine parse_node_create_branch (node, rule)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
    end subroutine parse_node_create_branch

<Parser: procedures>+≡
    module subroutine parse_node_create_branch (node, rule)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        allocate (node)
        node%rule => rule
    end subroutine parse_node_create_branch
```

Copy a node. This is a shallow copy. Note that we have to nullify the `next` pointer if we don't want to inherit the context of the original node.

```

(Parser: parse node: TBP)+≡
    procedure :: copy => parse_node_copy

(Parser: sub interfaces)+≡
    module subroutine parse_node_copy (node, copy)
        class(parse_node_t), intent(in) :: node
        type(parse_node_t), pointer, intent(out) :: copy
    end subroutine parse_node_copy

(Parser: procedures)+≡
    module subroutine parse_node_copy (node, copy)
        class(parse_node_t), intent(in) :: node
        type(parse_node_t), pointer, intent(out) :: copy
        allocate (copy)
        select type (node)
            type is (parse_node_t)
                copy = node
        end select
        copy%next => null ()
    end subroutine parse_node_copy

```

Append a sub-node. The sub-node must exist and be a valid target, otherwise nothing is done.

```

(Parser: public)+≡
    public :: parse_node_append_sub

(Parser: parse node: TBP)+≡
    procedure :: append_sub => parse_node_append_sub

(Parser: sub interfaces)+≡
    module subroutine parse_node_append_sub (node, sub)
        class(parse_node_t), intent(inout) :: node
        type(parse_node_t), pointer :: sub
    end subroutine parse_node_append_sub

(Parser: procedures)+≡
    module subroutine parse_node_append_sub (node, sub)
        class(parse_node_t), intent(inout) :: node
        type(parse_node_t), pointer :: sub
        if (associated (sub)) then
            if (associated (node%sub_last)) then
                node%sub_last%next => sub
            else
                node%sub_first => sub
            end if
            node%sub_last => sub
        end if
    end subroutine parse_node_append_sub

```

For easy access, once the list is complete we count the number of sub-nodes. If there are no subnodes, the whole node is deleted.

```

(Parser: public)+≡
    public :: parse_node_freeze_branch

```

```

(Parser: sub interfaces)+≡
    module subroutine parse_node_freeze_branch (node)
        type(parse_node_t), pointer :: node
    end subroutine parse_node_freeze_branch

(Parser: procedures)+≡
    module subroutine parse_node_freeze_branch (node)
        type(parse_node_t), pointer :: node
        type(parse_node_t), pointer :: current
        node%n_sub = 0
        current => node%sub_first
        do while (associated (current))
            node%n_sub = node%n_sub + 1
            current => current%next
        end do
        if (node%n_sub == 0) deallocate (node)
    end subroutine parse_node_freeze_branch

```

Replace the syntax rule. This makes sense only if the parse node adheres to the syntax of the new rule.

```

(Parser: public)+≡
    public :: parse_node_replace_rule

(Parser: sub interfaces)+≡
    module subroutine parse_node_replace_rule (node, rule)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
    end subroutine parse_node_replace_rule

(Parser: procedures)+≡
    module subroutine parse_node_replace_rule (node, rule)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        node%rule => rule
    end subroutine parse_node_replace_rule

```

Replace the last subnode by the target node. Since the subnodes are stored as a linked list, we can do this only if we copy the subnodes. Furthermore, the target node must also be copied, and the `next` pointer of the copy is nullified. This ensures that we cannot modify the originals at the subnode level.

All copies are shallow copies. This implies that further modifications at the sub-subnode level will affect the original nodes and must therefore be forbidden.

Use with care, this invites to memory mismanagement. The copy nodes can be deallocated, but not finalized, since its subnodes are the same objects as the subnodes of the target node.

```

(Parser: public)+≡
    public :: parse_node_replace_last_sub

(Parser: sub interfaces)+≡
    module subroutine parse_node_replace_last_sub (node, pn_target)
        type(parse_node_t), intent(inout), target :: node
        type(parse_node_t), intent(in), target :: pn_target
    end subroutine parse_node_replace_last_sub

```

```

<Parser: procedures>+≡
module subroutine parse_node_replace_last_sub (node, pn_target)
  type(parse_node_t), intent(inout), target :: node
  type(parse_node_t), intent(in), target :: pn_target
  type(parse_node_t), pointer :: current, current_copy, previous
  integer :: i
  select case (node%n_sub)
  case (1)
    allocate (current_copy)
    current_copy = pn_target
    node%sub_first => current_copy
  case (2:)
    current => node%sub_first
    allocate (current_copy)
    current_copy = current
    node%sub_first => current_copy
    previous => current_copy
    do i = 1, node%n_sub - 2
      current => current%next
      allocate (current_copy)
      current_copy = current
      previous%next => current_copy
      previous => current_copy
    end do
    allocate (current_copy)
    current_copy = pn_target
    previous%next => current_copy
  case default
    call parse_node_write (node)
    call msg_bug ("'replace_last_sub' called for non-branch parse node")
  end select
  current_copy%next => null ()
  node%sub_last => current_copy
end subroutine parse_node_replace_last_sub

```

7.4.5 Accessing nodes

Return the node contents. Check if pointers are associated. No check when accessing a sub-node; assume that `parse_node_n_sub` is always used for the upper bound.

The token extractor returns a pointer.

```

<Parser: public>+≡
public :: parse_node_get_rule_ptr
public :: parse_node_get_n_sub
public :: parse_node_get_sub_ptr
public :: parse_node_get_next_ptr
public :: parse_node_get_last_sub_ptr

<Parser: parse node: TBP>+≡
procedure :: get_rule_ptr => parse_node_get_rule_ptr
procedure :: get_n_sub => parse_node_get_n_sub
procedure :: get_sub_ptr => parse_node_get_sub_ptr
procedure :: get_next_ptr => parse_node_get_next_ptr

```

<Parser: sub interfaces>+≡

```

module function parse_node_get_rule_ptr (node) result (rule)
  class(parse_node_t), intent(in) :: node
  type(syntax_rule_t), pointer :: rule
end function parse_node_get_rule_ptr
module function parse_node_get_last_sub_ptr (node, tag, required) result (sub)
  type(parse_node_t), pointer :: sub
  type(parse_node_t), intent(in), target :: node
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
end function parse_node_get_last_sub_ptr
module function parse_node_get_n_sub (node) result (n)
  class(parse_node_t), intent(in) :: node
  integer :: n
end function parse_node_get_n_sub
module function parse_node_get_sub_ptr (node, n, tag, required) result (sub)
  class(parse_node_t), intent(in), target :: node
  type(parse_node_t), pointer :: sub
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
end function parse_node_get_sub_ptr
module function parse_node_get_next_ptr (sub, n, tag, required) result (next)
  class(parse_node_t), intent(in), target :: sub
  type(parse_node_t), pointer :: next
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
end function parse_node_get_next_ptr

```

<Parser: procedures>+≡

```

module function parse_node_get_rule_ptr (node) result (rule)
  class(parse_node_t), intent(in) :: node
  type(syntax_rule_t), pointer :: rule
  if (associated (node%rule)) then
    rule => node%rule
  else
    rule => null ()
    call parse_node_undefined (node, "rule")
  end if
end function parse_node_get_rule_ptr

module function parse_node_get_n_sub (node) result (n)
  class(parse_node_t), intent(in) :: node
  integer :: n
  n = node%n_sub
end function parse_node_get_n_sub

module function parse_node_get_sub_ptr (node, n, tag, required) result (sub)
  class(parse_node_t), intent(in), target :: node
  type(parse_node_t), pointer :: sub
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  integer :: i

```



```

sub => node%sub_first
if (present (n)) then
  do i = 2, n
    if (associated (sub)) then
      sub => sub%next
    else
      return
    end if
  end do
end if
call parse_node_check (sub, tag, required)
end function parse_node_get_sub_ptr

module function parse_node_get_next_ptr (sub, n, tag, required) result (next)
  class(parse_node_t), intent(in), target :: sub
  type(parse_node_t), pointer :: next
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  integer :: i
  next => sub%next
  if (present (n)) then
    do i = 2, n
      if (associated (next)) then
        next => next%next
      else
        exit
      end if
    end do
  end if
  call parse_node_check (next, tag, required)
end function parse_node_get_next_ptr

module function parse_node_get_last_sub_ptr (node, tag, required) result (sub)
  type(parse_node_t), pointer :: sub
  type(parse_node_t), intent(in), target :: node
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  sub => node%sub_last
  call parse_node_check (sub, tag, required)
end function parse_node_get_last_sub_ptr

```

<Parser: procedures>+≡

```

subroutine parse_node_undefined (node, obj)
  type(parse_node_t), intent(in) :: node
  character(*), intent(in) :: obj
  call parse_node_write (node, 6)
  call msg_bug (" Parse-tree node: " // obj // " requested, but undefined")
end subroutine parse_node_undefined

```

Check if a parse node has a particular tag, and if it is associated:

<Parser: public>+≡

```

public :: parse_node_check

```

```

(Parser: sub interfaces)+≡
    module subroutine parse_node_check (node, tag, required)
        type(parse_node_t), pointer :: node
        character(*), intent(in), optional :: tag
        logical, intent(in), optional :: required
    end subroutine parse_node_check

(Parser: procedures)+≡
    module subroutine parse_node_check (node, tag, required)
        type(parse_node_t), pointer :: node
        character(*), intent(in), optional :: tag
        logical, intent(in), optional :: required
        if (associated (node)) then
            if (present (tag)) then
                if (parse_node_get_rule_key (node) /= tag) &
                    call parse_node_mismatch (tag, node)
            end if
        else
            if (present (required)) then
                if (required) &
                    call msg_bug (" Missing node, expected <" // tag // ">")
            end if
        end if
    end subroutine parse_node_check

```

This is called by a parse-tree scanner if the expected and the actual nodes do not match

```

(Parser: public)+≡
    public :: parse_node_mismatch

(Parser: sub interfaces)+≡
    module subroutine parse_node_mismatch (string, parse_node)
        character(*), intent(in) :: string
        type(parse_node_t), intent(in) :: parse_node
    end subroutine parse_node_mismatch

(Parser: procedures)+≡
    module subroutine parse_node_mismatch (string, parse_node)
        character(*), intent(in) :: string
        type(parse_node_t), intent(in) :: parse_node
        call parse_node_write (parse_node)
        call msg_bug (" Syntax mismatch, expected <" // string // ">.")
    end subroutine parse_node_mismatch

```

The following functions are wrappers for extracting the token contents.

```

(Parser: public)+≡
    public :: parse_node_get_logical
    public :: parse_node_get_integer
    public :: parse_node_get_real
    public :: parse_node_get_cmplx
    public :: parse_node_get_string
    public :: parse_node_get_key
    public :: parse_node_get_rule_key

```

```

(Parser: parse node: TBP)+≡
  procedure :: get_logical => parse_node_get_logical
  procedure :: get_integer => parse_node_get_integer
  procedure :: get_real => parse_node_get_real
  procedure :: get_cmplx => parse_node_get_cmplx
  procedure :: get_string => parse_node_get_string
  procedure :: get_key => parse_node_get_key
  procedure :: get_rule_key => parse_node_get_rule_key

(Parser: sub interfaces)+≡
  module function parse_node_get_logical (node) result (lval)
    class(parse_node_t), intent(in), target :: node
    logical :: lval
  end function parse_node_get_logical
  module function parse_node_get_integer (node) result (ival)
    class(parse_node_t), intent(in), target :: node
    integer :: ival
  end function parse_node_get_integer
  module function parse_node_get_real (node) result (rval)
    class(parse_node_t), intent(in), target :: node
    real(default) :: rval
  end function parse_node_get_real
  module function parse_node_get_cmplx (node) result (cval)
    class(parse_node_t), intent(in), target :: node
    complex(default) :: cval
  end function parse_node_get_cmplx
  module function parse_node_get_string (node) result (sval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: sval
  end function parse_node_get_string
  module function parse_node_get_key (node) result (kval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: kval
  end function parse_node_get_key
  module function parse_node_get_rule_key (node) result (kval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: kval
  end function parse_node_get_rule_key
  module function parse_node_get_token_ptr (node) result (token)
    type(token_t), pointer :: token
    type(parse_node_t), intent(in), target :: node
  end function parse_node_get_token_ptr

(Parser: procedures)+≡
  module function parse_node_get_logical (node) result (lval)
    class(parse_node_t), intent(in), target :: node
    logical :: lval
    lval = token_get_logical (parse_node_get_token_ptr (node))
  end function parse_node_get_logical

  module function parse_node_get_integer (node) result (ival)
    class(parse_node_t), intent(in), target :: node
    integer :: ival
    ival = token_get_integer (parse_node_get_token_ptr (node))
  end function parse_node_get_integer

```

```

module function parse_node_get_real (node) result (rval)
  class(parse_node_t), intent(in), target :: node
  real(default) :: rval
  rval = token_get_real (parse_node_get_token_ptr (node))
end function parse_node_get_real

module function parse_node_get_cmplx (node) result (cval)
  class(parse_node_t), intent(in), target :: node
  complex(default) :: cval
  cval = token_get_cmplx (parse_node_get_token_ptr (node))
end function parse_node_get_cmplx

module function parse_node_get_string (node) result (sval)
  class(parse_node_t), intent(in), target :: node
  type(string_t) :: sval
  sval = token_get_string (parse_node_get_token_ptr (node))
end function parse_node_get_string

module function parse_node_get_key (node) result (kval)
  class(parse_node_t), intent(in), target :: node
  type(string_t) :: kval
  kval = token_get_key (parse_node_get_token_ptr (node))
end function parse_node_get_key

module function parse_node_get_rule_key (node) result (kval)
  class(parse_node_t), intent(in), target :: node
  type(string_t) :: kval
  kval = syntax_rule_get_key (parse_node_get_rule_ptr (node))
end function parse_node_get_rule_key

module function parse_node_get_token_ptr (node) result (token)
  type(token_t), pointer :: token
  type(parse_node_t), intent(in), target :: node
  if (token_is_valid (node%token)) then
    token => node%token
  else
    call parse_node_undefined (node, "token")
  end if
end function parse_node_get_token_ptr

```

Return a MD5 sum for a parse node. The method is to write the node to a scratch file and to evaluate the MD5 sum of that file.

```

(Parser: public)+≡
  public :: parse_node_get_md5sum

(Parser: sub interfaces)+≡
  module function parse_node_get_md5sum (pn) result (md5sum_pn)
    character(32) :: md5sum_pn
    type(parse_node_t), intent(in) :: pn
  end function parse_node_get_md5sum

(Parser: procedures)+≡
  module function parse_node_get_md5sum (pn) result (md5sum_pn)
    character(32) :: md5sum_pn

```

```

    type(parse_node_t), intent(in) :: pn
    integer :: u
    u = free_unit ()
    open (unit = u, status = "scratch", action = "readwrite")
    call parse_node_write_rec (pn, unit=u)
    rewind (u)
    md5sum_pn = md5sum (u)
    close (u)
end function parse_node_get_md5sum

```

7.4.6 The parse tree

The parse tree is a tree of nodes, where leaf nodes hold a valid token, while branch nodes point to a list of sub-nodes.

```

<Parser: public>+≡
    public :: parse_tree_t

<Parser: types>+≡
    type :: parse_tree_t
    private
        type(parse_node_t), pointer :: root_node => null ()
    contains
        <Parser: parse tree: TBP>
    end type parse_tree_t

```

The parser. Its arguments are the parse tree (which should be empty initially), the lexer (which should be already set up), the syntax table (which should be valid), and the input stream. The input stream is completely parsed, using the lexer setup and the syntax rules as given, and the parse tree is built accordingly.

If `check_eof` is absent or true, the parser will complain about trailing garbage. Otherwise, it will ignore it.

By default, the input stream is matched against the top rule in the specified syntax. If `key` is given, it is matched against the rule with the specified key instead.

Failure at the top level means that no rule could match at all; in this case the error message will show the top rule.

```

<Parser: public>+≡
    public :: parse_tree_init

<Parser: parse tree: TBP>≡
    procedure :: parse => parse_tree_init

<Parser: sub interfaces>+≡
    module subroutine parse_tree_init &
        (parse_tree, syntax, lexer, key, check_eof)
        class(parse_tree_t), intent(inout) :: parse_tree
        type(lexer_t), intent(inout) :: lexer
        type(syntax_t), intent(in), target :: syntax
        type(string_t), intent(in), optional :: key
        logical, intent(in), optional :: check_eof
    end subroutine parse_tree_init

```

```

<Parser: procedures>+≡
module subroutine parse_tree_init &
    (parse_tree, syntax, lexer, key, check_eof)
    class(parse_tree_t), intent(inout) :: parse_tree
    type(lexer_t), intent(inout) :: lexer
    type(syntax_t), intent(in), target :: syntax
    type(string_t), intent(in), optional :: key
    logical, intent(in), optional :: check_eof
    type(syntax_rule_t), pointer :: rule
    type(lexeme_t) :: lexeme
    type(parse_node_t), pointer :: node
    logical :: ok, check
    check = .true.; if (present (check_eof)) check = check_eof
    call lexer_clear (lexer)
    if (present (key)) then
        rule => syntax_get_rule_ptr (syntax, key)
    else
        rule => syntax_get_top_rule_ptr (syntax)
    end if
    if (associated (rule)) then
        call parse_node_match_rule (node, rule, ok)
        if (ok) then
            parse_tree%root_node => node
        else
            call parse_error (rule, lexeme)
        end if
        if (check) then
            call lex (lexeme, lexer)
            if (.not. lexeme_is_eof (lexeme)) then
                call lexer_show_location (lexer)
                call msg_fatal (" Syntax error " &
                    // "(at or before the location indicated above)")
            end if
        end if
    else
        call msg_bug (" Parser failed because syntax is empty")
    end if
contains
<Parser: internal subroutines of parse_tree_init>
end subroutine parse_tree_init

```

The parser works recursively, following the rule tree, building the tree of nodes on the fly. If the given rule matches, the node is filled on return. If not, the node remains empty.

```

<Parser: internal subroutines of parse_tree_init>≡
recursive subroutine parse_node_match_rule (node, rule, ok)
    type(parse_node_t), pointer :: node
    type(syntax_rule_t), intent(in), target :: rule
    logical, intent(out) :: ok
    logical, parameter :: debug = .false.
    integer :: type
    if (debug) write (6, "(A)", advance="no") "Parsing rule: "
    if (debug) call syntax_rule_write (rule, 6)

```

```

node => null ()
type = syntax_rule_get_type (rule)
if (syntax_rule_is_atomic (rule)) then
    call lex (lexeme, lexer)
    if (debug) write (6, "(A)", advance="no") "Token: "
    if (debug) call lexeme_write (lexeme, 6)
    call parse_node_create_leaf (node, rule, lexeme)
    ok = associated (node)
    if (.not. ok) call lexer_put_back (lexer, lexeme)
else
    select case (type)
    case (S_ALTERNATIVE); call parse_alternative (node, rule, ok)
    case (S_GROUP);       call parse_group (node, rule, ok)
    case (S_SEQUENCE);    call parse_sequence (node, rule, .false., ok)
    case (S_LIST);        call parse_sequence (node, rule, .true., ok)
    case (S_ARGS);        call parse_args (node, rule, ok)
    case (S_IGNORE);      call parse_ignore (node, ok)
    end select
end if
if (debug) then
    if (ok) then
        write (6, "(A)", advance="no") "Matched rule: "
    else
        write (6, "(A)", advance="no") "Failed rule: "
    end if
    call syntax_rule_write (rule)
    if (associated (node)) call parse_node_write (node)
end if
end subroutine parse_node_match_rule

```

Parse an alternative: try each case. If the match succeeds, the node has been filled, so return. If nothing works, return failure.

(Parser: internal subroutines of parse_tree_init)+≡

```

recursive subroutine parse_alternative (node, rule, ok)
    type(parse_node_t), pointer :: node
    type(syntax_rule_t), intent(in), target :: rule
    logical, intent(out) :: ok
    integer :: i
    do i = 1, syntax_rule_get_n_sub (rule)
        call parse_node_match_rule (node, syntax_rule_get_sub_ptr (rule, i), ok)
        if (ok) return
    end do
    ok = .false.
end subroutine parse_alternative

```

Parse a group: the first and third lexemes have to be the delimiters, the second one is parsed as the actual node, using now the child rule. If the first match fails, return with failure. If the other matches fail, issue an error, since we cannot lex back more than one item.

(Parser: internal subroutines of parse_tree_init)+≡

```

recursive subroutine parse_group (node, rule, ok)
    type(parse_node_t), pointer :: node
    type(syntax_rule_t), intent(in), target :: rule
    logical, intent(out) :: ok
    type(string_t), dimension(2) :: delimiter

```

```

delimiter = syntax_rule_get_delimiter (rule)
call lex (lexeme, lexer)
if (lexeme_get_string (lexeme) == delimiter(1)) then
  call parse_node_match_rule (node, syntax_rule_get_sub_ptr (rule, 1), ok)
  if (ok) then
    call lex (lexeme, lexer)
    if (lexeme_get_string (lexeme) == delimiter(2)) then
      ok = .true.
    else
      call parse_error (rule, lexeme)
    end if
  else
    call parse_error (rule, lexeme)
  end if
else
  call lexer_put_back (lexer, lexeme)
  ok = .false.
end if
end subroutine parse_group

```

Parsing a sequence. The last rule element may be special: optional and/or repetitive. Each sub-node that matches is appended to the sub-node list of the parent node.

If sep is true, we look for a separator after each element.

(Parser: internal subroutines of parse_tree_init)+≡

```

recursive subroutine parse_sequence (node, rule, sep, ok)
  type(parse_node_t), pointer :: node
  type(syntax_rule_t), intent(in), target :: rule
  logical, intent(in) :: sep
  logical, intent(out) :: ok
  type(parse_node_t), pointer :: current
  integer :: i, n
  logical :: opt, rep, cont
  type(string_t) :: separator
  call parse_node_create_branch (node, rule)
  if (sep) separator = syntax_rule_get_separator (rule)
  n = syntax_rule_get_n_sub (rule)
  opt = syntax_rule_last_optional (rule)
  rep = syntax_rule_last_repetitive (rule)
  ok = .true.
  cont = .true.
SCAN_RULE: do i = 1, n
  call parse_node_match_rule &
    (current, syntax_rule_get_sub_ptr (rule, i), cont)
  if (cont) then
    call parse_node_append_sub (node, current)
    if (sep .and. (i<n .or. rep)) then
      call lex (lexeme, lexer)
      if (lexeme_get_string (lexeme) /= separator) then
        call lexer_put_back (lexer, lexeme)
        cont = .false.
        exit SCAN_RULE
      end if
    end if
  end if
end if

```



```

else
    if (i == n .and. opt) then
        exit SCAN_RULE
    else if (i == 1) then
        ok = .false.
        exit SCAN_RULE
    else
        call parse_error (rule, lexeme)
    end if
end if
end do SCAN_RULE
if (rep) then
    do while (cont)
        call parse_node_match_rule &
            (current, syntax_rule_get_sub_ptr (rule, n), cont)
        if (cont) then
            call parse_node_append_sub (node, current)
            if (sep) then
                call lex (lexeme, lexer)
                if (lexeme_get_string (lexeme) /= separator) then
                    call lexer_put_back (lexer, lexeme)
                    cont = .false.
                end if
            end if
        else
            if (sep) call parse_error (rule, lexeme)
        end if
    end do
end if
call parse_node_freeze_branch (node)
end subroutine parse_sequence

```

Argument list: We use the `parse_group` code, but call `parse_sequence` inside.

(Parser: internal subroutines of parse_tree_init)+≡

```

recursive subroutine parse_args (node, rule, ok)
    type(parse_node_t), pointer :: node
    type(syntax_rule_t), intent(in), target :: rule
    logical, intent(out) :: ok
    type(string_t), dimension(2) :: delimiter
    delimiter = syntax_rule_get_delimiter (rule)
    call lex (lexeme, lexer)
    if (lexeme_get_string (lexeme) == delimiter(1)) then
        call parse_sequence (node, rule, .true., ok)
        if (ok) then
            call lex (lexeme, lexer)
            if (lexeme_get_string (lexeme) == delimiter(2)) then
                ok = .true.
            else
                call parse_error (rule, lexeme)
            end if
        else
            call parse_error (rule, lexeme)
        end if
    else
        call lexer_put_back (lexer, lexeme)
    end if
end subroutine parse_args

```

```

        ok = .false.
    end if
end subroutine parse_args

```

The IGNORE syntax reads one lexeme and discards it if it is numeric, logical or string/identifier (but not a keyword). This is a successful match. Otherwise, the match fails. The node pointer is returned disassociated in any case.

```

(Parser: internal subroutines of parse_tree_init)+≡
subroutine parse_ignore (node, ok)
    type(parse_node_t), pointer :: node
    logical, intent(out) :: ok
    call lex (lexeme, lexer)
    select case (lexeme_get_type (lexeme))
    case (T_NUMERIC, T_IDENTIFIER, T_QUOTED)
        ok = .true.
    case default
        ok = .false.
    end select
    node => null ()
end subroutine parse_ignore

```

If the match fails and we cannot step back:

```

(Parser: internal subroutines of parse_tree_init)+≡
subroutine parse_error (rule, lexeme)
    type(syntax_rule_t), intent(in) :: rule
    type(lexeme_t), intent(in) :: lexeme
    character(80) :: buffer
    integer :: u, iostat
    call lexer_show_location (lexer)
    u = free_unit ()
    open (u, status = "scratch")
    write (u, "(A)", advance="no") "Expected syntax:"
    call syntax_rule_write (rule, u)
    write (u, "(A)", advance="no") "Found token:"
    call lexeme_write (lexeme, u)
    rewind (u)
    do
        read (u, "(A)", iostat=iostat) buffer
        if (iostat /= 0) exit
        call msg_message (trim (buffer))
    end do
    call msg_fatal (" Syntax error " &
        // "(at or before the location indicated above)")
end subroutine parse_error

```

The finalizer recursively deallocates all nodes and their contents. For each node, `parse_node_final` is called on the sub-nodes, which in turn deallocates the token or sub-node array contained within each of them. At the end, only the top node remains to be deallocated.

```

(Parser: public)+≡
public :: parse_tree_final

(Parser: parse tree: TBP)+≡
procedure :: final => parse_tree_final

```

```

<Parser: sub interfaces>+≡
    module subroutine parse_tree_final (parse_tree)
        class(parse_tree_t), intent(inout) :: parse_tree
    end subroutine parse_tree_final

```

```

<Parser: procedures>+≡
    module subroutine parse_tree_final (parse_tree)
        class(parse_tree_t), intent(inout) :: parse_tree
        if (associated (parse_tree%root_node)) then
            call parse_node_final (parse_tree%root_node)
            deallocate (parse_tree%root_node)
        end if
    end subroutine parse_tree_final

```

Print the parse tree. Print one token per line, indented according to the depth of the node.

The **verbose** version includes type identifiers for the nodes.

```

<Parser: public>+≡
    public :: parse_tree_write

<Parser: parse tree: TBP>+≡
    procedure :: write => parse_tree_write

<Parser: sub interfaces>+≡
    module subroutine parse_tree_write (parse_tree, unit, verbose)
        class(parse_tree_t), intent(in) :: parse_tree
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine parse_tree_write

<Parser: procedures>+≡
    module subroutine parse_tree_write (parse_tree, unit, verbose)
        class(parse_tree_t), intent(in) :: parse_tree
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        logical :: short
        u = given_output_unit (unit); if (u < 0) return
        short = .true.; if (present (verbose)) short = .not. verbose
        write (u, "(A)") "Parse tree:"
        if (associated (parse_tree%root_node)) then
            call parse_node_write_rec (parse_tree%root_node, unit, short, 1)
        else
            write (u, *) "[empty]"
        end if
    end subroutine parse_tree_write

```

This is a generic error that can be issued if the parse tree does not meet the expectations of the parser. This most certainly indicates a bug.

```

<Parser: public>+≡
    public :: parse_tree_bug

<Parser: sub interfaces>+≡
    module subroutine parse_tree_bug (node, keys)
        type(parse_node_t), intent(in) :: node

```

```

        character(*), intent(in) :: keys
    end subroutine parse_tree_bug
<Parser: procedures>+≡
    module subroutine parse_tree_bug (node, keys)
        type(parse_node_t), intent(in) :: node
        character(*), intent(in) :: keys
        call parse_node_write (node)
        call msg_bug (" Inconsistency in parse tree: expected " // keys)
    end subroutine parse_tree_bug

```

7.4.7 Access the parser

For scanning the parse tree we give access to the top node, as a node pointer. Of course, there should be no write access.

```

<Parser: parse tree: TBP>+≡
    procedure :: get_root_ptr => parse_tree_get_root_ptr
<Parser: sub interfaces>+≡
    module function parse_tree_get_root_ptr (parse_tree) result (node)
        class(parse_tree_t), intent(in) :: parse_tree
        type(parse_node_t), pointer :: node
    end function parse_tree_get_root_ptr
<Parser: procedures>+≡
    module function parse_tree_get_root_ptr (parse_tree) result (node)
        class(parse_tree_t), intent(in) :: parse_tree
        type(parse_node_t), pointer :: node
        node => parse_tree%root_node
    end function parse_tree_get_root_ptr

```

7.4.8 Tools

This operation traverses the parse tree and simplifies any occurrences of a set of syntax rules. If such a parse node has only one sub-node, it is replaced by that subnode. (This makes sense only of the rules to eliminate have no meaningful token.)

```

<Parser: public>+≡
    public :: parse_tree_reduce
<Parser: sub interfaces>+≡
    module subroutine parse_tree_reduce (parse_tree, rule_key)
        type(parse_tree_t), intent(inout) :: parse_tree
        type(string_t), dimension(:), intent(in) :: rule_key
    end subroutine parse_tree_reduce
<Parser: procedures>+≡
    module subroutine parse_tree_reduce (parse_tree, rule_key)
        type(parse_tree_t), intent(inout) :: parse_tree
        type(string_t), dimension(:), intent(in) :: rule_key
        type(parse_node_t), pointer :: pn
        pn => parse_tree%root_node
        if (associated (pn)) then

```

```

        call parse_node_reduce (pn, null(), null())
    end if
contains
    recursive subroutine parse_node_reduce (pn, pn_prev, pn_parent)
        type(parse_node_t), intent(inout), pointer :: pn
        type(parse_node_t), intent(in), pointer :: pn_prev, pn_parent
        type(parse_node_t), pointer :: pn_sub, pn_sub_prev, pn_tmp
        pn_sub_prev => null ()
        pn_sub => pn%sub_first
        do while (associated (pn_sub))
            call parse_node_reduce (pn_sub, pn_sub_prev, pn)
            pn_sub_prev => pn_sub
            pn_sub => pn_sub%next
        end do
        if (parse_node_get_n_sub (pn) == 1) then
            if (matches (parse_node_get_rule_key (pn), rule_key)) then
                pn_tmp => pn
                pn => pn%sub_first
                if (associated (pn_prev)) then
                    pn_prev%next => pn
                else if (associated (pn_parent)) then
                    pn_parent%sub_first => pn
                else
                    parse_tree%root_node => pn
                end if
                if (associated (pn_tmp%next)) then
                    pn%next => pn_tmp%next
                else if (associated (pn_parent)) then
                    pn_parent%sub_last => pn
                end if
                call parse_node_final (pn_tmp, recursive=.false.)
                deallocate (pn_tmp)
            end if
        end if
    end subroutine parse_node_reduce
    function matches (key, key_list) result (flag)
        logical :: flag
        type(string_t), intent(in) :: key
        type(string_t), dimension(:), intent(in) :: key_list
        integer :: i
        flag = .true.
        do i = 1, size (key_list)
            if (key == key_list(i)) return
        end do
        flag = .false.
    end function matches
end subroutine parse_tree_reduce

```

7.4.9 Applications

For a file of the form

```
process foo, bar
```

```

    <something>
process xyz
    <something>

```

get the <something> entry node for the first matching process tag. If no matching entry is found, the node pointer remains unassociated.

```

(Parser: public)+≡
    public :: parse_tree_get_process_ptr

(Parser: sub interfaces)+≡
    module function parse_tree_get_process_ptr (parse_tree, process) result (node)
        type(parse_node_t), pointer :: node
        type(parse_tree_t), intent(in), target :: parse_tree
        type(string_t), intent(in) :: process
    end function parse_tree_get_process_ptr

(Parser: procedures)+≡
    module function parse_tree_get_process_ptr (parse_tree, process) result (node)
        type(parse_node_t), pointer :: node
        type(parse_tree_t), intent(in), target :: parse_tree
        type(string_t), intent(in) :: process
        type(parse_node_t), pointer :: node_root, node_process_def
        type(parse_node_t), pointer :: node_process_phs, node_process_list
        integer :: j
        node_root => parse_tree%get_root_ptr ()
        if (associated (node_root)) then
            node_process_phs => parse_node_get_sub_ptr (node_root)
            SCAN_FILE: do while (associated (node_process_phs))
                node_process_def => parse_node_get_sub_ptr (node_process_phs)
                node_process_list => parse_node_get_sub_ptr (node_process_def, 2)
                do j = 1, parse_node_get_n_sub (node_process_list)
                    if (parse_node_get_string &
                        (parse_node_get_sub_ptr (node_process_list, j)) &
                        == process) then
                        node => parse_node_get_next_ptr (node_process_def)
                        return
                    end if
                end do
                node_process_phs => parse_node_get_next_ptr (node_process_phs)
            end do SCAN_FILE
            node => null ()
        else
            node => null ()
        end if
    end function parse_tree_get_process_ptr

```

7.4.10 Unit tests

Test module, followed by the corresponding implementation module.

```

(parser_ut.f90)≡
    <File header>

    module parser_ut

```

```

        use unit_tests
        use parser_util

    <Standard module head>

    <Parser: public test>

contains

    <Parser: test driver>

end module parser_util
(parser_util.f90)≡
    <File header>

    module parser_util

        use syntax_rules

        use parser

    <Standard module head>

    <Parser: test declarations>

contains

    <Parser: tests>

end module parser_util
API: driver for the unit tests below.
    <Parser: public test>≡
        public :: parse_test
    <Parser: test driver>≡
        subroutine parse_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <Parser: execute tests>
        end subroutine parse_test

This checks the parser.
    <Parser: execute tests>≡
        call test (parse_1, "parse_1", &
            "check the parser", &
            u, results)
    <Parser: test declarations>≡
        public :: parse_1
    <Parser: tests>≡
        subroutine parse_1 (u)
            use ifiles
            use lexers

```

```

integer, intent(in) :: u

type(ifile_t) :: ifile
type(syntax_t), target :: syntax
type(lexer_t) :: lexer
type(stream_t), target :: stream
type(parse_tree_t), target :: parse_tree

write (u, "(A)")  "* Test output: Parsing"
write (u, "(A)")  "* Purpose: test parse routines"
write (u, "(A)")

call ifile_append (ifile, "SEQ expr = term addition*")
call ifile_append (ifile, "SEQ addition = plus_or_minus term")
call ifile_append (ifile, "SEQ term = factor multiplication*")
call ifile_append (ifile, "SEQ multiplication = times_or_over factor")
call ifile_append (ifile, "SEQ factor = atom exponentiation*")
call ifile_append (ifile, "SEQ exponentiation = '^' atom")
call ifile_append (ifile, "ALT atom = real | delimited_expr")
call ifile_append (ifile, "GRO delimited_expr = ( expr )")
call ifile_append (ifile, "ALT plus_or_minus = '+' | '-'")
call ifile_append (ifile, "ALT times_or_over = '*' | '/'")
call ifile_append (ifile, "KEY '+'")
call ifile_append (ifile, "KEY '-'")
call ifile_append (ifile, "KEY '*'")
call ifile_append (ifile, "KEY '/'")
call ifile_append (ifile, "KEY '^'")
call ifile_append (ifile, "REA real")

write (u, "(A)")  "* File contents (syntax definition):"
call ifile_write (ifile, u)
write (u, "(A)")  "EOF"
write (u, "(A)")

call syntax_init (syntax, ifile)
call ifile_final (ifile)
call syntax_write (syntax, u)
write (u, "(A)")

call lexer_init (lexer, &
    comment_chars = " ", &
    quote_chars = "\"", &
    quote_match = "\"", &
    single_chars = "+-*/^()", &
    special_class = [" "], &
    keyword_list = syntax_get_keyword_list_ptr (syntax))
call lexer_write_setup (lexer, u)
write (u, "(A)")

call ifile_append (ifile, "(27+8^3-2/3)*(4+7)^2*99")
write (u, "(A)")  "* File contents (input file):"
call ifile_write (ifile, u)
write (u, "(A)")  "EOF"
print *

```



```

call stream_init (stream, ifile)
call lexer_assign_stream (lexer, stream)
call parse_tree_init (parse_tree, syntax, lexer)
call stream_final (stream)
call parse_tree_write (parse_tree, u, .true.)
print *

write (u, "(A)")  "* Cleanup, everything should now be empty:"
write (u, "(A)")

call parse_tree_final (parse_tree)
call parse_tree_write (parse_tree, u, .true.)
write (u, "(A)")

call lexer_final (lexer)
call lexer_write_setup (lexer, u)
write (u, "(A)")

call ifile_final (ifile)
write (u, "(A)")  "* File contents:"
call ifile_write (ifile, u)
write (u, "(A)")  "EOF"
write (u, "(A)")

call syntax_final (syntax)
call syntax_write (syntax, u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: parser_1"

end subroutine parse_1

```

7.5 XML Parser

The XML parser is actually independent from the previous modules of `lexer` and `parser`. However, for a generic I/O interface we make use of the `stream_t` facility.

We need the XML parser for reading and writing LHEF data files. Only a subset of XML is actually relevant. The parser is of the “pull” type, i.e., the program steers the reading of XML data in a context-sensitive manner.

```
<xml.f90>≡
  <File header>

  module xml

    <Use strings>
      use lexers

    <Standard module head>

    <XML: public>

    <XML: types>

    interface
    <XML: sub interfaces>
      end interface

  end module xml

<xml_sub.f90>≡
  <File header>

  submodule (xml) xml_s

    use io_units
    use system_defs, only: BLANK, TAB
    use diagnostics
    use ifiles

    implicit none

  contains

    <XML: procedures>

  end submodule xml_s
```

7.5.1 Cached Stream

The `stream` type as defined in the `lexer` module is versatile regarding the choice of input channel, but it does not allow reading a section more than once. Here, we define an extension where we can return a string to the stream, which is

stored in a cache variable, and presented to the caller for the next read.

```

<XML: public>≡
    public :: cstream_t

<XML: types>≡
    type, extends (stream_t) :: cstream_t
        logical :: cache_is_empty = .true.
        type(string_t) :: cache
    contains
        <XML: cstream: TBP>
    end type cstream_t

```

The initializers are simply inherited.

Finalizer: also inherited, in essence:

```

<XML: cstream: TBP>≡
    procedure :: final => cstream_final

<XML: sub interfaces>≡
    module subroutine cstream_final (stream)
        class(cstream_t), intent(inout) :: stream
    end subroutine cstream_final

<XML: procedures>≡
    module subroutine cstream_final (stream)
        class(cstream_t), intent(inout) :: stream
        stream%cache_is_empty = .true.
        call stream%stream_t%final ()
    end subroutine cstream_final

```

Get record: now, if there is a cache string, return this instead of the record from the stream.

```

<XML: cstream: TBP>+≡
    procedure :: get_record => cstream_get_record

<XML: sub interfaces>+≡
    module subroutine cstream_get_record (cstream, string, iostat)
        class(cstream_t), intent(inout) :: cstream
        type(string_t), intent(out) :: string
        integer, intent(out) :: iostat
    end subroutine cstream_get_record

<XML: procedures>+≡
    module subroutine cstream_get_record (cstream, string, iostat)
        class(cstream_t), intent(inout) :: cstream
        type(string_t), intent(out) :: string
        integer, intent(out) :: iostat
        if (cstream%cache_is_empty) then
            call stream_get_record (cstream%stream_t, string, iostat)
        else
            string = cstream%cache
            cstream%cache_is_empty = .true.
            iostat = 0
        end if
    end subroutine cstream_get_record

```

Revert: return the (partially read) record to the stream, putting it in the cache.

```

<XML: cstream: TBP>+≡
    procedure :: revert_record => cstream_revert_record

<XML: sub interfaces>+≡
    module subroutine cstream_revert_record (cstream, string)
        class(cstream_t), intent(inout) :: cstream
        type(string_t), intent(in) :: string
    end subroutine cstream_revert_record

<XML: procedures>+≡
    module subroutine cstream_revert_record (cstream, string)
        class(cstream_t), intent(inout) :: cstream
        type(string_t), intent(in) :: string
        if (cstream%cache_is_empty) then
            cstream%cache = string
            cstream%cache_is_empty = .false.
        else
            call msg_bug ("CStream: attempt to revert twice")
        end if
    end subroutine cstream_revert_record

```

7.5.2 Attributes

A tag attribute has a name and a value; both are strings. When the attribute is defined, the known flag indicates this.

```

<XML: types>+≡
    type :: attribute_t
        type(string_t) :: name
        type(string_t) :: value
        logical :: known = .false.
    contains
        <XML: attribute: TBP>
    end type attribute_t

```

Output in standard format, non-advancing. (If the value is unknown, we indicate this by a question mark, which is non-standard.)

```

<XML: attribute: TBP>≡
    procedure :: write => attribute_write

<XML: sub interfaces>+≡
    module subroutine attribute_write (object, unit)
        class(attribute_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine attribute_write

<XML: procedures>+≡
    module subroutine attribute_write (object, unit)
        class(attribute_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A,'=')", advance = "no") char (object%name)
    end subroutine attribute_write

```

```

    if (object%known) then
        write (u, "(A,A,A)", advance = "no")  '''', char (object%value), '''
    else
        write (u, "(?'')", advance = "no")
    end if
end subroutine attribute_write

```

This is a genuine constructor. The value is optional.

```

<XML: public>+≡
    public :: xml_attribute

<XML: sub interfaces>+≡
    module function xml_attribute (name, value) result (attribute)
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: value
        type(attribute_t) :: attribute
    end function xml_attribute

<XML: procedures>+≡
    module function xml_attribute (name, value) result (attribute)
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: value
        type(attribute_t) :: attribute
        attribute%name = name
        if (present (value)) then
            attribute%value = value
            attribute%known = .true.
        else
            attribute%known = .false.
        end if
    end function xml_attribute

```

Set a value explicitly.

```

<XML: attribute: TBP>+≡
    procedure :: set_value => attribute_set_value

<XML: sub interfaces>+≡
    module subroutine attribute_set_value (attribute, value)
        class(attribute_t), intent(inout) :: attribute
        type(string_t), intent(in) :: value
    end subroutine attribute_set_value

<XML: procedures>+≡
    module subroutine attribute_set_value (attribute, value)
        class(attribute_t), intent(inout) :: attribute
        type(string_t), intent(in) :: value
        attribute%value = value
        attribute%known = .true.
    end subroutine attribute_set_value

```

Extract a value. If unset, return "?"

```

<XML: attribute: TBP>+≡
    procedure :: get_value => attribute_get_value

```

```

<XML: sub interfaces>+≡
    module function attribute_get_value (attribute) result (value)
        class(attribute_t), intent(in) :: attribute
        type(string_t) :: value
    end function attribute_get_value

<XML: procedures>+≡
    module function attribute_get_value (attribute) result (value)
        class(attribute_t), intent(in) :: attribute
        type(string_t) :: value
        if (attribute%known) then
            value = attribute%value
        else
            value = "?"
        end if
    end function attribute_get_value

```

7.5.3 The Tag Type

The basic entity is the internal representation of an XML tag. The tag has a name, a well-defined set of attributes which may be mandatory or optional, and a flag that determines whether there is content or not. The content itself is not stored in the data structure.

```

<XML: public>+≡
    public :: xml_tag_t

<XML: types>+≡
    type :: xml_tag_t
        type(string_t) :: name
        type(attribute_t), dimension(:), allocatable :: attribute
        logical :: has_content = .false.
    contains
        <XML: tag: TBP>
    end type xml_tag_t

```

Initialization. There are different versions, depending on content.

```

<XML: tag: TBP>≡
    generic :: init => init_no_attributes
    procedure :: init_no_attributes => xml_tag_init_no_attributes

<XML: sub interfaces>+≡
    module subroutine xml_tag_init_no_attributes (tag, name, has_content)
        class(xml_tag_t), intent(out) :: tag
        type(string_t), intent(in) :: name
        logical, intent(in), optional :: has_content
    end subroutine xml_tag_init_no_attributes

<XML: procedures>+≡
    module subroutine xml_tag_init_no_attributes (tag, name, has_content)
        class(xml_tag_t), intent(out) :: tag
        type(string_t), intent(in) :: name
        logical, intent(in), optional :: has_content
        tag%name = name
    end subroutine xml_tag_init_no_attributes

```

```

        allocate (tag%attribute (0))
        if (present (has_content)) tag%has_content = has_content
    end subroutine xml_tag_init_no_attributes

```

This version sets attributes.

<XML: tag: TBP>+≡

```

        generic :: init => init_with_attributes
        procedure :: init_with_attributes => xml_tag_init_with_attributes

```

<XML: sub interfaces>+≡

```

        module subroutine xml_tag_init_with_attributes (tag, name, attribute, has_content)
            class(xml_tag_t), intent(out) :: tag
            type(string_t), intent(in) :: name
            type(attribute_t), dimension(:), intent(in) :: attribute
            logical, intent(in), optional :: has_content
        end subroutine xml_tag_init_with_attributes

```

<XML: procedures>+≡

```

        module subroutine xml_tag_init_with_attributes (tag, name, attribute, has_content)
            class(xml_tag_t), intent(out) :: tag
            type(string_t), intent(in) :: name
            type(attribute_t), dimension(:), intent(in) :: attribute
            logical, intent(in), optional :: has_content
            tag%name = name
            allocate (tag%attribute (size (attribute)))
            tag%attribute = attribute
            if (present (has_content)) tag%has_content = has_content
        end subroutine xml_tag_init_with_attributes

```

Set an attribute value explicitly.

<XML: tag: TBP>+≡

```

        procedure :: set_attribute => xml_tag_set_attribute

```

<XML: sub interfaces>+≡

```

        module subroutine xml_tag_set_attribute (tag, i, value)
            class(xml_tag_t), intent(inout) :: tag
            integer, intent(in) :: i
            type(string_t), intent(in) :: value
        end subroutine xml_tag_set_attribute

```

<XML: procedures>+≡

```

        module subroutine xml_tag_set_attribute (tag, i, value)
            class(xml_tag_t), intent(inout) :: tag
            integer, intent(in) :: i
            type(string_t), intent(in) :: value
            call tag%attribute(i)%set_value (value)
        end subroutine xml_tag_set_attribute

```

Get an attribute value.

<XML: tag: TBP>+≡

```

        procedure :: get_attribute => xml_tag_get_attribute

```

```

<XML: sub interfaces>+≡
    module function xml_tag_get_attribute (tag, i) result (value)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in) :: i
        type(string_t) :: value
    end function xml_tag_get_attribute

<XML: procedures>+≡
    module function xml_tag_get_attribute (tag, i) result (value)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in) :: i
        type(string_t) :: value
        value = tag%attribute(i)%get_value ()
    end function xml_tag_get_attribute

```

Output to an I/O unit, default STDOUT. We use non-advancing output.

```

<XML: tag: TBP>+≡
    generic :: write => write_without_content
    procedure :: write_without_content => xml_tag_write

<XML: sub interfaces>+≡
    module subroutine xml_tag_write (tag, unit)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in), optional :: unit
    end subroutine xml_tag_write

<XML: procedures>+≡
    module subroutine xml_tag_write (tag, unit)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "('<',A)", advance = "no") char (tag%name)
        do i = 1, size (tag%attribute)
            write (u, "(1x)", advance = "no")
            call tag%attribute(i)%write (u)
        end do
        if (tag%has_content) then
            write (u, "('>')", advance = "no")
        else
            write (u, "(' />')", advance = "no")
        end if
    end subroutine xml_tag_write

```

If there is content, we should write the context next (arbitrary format), the write the corresponding closing tag. Again, non-advancing.

```

<XML: tag: TBP>+≡
    procedure :: close => xml_tag_close

<XML: sub interfaces>+≡
    module subroutine xml_tag_close (tag, unit)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in), optional :: unit
    end subroutine xml_tag_close

```



```

<XML: procedures>+≡
module subroutine xml_tag_close (tag, unit)
  class(xml_tag_t), intent(in) :: tag
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "('</',A,'>')", advance = "no") char (tag%name)
end subroutine xml_tag_close

```

Given content as a single string, we can write tag, content, and closing at once

```

<XML: tag: TBP>+≡
generic :: write => write_with_content
procedure :: write_with_content => xml_tag_write_with_content

<XML: sub interfaces>+≡
module subroutine xml_tag_write_with_content (tag, content, unit)
  class(xml_tag_t), intent(in) :: tag
  type(string_t), intent(in) :: content
  integer, intent(in), optional :: unit
end subroutine xml_tag_write_with_content

<XML: procedures>+≡
module subroutine xml_tag_write_with_content (tag, content, unit)
  class(xml_tag_t), intent(in) :: tag
  type(string_t), intent(in) :: content
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  call tag%write (u)
  write (u, "(A)", advance = "no") char (content)
  call tag%close (u)
end subroutine xml_tag_write_with_content

```

Input from stream. We know what we are looking for, so we check if the name matches, then fill attributes. We report an error if (a) an I/O error occurs, (b) we reach EOF before encountering the tag, (c) if the tag is incomplete.

Trailing text after reading a tag is put back to the input stream.

We assume that the tag is not broken across records, and that there is only one tag within the record. This is more restricted than standard XML.

```

<XML: tag: TBP>+≡
procedure :: read => xml_tag_read

<XML: sub interfaces>+≡
module subroutine xml_tag_read (tag, cstream, success)
  class(xml_tag_t), intent(inout) :: tag
  type(cstream_t), intent(inout) :: cstream
  logical, intent(out) :: success
end subroutine xml_tag_read

<XML: procedures>+≡
module subroutine xml_tag_read (tag, cstream, success)
  class(xml_tag_t), intent(inout) :: tag
  type(cstream_t), intent(inout) :: cstream
  logical, intent(out) :: success

```

```

type(string_t) :: string
integer :: iostat, p1, p2
character(2), parameter :: WS = BLANK // TAB
logical :: done

! Skip comments and blank lines
FIND_NON_COMMENT: do
  FIND_NONEMPTY_RECORD: do
    call cstream%get_record (string, iostat)
    if (iostat /= 0) call err_io ()
    p1 = verify (string, WS)
    if (p1 > 0) exit FIND_NONEMPTY_RECORD
  end do FIND_NONEMPTY_RECORD

  ! Look for comment beginning
  p2 = p1 + 3
  if (extract (string, p1, p2) /= "<!--") exit FIND_NON_COMMENT

  ! Look for comment end, then restart
  string = extract (string, p2 + 1)
  FIND_COMMENT_END: do
    do p1 = 1, len (string) - 2
      p2 = p1 + 2
      if (extract (string, p1, p2) == "-->") then

        ! Return trailing text to the stream
        string = extract (string, p2 + 1)
        if (string /= "") call cstream%revert_record (string)
        exit FIND_COMMENT_END

      end if
    end do
    call cstream%get_record (string, iostat)
    if (iostat /= 0) call err_io ()
  end do FIND_COMMENT_END
end do FIND_NON_COMMENT

! Look for opening <
p2 = p1
if (extract (string, p1, p2) /= "<") then
  call cstream%revert_record (string)
  success = .false.; return
else

  ! Look for tag name
  string = extract (string, p2 + 1)
  p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
  p2 = p1 + len (tag%name) - 1
  if (extract (string, p1, p2) /= tag%name) then
    call cstream%revert_record ("<" // string)
    success = .false.; return
  else

    ! Look for attributes

```

```

        string = extract (string, p2 + 1)
        READ_ATTRIBUTES: do
            call tag%read_attribute (string, done)
            if (done) exit READ_ATTRIBUTES
        end do READ_ATTRIBUTES

        ! Look for closing >
        p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
        p2 = p1
        if (extract (string, p1, p1) == ">") then
            tag%has_content = .true.
        else

            ! Look for closing />
            p2 = p1 + 1
            if (extract (string, p1, p2) /= ">") call err_incomplete ()
        end if

        ! Return trailing text to the stream
        string = extract (string, p2 + 1)
        if (string /= "") call cstream%revert_record (string)
        success = .true.

    end if
end if

contains

subroutine err_io ()
    select case (iostat)
    case (:-1)
        call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
            // "': end of file")
    case (1:)
        call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
            // "': I/O error")
    end select
    success = .false.
end subroutine err_io

subroutine err_incomplete ()
    call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
        // "': tag incomplete")
    success = .false.
end subroutine err_incomplete

end subroutine xml_tag_read

```

Read a single attribute. If the attribute is valid, assign the value. Setting a value twice should be an error, but is not detected. If the attribute is unknown, ignore it. If we reach the closing sign, report this.

<XML: tag: TBP>+≡

```
procedure :: read_attribute => xml_tag_read_attribute
```

```

<XML: sub interfaces>+≡
    module subroutine xml_tag_read_attribute (tag, string, done)
        class(xml_tag_t), intent(inout) :: tag
        type(string_t), intent(inout) :: string
        logical, intent(out) :: done
    end subroutine xml_tag_read_attribute

<XML: procedures>+≡
    module subroutine xml_tag_read_attribute (tag, string, done)
        class(xml_tag_t), intent(inout) :: tag
        type(string_t), intent(inout) :: string
        logical, intent(out) :: done
        character(2), parameter :: WS = BLANK // TAB
        type(string_t) :: name, value
        integer :: p1, p2, i

        p1 = verify (string, WS); if (p1 == 0) call err ()
        p2 = p1

        ! Look for first terminating '>' or '>/'
        if (extract (string, p1, p2) == ">") then
            done = .true.
        else
            p2 = p1 + 1
            if (extract (string, p1, p2) == ">/") then
                done = .true.
            else

                ! Look for '='
                p2 = scan (string, '=')
                if (p2 == 0) call err ()
                name = trim (extract (string, p1, p2 - 1))

                ! Look for '"'
                string = extract (string, p2 + 1)
                p1 = verify (string, WS); if (p1 == 0) call err ()
                p2 = p1
                if (extract (string, p1, p2) /= '"') call err ()

                ! Look for matching '"' and get value
                string = extract (string, p2 + 1)
                p1 = 1
                p2 = scan (string, '"')
                if (p2 == 0) call err ()
                value = extract (string, p1, p2 - 1)

                SCAN_KNOWN_ATTRIBUTES: do i = 1, size (tag%attribute)
                    if (name == tag%attribute(i)%name) then
                        call tag%attribute(i)%set_value (value)
                        exit SCAN_KNOWN_ATTRIBUTES
                    end if
                end do SCAN_KNOWN_ATTRIBUTES

                string = extract (string, p2 + 1)
                done = .false.
            end if
        end if
    end subroutine xml_tag_read_attribute

```

```

        end if
    end if

contains

    subroutine err ()
        call msg_fatal ("XML: Error reading attributes of '" // char (tag%name) &
            // "': syntax error")
    end subroutine err

end subroutine xml_tag_read_attribute

```

Read the content string of a tag. We check for the appropriate closing tag and report it. If a closing tag does not match in name, ignore it.

Note: this assumes that no tag with the same name is embedded in the current content. Also, we do not check for XML validity inside the content.

<XML: tag: TBP>+≡

```

    procedure :: read_content => xml_tag_read_content

```

<XML: sub interfaces>+≡

```

    module subroutine xml_tag_read_content (tag, cstream, content, closing)
        class(xml_tag_t), intent(in) :: tag
        type(cstream_t), intent(inout) :: cstream
        type(string_t), intent(out) :: content
        logical, intent(out) :: closing
    end subroutine xml_tag_read_content

```

<XML: procedures>+≡

```

    module subroutine xml_tag_read_content (tag, cstream, content, closing)
        class(xml_tag_t), intent(in) :: tag
        type(cstream_t), intent(inout) :: cstream
        type(string_t), intent(out) :: content
        type(string_t) :: string
        logical, intent(out) :: closing
        integer :: iostat
        integer :: p0, p1, p2
        character(2), parameter :: WS = BLANK // TAB
        call cstream%get_record (content, iostat)
        if (iostat /= 0) call err_io ()
        closing = .false.
        FIND_CLOSING: do p0 = 1, len (content) - 1

            ! Look for terminating </
            p1 = p0
            p2 = p1 + 1
            if (extract (content, p1, p2) == "</") then

                ! Look for closing tag name
                string = extract (content, p2 + 1)
                p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
                p2 = p1 + len (tag%name) - 1
                if (extract (string, p1, p2) == tag%name) then

                    ! Tag name matches: look for final >

```

```

        string = extract (string, p2 + 1)
        p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
        p2 = p1
        if (extract (string, p1, p2) /= ">") call err_incomplete ()

        ! Return trailing text to the stream
        string = extract (string, p2 + 1)
        if (string /= "") call cstream%revert_record (string)
        content = extract (content, 1, p0 -1)
        closing = .true.
        exit FIND_CLOSING

    end if
end if
end do FIND_CLOSING

contains

subroutine err_io ()
    select case (iostat)
    case (:-1)
        call msg_fatal ("XML: Error reading content of '" // char (tag%name) &
            // "': end of file")
    case (1:)
        call msg_fatal ("XML: Error reading content of '" // char (tag%name) &
            // "': I/O error")
    end select
    closing = .false.
end subroutine err_io

subroutine err_incomplete ()
    call msg_fatal ("XML: Error reading content '" // char (tag%name) &
        // "': closing tag incomplete")
    closing = .false.
end subroutine err_incomplete

end subroutine xml_tag_read_content

```

7.5.4 Unit tests

Test module, followed by the corresponding implementation module.

`<xml_ut.f90>`≡

<File header>

```

module xml_ut
    use unit_tests
    use xml_util

```

<Standard module head>

<XML: public test>

```

contains

  <XML: test driver>

end module xml_ut

<xml_uti.f90>≡
  <File header>

  module xml_uti

    <Use strings>
    use io_units

    use xml

    <Standard module head>

    <XML: test declarations>

contains

  <XML: tests>

  <XML: test auxiliary>

end module xml_uti
API: driver for the unit tests below.
<XML: public test>≡
  public :: xml_test
<XML: test driver>≡
  subroutine xml_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <XML: execute tests>
  end subroutine xml_test

```

7.5.5 Auxiliary Routines

Show the contents of a temporary file, i.e., open unit.

```

<XML: test auxiliary>≡
  subroutine show (u_tmp, u)
    integer, intent(in) :: u_tmp, u
    character (80) :: buffer
    integer :: iostat
    write (u, "(A)") "File content:"
    rewind (u_tmp)
    do
      read (u_tmp, "(A)", iostat = iostat) buffer
      if (iostat /= 0) exit
      write (u, "(A)") trim (buffer)
    end do
  end subroutine show

```

```

rewind (u_tmp)
end subroutine show

```

7.5.6 Basic Tag I/O

Write a tag and read it again, using a temporary file.

```

<XML: execute tests>≡
  call test (xml_1, "xml_1", &
    "basic I/O", &
    u, results)

<XML: test declarations>≡
  public :: xml_1

<XML: tests>≡
  subroutine xml_1 (u)
    integer, intent(in) :: u
    type(xml_tag_t), allocatable :: tag
    integer :: u_tmp
    type(cstream_t) :: cstream
    logical :: success

    write (u, "(A)")  "* Test output: xml_1"
    write (u, "(A)")  "* Purpose: write and read tag"
    write (u, "(A)")

    write (u, "(A)")  "* Empty tag"
    write (u, *)

    u_tmp = free_unit ()
    open (u_tmp, status = "scratch", action = "readwrite")

    allocate (tag)
    call tag%init (var_str ("tagname"))
    call tag%write (u_tmp)
    write (u_tmp, *)
    deallocate (tag)

    call show (u_tmp, u)

    write (u, *)
    write (u, "(A)")  "Result from read:"
    call cstream%init (u_tmp)
    allocate (tag)
    call tag%init (var_str ("tagname"))
    call tag%read (cstream, success)
    call tag%write (u)
    write (u, *)
    write (u, "(A,L1)")  "success = ", success
    deallocate (tag)
    close (u_tmp)
    call cstream%final ()

    write (u, *)

```



```

write (u, "(A)")  "* Tag with preceding blank lines"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"))
write (u_tmp, *)
write (u_tmp, "(A)")  "      "
write (u_tmp, "(2x)", advance = "no")
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)")  "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)")  "success = ", success
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, *)
write (u, "(A)")  "* Tag with preceding comments"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"))
write (u_tmp, "(A)")  "<!-- comment ->"
write (u_tmp, *)
write (u_tmp, "(A)")  "<!-- multiline"
write (u_tmp, "(A)")  "      comment ->"
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)")  "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))

```

```

call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
close (u_tmp)
deallocate (tag)

call cstream%final ()

write (u, *)
write (u, "(A)")  "* Tag with name mismatch"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("wrongname"))
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: xml_1"

end subroutine xml_1

```

7.5.7 Optional Tag

Write and read two tags, one of them optional.

```

<XML: execute tests>+≡
  call test (xml_2, "xml_2", &
    "optional tag", &
    u, results)

<XML: test declarations>+≡
  public :: xml_2

```

```

<XML: tests>+≡
subroutine xml_2 (u)
  integer, intent(in) :: u
  type(xml_tag_t), allocatable :: tag1, tag2
  integer :: u_tmp
  type(cstream_t) :: cstream
  logical :: success

  write (u, "(A)")  "* Test output: xml_2"
  write (u, "(A)")  "* Purpose: handle optional tag"
  write (u, "(A)")

  write (u, "(A)")  "* Optional tag present"
  write (u, *)

  u_tmp = free_unit ()
  open (u_tmp, status = "scratch", action = "readwrite")

  allocate (tag1)
  call tag1%init (var_str ("option"))
  call tag1%write (u_tmp)
  write (u_tmp, *)
  allocate (tag2)
  call tag2%init (var_str ("tagname"))
  call tag2%write (u_tmp)
  write (u_tmp, *)
  deallocate (tag1, tag2)

  call show (u_tmp, u)

  write (u, *)
  write (u, "(A)")  "Result from read:"
  call cstream%init (u_tmp)
  allocate (tag1)
  call tag1%init (var_str ("option"))
  call tag1%read (cstream, success)
  call tag1%write (u)
  write (u, *)
  write (u, "(A,L1)")  "success = ", success
  write (u, *)
  allocate (tag2)
  call tag2%init (var_str ("tagname"))
  call tag2%read (cstream, success)
  call tag2%write (u)
  write (u, *)
  write (u, "(A,L1)")  "success = ", success
  deallocate (tag1, tag2)
  close (u_tmp)
  call cstream%final ()

  write (u, *)
  write (u, "(A)")  "* Optional tag absent"
  write (u, *)

```

```

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%write (u_tmp)
write (u_tmp, *)
deallocate (tag2)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag1)
call tag1%init (var_str ("option"))
call tag1%read (cstream, success)
call tag1%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, *)
allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%read (cstream, success)
call tag2%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag1, tag2)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: xml_2"

end subroutine xml_2

```

7.5.8 Optional Tag

Write and read a tag with single-line content.

```

<XML: execute tests>+≡
  call test (xml_3, "xml_3", &
    "content", &
    u, results)

<XML: test declarations>+≡
  public :: xml_3

<XML: tests>+≡
  subroutine xml_3 (u)
    integer, intent(in) :: u
    type(xml_tag_t), allocatable :: tag
    integer :: u_tmp
    type(cstream_t) :: cstream

```

```

logical :: success, closing
type(string_t) :: content

write (u, "(A)")  "* Test output: xml_3"
write (u, "(A)")  "* Purpose: handle tag with content"
write (u, "(A)")

write (u, "(A)")  "* Tag without content"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"))
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)")  "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)")  "success = ", success
write (u, "(A,L1)")  "content = ", tag%has_content
write (u, *)
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)")  "* Tag with content"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"), has_content = .true.)
call tag%write (var_str ("Content text"), u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)")  "Result from read:"
call cstream%init (u_tmp)
allocate (tag)

```

```

call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%read_content (cstream, content, closing)
call tag%write (u)
write (u, "(A)", advance = "no") char (content)
call tag%close (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, "(A,L1)") "content = ", tag%has_content
write (u, "(A,L1)") "closing = ", closing
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, *)
write (u, "(A)")  "* Tag with multiline content"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"), has_content = .true.)
call tag%write (u_tmp)
write (u_tmp, *)
write (u_tmp, "(A)") "Line 1"
write (u_tmp, "(A)") "Line 2"
call tag%close (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
do
    call tag%read_content (cstream, content, closing)
    if (closing) exit
    write (u, "(A)") char (content)
end do
call tag%close (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, "(A,L1)") "content = ", tag%has_content
deallocate (tag)
close (u_tmp)
call cstream%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: xml_3"

end subroutine xml_3

```

7.5.9 Basic Tag I/O

Write a tag and read it again, using a temporary file.

```

<XML: execute tests>+≡
  call test (xml_4, "xml_4", &
    "attributes", &
    u, results)

<XML: test declarations>+≡
  public :: xml_4

<XML: tests>+≡
  subroutine xml_4 (u)
    integer, intent(in) :: u
    type(xml_tag_t), allocatable :: tag
    integer :: u_tmp
    type(cstream_t) :: cstream
    logical :: success

    write (u, "(A)")  "* Test output: xml_4"
    write (u, "(A)")  "* Purpose: handle tag with attributes"
    write (u, "(A)")

    write (u, "(A)")  "* Tag with one mandatory and one optional attribute,"
    write (u, "(A)")  "* unknown attribute ignored"
    write (u, *)

    u_tmp = free_unit ()
    open (u_tmp, status = "scratch", action = "readwrite")

    allocate (tag)
    call tag%init (var_str ("tagname"), &
      [xml_attribute (var_str ("a1"), var_str ("foo")), &
      xml_attribute (var_str ("a3"), var_str ("gee"))])
    call tag%write (u_tmp)
    deallocate (tag)

    call show (u_tmp, u)

    write (u, *)
    write (u, "(A)")  "Result from read:"
    call cstream%init (u_tmp)
    allocate (tag)
    call tag%init (var_str ("tagname"), &
      [xml_attribute (var_str ("a1")), &
      xml_attribute (var_str ("a2"), var_str ("bar"))])
    call tag%read (cstream, success)
    call tag%write (u)

```

```
write (u, *)
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: xml_4"

end subroutine xml_4
```


Chapter 8

Random-Number Generator

These modules implement abstract types and tools for random-number generation.

rng_base Abstract random-number generator and factory

selectors Selection depending on weights and random numbers

Implementation of the RNG abstract types:

Module rng_tao: Interface to the TAO random number generator which the VAMP package provides. Note that VAMP explicitly requests this generator.

Module rng_stream: Implementation of RNGstream proposed by L'Ecuyer. The RNGStream provides access to different streams and/or substream of random numbers.

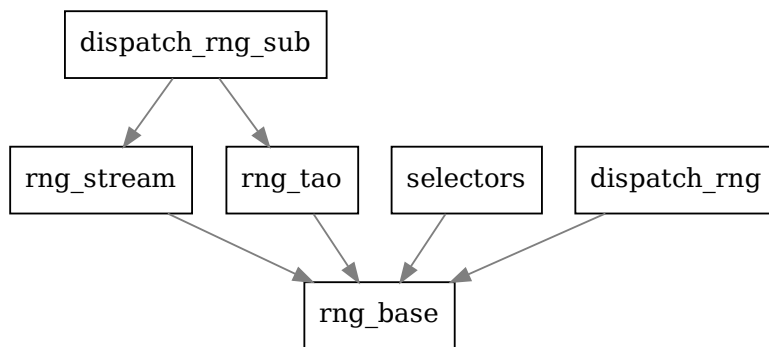


Figure 8.1: Module dependencies in `src/rng`.

8.1 Generic Random-Number Generator

For all generator implementations, we define a `rng` type which represents the state of a random-number generator with the associated methods that produce a random number. Furthermore, we define a `rng_factory` type. An object of this type is capable of allocating a sequence of `rng` objects. These generator states should be, if possible, statistically independent, so they can be used in parallel in different places of the event-generation chain.

```
<rng_base.f90>≡  
  <File header>  
  
  module rng_base  
  
    <Use kinds>  
    use kinds, only: i16  
  
    <Standard module head>  
  
    <RNG base: public>  
  
    <RNG base: types>  
  
    <RNG base: interfaces>  
  
    interface  
    <RNG base: sub interfaces>  
    end interface  
  
  end module rng_base  
<rng_base_sub.f90>≡  
  <File header>  
  
  submodule (rng_base) rng_base_s  
  
    use constants, only: TWOPI  
  
    implicit none  
  
    contains  
  
    <RNG base: procedures>  
  
  end submodule rng_base_s
```

8.1.1 Generator type

The `rng` object is actually the state of the random-number generator. The methods `initialize/reset` and `call` the generator for this state.

```
<RNG base: public>≡  
  public :: rng_t
```

```

<RNG base: types>≡
  type, abstract :: rng_t
  contains
    <RNG base: rng: TBP>
  end type rng_t

```

The `init` method initializes the generator and sets a seed. We should implement the interface such that a single integer is sufficient for a seed.

The seed may be omitted. The behavior without seed is not defined, however.

```

<RNG base: rng: TBP>≡
  procedure (rng_init), deferred :: init
<RNG base: interfaces>≡
  abstract interface
    subroutine rng_init (rng, seed)
      import
        class(rng_t), intent(out) :: rng
        integer, intent(in), optional :: seed
    end subroutine rng_init
  end interface

```

The `final` method deallocates memory where necessary and allows for another call of `init` to reset the generator.

```

<RNG base: rng: TBP>+≡
  procedure (rng_final), deferred :: final
<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_final (rng)
      import
        class(rng_t), intent(inout) :: rng
    end subroutine rng_final
  end interface

```

Output. We should, at least, identify the generator.

```

<RNG base: rng: TBP>+≡
  procedure (rng_write), deferred :: write
<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_write (rng, unit, indent)
      import
        class(rng_t), intent(in) :: rng
        integer, intent(in), optional :: unit, indent
    end subroutine rng_write
  end interface

```

These routines generate a single and an array of uniformly distributed default-precision random numbers, respectively.

```

<RNG base: rng: TBP>+≡
  generic :: generate => generate_single, generate_array
  procedure (rng_generate_single), deferred :: generate_single
  procedure (rng_generate_array), deferred :: generate_array

```

```

(RNG base: interfaces)+≡
  abstract interface
    subroutine rng_generate_single (rng, x)
      import
      class(rng_t), intent(inout) :: rng
      real(default), intent(out) :: x
    end subroutine rng_generate_single
  end interface

  abstract interface
    subroutine rng_generate_array (rng, x)
      import
      class(rng_t), intent(inout) :: rng
      real(default), dimension(:), intent(out) :: x
    end subroutine rng_generate_array
  end interface

```

These routines generate a single and an array of Gaussian (normal) distributed default-precision random numbers, respectively. Mean is 0 and $\sigma = 1$. Note that $z = \mu + \sigma x$ then distributes with mean μ and variance σ^2 .

The algorithm uses twice as much uniformly distributed random numbers, taken from the PDG review.

```

(RNG base: rng: TBP)+≡
  generic :: generate_gaussian => &
    rng_generate_gaussian_single, rng_generate_gaussian_array
  procedure, private :: rng_generate_gaussian_single
  procedure, private :: rng_generate_gaussian_array

(RNG base: sub interfaces)≡
  module subroutine rng_generate_gaussian_single (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), intent(out) :: x
  end subroutine rng_generate_gaussian_single
  module subroutine rng_generate_gaussian_array (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
  end subroutine rng_generate_gaussian_array

(RNG base: procedures)≡
  module subroutine rng_generate_gaussian_single (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), intent(out) :: x
    real(default), dimension(2) :: u
    call rng%generate (u)
    x = sin (twopi * u(1)) * sqrt (- 2 * log (u(2)))
  end subroutine rng_generate_gaussian_single

  module subroutine rng_generate_gaussian_array (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
    integer :: i
    do i = 1, size (x)
      call rng%generate_gaussian (x(i))
    end do
  end do

```

```
end subroutine rng_generate_gaussian_array
```

8.1.2 RNG Factory

A factory object has a `make` method that allocates and initializes a new generator of appropriate type. It uses a 16-bit integer for initialization. For a real-life implementation, the factory should return a sequence of statistically independent generators, and for different seeds, the sequences should also be independent.

```
<RNG base: public>+≡
  public :: rng_factory_t

<RNG base: types>+≡
  type, abstract :: rng_factory_t
    contains
      <RNG base: rng factory: TBP>
    end type rng_factory_t
```

Output. Should be short, just report the seed and current state of the factory.

```
<RNG base: rng factory: TBP>≡
  procedure (rng_factory_write), deferred :: write

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_write (object, unit)
      import
        class(rng_factory_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine rng_factory_write
  end interface
```

Initialize. It should be possible to do this repeatedly, resetting the state. The default seed should be 0.

```
<RNG base: rng factory: TBP>+≡
  procedure (rng_factory_init), deferred :: init

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_init (factory, seed)
      import
        class(rng_factory_t), intent(out) :: factory
        integer(i16), intent(in), optional :: seed
    end subroutine rng_factory_init
  end interface
```

Spawn a new generator.

```
<RNG base: rng factory: TBP>+≡
  procedure (rng_factory_make), deferred :: make
```

```

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_make (factory, rng)
      import
      class(rng_factory_t), intent(inout) :: factory
      class(rng_t), intent(out), allocatable :: rng
    end subroutine rng_factory_make
  end interface

```

8.1.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<rng_base_ut.f90>≡
  <File header>

  module rng_base_ut
    use unit_tests
    use rng_base_utl

    <Standard module head>

    <RNG base: public test>

    <RNG base: public test auxiliary>

    contains

    <RNG base: test driver>

  end module rng_base_ut

<rng_base_uti.f90>≡
  <File header>

  module rng_base_uti

    <Use kinds>
    use kinds, only: i16
    use format_utils, only: write_indent
    use io_units

    use rng_base

    <Standard module head>

    <RNG base: public test auxiliary>

    <RNG base: test declarations>

    <RNG base: test types>

    contains

```

<RNG base: tests>

<RNG base: test auxiliary>

end module rng_base_util

API: driver for the unit tests below.

<RNG base: public test>≡

public :: rng_base_test

<RNG base: test driver>≡

subroutine rng_base_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<RNG base: execute tests>

end subroutine rng_base_test

Test generator

The test 'mock' random generator generates a repeating series with the numbers 0.1, 0.3, 0.5, 0.7, 0.9. It has an integer stored as state. The integer must be one of 1, 3, 5, 7, 9.

<RNG base: public test auxiliary>≡

public :: rng_test_t

<RNG base: test types>≡

type, extends (rng_t) :: rng_test_t

integer :: state = 1

contains

procedure :: write => rng_test_write

procedure :: init => rng_test_init

procedure :: final => rng_test_final

procedure :: generate_single => rng_test_generate_single

procedure :: generate_array => rng_test_generate_array

end type rng_test_t

Output. The state is a single number, so print it.

<RNG base: test auxiliary>≡

subroutine rng_test_write (rng, unit, indent)

class(rng_test_t), intent(in) :: rng

integer, intent(in), optional :: unit, indent

integer :: u, ind

u = given_output_unit (unit)

ind = 0; if (present (indent)) ind = indent

call write_indent (u, ind)

write (u, "(A,IO,A)") "Random-number generator: &

&test (state = ", rng%state, ")"

end subroutine rng_test_write

The default seed is 1.

<RNG base: test auxiliary>+≡

subroutine rng_test_init (rng, seed)


```

class(rng_test_t), intent(out) :: rng
integer, intent(in), optional :: seed
if (present (seed)) rng%state = seed
end subroutine rng_test_init

```

Nothing to finalize:

```

<RNG base: test auxiliary>+≡
subroutine rng_test_final (rng)
class(rng_test_t), intent(inout) :: rng
end subroutine rng_test_final

```

Generate a single number and advance the state.

```

<RNG base: test auxiliary>+≡
subroutine rng_test_generate_single (rng, x)
class(rng_test_t), intent(inout) :: rng
real(default), intent(out) :: x
x = rng%state / 10._default
rng%state = mod (rng%state + 2, 10)
end subroutine rng_test_generate_single

```

The array generator calls the single-item generator multiple times.

```

<RNG base: test auxiliary>+≡
subroutine rng_test_generate_array (rng, x)
class(rng_test_t), intent(inout) :: rng
real(default), dimension(:), intent(out) :: x
integer :: i
do i = 1, size (x)
call rng%generate (x(i))
end do
end subroutine rng_test_generate_array

```

Test Factory

This factory makes `rng_test_t` generators, initialized with integers 1, 3, 5, 7, 9 if given the input 0, 1, 2, 3, 4. The generators within one sequence are all identical, however.

```

<RNG base: public test auxiliary>+≡
public :: rng_test_factory_t

<RNG base: test types>+≡
type, extends (rng_factory_t) :: rng_test_factory_t
integer :: seed = 1
contains
<RNG base: rng test factory: TBP>
end type rng_test_factory_t

```

Output.

```

<RNG base: rng test factory: TBP>≡
procedure :: write => rng_test_factory_write

```

```

<RNG base: test auxiliary>+≡
  subroutine rng_test_factory_write (object, unit)
    class(rng_test_factory_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,I0,A)") "RNG factory: test (", object%seed, ")"
  end subroutine rng_test_factory_write

```

Initialize, translating the given seed.

```

<RNG base: rng test factory: TBP>+≡
  procedure :: init => rng_test_factory_init

<RNG base: test auxiliary>+≡
  subroutine rng_test_factory_init (factory, seed)
    class(rng_test_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
    if (present (seed)) factory%seed = mod (seed * 2 + 1, 10)
  end subroutine rng_test_factory_init

```

```

<RNG base: rng test factory: TBP>+≡
  procedure :: make => rng_test_factory_make

<RNG base: test auxiliary>+≡
  subroutine rng_test_factory_make (factory, rng)
    class(rng_test_factory_t), intent(inout) :: factory
    class(rng_t), intent(out), allocatable :: rng
    allocate (rng_test_t :: rng)
    select type (rng)
    type is (rng_test_t)
      call rng%init (int (factory%seed))
    end select
  end subroutine rng_test_factory_make

```

Generator check

Initialize the generator and draw random numbers.

```

<RNG base: execute tests>≡
  call test (rng_base_1, "rng_base_1", &
    "rng initialization and call", &
    u, results)

<RNG base: test declarations>≡
  public :: rng_base_1

<RNG base: tests>≡
  subroutine rng_base_1 (u)
    integer, intent(in) :: u
    class(rng_t), allocatable :: rng

    real(default) :: x
    real(default), dimension(2) :: x2

```

```

write (u, "(A)")  "* Test output: rng_base_1"
write (u, "(A)")  "* Purpose: initialize and call a test random-number &
&generator"
write (u, "(A)")

write (u, "(A)")  "* Initialize generator"
write (u, "(A)")

allocate (rng_test_t :: rng)
call rng%init (3)

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get random number"
write (u, "(A)")

call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
write (u, "(A)")  "* Get random number pair"
write (u, "(A)")

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))")  "x =", x2

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_base_1"

end subroutine rng_base_1

```

Factory check

Set up a factory and spawn generators.

```

<RNG base: execute tests>+≡
  call test (rng_base_2, "rng_base_2", &
    "rng factory", &
    u, results)

<RNG base: test declarations>+≡
  public :: rng_base_2

<RNG base: tests>+≡
  subroutine rng_base_2 (u)
    integer, intent(in) :: u
    type(rng_test_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng

```

```

write (u, "(A)")  "* Test output: rng_base_2"
write (u, "(A)")  "* Purpose: initialize and use a rng factory"
write (u, "(A)")

write (u, "(A)")  "* Initialize factory"
write (u, "(A)")

call rng_factory%init ()
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Make a generator"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_base_2"

end subroutine rng_base_2

```

8.2 Select from a weighted sample

```
<selectors.f90>≡  
  <File header>  
  
  module selectors  
  
    <Use kinds>  
    use rng_base  
  
    <Standard module head>  
  
    <Selectors: public>  
  
    <Selectors: types>  
  
    interface  
    <Selectors: sub interfaces>  
    end interface  
  
  end module selectors  
  
<selectors_sub.f90>≡  
  <File header>  
  
  submodule (selectors) selectors_s  
  
    use io_units  
    use diagnostics  
    use format_defs, only: FMT_14, FMT_19  
  
    implicit none  
  
    contains  
  
    <Selectors: procedures>  
  
  end submodule selectors_s
```

8.2.1 Selector type

The rng object is actually the state of the random-number generator. The methods initialize/reset and call the generator for this state.

```
<Selectors: public>≡  
  public :: selector_t  
  
<Selectors: types>≡  
  type :: selector_t  
    integer :: offset = 0  
    integer, dimension(:), allocatable :: map  
    real(default), dimension(:), allocatable :: weight  
    real(default), dimension(:), allocatable :: acc  
  contains
```

```

    <Selectors: selector: TBP>
end type selector_t

```

Display contents.

```

<Selectors: selector: TBP>≡
    procedure :: write => selector_write

<Selectors: sub interfaces>≡
    module subroutine selector_write (object, unit, testflag)
        class(selector_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine selector_write

<Selectors: procedures>≡
    module subroutine selector_write (object, unit, testflag)
        class(selector_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u, i
        logical :: truncate
        u = given_output_unit (unit)
        truncate = .false.; if (present (testflag)) truncate = testflag
        write (u, "(1x,A)") "Selector: i, weight, acc. weight"
        if (allocated (object%weight)) then
            do i = 1, size (object%weight)
                if (truncate) then
                    write (u, "(3x,I0,2(1x," // FMT_14 // ")") &
                        object%map(i), object%weight(i), object%acc(i)
                else
                    write (u, "(3x,I0,2(1x," // FMT_19 // ")") &
                        object%map(i), object%weight(i), object%acc(i)
                end if
            end do
        else
            write (u, "(3x,A)") "[undefined]"
        end if
    end subroutine selector_write

```

We pack the input weight array such that zero-weight entries are removed. We also normalize it. This makes a map array for mapping the selected weight to the actual entry necessary.

We may encounter a case where all weights are zero. We do not reject this, but set up the selector so that it always returns the first entry.

```

<Selectors: selector: TBP>+≡
    procedure :: init => selector_init

<Selectors: sub interfaces>+≡
    module subroutine selector_init (selector, weight, negative_weights, offset)
        class(selector_t), intent(out) :: selector
        real(default), dimension(:), intent(in) :: weight
        logical, intent(in), optional :: negative_weights
        integer, intent(in), optional :: offset
    end subroutine selector_init

```

<Selectors: procedures>+≡

```

module subroutine selector_init (selector, weight, negative_weights, offset)
  class(selector_t), intent(out) :: selector
  real(default), dimension(:), intent(in) :: weight
  logical, intent(in), optional :: negative_weights
  integer, intent(in), optional :: offset
  real(default) :: s
  integer :: n, i
  logical :: neg_wgt
  logical, dimension(:), allocatable :: mask
  if (present (offset)) selector%offset = offset
  if (size (weight) == 0) &
    call msg_bug ("Selector init: zero-size weight array")
  neg_wgt = .false.
  if (present (negative_weights)) neg_wgt = negative_weights
  if (.not. neg_wgt .and. any (weight < 0)) &
    call msg_fatal ("Selector init: negative weight encountered")
  s = sum (weight)
  allocate (mask (size (weight)), &
    source = weight /= 0)
  n = count (mask)
  if (n > 0) then
    allocate (selector%map (n), &
      source = pack ([ (i + selector%offset, i = 1, size (weight)) ], mask))
    allocate (selector%weight (n), &
      source = pack (abs (weight) / s, mask))
    allocate (selector%acc (n))
    selector%acc(1) = selector%weight(1)
    do i = 2, n - 1
      selector%acc(i) = selector%acc(i-1) + selector%weight(i)
    end do
    selector%acc(n) = 1
  else
    allocate (selector%map (1), source = 1)
    allocate (selector%weight (1), source = 0._default)
    allocate (selector%acc (1), source = 1._default)
  end if
end subroutine selector_init

```

Select an entry based upon the number *x*, which should be a uniformly distributed random number between 0 and 1.

<Selectors: selector: TBP>+≡

```

procedure :: select => selector_select

```

<Selectors: sub interfaces>+≡

```

module function selector_select (selector, x) result (n)
  class(selector_t), intent(in) :: selector
  real(default), intent(in) :: x
  integer :: n
end function selector_select

```

<Selectors: procedures>+≡

```

module function selector_select (selector, x) result (n)
  class(selector_t), intent(in) :: selector
  real(default), intent(in) :: x

```

```

integer :: n
integer :: i
if (x < 0 .or. x > 1) &
    call msg_bug ("Selector: random number out of range")
do i = 1, size (selector%acc)
    if (x <= selector%acc(i)) exit
end do
n = selector%map(i)
end function selector_select

```

Use the provided random-number generator to select an entry. (Unless there is only one entry.)

```

⟨Selectors: selector: TBP⟩+=
    procedure :: generate => selector_generate

⟨Selectors: sub interfaces⟩+=
    module subroutine selector_generate (selector, rng, n)
        class(selector_t), intent(in) :: selector
        class(rng_t), intent(inout) :: rng
        integer, intent(out) :: n
    end subroutine selector_generate

⟨Selectors: procedures⟩+=
    module subroutine selector_generate (selector, rng, n)
        class(selector_t), intent(in) :: selector
        class(rng_t), intent(inout) :: rng
        integer, intent(out) :: n
        real(default) :: x
        select case (size (selector%acc))
        case (1)
            n = selector%map(1)
        case default
            call rng%generate (x)
            n = selector%select (x)
        end select
    end subroutine selector_generate

```

Determine the normalized weight for a selected entry. We use a linear search for the inverse lookup, assuming that efficiency is not an issue for this function.

```

⟨Selectors: selector: TBP⟩+=
    procedure :: get_weight => selector_get_weight

⟨Selectors: sub interfaces⟩+=
    module function selector_get_weight (selector, n) result (weight)
        class(selector_t), intent(in) :: selector
        integer, intent(in) :: n
        real(default) :: weight
    end function selector_get_weight

⟨Selectors: procedures⟩+=
    module function selector_get_weight (selector, n) result (weight)
        class(selector_t), intent(in) :: selector
        integer, intent(in) :: n
        real(default) :: weight
        integer :: i

```



```

do i = 1, size (selector%weight)
  if (selector%map(i) == n) then
    weight = selector%weight(i)
    return
  end if
end do
weight = 0
end function selector_get_weight

```

8.2.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨selectors_ut.f90⟩≡
  ⟨File header⟩

  module selectors_ut
    use unit_tests
    use selectors_ut

    ⟨Standard module head⟩

    ⟨Selectors: public test⟩

    contains

    ⟨Selectors: test driver⟩

  end module selectors_ut
⟨selectors_uti.f90⟩≡
  ⟨File header⟩

  module selectors_uti

    ⟨Use kinds⟩
    use rng_base

    use selectors

    use rng_base_ut, only: rng_test_t

    ⟨Standard module head⟩

    ⟨Selectors: test declarations⟩

    contains

    ⟨Selectors: tests⟩

  end module selectors_uti
API: driver for the unit tests below.
⟨Selectors: public test⟩≡
  public :: selectors_test

```

```

<Selectors: test driver>≡
  subroutine selectors_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Selectors: execute tests>
  end subroutine selectors_test

```

Basic check

Initialize the selector and draw random numbers.

```

<Selectors: execute tests>≡
  call test (selectors_1, "selectors_1", &
    "initialize, generate, query", &
    u, results)

<Selectors: test declarations>≡
  public :: selectors_1

<Selectors: tests>≡
  subroutine selectors_1 (u)
    integer, intent(in) :: u
    type(selector_t) :: selector
    class(rng_t), allocatable, target :: rng
    integer :: i, n

    write (u, "(A)")  "* Test output: selectors_1"
    write (u, "(A)")  "* Purpose: initialize a selector and test it"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize selector"
    write (u, "(A)")

    call selector%init &
      ([2._default, 3.5_default, 0._default, &
        2._default, 0.5_default, 2._default])
    call selector%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Select numbers using predictable test generator"
    write (u, "(A)")

    allocate (rng_test_t :: rng)
    call rng%init (1)

    do i = 1, 5
      call selector%generate (rng, n)
      write (u, "(1x,I0)")  n
    end do

    write (u, "(A)")
    write (u, "(A)")  "* Select numbers using real input number"
    write (u, "(A)")

    write (u, "(1x,A,I0)")  "select(0.00) = ", selector%select (0._default)

```

```

write (u, "(1x,A,I0)") "select(0.77) = ", selector%select (0.77_default)
write (u, "(1x,A,I0)") "select(1.00) = ", selector%select (1._default)

write (u, "(A)")
write (u, "(A)")  "* Get weight"
write (u, "(A)")

write (u, "(1x,A,ES19.12)") "weight(2) =", selector%get_weight(2)
write (u, "(1x,A,ES19.12)") "weight(3) =", selector%get_weight(3)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: selectors_1"

end subroutine selectors_1

```

Offset

Same tests with a -1 offset on all indices, i.e., counting from zero.

```

<Selectors: execute tests>+≡
  call test (selectors_2, "selectors_2", &
    "handle index offset", &
    u, results)

<Selectors: test declarations>+≡
  public :: selectors_2

<Selectors: tests>+≡
  subroutine selectors_2 (u)
    integer, intent(in) :: u
    type(selector_t) :: selector
    class(rng_t), allocatable, target :: rng
    integer :: i, n

    write (u, "(A)")  "* Test output: selectors_2"
    write (u, "(A)")  "* Purpose: initialize and use a selector &
      &with offset index"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize selector"
    write (u, "(A)")

    call selector%init &
      ([2._default, 3.5_default, 0._default, &
        2._default, 0.5_default, 2._default], &
        offset = -1)
    call selector%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Select numbers using predictable test generator"

```

```

write (u, "(A)")

allocate (rng_test_t :: rng)
call rng%init (1)

do i = 1, 5
    call selector%generate (rng, n)
    write (u, "(1x,I0)") n
end do

write (u, "(A)")
write (u, "(A)")  "* Select numbers using real input number"
write (u, "(A)")

write (u, "(1x,A,I0)") "select(0.00) = ", selector%select (0._default)
write (u, "(1x,A,I0)") "select(0.77) = ", selector%select (0.77_default)
write (u, "(1x,A,I0)") "select(1.00) = ", selector%select (1._default)

write (u, "(A)")
write (u, "(A)")  "* Get weight"
write (u, "(A)")

write (u, "(1x,A,ES19.12)") "weight(1) =", selector%get_weight(1)
write (u, "(1x,A,ES19.12)") "weight(2) =", selector%get_weight(2)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: selectors_2"

end subroutine selectors_2

```

8.3 TAO Random-Number Generator

This module provides an implementation for the generic random-number generator. Actually, we interface the TAO random-number generator which is available via the VAMP package.

```

<rng_tao.f90>≡
  <File header>

  module rng_tao

    <Use kinds>
    use tao_random_numbers !NODEP!

    use rng_base

    <Standard module head>

```

```

    <RNG tao: public>

    <RNG tao: types>

        interface
    <RNG tao: sub interfaces>
        end interface

    contains

    <RNG tao: main procedures>

    end module rng_tao
<rng_tao_sub.f90>≡
    <File header>

    submodule (rng_tao) rng_tao_s

        use io_units
        use format_utils, only: write_indent

        implicit none

    contains

    <RNG tao: procedures>

    end submodule rng_tao_s

```

8.3.1 Generator type

The rng object is actually the state of the random-number generator. The methods initialize/reset and call the generator for this state.

We keep the seed, in case we want to recover it later, and count the number of calls since seeding.

```

<RNG tao: public>≡
    public :: rng_tao_t

<RNG tao: types>≡
    type, extends (rng_t) :: rng_tao_t
        integer :: seed = 0
        integer :: n_calls = 0
        type(tao_random_state) :: state
    contains
    <RNG tao: rng tao: TBP>
    end type rng_tao_t

```

Output: Display seed and number of calls.

```

<RNG tao: rng tao: TBP>≡
    procedure :: write => rng_tao_write

```

```

<RNG tao: sub interfaces>≡
  module subroutine rng_tao_write (rng, unit, indent)
    class(rng_tao_t), intent(in) :: rng
    integer, intent(in), optional :: unit, indent
  end subroutine rng_tao_write

```

```

<RNG tao: procedures>≡
  module subroutine rng_tao_write (rng, unit, indent)
    class(rng_tao_t), intent(in) :: rng
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(A)") "TA0 random-number generator:"
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") "seed = ", rng%seed
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") "calls = ", rng%n_calls
  end subroutine rng_tao_write

```

The `init` method initializes the generator and sets a seed. We should implement the interface such that a single integer is sufficient for a seed.

The seed may be omitted. The default seed is 0.

```

<RNG tao: rng tao: TBP>+≡
  procedure :: init => rng_tao_init

<RNG tao: sub interfaces>+≡
  module subroutine rng_tao_init (rng, seed)
    class(rng_tao_t), intent(out) :: rng
    integer, intent(in), optional :: seed
  end subroutine rng_tao_init

<RNG tao: procedures>+≡
  module subroutine rng_tao_init (rng, seed)
    class(rng_tao_t), intent(out) :: rng
    integer, intent(in), optional :: seed
    if (present (seed)) rng%seed = seed
    call tao_random_create (rng%state, rng%seed)
  end subroutine rng_tao_init

```

The `final` method deallocates memory where necessary and allows for another call of `init` to reset the generator.

```

<RNG tao: rng tao: TBP>+≡
  procedure :: final => rng_tao_final

<RNG tao: sub interfaces>+≡
  module subroutine rng_tao_final (rng)
    class(rng_tao_t), intent(inout) :: rng
  end subroutine rng_tao_final

<RNG tao: procedures>+≡
  module subroutine rng_tao_final (rng)
    class(rng_tao_t), intent(inout) :: rng
    call tao_random_destroy (rng%state)
  end subroutine rng_tao_final

```

```
end subroutine rng_tao_final
```

These routines generate a single and an array of default-precision random numbers, respectively.

We have to convert from explicit double to abstract default precision. Under normal conditions, both are equivalent, however. Unless, someone decides to do single precision, there is always an interface for `tao_random_numbers`.

```
<RNG tao: rng tao: TBP>+≡
  procedure :: generate_single => rng_tao_generate_single
  procedure :: generate_array => rng_tao_generate_array

<RNG tao: sub interfaces>+≡
  module subroutine rng_tao_generate_single (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), intent(out) :: x
  end subroutine rng_tao_generate_single
  module subroutine rng_tao_generate_array (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
  end subroutine rng_tao_generate_array

<RNG tao: procedures>+≡
  module subroutine rng_tao_generate_single (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), intent(out) :: x
    real(default) :: r
    call tao_random_number (rng%state, r)
    x = r
    rng%n_calls = rng%n_calls + 1
  end subroutine rng_tao_generate_single

  module subroutine rng_tao_generate_array (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
    real(default) :: r
    integer :: i
    do i = 1, size (x)
      call tao_random_number (rng%state, r)
      x(i) = r
    end do
    rng%n_calls = rng%n_calls + size (x)
  end subroutine rng_tao_generate_array
```

Factory

This factory makes `rng_tao_t` generators, initialized with the seeds

$$s_i = s_0 * 2^{16} + i \quad (8.1)$$

where s_0 is the seed (a 16-bit integer) given to the factory object, and i is the index in the generated sequence of generators, starting with zero.

```
<RNG tao: public>+≡
  public :: rng_tao_factory_t
```

```

<RNG tao: types>+≡
  type, extends (rng_factory_t) :: rng_tao_factory_t
    integer(i16) :: s = 0
    integer(i16) :: i = 0
  contains
    <RNG tao: rng tao factory: TBP>
  end type rng_tao_factory_t

```

Output.

```

<RNG tao: rng tao factory: TBP>≡
  procedure :: write => rng_tao_factory_write

<RNG tao: sub interfaces>+≡
  module subroutine rng_tao_factory_write (object, unit)
    class(rng_tao_factory_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine rng_tao_factory_write

<RNG tao: procedures>+≡
  module subroutine rng_tao_factory_write (object, unit)
    class(rng_tao_factory_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,2(I0,A))") &
      "RNG factory: tao (", object%s, ",", object%i, ")"
  end subroutine rng_tao_factory_write

```

Initialize, translating the given seed.

```

<RNG tao: rng tao factory: TBP>+≡
  procedure :: init => rng_tao_factory_init

<RNG tao: sub interfaces>+≡
  module subroutine rng_tao_factory_init (factory, seed)
    class(rng_tao_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
  end subroutine rng_tao_factory_init

<RNG tao: procedures>+≡
  module subroutine rng_tao_factory_init (factory, seed)
    class(rng_tao_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
    if (present (seed)) factory%s = seed
  end subroutine rng_tao_factory_init

```

Due to a bug of allocating polymorphic types with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

<RNG tao: rng tao factory: TBP>+≡
  procedure :: make => rng_tao_factory_make

<RNG tao: main procedures>≡
  subroutine rng_tao_factory_make (factory, rng)
    class(rng_tao_factory_t), intent(inout) :: factory

```



```

class(rng_t), intent(out), allocatable :: rng
allocate (rng_tao_t :: rng)
select type (rng)
type is (rng_tao_t)
    call rng%init (factory%s * 65536 + factory%i)
    factory%i = int (factory%i + 1, kind = i16)
end select
end subroutine rng_tao_factory_make

```

8.3.2 Unit tests

Test module, followed by the corresponding implementation module.

<rng_tao_ut.f90>≡
<File header>

```

module rng_tao_ut
    use unit_tests
    use rng_tao_uti

```

<Standard module head>

<RNG tao: public test>

contains

<RNG tao: test driver>

```

end module rng_tao_ut

```

<rng_tao_uti.f90>≡
<File header>

```

module rng_tao_uti

```

<Use kinds>

```

    use kinds, only: i16
    use rng_base

```

```

    use rng_tao

```

<Standard module head>

<RNG tao: test declarations>

contains

<RNG tao: tests>

```

end module rng_tao_uti

```

API: driver for the unit tests below.

<RNG tao: public test>≡
 public :: rng_tao_test

```

<RNG tao: test driver>≡
  subroutine rng_tao_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <RNG tao: execute tests>
  end subroutine rng_tao_test

```

Generator check

Initialize the generator and draw random numbers.

```

<RNG tao: execute tests>≡
  call test (rng_tao_1, "rng_tao_1", &
    "rng initialization and call", &
    u, results)

<RNG tao: test declarations>≡
  public :: rng_tao_1

<RNG tao: tests>≡
  subroutine rng_tao_1 (u)
    integer, intent(in) :: u
    class(rng_t), allocatable, target :: rng

    real(default) :: x
    real(default), dimension(2) :: x2

    write (u, "(A)")  "* Test output: rng_tao_1"
    write (u, "(A)")  "*   Purpose: initialize and call the TAO random-number &
      &generator"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize generator (default seed)"
    write (u, "(A)")

    allocate (rng_tao_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Get random number"
    write (u, "(A)")

    call rng%generate (x)
    write (u, "(A,2(1x,F9.7))")  "x =", x

    write (u, "(A)")
    write (u, "(A)")  "* Get random number pair"
    write (u, "(A)")

    call rng%generate (x2)
    write (u, "(A,2(1x,F9.7))")  "x =", x2

    write (u, "(A)")

```

```

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_tao_1"

end subroutine rng_tao_1

```

Factory check

Set up a factory and spawn generators.

```

<RNG tao: execute tests>+≡
  call test (rng_tao_2, "rng_tao_2", &
    "rng factory", &
    u, results)
<RNG tao: test declarations>+≡
  public :: rng_tao_2
<RNG tao: tests>+≡
  subroutine rng_tao_2 (u)
    integer, intent(in) :: u
    type(rng_tao_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng
    real(default) :: x

    write (u, "(A)")  "* Test output: rng_tao_2"
    write (u, "(A)")  "* Purpose: initialize and use a rng factory"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize factory"
    write (u, "(A)")

    call rng_factory%init ()
    call rng_factory%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Make a generator"
    write (u, "(A)")

    call rng_factory%make (rng)
    call rng%write (u)
    call rng%generate (x)
    write (u, *)
    write (u, "(1x,A,F7.5)")  "x = ", x
    call rng%final ()
    deallocate (rng)

    write (u, "(A)")
    write (u, "(A)")  "* Repeat"

```

```

write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)") "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize factory with different seed"
write (u, "(A)")

call rng_factory%init (1_i16)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Make a generator"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)") "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_tao_2"

end subroutine rng_tao_2

```

8.4 RNG Stream

We implement the RNGstream proposed and implemented in C++, C and Java by L'Ecuyer et al. (L'Ecuyer, Pierre, Richard Simard, E. Jack Chen, and W. David Kelton. "An Object-Oriented Random-Number Package with Many Long Streams and Substreams." *Operations Research* 50, no. 6 (December 2002): 1073–1075. doi:10.1287/opre.50.6.1073.358.). RNGstream allows us to access multiple independent streams of random numbers.

```

⟨rng_stream.f90⟩≡
  ⟨File header⟩

```

```

module rng_stream

  <Use kinds>
    use kinds, only: i16
    use rng_base

  <Standard module head>

  <RNG stream: public>

  <RNG stream: types>

    interface
  <RNG stream: sub interfaces>
    end interface

  contains

  <RNG stream: main procedures>

end module rng_stream

<rng_stream_sub.f90>≡
  <File header>

  submodule (rng_stream) rng_stream_s

    use io_units
    use format_utils, only: write_indent
    use diagnostics

    implicit none

  <RNG stream: parameters>

  contains

  <RNG stream: procedures>

end submodule rng_stream_s

```

We store the current position in the stream of random numbers. Furthermore, we store the beginning of the (latest) substream and the initial starting point of the stream, which corresponds to the “seed”. The default seed is 1234.

```

<RNG stream: public>≡
  public :: rng_stream_t

<RNG stream: types>≡
  type, extends(rng_t) :: rng_stream_t
    private
    logical :: antithetic = .false.
    logical :: increased_precision = .false.
    real(default), dimension(3, 2) :: current_position = 1234._default
    real(default), dimension(3, 2) :: beginning_substream = 1234._default

```

```

    real(default), dimension(3, 2) :: initial_stream = 1234._default
contains
  (RNG stream: rng stream: TBP)
end type rng_stream_t

```

Output. Display current position and the (sub-)stream positions.

```

(RNG stream: rng stream: TBP)≡
  procedure, public :: write => rng_stream_write

(RNG stream: sub interfaces)≡
  module subroutine rng_stream_write (rng, unit, indent)
    class(rng_stream_t), intent(in) :: rng
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
  end subroutine rng_stream_write

(RNG stream: procedures)≡
  module subroutine rng_stream_write (rng, unit, indent)
    class(rng_stream_t), intent(in) :: rng
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: j, u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(A)") "RNG Stream generator"
    call write_indent (u, ind)
    write (u, "(A)") "Current position = [ "
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%current_position(:, 1)
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%current_position(:, 2)
    call write_indent (u, ind)
    write (u, "(A)") "]"
    call write_indent (u, ind)
    write (u, "(A)") "Beginning substream = [ "
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%beginning_substream(:, 1)
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%beginning_substream(:, 2)
    call write_indent (u, ind)
    write (u, "(A)") "]"
    call write_indent (u, ind)
    write (u, "(A)") "Initial stream = [ "
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%initial_stream(:, 1)
    call write_indent (u, ind)
    write (u, "(3(F20.1,' ',1X))") rng%initial_stream(:, 2)
    call write_indent (u, ind)
    write (u, "(A)") "]"
  end subroutine rng_stream_write

```

Initialise the generator. Set the states to the (optional) seed.

```

(RNG stream: rng stream: TBP)+≡

```

```

    procedure, public :: init => rng_stream_init
  <RNG stream: sub interfaces>+≡
    module subroutine rng_stream_init (rng, seed)
      class(rng_stream_t), intent(out) :: rng
      integer, intent(in), optional :: seed
    end subroutine rng_stream_init
  <RNG stream: procedures>+≡
    module subroutine rng_stream_init (rng, seed)
      class(rng_stream_t), intent(out) :: rng
      integer, intent(in), optional :: seed
      real(default), dimension(3, 2) :: real_seed
      if (present (seed)) then
        real_seed = real(seed, default)
        call rng%set_initial_stream (real_seed)
      end if
    end subroutine rng_stream_init

```

Finalize. Nothing to do.

```

  <RNG stream: rng stream: TBP>+≡
    procedure, public :: final => rng_stream_final
  <RNG stream: sub interfaces>+≡
    module subroutine rng_stream_final (rng)
      class(rng_stream_t), intent(inout) :: rng
    end subroutine rng_stream_final
  <RNG stream: procedures>+≡
    module subroutine rng_stream_final (rng)
      class(rng_stream_t), intent(inout) :: rng
    end subroutine rng_stream_final

```

Set the initial stream, but test the seed before. They are not allowed to be 0 or larger than m_1 or m_2 .

```

  <RNG stream: rng stream: TBP>+≡
    procedure, public :: set_initial_stream => rng_stream_set_initial_stream
  <RNG stream: sub interfaces>+≡
    module subroutine rng_stream_set_initial_stream (rng, seed)
      class(rng_stream_t), intent(inout) :: rng
      real(default), dimension(3, 2), intent(in) :: seed
    end subroutine rng_stream_set_initial_stream
  <RNG stream: procedures>+≡
    module subroutine rng_stream_set_initial_stream (rng, seed)
      class(rng_stream_t), intent(inout) :: rng
      real(default), dimension(3, 2), intent(in) :: seed
      if (any (seed(:, 1) > m1)) then
        write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: seed(:, 1) >= ", m1, ",&
          & Seed is not set."
        call msg_fatal ()
      end if
      if (any (seed(:, 2) > m2)) then
        write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: seed(:, 2) >= ", m2, ",&
          & Seed is not set."
      end if
    end subroutine rng_stream_set_initial_stream

```

```

        call msg_fatal ()
    end if
    if (any (seed(:, 1) == 0)) then
        write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: First 3 seed = 0."
        call msg_fatal ()
    end if
    if (any (seed(:, 2) == 0)) then
        write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: Last 3 seed = 0."
        call msg_fatal ()
    end if
    rng%initial_stream = seed
    call rng%reset_stream ()
end subroutine rng_stream_set_initial_stream

```

Generate a single real random number from the current state of (sub-)stream.

The machine representation of the result can lead to negative numbers. We add m_1 or m_2 to the respective number to ensure they are all positive and are still congruent to $\text{mod } m_1$ or $\text{mod } m_2$.

The final formula $x = y(3,1) - y(3,2) \pmod{m_1}$ can lead to negative random numbers. Instead of directly calculating the modulo, we check whether $y(3,1)$ is larger than $y(3,2)$, or not. If $x(3,1) > y(3,2)$, then $y(3,1) - y(3,2)$ is congruent to $y(3,1) - y(3,2) \pmod{m_1}$. If $y(3,1) < y(3,2)$, then $y(3,1) - y(3,2) + m_1$ is congruent to $y(3,1) - y(3,2) \pmod{m_1}$.

(RNG stream: parameters)≡

```

real(default), parameter :: &
    m1 = 4294967087.0_default, &
    m2 = 4294944443.0_default, &
    norm = 1.0_default / (m1 + 1.0_default)
real(default), dimension(3, 3), parameter :: A1p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -810728.0_default, 1403580.0_default, 0.0_default], &
    shape (A1p0), order = [2, 1])
real(default), dimension(3, 3), parameter :: A2p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -1370589.0_default, 0.0_default, 527612.0_default], &
    shape (A2p0), order = [2, 1])

```

(RNG stream: rng stream: TBP)+≡

```

procedure, public :: generate_single => rng_stream_generate_single

```

(RNG stream: sub interfaces)+≡

```

module subroutine rng_stream_generate_single (rng, x)
    class(rng_stream_t), intent(inout) :: rng
    real(default), intent(out) :: x
end subroutine rng_stream_generate_single

```

(RNG stream: procedures)+≡

```

module subroutine rng_stream_generate_single (rng, x)
    class(rng_stream_t), intent(inout) :: rng
    real(default), intent(out) :: x
    associate (y => rng%current_position)
        y(:, 1) = mod (matmul (A1p0, y(:, 1)), m1)
    end associate

```



```

        if (y(3, 1) < 0._default) y(3, 1) = y(3, 1) + m1
        y(:, 2) = mod (matmul (A2p0, y(:, 2)), m2)
        if (y(3, 2) < 0._default) y(3, 2) = y(3, 2) + m2
        x = y(3, 1) - y(3, 2)
        if (x < 0._default) x = x + m1
        x = x * norm
    end associate
    if (rng%antithetic) x = 1. - x
end subroutine rng_stream_generate_single

```

Generate an array of real random numbers.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: generate_array => rng_stream_generate_array

<RNG stream: sub interfaces>+≡
    module subroutine rng_stream_generate_array (rng, x)
        class(rng_stream_t), intent(inout) :: rng
        real(default), dimension(:), intent(out) :: x
    end subroutine rng_stream_generate_array

<RNG stream: procedures>+≡
    module subroutine rng_stream_generate_array (rng, x)
        class(rng_stream_t), intent(inout) :: rng
        real(default), dimension(:), intent(out) :: x
        integer :: j
        do j = 1, size (x)
            call rng%generate_single(x(j))
        end do
    end subroutine rng_stream_generate_array

```

Reset to initial stream.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: reset_stream => rng_stream_reset_stream

<RNG stream: sub interfaces>+≡
    module subroutine rng_stream_reset_stream (rng)
        class(rng_stream_t), intent(inout) :: rng
    end subroutine rng_stream_reset_stream

<RNG stream: procedures>+≡
    module subroutine rng_stream_reset_stream (rng)
        class(rng_stream_t), intent(inout) :: rng
        rng%current_position = rng%initial_stream
        rng%beginning_substream = rng%initial_stream
    end subroutine rng_stream_reset_stream

```

Reset to beginning of substream.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: reset_substream => rng_stream_reset_substream

<RNG stream: sub interfaces>+≡
    module subroutine rng_stream_reset_substream (rng)
        class(rng_stream_t), intent(inout) :: rng
    end subroutine rng_stream_reset_substream

```

```

<RNG stream: procedures>+≡
  module subroutine rng_stream_reset_substream (rng)
    class(rng_stream_t), intent(inout) :: rng
    rng%current_position = rng%beginning_substream
  end subroutine rng_stream_reset_substream

```

Advance to next substream.

```

<RNG stream: parameters>+≡
  real(default), dimension(3, 3), parameter :: A1p76 = reshape (&
    [82758667.0_default, 1871391091.0_default, 4127413238.0_default, &
    3672831523.0_default, 69195019.0_default, 1871391091.0_default, &
    3672091415.0_default, 352874325.0_default, 69195019.0_default], &
    shape(A1p76), order = [2, 1])
  real(default), dimension(3, 3), parameter :: A2p76 = reshape (&
    [1511326704.0_default, 3759209742.0_default, 1610795712.0_default, &
    4292754251.0_default, 1511326704.0_default, 3889917532.0_default, &
    3859662829.0_default, 4292754251.0_default, 3708466080.0_default], &
    shape(A2p76), order = [2, 1])

```

```

<RNG stream: rng stream: TBP>+≡
  procedure, public :: next_substream => rng_stream_next_substream

```

```

<RNG stream: sub interfaces>+≡
  module subroutine rng_stream_next_substream (rng)
    class(rng_stream_t), intent(inout) :: rng
  end subroutine rng_stream_next_substream

```

```

<RNG stream: procedures>+≡
  module subroutine rng_stream_next_substream (rng)
    class(rng_stream_t), intent(inout) :: rng
    associate (x => rng%beginning_substream)
      x(:,1) = matmul_mod (A1p76, x(:,1), m1)
      x(:,2) = matmul_mod (A2p76, x(:,2), m2)
    end associate
    call rng%reset_substream ()
  end subroutine rng_stream_next_substream

```

Advance state of the current stream by n steps. We do not touch the beginning of the substream nor the initial stream. The purpose of the procedure is to reproduce the same random number (streams) among multiple workers without additional communication cost. E.g. worker 1 needs the first 5000 random numbers and the second one needs the next 5000 random numbers. In such a way we can exactly reproduce results (upon numerical noise) in single or parallel runs with the RngStream. The procedure must only be used with care! Misuse can lead to wrong results!

```

<RNG stream: parameter>≡
  real(default), dimension(3, 3), parameter :: A1p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -810728.0_default, 1403580.0_default, 0.0_default], &
    shape(A1p0), order = [2, 1])
  real(default), dimension(3, 3), parameter :: A2p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &

```

```

-1370589.0_default, 0.0_default, 527612.0_default], &
shape(A2p0), order = [2, 1])
<RNG stream: rng stream: TBP>+≡
  procedure, public :: advance_state => rng_stream_advance_state
<RNG stream: sub interfaces>+≡
  module subroutine rng_stream_advance_state (rng, n)
    class(rng_stream_t), intent(inout) :: rng
    integer, intent(in) :: n
  end subroutine rng_stream_advance_state
<RNG stream: procedures>+≡
  module subroutine rng_stream_advance_state (rng, n)
    class(rng_stream_t), intent(inout) :: rng
    integer, intent(in) :: n
    real(default), dimension(3, 3) :: A1pn, A2pn
    associate (x => rng%current_position)
      A1pn = matpow_mod (A1p0, m1, n)
      A2pn = matpow_mod (A2p0, m2, n)
      x(:,1) = matmul_mod (A1pn, x(:,1), m1)
      x(:,2) = matmul_mod (A2pn, x(:,2), m2)
    end associate
  end subroutine rng_stream_advance_state

```

A divide and conquer algorithm is applied to calculate $A^n \bmod m$. We refer to the original paper from L'Ecuyer for further reading.

```

<RNG stream: procedures>+≡
  function matpow_mod (a, m, n) result (c)
    real(default), dimension(3, 3), intent(in) :: a
    real(default), intent(in) :: m
    integer, intent(in) :: n
    real(default), dimension(3, 3) :: c
    real(default), dimension(3, 3) :: w
    integer :: i
    w = a
    c = 0._default; forall (i = 1:3) c(i, i) = 1._default
    i = n
    do while (i > 0)
      if (mod(i, 2) /= 0) c = matmat_mod (w, c, m)
      w = matmat_mod (w, w, m)
      i = i / 2
    end do
  end function matpow_mod

  function matmat_mod (a, b, m) result (c)
    real(default), dimension(3, 3), intent(in) :: a
    real(default), dimension(3, 3), intent(in) :: b
    real(default), dimension(3, 3) :: c
    real(default), intent(in) :: m
    integer :: i
    do i = 1, 3
      c(:, i) = matmul_mod (a, b(:, i), m)
    end do
  end function matmat_mod

```

8.4.1 Factory

We utilize the streams proposed by L'Ecuyer where we use precalculated transition matrices to jump between different (sub-)streams.

The random generator has the period ρ and the transition function $T : s_n \rightarrow s_{n+1}$ whereas s_n is the generator's state after n steps. Furthermore, it is $T^\rho(s) = s$. The stream of random number then is disjoint into streams and substreams. The length of the streams, which divide the overall stream, should be $Z = 2^z$ and partition those streams again in $V = 2^v$ substreams of length $W = 2^w$.

We store the seed and the initial stream, also, the beginning of the substream.

```

(RNG stream: public)+≡
    public :: rng_stream_factory_t

(RNG stream: types)+≡
    type, extends(rng_factory_t) :: rng_stream_factory_t
        real(default), dimension(3, 2) :: seed = 1234._default
        contains
        (RNG stream: rng stream factory: TBP)
    end type rng_stream_factory_t

```

Output.

```

(RNG stream: rng stream factory: TBP)≡
    procedure, public :: write => rng_stream_factory_write

(RNG stream: sub interfaces)+≡
    module subroutine rng_stream_factory_write (object, unit)
        class(rng_stream_factory_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine rng_stream_factory_write

(RNG stream: procedures)+≡
    module subroutine rng_stream_factory_write (object, unit)
        class(rng_stream_factory_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "RNG Stream factory"
        write (u, "(1x,A,6(F20.1,' ',1X),A)") "Next seed = [ "
        write (u, "(1x,3(F20.1,' ',1X))") object%seed(:, 1)
        write (u, "(1x,3(F20.1,' ',1X))") object%seed(:, 2)
        write (u, "(1x,A)") "]"
    end subroutine rng_stream_factory_write

```

Initialize. Default seed is 1234. We do not check whether the seed is valid, this is later done in `rng_stream_init`.

Additionally, we have to explicitly convert from `integer` to `real` because we are using floating-point arithmetic and not integer arithmetic due to a larger set of number in the representation of real numbers.

```

(RNG stream: rng stream factory: TBP)+≡
    procedure, public :: init => rng_stream_factory_init

```

```

(RNG stream: sub interfaces)+≡
  module subroutine rng_stream_factory_init (factory, seed)
    class(rng_stream_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
  end subroutine rng_stream_factory_init

```

```

(RNG stream: procedures)+≡
  module subroutine rng_stream_factory_init (factory, seed)
    class(rng_stream_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
    real(default), dimension(3, 2) :: real_seed
    if (present (seed)) then
      factory%seed = real(seed, default)
    end if
  end subroutine rng_stream_factory_init

```

Allocate a new RNG and different stream states, accordingly. Due to a bug of allocating polymorphic types with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

(RNG stream: rng stream factory: TBP)+≡
  procedure, public :: make => rng_stream_factory_make

```

```

(RNG stream: main procedures)≡
  subroutine rng_stream_factory_make (factory, rng)
    class(rng_stream_factory_t), intent(inout) :: factory
    class(rng_t), intent(out), allocatable :: rng
    allocate (rng_stream_t :: rng)
    select type (rng)
    type is (rng_stream_t)
      call rng%init ()
      call rng%set_initial_stream (factory%seed)
    end select
    call factory%advance_seed ()
  end subroutine rng_stream_factory_make

```

Advance seed. Use the precalculated transistion matrices for the streams.

```

(RNG stream: parameters)+≡
  real(default), dimension(3, 3), parameter :: A1p127 = reshape (&
    [2427906178.0_default, 3580155704.0_default, 949770784.0_default, &
    226153695.0_default, 1230515664.0_default, 3580155704.0_default, &
    1988835001.0_default, 986791581.0_default, 1230515664.0_default], &
    shape(A1p127), order = [2, 1])
  real(default), dimension(3, 3), parameter :: A2p127 = reshape (&
    [1464411153.0_default, 277697599.0_default, 1610723613.0_default, &
    32183930.0_default, 1464411153.0_default, 1022607788.0_default, &
    2824425944.0_default, 32183930.0_default, 2093834863.0_default], &
    shape(A2p127), order = [2, 1])

```

```

(RNG stream: rng stream factory: TBP)+≡
  procedure, private :: advance_seed => rng_stream_factory_advance_seed

```

```

(RNG stream: sub interfaces)+≡
  module subroutine rng_stream_factory_advance_seed (factory)
    class(rng_stream_factory_t), intent(inout) :: factory
  end subroutine rng_stream_factory_advance_seed

```

```

<RNG stream: procedures>+≡
module subroutine rng_stream_factory_advance_seed (factory)
  class(rng_stream_factory_t), intent(inout) :: factory
  factory%seed(:,1) = matmul_mod (A1p127, factory%seed(:,1), m1)
  factory%seed(:,2) = matmul_mod (A2p127, factory%seed(:,2), m2)
end subroutine rng_stream_factory_advance_seed

```

Matrix modulo calculation optimized for 2^{53} representation of floating numbers. Speed efficiency is not a requirement, because the streams should not be advanced that often.

```

<RNG stream: procedures>+≡
function matmul_mod (a, u, m) result (v)
  real(default), dimension(:, :), intent(in) :: a
  real(default), dimension(:, :), intent(in) :: u
  real(default), intent(in) :: m
  real(default), dimension(size (u)) :: v
  integer :: i
  do i = 1, 3
    v(i) = mult_mod (a(i, 1), u(1), 0.0_default, m)
    v(i) = mult_mod (a(i, 2), u(2), v(i), m)
    v(i) = mult_mod (a(i, 3), u(3), v(i), m)
  end do
end function matmul_mod

```

Decompose.

Decomposition to ensure exact accuracy for the case v exceeds 2^{53} .

$$a \cdot smodm = ((a1 \cdot s \bmod m) * 2^{17} + a2 \cdot s) \bmod m.$$

```

<RNG stream: parameters>+≡
real(default), parameter :: &
  a12 = 1403580.0_default, &
  a13n = 810728.0_default, &
  a21 = 527612.0_default, &
  a23n = 1370589.0_default, &
  two53 = 9007199254740992.0_default, &
  two17 = 131072.0_default

```

```

<RNG stream: procedures>+≡
function mult_mod (a, b, c, m) result (v)
  real(default), intent(in) :: a
  real(default), intent(in) :: b
  real(default), intent(in) :: c
  real(default), intent(in) :: m
  real(default) :: v
  integer :: a1
  real(default) :: a2
  v = a * b + c
  if (v >= two53 .or. v <= -two53) then
    a1 = int (a / two17)
    a2 = a - a1 * two17
    v = mod (a1 * b, m)
    v = v * two17 + a2 * b + c
  end if

```

```

    v = mod (v, m)
    if (v < 0.0_default) v = v + m
end function mult_mod

```

8.4.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨rng_stream_ut.f90⟩≡
  ⟨File header⟩

  module rng_stream_ut
    use unit_tests
    use rng_stream_uti

    ⟨Standard module head⟩

    ⟨RNG stream: public test⟩

    contains

    ⟨RNG stream: test driver⟩

  end module rng_stream_ut

⟨rng_stream_uti.f90⟩≡
  ⟨File header⟩

  module rng_stream_uti

    ⟨Use kinds⟩
    use kinds, only: i16
    use rng_base

    use rng_stream

    ⟨Standard module head⟩

    ⟨RNG stream: test declarations⟩

    contains

    ⟨RNG stream: tests⟩

  end module rng_stream_uti
API: driver for the unit tests below.
⟨RNG stream: public test⟩≡
  public :: rng_stream_test
⟨RNG stream: test driver⟩≡
  subroutine rng_stream_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  ⟨RNG stream: execute tests⟩

```

```
end subroutine rng_stream_test
```

Generator check

Initialize the generator and draw random numbers.

```
<RNG stream: execute tests>≡
  call test (rng_stream_1, "rng_stream_1", &
    "rng initialization and call", &
    u, results)

<RNG stream: test declarations>≡
  public :: rng_stream_1

<RNG stream: tests>≡
  subroutine rng_stream_1 (u)
    integer, intent(in) :: u
    class(rng_t), allocatable, target :: rng

    real(default) :: x
    real(default), dimension(2) :: x2

    write (u, "(A)")  "* Test output: rng_stream_1"
    write (u, "(A)")  "* Purpose: initialize and call the RNGstream random-number &
      &generator"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Get random number"
    write (u, "(A)")

    call rng%generate (x)
    write (u, "(A,2(1x,F9.7))")  "x =", x

    write (u, "(A)")
    write (u, "(A)")  "* Get random number pair"
    write (u, "(A)")

    call rng%generate (x2)
    write (u, "(A,2(1x,F9.7))")  "x =", x2

    write (u, "(A)")
    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Jump to next substream and get random number"
    write (u, "(A)")
```



```

select type (rng)
type is (rng_stream_t)
  call rng%next_substream ()
end select
call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_1"

end subroutine rng_stream_1

```

Factory check

Set up a factory and spawn generators.

```

<RNG stream: execute tests>+≡
  call test (rng_stream_2, "rng_stream_2", &
    "rng factory", &
    u, results)

<RNG stream: test declarations>+≡
  public :: rng_stream_2

<RNG stream: tests>+≡
  subroutine rng_stream_2 (u)
    integer, intent(in) :: u
    type(rng_stream_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng
    real(default) :: x

    write (u, "(A)")  "* Test output: rng_stream_2"
    write (u, "(A)")  "* Purpose: initialize and use a rng factory"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize factory"
    write (u, "(A)")

    call rng_factory%init ()
    call rng_factory%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Make a generator"
    write (u, "(A)")

    call rng_factory%make (rng)

```

```

call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)") "x = ", x
call rng%final ()
deallocate (rng)

write (u, "(A)")
write (u, "(A)")  "* Repeat"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)") "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize factory with different seed"
write (u, "(A)")

call rng_factory%init (1_i16)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Make a generator"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)") "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_2"

end subroutine rng_stream_2

```

RNG Stream extension

Initialize the generator and advance state by 15389 steps and compare with regular advanced stream position.

```

<RNG stream: execute tests>+≡
    call test (rng_stream_3, "rng_stream_3", &
        "rng initialization and advance state", &
        u, results)

<RNG stream: test declarations>+≡
    public :: rng_stream_3

<RNG stream: tests>+≡
    subroutine rng_stream_3 (u)
        integer, intent(in) :: u
        class(rng_t), allocatable, target :: rng

        integer :: i
        real(default) :: x
        real(default), dimension(2) :: x2

        write (u, "(A)")  "* Test output: rng_stream_3"
        write (u, "(A)")  "* Purpose: initialize and advance the state of the random-number &
            &generator"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize generator (default seed)"
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Advance state by 15389 by iteration"
        write (u, "(A)")

        do i = 1, 15389
            call rng%generate (x)
        end do

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Get random number"
        write (u, "(A)")

        call rng%generate (x)
        write (u, "(A,2(1x,F9.7))")  "x =", x

        write (u, "(A)")
        write (u, "(A)")  "* Advance state by 15389 by procedure"
        write (u, "(A)")

        select type (rng)
        type is (rng_stream_t)
            call rng%reset_substream ()
            call rng%advance_state (15389)

```

```

end select

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get random number"
write (u, "(A)")

call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
write (u, "(A)")  "* Get random number pair"
write (u, "(A)")

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))")  "x =", x2

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Jump to next substream and get random number"
write (u, "(A)")

select type (rng)
type is (rng_stream_t)
  call rng%next_substream ()
end select
call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_3"

end subroutine rng_stream_3

```

8.5 Dispatch

```

⟨dispatch_rng.f90⟩≡
  ⟨File header⟩

module dispatch_rng

```

```

    use kinds, only: i16
  <Use strings>
    use variables
    use rng_base

  <Standard module head>

  <Dispatch rng: public>

  <Dispatch rng: variables>

  interface
  <Dispatch rng: sub interfaces>
    end interface

  end module dispatch_rng

  <dispatch_rng_sub.f90>≡
  <File header>

  submodule (dispatch_rng) dispatch_rng_s

    use diagnostics
    use rng_tao
    use rng_stream

    implicit none

  <Dispatch rng: parameters>

  contains

  <Dispatch rng: procedures>

  end submodule dispatch_rng_s

```

Allocate a random-number generator factory according to the variable `$rng_method`, using the current seed in the global record. (If the variable does not exist, the lookup will return the value 0.) We take only the lower 15 bits of the seed, so the actual value fits into a positive 16-bit signed integer.

Since we want to guarantee that all random-number generators in a run are independent, we increment the global seed by one after creating the rng factory and return it to the caller. If the user wants to have identical sequences, he can always set the seed manually, before it is used.

```

  <Dispatch rng: public>≡
    public :: dispatch_rng_factory

  <Dispatch rng: sub interfaces>≡
    module subroutine dispatch_rng_factory &
      (rng_factory, var_list, next_rng_seed)
      class(rng_factory_t), allocatable, intent(inout) :: rng_factory
      type(var_list_t), intent(in) :: var_list
      integer, intent(out) :: next_rng_seed
    end subroutine dispatch_rng_factory

```

```

end subroutine dispatch_rng_factory

<Dispatch rng: procedures>≡
module subroutine dispatch_rng_factory &
  (rng_factory, var_list, next_rng_seed)
  class(rng_factory_t), allocatable, intent(inout) :: rng_factory
  type(var_list_t), intent(in) :: var_list
  integer, intent(out) :: next_rng_seed
  type(var_list_t) :: local
  type(string_t) :: rng_method
  integer :: seed
  character(30) :: buffer
  integer(i16) :: s
  rng_method = var_list%get_sval (var_str ("rng_method"))
  seed = var_list%get_ival (var_str ("seed"))
  s = int (mod (seed, 32768), i16)
  select case (char (rng_method))
  case ("tao")
    allocate (rng_tao_factory_t :: rng_factory)
    call msg_message ("RNG: Initializing TAO random-number generator")
    next_rng_seed = seed + 1
  case ("rng_stream")
    allocate (rng_stream_factory_t :: rng_factory)
    call msg_message ("RNG: Initializing RNG Stream random-number generator")
    next_rng_seed = seed + 1
  case default
    if (associated (dispatch_rng_factory_fallback)) then
      call dispatch_rng_factory_fallback &
        (rng_factory, var_list, next_rng_seed)
    end if
    if (.not. allocated (rng_factory)) then
      call msg_fatal ("Random-number generator '" &
        // char (rng_method) // "' not implemented")
    end if
  end select
  write (buffer, "(I0)") s
  call msg_message ("RNG: Setting seed for random-number generator to " &
    // trim (buffer))
  call rng_factory%init (s)
end subroutine dispatch_rng_factory

```

This is a hook that allows us to inject further handlers for RNG factory objects, in particular a test RNG.

```

<Dispatch rng: public>+≡
  public :: dispatch_rng_factory_fallback

<Dispatch rng: variables>≡
  procedure (dispatch_rng_factory), pointer :: &
    dispatch_rng_factory_fallback => null ()

```

If the RNG factory dispatcher has used up a seed, we should reset it in the variable list. Separate subroutine with optional argument for more flexibility.

```

<Dispatch rng: public>+≡
  public :: update_rng_seed_in_var_list

```

```

<Dispatch rng: sub interfaces>+≡
    module subroutine update_rng_seed_in_var_list (var_list, next_rng_seed)
        type(var_list_t), intent(inout), optional :: var_list
        integer, intent(in) :: next_rng_seed
    end subroutine update_rng_seed_in_var_list

<Dispatch rng: procedures>+≡
    module subroutine update_rng_seed_in_var_list (var_list, next_rng_seed)
        type(var_list_t), intent(inout), optional :: var_list
        integer, intent(in) :: next_rng_seed
        if (present (var_list)) then
            call var_list%set_int (var_str ("seed"), next_rng_seed, is_known=.true.)
        end if
    end subroutine update_rng_seed_in_var_list

```

8.5.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_rng_ut.f90>≡
    <File header>

    module dispatch_rng_ut
        use unit_tests
        use dispatch_rng_util

    <Standard module head>

    <Dispatch rng: public test>

    <Dispatch rng: public test auxiliary>

    contains

    <Dispatch rng: test driver>

    end module dispatch_rng_ut

<dispatch_rng_util.f90>≡
    <File header>

    module dispatch_rng_util

    <Use strings>
        use variables
        use diagnostics
        use rng_base
        use dispatch_rng

    <Standard module head>

    <Dispatch rng: public test auxiliary>

    <Dispatch rng: test declarations>

```

contains

⟨Dispatch rng: tests⟩

⟨Dispatch rng: test auxiliary⟩

end module dispatch_rng_util

API: driver for the unit tests below.

⟨Dispatch rng: public test⟩≡

public :: dispatch_rng_test

⟨Dispatch rng: test driver⟩≡

subroutine dispatch_rng_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

⟨Dispatch rng: execute tests⟩

end subroutine dispatch_rng_test

Select type: random number generator

This is an extra dispatcher that enables the test RNG. This procedure should be assigned to the `dispatch_rng_factory_fallback` hook before any tests are executed.

The test generator does not use the seed at all, but it does increment it to be consistent with the other implementations.

⟨Dispatch rng: public test auxiliary⟩≡

public :: dispatch_rng_factory_test

⟨Dispatch rng: test auxiliary⟩≡

subroutine dispatch_rng_factory_test (rng_factory, var_list, next_rng_seed)

use rng_base

use rng_base_util, only: rng_test_factory_t

class(rng_factory_t), allocatable, intent(inout) :: rng_factory

type(var_list_t), intent(in) :: var_list

integer, intent(out) :: next_rng_seed

type(string_t) :: rng_method

if (var_list%contains (var_str ("rng_method"))) then

 rng_method = var_list%get_sval (var_str ("rng_method"))

else

 rng_method = "unit_test"

end if

next_rng_seed = &

 var_list%get_ival (var_str ("seed")) + 1

select case (char (rng_method))

case ("unit_test")

 allocate (rng_test_factory_t :: rng_factory)

 call msg_message ("RNG: Initializing Test random-number generator")

end select

end subroutine dispatch_rng_factory_test

This is the analog for the TAO RNG, for the unit tests we need a full generator.
(The seed is to be zero or a small integer.)

```

<Dispatch rng: public test auxiliary>+≡
    public :: dispatch_rng_factory_tao

<Dispatch rng: test auxiliary>+≡
    subroutine dispatch_rng_factory_tao (rng_factory, var_list, next_rng_seed)
        use kinds, only: i16
        use rng_base
        use rng_tao, only: rng_tao_factory_t
        class(rng_factory_t), allocatable, intent(inout) :: rng_factory
        type(var_list_t), intent(in) :: var_list
        integer, intent(out) :: next_rng_seed
        type(string_t) :: rng_method
        integer(i16) :: s
        if (var_list%contains (var_str ("rng_method"))) then
            rng_method = var_list%get_sval (var_str ("rng_method"))
        else
            rng_method = "tao"
        end if
        s = var_list%get_ival (var_str ("seed"))
        select case (char (rng_method))
        case ("tao")
            allocate (rng_tao_factory_t :: rng_factory)
            call rng_factory%init (s)
        end select
        next_rng_seed = s + 1
    end subroutine dispatch_rng_factory_tao

```

Create RNG factories for different algorithms. Note that the seed is updated after each rng factory call.

```

<Dispatch rng: execute tests>≡
    call test (dispatch_rng_1, "dispatch_rng_1", &
        "random-number generator", &
        u, results)

<Dispatch rng: test declarations>≡
    public :: dispatch_rng_1

<Dispatch rng: tests>≡
    subroutine dispatch_rng_1 (u)
        integer, intent(in) :: u
        type(var_list_t) :: var_list
        integer :: next_rng_seed
        class(rng_factory_t), allocatable :: rng_factory

        write (u, "(A)")  "* Test output: dispatch_rng_1"
        write (u, "(A)")  "* Purpose: select random-number generator"
        write (u, "(A)")

        call var_list%init_defaults (0)

        write (u, "(A)")  "* Allocate RNG factory as rng_test_factory_t"
        write (u, "(A)")
    end subroutine dispatch_rng_1

```

```

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("unit_test"), is_known = .true.)
call var_list%set_int (&
    var_str ("seed"), 1, is_known = .true.)

call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

write (u, "(A)")
write (u, "(A)")  "* Allocate RNG factory as rng_tao_factory_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("tao"), is_known = .true.)
call update_rng_seed_in_var_list (var_list, next_rng_seed)
call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

write (u, "(A)")
write (u, "(A)")  "* Allocate RNG factory as rng_stream_factory_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("rng_stream"), is_known = .true.)
call update_rng_seed_in_var_list (var_list, next_rng_seed)
call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_rng_1"

end subroutine dispatch_rng_1

```

Chapter 9

Physics

Here we collect definitions and functions that we need for (particle) physics in general, to make them available for the more specific needs of WHIZARD.

physics_defs Physical constants.

c_particles A simple data type for particles which is C compatible.

lorentz Define three-vectors, four-vectors and Lorentz transformations and common operations for them.

phs_point Collections of Lorentz vectors.

sm_physics Here, running functions are stored for special kinematical setup like running coupling constants, Catani-Seymour dipoles, or Sudakov factors.

sm_qcd Definitions and methods for dealing with the running QCD coupling.

shower_algorithms Algorithms typically used in Parton Showers as well as in their matching to NLO computations, e.g. with the POWHEG method.

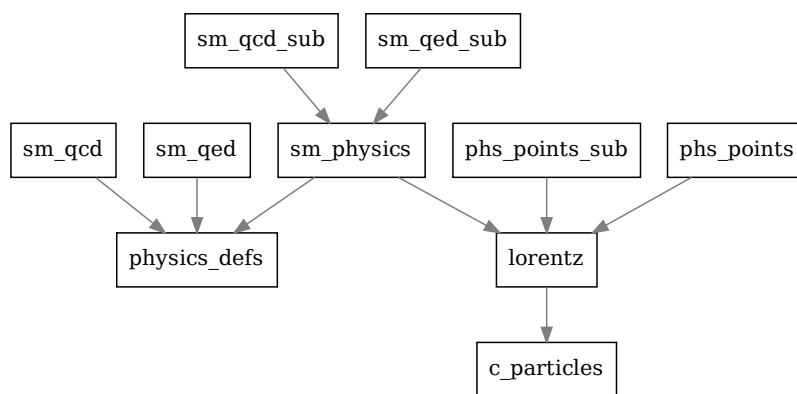


Figure 9.1: Module dependencies in `src/physics`.

9.1 Physics Constants

There is also the generic `constants` module. The constants listed here are more specific for particle physics.

```
(physics_defs.f90)≡  
  <File header>  
  
  module physics_defs  
  
    <Use kinds>  
    <Use strings>  
    use constants, only: one, two, three  
  
    <Standard module head>  
  
    <Physics defs: public parameters>  
  
    <Physics defs: public>  
  
    <Physics defs: interfaces>  
  
    interface  
    <Physics defs: sub interfaces>  
    end interface  
  
  end module physics_defs  
(physics_defs_sub.f90)≡  
  <File header>  
  
  submodule (physics_defs) physics_defs_s  
  
    implicit none  
  
    contains  
  
    <Physics defs: procedures>  
  
  end submodule physics_defs_s
```

9.1.1 Units

Conversion from energy units to cross-section units.

```
<Physics defs: public parameters>≡  
  real(default), parameter, public :: &  
    conv = 0.38937966e12_default
```

Conversion from millimeter to nanoseconds for lifetimes.

```
<Physics defs: public parameters>+≡  
  real(default), parameter, public :: &  
    ns_per_mm = 1.e6_default / 299792458._default
```

Rescaling factor.

```
<Physics defs: public parameters>+=  
    real(default), parameter, public :: &  
        pb_per_fb = 1.e-3_default
```

String for the default energy and cross-section units.

```
<Physics defs: public parameters>+=  
    character(*), parameter, public :: &  
        energy_unit = "GeV"  
    character(*), parameter, public :: &  
        cross_section_unit = "fb"
```

9.1.2 SM and QCD constants

```
<Physics defs: public parameters>+=  
    real(default), parameter, public :: &  
        NC = three, &  
        CF = (NC**2 - one) / two / NC, &  
        CA = NC, &  
        TR = one / two
```

9.1.3 Parameter Reference values

These are used exclusively in the context of running QCD parameters. In other contexts, we rely on the uniform parameter set as provided by the model definition, modifiable by the user.

```
<Physics defs: public parameters>+=  
    real(default), public, parameter :: MZ_REF = 91.188_default  
    real(default), public, parameter :: ME_REF = 0.000510998928_default  
    real(default), public, parameter :: ALPHA_QCD_MZ_REF = 0.1178_default  
    real(default), public, parameter :: ALPHA_QED_ME_REF = 0.0072973525693_default  
    real(default), public, parameter :: LAMBDA_QCD_REF = 200.e-3_default
```

9.1.4 Particle codes

Let us define a few particle codes independent of the model.

We need an UNDEFINED value:

```
<Physics defs: public parameters>+=  
    integer, parameter, public :: UNDEFINED = 0
```

SM fermions:

```
<Physics defs: public parameters>+=  
    integer, parameter, public :: DOWN_Q = 1  
    integer, parameter, public :: UP_Q = 2  
    integer, parameter, public :: STRANGE_Q = 3  
    integer, parameter, public :: CHARM_Q = 4  
    integer, parameter, public :: BOTTOM_Q = 5  
    integer, parameter, public :: TOP_Q = 6  
    integer, parameter, public :: ELECTRON = 11  
    integer, parameter, public :: ELECTRON_NEUTRINO = 12  
    integer, parameter, public :: MUON = 13
```

```

integer, parameter, public :: MUON_NEUTRINO = 14
integer, parameter, public :: TAU = 15
integer, parameter, public :: TAU_NEUTRINO = 16

```

Gauge bosons:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: GLUON = 21
integer, parameter, public :: PHOTON = 22
integer, parameter, public :: PHOTON_OFFSHELL = -2002
integer, parameter, public :: PHOTON_ONSHELL = 2002
integer, parameter, public :: Z_BOSON = 23
integer, parameter, public :: W_BOSON = 24

```

Light mesons:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: PION = 111
integer, parameter, public :: PIPLUS = 211
integer, parameter, public :: PIMINUS = - PIPLUS

```

Di-Quarks:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: UDO = 2101
integer, parameter, public :: UD1 = 2103
integer, parameter, public :: UU1 = 2203

```

Mesons:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: KOL = 130
integer, parameter, public :: KOS = 310
integer, parameter, public :: KO = 311
integer, parameter, public :: KPLUS = 321
integer, parameter, public :: DPLUS = 411
integer, parameter, public :: DO = 421
integer, parameter, public :: BO = 511
integer, parameter, public :: BPLUS = 521

```

Light baryons:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: PROTON = 2212
integer, parameter, public :: NEUTRON = 2112
integer, parameter, public :: DELTAPLUSPLUS = 2224
integer, parameter, public :: DELTAPLUS = 2214
integer, parameter, public :: DELTAO = 2114
integer, parameter, public :: DELTAMINUS = 1114

```

Strange baryons:

```

<Physics defs: public parameters>+≡
integer, parameter, public :: SIGMAPLUS = 3222
integer, parameter, public :: SIGMAO = 3212
integer, parameter, public :: SIGMAMINUS = 3112

```

Charmed baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: SIGMACPLUSPLUS = 4222  
  integer, parameter, public :: SIGMACPLUS = 4212  
  integer, parameter, public :: SIGMACO = 4112
```

Bottom baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: SIGMABO = 5212  
  integer, parameter, public :: SIGMABPLUS = 5222
```

81-100 are reserved for internal codes. Hadron and beam remnants:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: BEAM_REMNANT = 9999  
  integer, parameter, public :: HADRON_REMNANT = 90  
  integer, parameter, public :: HADRON_REMNANT_SINGLET = 91  
  integer, parameter, public :: HADRON_REMNANT_TRIPLET = 92  
  integer, parameter, public :: HADRON_REMNANT_OCTET = 93
```

Further particle codes for internal use:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: INTERNAL = 94  
  integer, parameter, public :: INVALID = 97  
  
  integer, parameter, public :: COMPOSITE = 99
```

9.1.5 Spin codes

Somewhat redundant, but for better readability we define named constants for spin types. If the mass is nonzero, this is equal to the number of degrees of freedom.

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: UNKNOWN = 0  
  integer, parameter, public :: SCALAR = 1, SPINOR = 2, VECTOR = 3, &  
    VECTORSPINOR = 4, TENSOR = 5
```

Isospin types and charge types are counted in an analogous way, where charge type 1 is charge 0, 2 is charge 1/3, and so on. Zero always means unknown. Note that charge and isospin types have an explicit sign.

Color types are defined as the dimension of the representation.

9.1.6 NLO status codes

Used to specify whether a `term_instance_t` of a `process_instance_t` is associated with a Born, real-subtracted, virtual-subtracted or subtraction-dummy matrix element.

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: BORN = 0  
  integer, parameter, public :: NLO_REAL = 1
```



```

integer, parameter, public :: NLO_VIRTUAL = 2
integer, parameter, public :: NLO_MISMATCH = 3
integer, parameter, public :: NLO_DGLAP = 4
integer, parameter, public :: NLO_SUBTRACTION = 5
integer, parameter, public :: NLO_FULL = 6
integer, parameter, public :: GKS = 7
integer, parameter, public :: COMPONENT_UNDEFINED = 99

```

NLO_FULL is not strictly a component status code but having it is convenient. We define the number of additional subtractions for beam-involved NLO calculations. Each subtraction refers to a rescaling of one of two beams. Obviously, this approach is not flexible enough to support setups with just a single beam described by a structure function.

```

<Physics defs: public parameters>+=
  integer, parameter, public :: n_beams_rescaled = 2

```

Orders of the electron PDFs.

```

<Physics defs: public parameters>+=
  integer, parameter, public :: EPDF_LL = 0
  integer, parameter, public :: EPDF_NLL = 1

```

```

<Physics defs: public>=
  public :: component_status

```

```

<Physics defs: interfaces>=
  interface component_status
    module procedure component_status_of_string
    module procedure component_status_to_string
  end interface

```

```

<Physics defs: sub interfaces>=
  elemental module function component_status_of_string (string) result (i)
    integer :: i
    type(string_t), intent(in) :: string
  end function component_status_of_string
  elemental module function component_status_to_string (i) result (string)
    type(string_t) :: string
    integer, intent(in) :: i
  end function component_status_to_string

```

```

<Physics defs: procedures>=
  elemental module function component_status_of_string (string) result (i)
    integer :: i
    type(string_t), intent(in) :: string
    select case (char(string))
    case ("born")
      i = BORN
    case ("real")
      i = NLO_REAL
    case ("virtual")
      i = NLO_VIRTUAL
    case ("mismatch")
      i = NLO_MISMATCH
    case ("dglap")

```

```

        i = NLO_DGLAP
    case ("subtraction")
        i = NLO_SUBTRACTION
    case ("full")
        i = NLO_FULL
    case ("GKS")
        i = GKS
    case default
        i = COMPONENT_UNDEFINED
    end select
end function component_status_of_string

elemental module function component_status_to_string (i) result (string)
    type(string_t) :: string
    integer, intent(in) :: i
    select case (i)
    case (BORN)
        string = "born"
    case (NLO_REAL)
        string = "real"
    case (NLO_VIRTUAL)
        string = "virtual"
    case (NLO_MISMATCH)
        string = "mismatch"
    case (NLO_DGLAP)
        string = "dglap"
    case (NLO_SUBTRACTION)
        string = "subtraction"
    case (NLO_FULL)
        string = "full"
    case (GKS)
        string = "GKS"
    case default
        string = "undefined"
    end select
end function component_status_to_string

<Physics defs: public>+≡
    public :: is_nlo_component

<Physics defs: sub interfaces>+≡
    elemental module function is_nlo_component (comp) result (is_nlo)
        logical :: is_nlo
        integer, intent(in) :: comp
    end function is_nlo_component

<Physics defs: procedures>+≡
    elemental module function is_nlo_component (comp) result (is_nlo)
        logical :: is_nlo
        integer, intent(in) :: comp
        select case (comp)
        case (BORN : GKS)
            is_nlo = .true.
        case default
            is_nlo = .false.

```

```

        end select
    end function is_nlo_component

<Physics defs: public>+≡
    public :: is_subtraction_component

<Physics defs: sub interfaces>+≡
    module function is_subtraction_component (emitter, nlo_type) result (is_subtraction)
        logical :: is_subtraction
        integer, intent(in) :: emitter, nlo_type
    end function is_subtraction_component

<Physics defs: procedures>+≡
    module function is_subtraction_component (emitter, nlo_type) result (is_subtraction)
        logical :: is_subtraction
        integer, intent(in) :: emitter, nlo_type
        is_subtraction = nlo_type == NLO_REAL .and. emitter < 0
    end function is_subtraction_component

```

9.1.7 Threshold

Some commonly used variables for the threshold computation

```

<Physics defs: public parameters>+≡
    integer, parameter, public :: THR_POS_WP = 3
    integer, parameter, public :: THR_POS_WM = 4
    integer, parameter, public :: THR_POS_B = 5
    integer, parameter, public :: THR_POS_BBAR = 6
    integer, parameter, public :: THR_POS_GLUON = 7

    integer, parameter, public :: THR_EMITTER_OFFSET = 4

    integer, parameter, public :: NO_FACTORIZATION = 0
    integer, parameter, public :: FACTORIZATION_THRESHOLD = 1

    integer, dimension(2), parameter, public :: ass_quark = [5, 6]
    integer, dimension(2), parameter, public :: ass_boson = [3, 4]

    integer, parameter, public :: PROC_MODE_UNDEFINED = 0
    integer, parameter, public :: PROC_MODE_TT = 1
    integer, parameter, public :: PROC_MODE_WBWB = 2

<Physics defs: public>+≡
    public :: thr_leg

<Physics defs: sub interfaces>+≡
    module function thr_leg (emitter) result (leg)
        integer :: leg
        integer, intent(in) :: emitter
    end function thr_leg

```

```

(Physics defs: procedures) +=
  module function thr_leg (emitter) result (leg)
    integer :: leg
    integer, intent(in) :: emitter
    leg = emitter - THR_EMITTER_OFFSET
  end function thr_leg

```

9.2 C-compatible Particle Type

For easy communication with C code, we introduce a simple C-compatible type for particles. The components are either default C integers or default C doubles.

The `c_prt` type is transparent, and its contents should be regarded as part of the interface.

```
<c_particles.f90>≡
  <File header>

  module c_particles

    use, intrinsic :: iso_c_binding !NODEP!

    <Standard module head>

    <C Particles: public>

    <C Particles: types>

    interface
    <C Particles: sub interfaces>
    end interface

  end module c_particles

<c_particles_sub.f90>≡
  <File header>

  submodule (c_particles) c_particles_s

    use io_units
    use format_defs, only: FMT_14, FMT_19

    implicit none

    contains

    <C Particles: procedures>

  end submodule c_particles_s

<C Particles: public>≡
  public :: c_prt_t

<C Particles: types>≡
  type, bind(C) :: c_prt_t
    integer(c_int) :: type = 0
    integer(c_int) :: pdg = 0
    integer(c_int) :: polarized = 0
    integer(c_int) :: h = 0
    real(c_double) :: pe = 0
    real(c_double) :: px = 0
    real(c_double) :: py = 0
    real(c_double) :: pz = 0
```

```

        real(c_double) :: p2 = 0
    end type c_prt_t

```

This is for debugging only, there is no C binding. It is a simplified version of `prt_write`.

```

<C Particles: public>+≡
    public :: c_prt_write

<C Particles: sub interfaces>≡
    module subroutine c_prt_write (prt, unit)
        type(c_prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
    end subroutine c_prt_write

<C Particles: procedures>≡
    module subroutine c_prt_write (prt, unit)
        type(c_prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)", advance="no") "prt("
        write (u, "(I0,':')", advance="no") prt%type
        if (prt%polarized /= 0) then
            write (u, "(I0,'/',I0,'|')", advance="no") prt%pdg, prt%h
        else
            write (u, "(I0,'|')", advance="no") prt%pdg
        end if
        write (u, "(" // FMT_14 // ",','," // FMT_14 // ",','," // &
            FMT_14 // ",','," // FMT_14 // ")", advance="no") &
            prt%pe, prt%px, prt%py, prt%pz
        write (u, "( '|'," // FMT_19 // ")", advance="no") prt%p2
        write (u, "(A)" " )"
    end subroutine c_prt_write

```

9.3 Lorentz algebra

Define Lorentz vectors, three-vectors, boosts, and some functions to manipulate them.

To make maximum use of this, all functions, if possible, are declared elemental (or pure, if this is not possible).

```
<lorentz.f90>≡  
  <File header>  
  
  module lorentz  
  
    <Use kinds with double>  
    use constants, only: zero, one  
    use c_particles  
  
    <Standard module head>  
  
    <Lorentz: public>  
  
    <Lorentz: public operators>  
  
    <Lorentz: public functions>  
  
    <Lorentz: types>  
  
    <Lorentz: parameters>  
  
    <Lorentz: interfaces>  
  
    interface  
    <Lorentz: sub interfaces>  
    end interface  
  
  end module lorentz  
<lorentz_sub.f90>≡  
  <File header>  
  
  submodule (lorentz) lorentz_s  
  
    use constants, only: pi, twopi, degree, two, tiny_07, eps0  
    use numeric_utils  
    use io_units  
    use format_defs, only: FMT_11, FMT_13, FMT_15, FMT_19  
    use format_utils, only: pac_fmt  
    use diagnostics  
  
    implicit none  
  
  contains  
  
    <Lorentz: procedures>  
  
  end submodule lorentz_s
```

9.3.1 Three-vectors

First of all, let us introduce three-vectors in a trivial way. The functions and overloaded elementary operations clearly are too much overhead, but we like to keep the interface for three-vectors and four-vectors exactly parallel. By the way, we might attach a label to a vector by extending the type definition later.

```

(Lorentz: public)≡
    public :: vector3_t

(Lorentz: types)≡
    type :: vector3_t
        real(default), dimension(3) :: p
    end type vector3_t

```

Output a vector

```

(Lorentz: public)+≡
    public :: vector3_write

(Lorentz: sub interfaces)≡
    module subroutine vector3_write (p, unit, testflag)
        type(vector3_t), intent(in) :: p
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine vector3_write

(Lorentz: procedures)≡
    module subroutine vector3_write (p, unit, testflag)
        type(vector3_t), intent(in) :: p
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        character(len=7) :: fmt
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call pac_fmt (fmt, FMT_19, FMT_15, testflag)
        write(u, "(1x,A,3(1x," // fmt // "))" ) 'P = ', p%p
    end subroutine vector3_write

```

This is a three-vector with zero components

```

(Lorentz: public)+≡
    public :: vector3_null

(Lorentz: parameters)≡
    type(vector3_t), parameter :: vector3_null = &
        vector3_t ([ zero, zero, zero ])

```

Canonical three-vector:

```

(Lorentz: public)+≡
    public :: vector3_canonical

```



```

<Lorentz: sub interfaces>+≡
    elemental module function vector3_canonical (k) result (p)
        type(vector3_t) :: p
        integer, intent(in) :: k
    end function vector3_canonical

```

```

<Lorentz: procedures>+≡
    elemental module function vector3_canonical (k) result (p)
        type(vector3_t) :: p
        integer, intent(in) :: k
        p = vector3_null
        p%p(k) = 1
    end function vector3_canonical

```

A moving particle (k -axis, or arbitrary axis). Note that the function for the generic momentum cannot be elemental.

```

<Lorentz: public>+≡
    public :: vector3_moving

<Lorentz: interfaces>≡
    interface vector3_moving
        module procedure vector3_moving_canonical
        module procedure vector3_moving_generic
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_moving_canonical (p, k) result(q)
        type(vector3_t) :: q
        real(default), intent(in) :: p
        integer, intent(in) :: k
    end function vector3_moving_canonical
    pure module function vector3_moving_generic (p) result(q)
        real(default), dimension(3), intent(in) :: p
        type(vector3_t) :: q
    end function vector3_moving_generic

<Lorentz: procedures>+≡
    elemental module function vector3_moving_canonical (p, k) result(q)
        type(vector3_t) :: q
        real(default), intent(in) :: p
        integer, intent(in) :: k
        q = vector3_null
        q%p(k) = p
    end function vector3_moving_canonical
    pure module function vector3_moving_generic (p) result(q)
        real(default), dimension(3), intent(in) :: p
        type(vector3_t) :: q
        q%p = p
    end function vector3_moving_generic

```

Equality and inequality

```

<Lorentz: public operators>≡
    public :: operator(==), operator(/=)

```

```

<Lorentz: interfaces>+≡
  interface operator(==)
    module procedure vector3_eq
  end interface
  interface operator(/=)
    module procedure vector3_neq
  end interface
<Lorentz: sub interfaces>+≡
  elemental module function vector3_eq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
  end function vector3_eq
  elemental module function vector3_neq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
  end function vector3_neq
<Lorentz: procedures>+≡
  elemental module function vector3_eq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
    r = all (abs (p%p - q%p) < eps0)
  end function vector3_eq
  elemental module function vector3_neq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
    r = any (abs(p%p - q%p) > eps0)
  end function vector3_neq

```

Define addition and subtraction

```

<Lorentz: public operators>+≡
  public :: operator(+), operator(-)
<Lorentz: interfaces>+≡
  interface operator(+)
    module procedure add_vector3
  end interface
  interface operator(-)
    module procedure sub_vector3
  end interface
<Lorentz: sub interfaces>+≡
  elemental module function add_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
  end function add_vector3
  elemental module function sub_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
  end function sub_vector3
<Lorentz: procedures>+≡
  elemental module function add_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q

```

```

    r%p = p%p + q%p
end function add_vector3
elemental module function sub_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
    r%p = p%p - q%p
end function sub_vector3

```

The multiplication sign is overloaded with scalar multiplication; similarly division:

```

<Lorentz: public operators>+≡
    public :: operator(*), operator(/)

<Lorentz: interfaces>+≡
    interface operator(*)
        module procedure prod_integer_vector3, prod_vector3_integer
        module procedure prod_real_vector3, prod_vector3_real
    end interface
    interface operator(/)
        module procedure div_vector3_real, div_vector3_integer
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function prod_real_vector3 (s, p) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function prod_real_vector3
    elemental module function prod_vector3_real (p, s) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function prod_vector3_real
    elemental module function div_vector3_real (p, s) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function div_vector3_real
    elemental module function prod_integer_vector3 (s, p) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function prod_integer_vector3
    elemental module function prod_vector3_integer (p, s) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function prod_vector3_integer
    elemental module function div_vector3_integer (p, s) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
    end function div_vector3_integer

<Lorentz: procedures>+≡

```

```

elemental module function prod_real_vector3 (s, p) result (q)
  type(vector3_t) :: q
  real(default), intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = s * p%p
end function prod_real_vector3
elemental module function prod_vector3_real (p, s) result (q)
  type(vector3_t) :: q
  real(default), intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = s * p%p
end function prod_vector3_real
elemental module function div_vector3_real (p, s) result (q)
  type(vector3_t) :: q
  real(default), intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = p%p/s
end function div_vector3_real
elemental module function prod_integer_vector3 (s, p) result (q)
  type(vector3_t) :: q
  integer, intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = s * p%p
end function prod_integer_vector3
elemental module function prod_vector3_integer (p, s) result (q)
  type(vector3_t) :: q
  integer, intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = s * p%p
end function prod_vector3_integer
elemental module function div_vector3_integer (p, s) result (q)
  type(vector3_t) :: q
  integer, intent(in) :: s
  type(vector3_t), intent(in) :: p
  q%p = p%p/s
end function div_vector3_integer

```

The multiplication sign can also indicate scalar products:

```

(Lorentz: interfaces)+≡
  interface operator(*)
    module procedure prod_vector3
  end interface

(Lorentz: sub interfaces)+≡
  elemental module function prod_vector3 (p, q) result (s)
    real(default) :: s
    type(vector3_t), intent(in) :: p,q
  end function prod_vector3

(Lorentz: procedures)+≡
  elemental module function prod_vector3 (p, q) result (s)
    real(default) :: s
    type(vector3_t), intent(in) :: p,q
    s = dot_product (p%p, q%p)
  end function prod_vector3

```

```

<Lorentz: public functions>≡
    public :: cross_product

<Lorentz: interfaces>+≡
    interface cross_product
        module procedure vector3_cross_product
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_cross_product (p, q) result (r)
        type(vector3_t) :: r
        type(vector3_t), intent(in) :: p,q
    end function vector3_cross_product

<Lorentz: procedures>+≡
    elemental module function vector3_cross_product (p, q) result (r)
        type(vector3_t) :: r
        type(vector3_t), intent(in) :: p,q
        integer :: i
        do i=1,3
            r%p(i) = dot_product (p%p, matmul(epsilon_three(i, :, :), q%p))
        end do
    end function vector3_cross_product

```

Exponentiation is defined only for integer powers. Odd powers mean take the square root; so `p**1` is the length of `p`.

```

<Lorentz: public operators>+≡
    public :: operator(**)

<Lorentz: interfaces>+≡
    interface operator(**)
        module procedure power_vector3
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function power_vector3 (p, e) result (s)
        real(default) :: s
        type(vector3_t), intent(in) :: p
        integer, intent(in) :: e
    end function power_vector3

<Lorentz: procedures>+≡
    elemental module function power_vector3 (p, e) result (s)
        real(default) :: s
        type(vector3_t), intent(in) :: p
        integer, intent(in) :: e
        s = dot_product (p%p, p%p)
        if (e/=2) then
            if (mod(e,2)==0) then
                s = s**(e/2)
            else
                s = sqrt(s)**e
            end if
        end if
    end function power_vector3

```

Finally, we need a negation.

```

<Lorentz: interfaces>+≡
    interface operator(-)
        module procedure negate_vector3
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function negate_vector3 (p) result (q)
        type(vector3_t) :: q
        type(vector3_t), intent(in) :: p
    end function negate_vector3

<Lorentz: procedures>+≡
    elemental module function negate_vector3 (p) result (q)
        type(vector3_t) :: q
        type(vector3_t), intent(in) :: p
        integer :: i
        do i = 1, 3
            if (abs (p%p(i)) < eps0) then
                q%p(i) = 0
            else
                q%p(i) = -p%p(i)
            end if
        end do
    end function negate_vector3

```

The sum function can be useful:

```

<Lorentz: public functions>+≡
    public :: sum

<Lorentz: interfaces>+≡
    interface sum
        module procedure sum_vector3
    end interface

<Lorentz: public>+≡
    public :: vector3_set_component

<Lorentz: sub interfaces>+≡
    module subroutine vector3_set_component (p, i, value)
        type(vector3_t), intent(inout) :: p
        integer, intent(in) :: i
        real(default), intent(in) :: value
    end subroutine vector3_set_component

<Lorentz: procedures>+≡
    module subroutine vector3_set_component (p, i, value)
        type(vector3_t), intent(inout) :: p
        integer, intent(in) :: i
        real(default), intent(in) :: value
        p%p(i) = value
    end subroutine vector3_set_component

```

```

<Lorentz: sub interfaces>+≡
  pure module function sum_vector3 (p) result (q)
    type(vector3_t) :: q
    type(vector3_t), dimension(:), intent(in) :: p
  end function sum_vector3

```

```

<Lorentz: procedures>+≡
  pure module function sum_vector3 (p) result (q)
    type(vector3_t) :: q
    type(vector3_t), dimension(:), intent(in) :: p
    integer :: i
    do i=1, 3
      q%p(i) = sum (p%p(i))
    end do
  end function sum_vector3

```

Any component:

```

<Lorentz: public>+≡
  public :: vector3_get_component

<Lorentz: sub interfaces>+≡
  elemental module function vector3_get_component (p, k) result (c)
    type(vector3_t), intent(in) :: p
    integer, intent(in) :: k
    real(default) :: c
  end function vector3_get_component

<Lorentz: procedures>+≡
  elemental module function vector3_get_component (p, k) result (c)
    type(vector3_t), intent(in) :: p
    integer, intent(in) :: k
    real(default) :: c
    c = p%p(k)
  end function vector3_get_component

```

Extract all components. This is not elemental.

```

<Lorentz: public>+≡
  public :: vector3_get_components

<Lorentz: sub interfaces>+≡
  pure module function vector3_get_components (p) result (a)
    type(vector3_t), intent(in) :: p
    real(default), dimension(3) :: a
  end function vector3_get_components

<Lorentz: procedures>+≡
  pure module function vector3_get_components (p) result (a)
    type(vector3_t), intent(in) :: p
    real(default), dimension(3) :: a
    a = p%p
  end function vector3_get_components

```

This function returns the direction of a three-vector, i.e., a normalized three-vector. If the vector is null, we return a null vector.

```

<Lorentz: public functions>+≡
  public :: direction

```

```

<Lorentz: interfaces>+≡
  interface direction
    module procedure vector3_get_direction
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function vector3_get_direction (p) result (q)
    type(vector3_t) :: q
    type(vector3_t), intent(in) :: p
  end function vector3_get_direction

<Lorentz: procedures>+≡
  elemental module function vector3_get_direction (p) result (q)
    type(vector3_t) :: q
    type(vector3_t), intent(in) :: p
    real(default) :: pp
    pp = p**1
    if (pp > eps0) then
      q%p = p%p / pp
    else
      q%p = 0
    end if
  end function vector3_get_direction

```

9.3.2 Four-vectors

In four-vectors the zero-component needs special treatment, therefore we do not use the standard operations. Sure, we pay for the extra layer of abstraction by losing efficiency; so we have to assume that the time-critical applications do not involve four-vector operations.

```

<Lorentz: public>+≡
  public :: vector4_t

<Lorentz: types>+≡
  type :: vector4_t
    real(default), dimension(0:3) :: p = &
      [zero, zero, zero, zero]
  contains
    <Lorentz: vector4: TBP>
  end type vector4_t

```

Output a vector

```

<Lorentz: public>+≡
  public :: vector4_write

<Lorentz: vector4: TBP>≡
  procedure :: write => vector4_write

<Lorentz: sub interfaces>+≡
  module subroutine vector4_write &
    (p, unit, show_mass, testflag, compressed, ultra)
    class(vector4_t), intent(in) :: p
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_mass, testflag, compressed, ultra
  end subroutine vector4_write

```


<Lorentz: procedures>+≡

```

module subroutine vector4_write &
    (p, unit, show_mass, testflag, compressed, ultra)
    class(vector4_t), intent(in) :: p
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_mass, testflag, compressed, ultra
    logical :: comp, sm, tf, extreme
    integer :: u
    character(len=7) :: fmt
    real(default) :: m
    comp = .false.; if (present (compressed)) comp = compressed
    sm = .false.; if (present (show_mass)) sm = show_mass
    tf = .false.; if (present (testflag)) tf = testflag
    extreme = .false.; if (present (ultra)) extreme = ultra
    if (extreme) then
        call pac_fmt (fmt, FMT_19, FMT_11, testflag)
    else
        call pac_fmt (fmt, FMT_19, FMT_13, testflag)
    end if
    u = given_output_unit (unit); if (u < 0) return
    if (comp) then
        write (u, "(4(F12.3,1X))", advance="no") p%p(0:3)
    else
        write (u, "(1x,A,1x," // fmt // ")") 'E = ', p%p(0)
        write (u, "(1x,A,3(1x," // fmt // ")") 'P = ', p%p(1:)
        if (sm) then
            m = p**1
            if (tf) call pacify (m, tolerance = 1E-6_default)
            write (u, "(1x,A,1x," // fmt // ")") 'M = ', m
        end if
    end if
end if
end subroutine vector4_write

```

Binary I/O

<Lorentz: public>+≡

```

public :: vector4_write_raw
public :: vector4_read_raw

```

<Lorentz: sub interfaces>+≡

```

module subroutine vector4_write_raw (p, u)
    type(vector4_t), intent(in) :: p
    integer, intent(in) :: u
end subroutine vector4_write_raw
module subroutine vector4_read_raw (p, u, iostat)
    type(vector4_t), intent(out) :: p
    integer, intent(in) :: u
    integer, intent(out), optional :: iostat
end subroutine vector4_read_raw

```

<Lorentz: procedures>+≡

```

module subroutine vector4_write_raw (p, u)
    type(vector4_t), intent(in) :: p
    integer, intent(in) :: u
    write (u) p%p
end subroutine vector4_write_raw

```

```

module subroutine vector4_read_raw (p, u, iostat)
  type(vector4_t), intent(out) :: p
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
  read (u, iostat=iostat) p%p
end subroutine vector4_read_raw

```

This is a four-vector with zero components

```

(Lorentz: public)+≡
  public :: vector4_null

(Lorentz: parameters)+≡
  type(vector4_t), parameter :: vector4_null = &
    vector4_t ([ zero, zero, zero, zero ])

```

Canonical four-vector:

```

(Lorentz: public)+≡
  public :: vector4_canonical

(Lorentz: sub interfaces)+≡
  elemental module function vector4_canonical (k) result (p)
    type(vector4_t) :: p
    integer, intent(in) :: k
  end function vector4_canonical

(Lorentz: procedures)+≡
  elemental module function vector4_canonical (k) result (p)
    type(vector4_t) :: p
    integer, intent(in) :: k
    p = vector4_null
    p%p(k) = 1
  end function vector4_canonical

```

A particle at rest:

```

(Lorentz: public)+≡
  public :: vector4_at_rest

(Lorentz: sub interfaces)+≡
  elemental module function vector4_at_rest (m) result (p)
    type(vector4_t) :: p
    real(default), intent(in) :: m
  end function vector4_at_rest

(Lorentz: procedures)+≡
  elemental module function vector4_at_rest (m) result (p)
    type(vector4_t) :: p
    real(default), intent(in) :: m
    p = vector4_t ([ m, zero, zero, zero ])
  end function vector4_at_rest

```

A moving particle (k -axis, or arbitrary axis)

```

(Lorentz: public)+≡
  public :: vector4_moving

```

```

<Lorentz: interfaces>+≡
  interface vector4_moving
    module procedure vector4_moving_canonical
    module procedure vector4_moving_generic
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function vector4_moving_canonical (E, p, k) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E, p
    integer, intent(in) :: k
  end function vector4_moving_canonical
  elemental module function vector4_moving_generic (E, p) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E
    type(vector3_t), intent(in) :: p
  end function vector4_moving_generic

<Lorentz: procedures>+≡
  elemental module function vector4_moving_canonical (E, p, k) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E, p
    integer, intent(in) :: k
    q = vector4_at_rest(E)
    q%p(k) = p
  end function vector4_moving_canonical
  elemental module function vector4_moving_generic (E, p) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E
    type(vector3_t), intent(in) :: p
    q%p(0) = E
    q%p(1:) = p%p
  end function vector4_moving_generic

```

Equality and inequality

```

<Lorentz: interfaces>+≡
  interface operator(==)
    module procedure vector4_eq
  end interface
  interface operator(/=)
    module procedure vector4_neq
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function vector4_eq (p, q) result (r)
    logical :: r
    type(vector4_t), intent(in) :: p,q
  end function vector4_eq
  elemental module function vector4_neq (p, q) result (r)
    logical :: r
    type(vector4_t), intent(in) :: p,q
  end function vector4_neq

<Lorentz: procedures>+≡
  elemental module function vector4_eq (p, q) result (r)
    logical :: r

```

```

    type(vector4_t), intent(in) :: p,q
    r = all (abs (p%p - q%p) < eps0)
end function vector4_eq
elemental module function vector4_neq (p, q) result (r)
    logical :: r
    type(vector4_t), intent(in) :: p,q
    r = any (abs (p%p - q%p) > eps0)
end function vector4_neq

```

Addition and subtraction:

```

<Lorentz: interfaces>+≡
    interface operator(+)
        module procedure add_vector4
    end interface
    interface operator(-)
        module procedure sub_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function add_vector4 (p,q) result (r)
        type(vector4_t) :: r
        type(vector4_t), intent(in) :: p,q
    end function add_vector4
    elemental module function sub_vector4 (p,q) result (r)
        type(vector4_t) :: r
        type(vector4_t), intent(in) :: p,q
    end function sub_vector4

<Lorentz: procedures>+≡
    elemental module function add_vector4 (p,q) result (r)
        type(vector4_t) :: r
        type(vector4_t), intent(in) :: p,q
        r%p = p%p + q%p
    end function add_vector4
    elemental module function sub_vector4 (p,q) result (r)
        type(vector4_t) :: r
        type(vector4_t), intent(in) :: p,q
        r%p = p%p - q%p
    end function sub_vector4

```

We also need scalar multiplication and division:

```

<Lorentz: interfaces>+≡
    interface operator(*)
        module procedure prod_real_vector4, prod_vector4_real
        module procedure prod_integer_vector4, prod_vector4_integer
    end interface
    interface operator(/)
        module procedure div_vector4_real
        module procedure div_vector4_integer
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function prod_real_vector4 (s, p) result (q)
        type(vector4_t) :: q

```

```

    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
end function prod_real_vector4
elemental module function prod_vector4_real (p, s) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
end function prod_vector4_real
elemental module function div_vector4_real (p, s) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
end function div_vector4_real
elemental module function prod_integer_vector4 (s, p) result (q)
    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
end function prod_integer_vector4
elemental module function prod_vector4_integer (p, s) result (q)
    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
end function prod_vector4_integer
elemental module function div_vector4_integer (p, s) result (q)
    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
end function div_vector4_integer

```

(Lorentz: procedures) +=

```

elemental module function prod_real_vector4 (s, p) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = s * p%p
end function prod_real_vector4
elemental module function prod_vector4_real (p, s) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = s * p%p
end function prod_vector4_real
elemental module function div_vector4_real (p, s) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = p%p/s
end function div_vector4_real
elemental module function prod_integer_vector4 (s, p) result (q)
    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = s * p%p
end function prod_integer_vector4
elemental module function prod_vector4_integer (p, s) result (q)

```

```

    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = s * p%p
end function prod_vector4_integer
elemental module function div_vector4_integer (p, s) result (q)
    type(vector4_t) :: q
    integer, intent(in) :: s
    type(vector4_t), intent(in) :: p
    q%p = p%p/s
end function div_vector4_integer

```

Scalar products and squares in the Minkowski sense:

```

<Lorentz: interfaces>+≡
    interface operator(*)
        module procedure prod_vector4
    end interface
    interface operator(**)
        module procedure power_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function prod_vector4 (p, q) result (s)
        real(default) :: s
        type(vector4_t), intent(in) :: p,q
    end function prod_vector4

<Lorentz: procedures>+≡
    elemental module function prod_vector4 (p, q) result (s)
        real(default) :: s
        type(vector4_t), intent(in) :: p,q
        s = p%p(0)*q%p(0) - dot_product(p%p(1:), q%p(1:))
    end function prod_vector4

```

The power operation for four-vectors is signed, i.e., p^{**1} is positive for timelike and negative for spacelike vectors. Note that $(p^{**1})^{**2}$ is not necessarily equal to p^{**2} .

```

<Lorentz: sub interfaces>+≡
    elemental module function power_vector4 (p, e) result (s)
        real(default) :: s
        type(vector4_t), intent(in) :: p
        integer, intent(in) :: e
    end function power_vector4

<Lorentz: procedures>+≡
    elemental module function power_vector4 (p, e) result (s)
        real(default) :: s
        type(vector4_t), intent(in) :: p
        integer, intent(in) :: e
        s = p * p
        if (e /= 2) then
            if (mod(e, 2) == 0) then
                s = s**(e / 2)
            else if (s >= 0) then

```

```

        s = sqrt(s)**e
    else
        s = -(sqrt(abs(s))**e)
    end if
end if
end function power_vector4

```

Finally, we introduce a negation

```

<Lorentz: interfaces>+=
    interface operator(-)
        module procedure negate_vector4
    end interface

<Lorentz: sub interfaces>+=
    elemental module function negate_vector4 (p) result (q)
        type(vector4_t) :: q
        type(vector4_t), intent(in) :: p
    end function negate_vector4

<Lorentz: procedures>+=
    elemental module function negate_vector4 (p) result (q)
        type(vector4_t) :: q
        type(vector4_t), intent(in) :: p
        integer :: i
        do i = 0, 3
            if (abs (p%p(i)) < eps0) then
                q%p(i) = 0
            else
                q%p(i) = -p%p(i)
            end if
        end do
    end function negate_vector4

```

The sum function can be useful:

```

<Lorentz: interfaces>+=
    interface sum
        module procedure sum_vector4, sum_vector4_mask
    end interface

<Lorentz: sub interfaces>+=
    pure module function sum_vector4 (p) result (q)
        type(vector4_t) :: q
        type(vector4_t), dimension(:), intent(in) :: p
    end function sum_vector4
    pure module function sum_vector4_mask (p, mask) result (q)
        type(vector4_t) :: q
        type(vector4_t), dimension(:), intent(in) :: p
        logical, dimension(:), intent(in) :: mask
    end function sum_vector4_mask

<Lorentz: procedures>+=
    pure module function sum_vector4 (p) result (q)
        type(vector4_t) :: q
        type(vector4_t), dimension(:), intent(in) :: p
        integer :: i

```

```

do i = 0, 3
  q%p(i) = sum (p%p(i))
end do
end function sum_vector4

pure module function sum_vector4_mask (p, mask) result (q)
  type(vector4_t) :: q
  type(vector4_t), dimension(:), intent(in) :: p
  logical, dimension(:), intent(in) :: mask
  integer :: i
  do i = 0, 3
    q%p(i) = sum (p%p(i), mask=mask)
  end do
end function sum_vector4_mask

```

9.3.3 Conversions

Manually set a component of the four-vector:

```

<Lorentz: public>+≡
  public :: vector4_set_component

<Lorentz: sub interfaces>+≡
  module subroutine vector4_set_component (p, k, c)
    type(vector4_t), intent(inout) :: p
    integer, intent(in) :: k
    real(default), intent(in) :: c
  end subroutine vector4_set_component

<Lorentz: procedures>+≡
  module subroutine vector4_set_component (p, k, c)
    type(vector4_t), intent(inout) :: p
    integer, intent(in) :: k
    real(default), intent(in) :: c
    p%p(k) = c
  end subroutine vector4_set_component

```

Any component:

```

<Lorentz: public>+≡
  public :: vector4_get_component

<Lorentz: sub interfaces>+≡
  elemental module function vector4_get_component (p, k) result (c)
    real(default) :: c
    type(vector4_t), intent(in) :: p
    integer, intent(in) :: k
  end function vector4_get_component

<Lorentz: procedures>+≡
  elemental module function vector4_get_component (p, k) result (c)
    real(default) :: c
    type(vector4_t), intent(in) :: p
    integer, intent(in) :: k
    c = p%p(k)
  end function vector4_get_component

```


Extract all components. This is not elemental.

```

(Lorentz: public)+≡
    public :: vector4_get_components

(Lorentz: sub interfaces)+≡
    pure module function vector4_get_components (p) result (a)
        real(default), dimension(0:3) :: a
        type(vector4_t), intent(in) :: p
    end function vector4_get_components

(Lorentz: procedures)+≡
    pure module function vector4_get_components (p) result (a)
        real(default), dimension(0:3) :: a
        type(vector4_t), intent(in) :: p
        a = p%p
    end function vector4_get_components

```

This function returns the space part of a four-vector, such that we can apply three-vector operations on it:

```

(Lorentz: public functions)+≡
    public :: space_part

(Lorentz: interfaces)+≡
    interface space_part
        module procedure vector4_get_space_part
    end interface

(Lorentz: sub interfaces)+≡
    elemental module function vector4_get_space_part (p) result (q)
        type(vector3_t) :: q
        type(vector4_t), intent(in) :: p
    end function vector4_get_space_part

(Lorentz: procedures)+≡
    elemental module function vector4_get_space_part (p) result (q)
        type(vector3_t) :: q
        type(vector4_t), intent(in) :: p
        q%p = p%p(1:)
    end function vector4_get_space_part

```

This function returns the direction of a four-vector, i.e., a normalized three-vector. If the four-vector has zero space part, we return a null vector.

```

(Lorentz: interfaces)+≡
    interface direction
        module procedure vector4_get_direction
    end interface

(Lorentz: sub interfaces)+≡
    elemental module function vector4_get_direction (p) result (q)
        type(vector3_t) :: q
        type(vector4_t), intent(in) :: p
    end function vector4_get_direction

```

```

(Lorentz: procedures)+≡
  elemental module function vector4_get_direction (p) result (q)
    type(vector3_t) :: q
    type(vector4_t), intent(in) :: p
    real(default) :: qq
    q%p = p%p(1:)
    qq = q**1
    if (abs(qq) > eps0) then
      q%p = q%p / qq
    else
      q%p = 0
    end if
  end function vector4_get_direction

```

Change the sign of the spatial part of a four-vector

```

(Lorentz: public)+≡
  public :: vector4_invert_direction

(Lorentz: sub interfaces)+≡
  elemental module subroutine vector4_invert_direction (p)
    type(vector4_t), intent(inout) :: p
  end subroutine vector4_invert_direction

(Lorentz: procedures)+≡
  elemental module subroutine vector4_invert_direction (p)
    type(vector4_t), intent(inout) :: p
    p%p(1:3) = -p%p(1:3)
  end subroutine vector4_invert_direction

```

This function returns the four-vector as an ordinary array. A second version for an array of four-vectors.

```

(Lorentz: public)+≡
  public :: assignment (=)

(Lorentz: interfaces)+≡
  interface assignment (=)
    module procedure array_from_vector4_1, array_from_vector4_2, &
      array_from_vector3_1, array_from_vector3_2, &
      vector4_from_array, vector3_from_array
  end interface

(Lorentz: sub interfaces)+≡
  pure module subroutine array_from_vector4_1 (a, p)
    real(default), dimension(:), intent(out) :: a
    type(vector4_t), intent(in) :: p
  end subroutine array_from_vector4_1
  pure module subroutine array_from_vector4_2 (a, p)
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), dimension(:, :), intent(out) :: a
  end subroutine array_from_vector4_2
  pure module subroutine array_from_vector3_1 (a, p)
    real(default), dimension(:), intent(out) :: a
    type(vector3_t), intent(in) :: p
  end subroutine array_from_vector3_1
  pure module subroutine array_from_vector3_2 (a, p)

```

```

        type(vector3_t), dimension(:), intent(in) :: p
        real(default), dimension(:,:), intent(out) :: a
    end subroutine array_from_vector3_2
    pure module subroutine vector4_from_array (p, a)
        type(vector4_t), intent(out) :: p
        real(default), dimension(:), intent(in) :: a
    end subroutine vector4_from_array
    pure module subroutine vector3_from_array (p, a)
        type(vector3_t), intent(out) :: p
        real(default), dimension(:), intent(in) :: a
    end subroutine vector3_from_array
    (Lorentz: procedures)+≡
    pure module subroutine array_from_vector4_1 (a, p)
        real(default), dimension(:), intent(out) :: a
        type(vector4_t), intent(in) :: p
        a = p%p
    end subroutine array_from_vector4_1

    pure module subroutine array_from_vector4_2 (a, p)
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), dimension(:,:), intent(out) :: a
        integer :: i
        forall (i=1:size(p))
            a(:,i) = p(i)%p
        end forall
    end subroutine array_from_vector4_2

    pure module subroutine array_from_vector3_1 (a, p)
        real(default), dimension(:), intent(out) :: a
        type(vector3_t), intent(in) :: p
        a = p%p
    end subroutine array_from_vector3_1

    pure module subroutine array_from_vector3_2 (a, p)
        type(vector3_t), dimension(:), intent(in) :: p
        real(default), dimension(:,:), intent(out) :: a
        integer :: i
        forall (i=1:size(p))
            a(:,i) = p(i)%p
        end forall
    end subroutine array_from_vector3_2

    pure module subroutine vector4_from_array (p, a)
        type(vector4_t), intent(out) :: p
        real(default), dimension(:), intent(in) :: a
        p%p(0:3) = a
    end subroutine vector4_from_array

    pure module subroutine vector3_from_array (p, a)
        type(vector3_t), intent(out) :: p
        real(default), dimension(:), intent(in) :: a
        p%p(1:3) = a
    end subroutine vector3_from_array

```

```

<Lorentz: public>+≡
    public :: vector4

<Lorentz: sub interfaces>+≡
    pure module function vector4 (a) result (p)
        type(vector4_t) :: p
        real(default), intent(in), dimension(4) :: a
    end function vector4

<Lorentz: procedures>+≡
    pure module function vector4 (a) result (p)
        type(vector4_t) :: p
        real(default), intent(in), dimension(4) :: a
        p%p = a
    end function vector4

<Lorentz: vector4: TBP>+≡
    procedure :: to_pythia6 => vector4_to_pythia6

<Lorentz: sub interfaces>+≡
    pure module function vector4_to_pythia6 (vector4, m) result (p)
        real(double), dimension(1:5) :: p
        class(vector4_t), intent(in) :: vector4
        real(default), intent(in), optional :: m
    end function vector4_to_pythia6

<Lorentz: procedures>+≡
    pure module function vector4_to_pythia6 (vector4, m) result (p)
        real(double), dimension(1:5) :: p
        class(vector4_t), intent(in) :: vector4
        real(default), intent(in), optional :: m
        p(1:3) = vector4%p(1:3)
        p(4) = vector4%p(0)
        if (present (m)) then
            p(5) = m
        else
            p(5) = vector4 ** 1
        end if
    end function vector4_to_pythia6

```

9.3.4 Interface to c_prt

Transform the momentum of a c_prt object into a four-vector and vice versa:

```

<Lorentz: interfaces>+≡
    interface assignment (=)
        module procedure vector4_from_c_prt, c_prt_from_vector4
    end interface

<Lorentz: sub interfaces>+≡
    pure module subroutine vector4_from_c_prt (p, c_prt)
        type(vector4_t), intent(out) :: p
        type(c_prt_t), intent(in) :: c_prt
    end subroutine vector4_from_c_prt
    pure module subroutine c_prt_from_vector4 (c_prt, p)

```

```

        type(c_prt_t), intent(out) :: c_prt
        type(vector4_t), intent(in) :: p
    end subroutine c_prt_from_vector4

<Lorentz: procedures>+≡
    pure module subroutine vector4_from_c_prt (p, c_prt)
        type(vector4_t), intent(out) :: p
        type(c_prt_t), intent(in) :: c_prt
        p%p(0) = c_prt%pe
        p%p(1) = c_prt%px
        p%p(2) = c_prt%py
        p%p(3) = c_prt%pz
    end subroutine vector4_from_c_prt

    pure module subroutine c_prt_from_vector4 (c_prt, p)
        type(c_prt_t), intent(out) :: c_prt
        type(vector4_t), intent(in) :: p
        c_prt%pe = p%p(0)
        c_prt%px = p%p(1)
        c_prt%py = p%p(2)
        c_prt%pz = p%p(3)
        c_prt%p2 = p ** 2
    end subroutine c_prt_from_vector4

Initialize a c_prt_t object with the components of a four-vector as its kinematical entries. Compute the invariant mass, or use the optional mass-squared value instead.

<Lorentz: public>+≡
    public :: vector4_to_c_prt

<Lorentz: sub interfaces>+≡
    elemental module function vector4_to_c_prt (p, p2) result (c_prt)
        type(c_prt_t) :: c_prt
        type(vector4_t), intent(in) :: p
        real(default), intent(in), optional :: p2
    end function vector4_to_c_prt

<Lorentz: procedures>+≡
    elemental module function vector4_to_c_prt (p, p2) result (c_prt)
        type(c_prt_t) :: c_prt
        type(vector4_t), intent(in) :: p
        real(default), intent(in), optional :: p2
        c_prt%pe = p%p(0)
        c_prt%px = p%p(1)
        c_prt%py = p%p(2)
        c_prt%pz = p%p(3)
        if (present (p2)) then
            c_prt%p2 = p2
        else
            c_prt%p2 = p ** 2
        end if
    end function vector4_to_c_prt

```

9.3.5 Angles

Return the angles in a canonical system. The angle ϕ is defined between $0 \leq \phi < 2\pi$. In degenerate cases, return zero.

```
<Lorentz: public functions>+≡
    public :: azimuthal_angle

<Lorentz: interfaces>+≡
    interface azimuthal_angle
        module procedure vector3_azimuthal_angle
        module procedure vector4_azimuthal_angle
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_azimuthal_angle (p) result (phi)
        real(default) :: phi
        type(vector3_t), intent(in) :: p
    end function vector3_azimuthal_angle
    elemental module function vector4_azimuthal_angle (p) result (phi)
        real(default) :: phi
        type(vector4_t), intent(in) :: p
    end function vector4_azimuthal_angle

<Lorentz: procedures>+≡
    elemental module function vector3_azimuthal_angle (p) result (phi)
        real(default) :: phi
        type(vector3_t), intent(in) :: p
        if (any (abs (p%p(1:2)) > 0)) then
            phi = atan2(p%p(2), p%p(1))
            if (phi < 0) phi = phi + twopi
        else
            phi = 0
        end if
    end function vector3_azimuthal_angle
    elemental module function vector4_azimuthal_angle (p) result (phi)
        real(default) :: phi
        type(vector4_t), intent(in) :: p
        phi = vector3_azimuthal_angle (space_part (p))
    end function vector4_azimuthal_angle

Azimuthal angle in degrees

<Lorentz: public functions>+≡
    public :: azimuthal_angle_deg

<Lorentz: interfaces>+≡
    interface azimuthal_angle_deg
        module procedure vector3_azimuthal_angle_deg
        module procedure vector4_azimuthal_angle_deg
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_azimuthal_angle_deg (p) result (phi)
        real(default) :: phi
        type(vector3_t), intent(in) :: p
    end function vector3_azimuthal_angle_deg
    elemental module function vector4_azimuthal_angle_deg (p) result (phi)
```

```

        real(default) :: phi
        type(vector4_t), intent(in) :: p
    end function vector4_azimuthal_angle_deg

<Lorentz: procedures>+≡
    elemental module function vector3_azimuthal_angle_deg (p) result (phi)
        real(default) :: phi
        type(vector3_t), intent(in) :: p
        phi = vector3_azimuthal_angle (p) / degree
    end function vector3_azimuthal_angle_deg
    elemental module function vector4_azimuthal_angle_deg (p) result (phi)
        real(default) :: phi
        type(vector4_t), intent(in) :: p
        phi = vector4_azimuthal_angle (p) / degree
    end function vector4_azimuthal_angle_deg

```

The azimuthal distance of two vectors. This is the difference of the azimuthal angles, but cannot be larger than π : The result is between $-\pi < \Delta\phi \leq \pi$.

```

<Lorentz: public functions>+≡
    public :: azimuthal_distance

<Lorentz: interfaces>+≡
    interface azimuthal_distance
        module procedure vector3_azimuthal_distance
        module procedure vector4_azimuthal_distance
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_azimuthal_distance (p, q) result (dphi)
        real(default) :: dphi
        type(vector3_t), intent(in) :: p,q
    end function vector3_azimuthal_distance
    elemental module function vector4_azimuthal_distance (p, q) result (dphi)
        real(default) :: dphi
        type(vector4_t), intent(in) :: p,q
    end function vector4_azimuthal_distance

<Lorentz: procedures>+≡
    elemental module function vector3_azimuthal_distance (p, q) result (dphi)
        real(default) :: dphi
        type(vector3_t), intent(in) :: p,q
        dphi = vector3_azimuthal_angle (q) - vector3_azimuthal_angle (p)
        if (dphi <= -pi) then
            dphi = dphi + twopi
        else if (dphi > pi) then
            dphi = dphi - twopi
        end if
    end function vector3_azimuthal_distance
    elemental module function vector4_azimuthal_distance (p, q) result (dphi)
        real(default) :: dphi
        type(vector4_t), intent(in) :: p,q
        dphi = vector3_azimuthal_distance &
            (space_part (p), space_part (q))
    end function vector4_azimuthal_distance

```

The same in degrees:

```

<Lorentz: public functions>+≡
    public :: azimuthal_distance_deg

<Lorentz: interfaces>+≡
    interface azimuthal_distance_deg
        module procedure vector3_azimuthal_distance_deg
        module procedure vector4_azimuthal_distance_deg
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function vector3_azimuthal_distance_deg (p, q) result (dphi)
        real(default) :: dphi
        type(vector3_t), intent(in) :: p,q
    end function vector3_azimuthal_distance_deg
    elemental module function vector4_azimuthal_distance_deg (p, q) result (dphi)
        real(default) :: dphi
        type(vector4_t), intent(in) :: p,q
    end function vector4_azimuthal_distance_deg

<Lorentz: procedures>+≡
    elemental module function vector3_azimuthal_distance_deg (p, q) result (dphi)
        real(default) :: dphi
        type(vector3_t), intent(in) :: p,q
        dphi = vector3_azimuthal_distance (p, q) / degree
    end function vector3_azimuthal_distance_deg
    elemental module function vector4_azimuthal_distance_deg (p, q) result (dphi)
        real(default) :: dphi
        type(vector4_t), intent(in) :: p,q
        dphi = vector4_azimuthal_distance (p, q) / degree
    end function vector4_azimuthal_distance_deg

```

The polar angle is defined $0 \leq \theta \leq \pi$. Note that ATAN2 has the reversed order of arguments: ATAN2(Y,X). Here, x is the 3-component while y is the transverse momentum which is always nonnegative. Therefore, the result is nonnegative as well.

```

<Lorentz: public functions>+≡
    public :: polar_angle

<Lorentz: interfaces>+≡
    interface polar_angle
        module procedure polar_angle_vector3
        module procedure polar_angle_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function polar_angle_vector3 (p) result (theta)
        real(default) :: theta
        type(vector3_t), intent(in) :: p
    end function polar_angle_vector3
    elemental module function polar_angle_vector4 (p) result (theta)
        real(default) :: theta
        type(vector4_t), intent(in) :: p
    end function polar_angle_vector4

```



```

<Lorentz: procedures>+≡
  elemental module function polar_angle_vector3 (p) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p
    if (any (abs (p%p) > 0)) then
      theta = atan2 (sqrt(p%p(1)**2 + p%p(2)**2), p%p(3))
    else
      theta = 0
    end if
  end function polar_angle_vector3
  elemental module function polar_angle_vector4 (p) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p
    theta = polar_angle (space_part (p))
  end function polar_angle_vector4

```

This is the cosine of the polar angle: $-1 \leq \cos \theta \leq 1$.

```

<Lorentz: public functions>+≡
  public :: polar_angle_ct

<Lorentz: interfaces>+≡
  interface polar_angle_ct
    module procedure polar_angle_ct_vector3
    module procedure polar_angle_ct_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function polar_angle_ct_vector3 (p) result (ct)
    real(default) :: ct
    type(vector3_t), intent(in) :: p
  end function polar_angle_ct_vector3
  elemental module function polar_angle_ct_vector4 (p) result (ct)
    real(default) :: ct
    type(vector4_t), intent(in) :: p
  end function polar_angle_ct_vector4

<Lorentz: procedures>+≡
  elemental module function polar_angle_ct_vector3 (p) result (ct)
    real(default) :: ct
    type(vector3_t), intent(in) :: p
    if (any (abs (p%p) > 0)) then
      ct = p%p(3) / p**1
    else
      ct = 1
    end if
  end function polar_angle_ct_vector3
  elemental module function polar_angle_ct_vector4 (p) result (ct)
    real(default) :: ct
    type(vector4_t), intent(in) :: p
    ct = polar_angle_ct (space_part (p))
  end function polar_angle_ct_vector4

```

The polar angle in degrees.

```

<Lorentz: public functions>+≡
  public :: polar_angle_deg

```

```

<Lorentz: interfaces>+≡
  interface polar_angle_deg
    module procedure polar_angle_deg_vector3
    module procedure polar_angle_deg_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function polar_angle_deg_vector3 (p) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p
  end function polar_angle_deg_vector3
  elemental module function polar_angle_deg_vector4 (p) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p
  end function polar_angle_deg_vector4

<Lorentz: procedures>+≡
  elemental module function polar_angle_deg_vector3 (p) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p
    theta = polar_angle (p) / degree
  end function polar_angle_deg_vector3
  elemental module function polar_angle_deg_vector4 (p) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p
    theta = polar_angle (p) / degree
  end function polar_angle_deg_vector4

```

This is the angle enclosed between two three-momenta. If one of the momenta is zero, we return an angle of zero. The range of the result is $0 \leq \theta \leq \pi$. If there is only one argument, take the positive z axis as reference.

```

<Lorentz: public functions>+≡
  public :: enclosed_angle

<Lorentz: interfaces>+≡
  interface enclosed_angle
    module procedure enclosed_angle_vector3
    module procedure enclosed_angle_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function enclosed_angle_vector3 (p, q) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p, q
  end function enclosed_angle_vector3
  elemental module function enclosed_angle_vector4 (p, q) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p, q
  end function enclosed_angle_vector4

<Lorentz: procedures>+≡
  elemental module function enclosed_angle_vector3 (p, q) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p, q
    theta = acos (enclosed_angle_ct (p, q))
  end function enclosed_angle_vector3

```

```

elemental module function enclosed_angle_vector4 (p, q) result (theta)
  real(default) :: theta
  type(vector4_t), intent(in) :: p, q
  theta = enclosed_angle (space_part (p), space_part (q))
end function enclosed_angle_vector4

```

The cosine of the enclosed angle.

```

<Lorentz: public functions>+≡
  public :: enclosed_angle_ct

<Lorentz: interfaces>+≡
  interface enclosed_angle_ct
    module procedure enclosed_angle_ct_vector3
    module procedure enclosed_angle_ct_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function enclosed_angle_ct_vector3 (p, q) result (ct)
    real(default) :: ct
    type(vector3_t), intent(in) :: p, q
  end function enclosed_angle_ct_vector3
  elemental module function enclosed_angle_ct_vector4 (p, q) result (ct)
    real(default) :: ct
    type(vector4_t), intent(in) :: p, q
  end function enclosed_angle_ct_vector4

<Lorentz: procedures>+≡
  elemental module function enclosed_angle_ct_vector3 (p, q) result (ct)
    real(default) :: ct
    type(vector3_t), intent(in) :: p, q
    if (any (abs (p%p) > 0) .and. any (abs (q%p) > 0)) then
      ct = p*q / (p**1 * q**1)
      if (ct>1) then
        ct = 1
      else if (ct<-1) then
        ct = -1
      end if
    else
      ct = 1
    end if
  end function enclosed_angle_ct_vector3
  elemental module function enclosed_angle_ct_vector4 (p, q) result (ct)
    real(default) :: ct
    type(vector4_t), intent(in) :: p, q
    ct = enclosed_angle_ct (space_part (p), space_part (q))
  end function enclosed_angle_ct_vector4

```

The enclosed angle in degrees.

```

<Lorentz: public functions>+≡
  public :: enclosed_angle_deg

<Lorentz: interfaces>+≡
  interface enclosed_angle_deg
    module procedure enclosed_angle_deg_vector3
    module procedure enclosed_angle_deg_vector4
  end interface

```

```

(Lorentz: sub interfaces)+≡
  elemental module function enclosed_angle_deg_vector3 (p, q) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p, q
  end function enclosed_angle_deg_vector3
  elemental module function enclosed_angle_deg_vector4 (p, q) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p, q
  end function enclosed_angle_deg_vector4

(Lorentz: procedures)+≡
  elemental module function enclosed_angle_deg_vector3 (p, q) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p, q
    theta = enclosed_angle (p, q) / degree
  end function enclosed_angle_deg_vector3
  elemental module function enclosed_angle_deg_vector4 (p, q) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p, q
    theta = enclosed_angle (p, q) / degree
  end function enclosed_angle_deg_vector4

```

The polar angle of the first momentum w.r.t. the second momentum, evaluated in the rest frame of the second momentum. If the second four-momentum is not timelike, return zero.

```

(Lorentz: public functions)+≡
  public :: enclosed_angle_rest_frame
  public :: enclosed_angle_ct_rest_frame
  public :: enclosed_angle_deg_rest_frame

(Lorentz: interfaces)+≡
  interface enclosed_angle_rest_frame
    module procedure enclosed_angle_rest_frame_vector4
  end interface
  interface enclosed_angle_ct_rest_frame
    module procedure enclosed_angle_ct_rest_frame_vector4
  end interface
  interface enclosed_angle_deg_rest_frame
    module procedure enclosed_angle_deg_rest_frame_vector4
  end interface

(Lorentz: sub interfaces)+≡
  elemental module function enclosed_angle_rest_frame_vector4 (p, q) result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
  end function enclosed_angle_rest_frame_vector4
  elemental module function enclosed_angle_ct_rest_frame_vector4 (p, q) result (ct)
    type(vector4_t), intent(in) :: p, q
    real(default) :: ct
  end function enclosed_angle_ct_rest_frame_vector4
  elemental module function enclosed_angle_deg_rest_frame_vector4 (p, q) &
    result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
  end function enclosed_angle_deg_rest_frame_vector4

```

```

<Lorentz: procedures>+≡
  elemental module function enclosed_angle_rest_frame_vector4 (p, q) result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
    theta = acos (enclosed_angle_ct_rest_frame (p, q))
  end function enclosed_angle_rest_frame_vector4
  elemental module function enclosed_angle_ct_rest_frame_vector4 (p, q) result (ct)
    type(vector4_t), intent(in) :: p, q
    real(default) :: ct
    if (invariant_mass(q) > 0) then
      ct = enclosed_angle_ct ( &
        space_part (boost(-q, invariant_mass (q)) * p), &
        space_part (q))
    else
      ct = 1
    end if
  end function enclosed_angle_ct_rest_frame_vector4
  elemental module function enclosed_angle_deg_rest_frame_vector4 (p, q) &
    result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
    theta = enclosed_angle_rest_frame (p, q) / degree
  end function enclosed_angle_deg_rest_frame_vector4

```

9.3.6 More kinematical functions (some redundant)

The scalar transverse momentum (assuming the z axis is longitudinal)

```

<Lorentz: public functions>+≡
  public :: transverse_part

<Lorentz: interfaces>+≡
  interface transverse_part
    module procedure transverse_part_vector4_beam_axis
    module procedure transverse_part_vector4_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function transverse_part_vector4_beam_axis (p) result (pT)
    real(default) :: pT
    type(vector4_t), intent(in) :: p
  end function transverse_part_vector4_beam_axis
  elemental module function transverse_part_vector4_vector4 (p1, p2) result (pT)
    real(default) :: pT
    type(vector4_t), intent(in) :: p1, p2
  end function transverse_part_vector4_vector4

<Lorentz: procedures>+≡
  elemental module function transverse_part_vector4_beam_axis (p) result (pT)
    real(default) :: pT
    type(vector4_t), intent(in) :: p
    pT = sqrt(p%p(1)**2 + p%p(2)**2)
  end function transverse_part_vector4_beam_axis

  elemental module function transverse_part_vector4_vector4 (p1, p2) result (pT)

```

```

real(default) :: pT
type(vector4_t), intent(in) :: p1, p2
real(default) :: p1_norm, p2_norm, p1p2, pT2
p1_norm = space_part_norm(p1)**2
p2_norm = space_part_norm(p2)**2
!   p1p2 = p1%p(1:3)*p2%p(1:3)
p1p2 = vector4_get_space_part(p1) * vector4_get_space_part(p2)
pT2 = (p1_norm*p2_norm - p1p2)/p1_norm
pT = sqrt (pT2)
end function transverse_part_vector4_vector4

```

The scalar longitudinal momentum (assuming the z axis is longitudinal). Identical to `momentum_z_component`.

```

<Lorentz: public functions>+≡
  public :: longitudinal_part

<Lorentz: interfaces>+≡
  interface longitudinal_part
    module procedure longitudinal_part_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function longitudinal_part_vector4 (p) result (pL)
    real(default) :: pL
    type(vector4_t), intent(in) :: p
  end function longitudinal_part_vector4

<Lorentz: procedures>+≡
  elemental module function longitudinal_part_vector4 (p) result (pL)
    real(default) :: pL
    type(vector4_t), intent(in) :: p
    pL = p%p(3)
  end function longitudinal_part_vector4

```

Absolute value of three-momentum

```

<Lorentz: public functions>+≡
  public :: space_part_norm

<Lorentz: interfaces>+≡
  interface space_part_norm
    module procedure space_part_norm_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function space_part_norm_vector4 (p) result (p3)
    real(default) :: p3
    type(vector4_t), intent(in) :: p
  end function space_part_norm_vector4

<Lorentz: procedures>+≡
  elemental module function space_part_norm_vector4 (p) result (p3)
    real(default) :: p3
    type(vector4_t), intent(in) :: p
    p3 = sqrt (p%p(1)**2 + p%p(2)**2 + p%p(3)**2)
  end function space_part_norm_vector4

```

The energy (the zeroth component)

```

(Lorentz: public functions)+≡
    public :: energy

(Lorentz: interfaces)+≡
    interface energy
        module procedure energy_vector4
        module procedure energy_vector3
        module procedure energy_real
    end interface

(Lorentz: sub interfaces)+≡
    elemental module function energy_vector4 (p) result (E)
        real(default) :: E
        type(vector4_t), intent(in) :: p
    end function energy_vector4
    elemental module function energy_vector3 (p, mass) result (E)
        real(default) :: E
        type(vector3_t), intent(in) :: p
        real(default), intent(in), optional :: mass
    end function energy_vector3
    elemental module function energy_real (p, mass) result (E)
        real(default) :: E
        real(default), intent(in) :: p
        real(default), intent(in), optional :: mass
    end function energy_real

(Lorentz: procedures)+≡
    elemental module function energy_vector4 (p) result (E)
        real(default) :: E
        type(vector4_t), intent(in) :: p
        E = p%p(0)
    end function energy_vector4

```

Alternative: The energy corresponding to a given momentum and mass. If the mass is omitted, it is zero

```

(Lorentz: procedures)+≡
    elemental module function energy_vector3 (p, mass) result (E)
        real(default) :: E
        type(vector3_t), intent(in) :: p
        real(default), intent(in), optional :: mass
        if (present (mass)) then
            E = sqrt (p**2 + mass**2)
        else
            E = p**1
        end if
    end function energy_vector3

    elemental module function energy_real (p, mass) result (E)
        real(default) :: E
        real(default), intent(in) :: p
        real(default), intent(in), optional :: mass
        if (present (mass)) then
            E = sqrt (p**2 + mass**2)
        else

```

```

        E = abs (p)
    end if
end function energy_real

```

The invariant mass of four-momenta. Zero for lightlike, negative for spacelike momenta.

```

<Lorentz: public functions>+≡
    public :: invariant_mass

<Lorentz: interfaces>+≡
    interface invariant_mass
        module procedure invariant_mass_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function invariant_mass_vector4 (p) result (m)
        real(default) :: m
        type(vector4_t), intent(in) :: p
    end function invariant_mass_vector4

<Lorentz: procedures>+≡
    elemental module function invariant_mass_vector4 (p) result (m)
        real(default) :: m
        type(vector4_t), intent(in) :: p
        real(default) :: msq
        msq = p*p
        if (msq >= 0) then
            m = sqrt (msq)
        else
            m = - sqrt (abs (msq))
        end if
    end function invariant_mass_vector4

```

The invariant mass squared. Zero for lightlike, negative for spacelike momenta.

```

<Lorentz: public functions>+≡
    public :: invariant_mass_squared

<Lorentz: interfaces>+≡
    interface invariant_mass_squared
        module procedure invariant_mass_squared_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function invariant_mass_squared_vector4 (p) result (msq)
        real(default) :: msq
        type(vector4_t), intent(in) :: p
    end function invariant_mass_squared_vector4

<Lorentz: procedures>+≡
    elemental module function invariant_mass_squared_vector4 (p) result (msq)
        real(default) :: msq
        type(vector4_t), intent(in) :: p
        msq = p*p
    end function invariant_mass_squared_vector4

```

The transverse mass. If the mass squared is negative, this value also is negative.

```

<Lorentz: public functions>+≡
    public :: transverse_mass

```



```

<Lorentz: interfaces>+≡
  interface transverse_mass
    module procedure transverse_mass_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function transverse_mass_vector4 (p) result (m)
    real(default) :: m
    type(vector4_t), intent(in) :: p
  end function transverse_mass_vector4

<Lorentz: procedures>+≡
  elemental module function transverse_mass_vector4 (p) result (m)
    real(default) :: m
    type(vector4_t), intent(in) :: p
    real(default) :: msq
    msq = p%p(0)**2 - p%p(1)**2 - p%p(2)**2
    if (msq >= 0) then
      m = sqrt (msq)
    else
      m = - sqrt (abs (msq))
    end if
  end function transverse_mass_vector4

```

The rapidity (defined if particle is massive or $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
  public :: rapidity

<Lorentz: interfaces>+≡
  interface rapidity
    module procedure rapidity_vector4
  end interface

<Lorentz: sub interfaces>+≡
  elemental module function rapidity_vector4 (p) result (y)
    real(default) :: y
    type(vector4_t), intent(in) :: p
  end function rapidity_vector4

<Lorentz: procedures>+≡
  elemental module function rapidity_vector4 (p) result (y)
    real(default) :: y
    type(vector4_t), intent(in) :: p
    y = .5 * log( (energy (p) + longitudinal_part (p)) &
      &          / (energy (p) - longitudinal_part (p)))
  end function rapidity_vector4

```

The pseudorapidity (defined if $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
  public :: pseudorapidity

<Lorentz: interfaces>+≡
  interface pseudorapidity
    module procedure pseudorapidity_vector4
  end interface

```

```

<Lorentz: sub interfaces>+≡
    elemental module function pseudorapidity_vector4 (p) result (eta)
        real(default) :: eta
        type(vector4_t), intent(in) :: p
    end function pseudorapidity_vector4

```

```

<Lorentz: procedures>+≡
    elemental module function pseudorapidity_vector4 (p) result (eta)
        real(default) :: eta
        type(vector4_t), intent(in) :: p
        eta = -log( tan (.5 * polar_angle (p)))
    end function pseudorapidity_vector4

```

The rapidity distance (defined if both $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
    public :: rapidity_distance

<Lorentz: interfaces>+≡
    interface rapidity_distance
        module procedure rapidity_distance_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function rapidity_distance_vector4 (p, q) result (dy)
        type(vector4_t), intent(in) :: p, q
        real(default) :: dy
    end function rapidity_distance_vector4

<Lorentz: procedures>+≡
    elemental module function rapidity_distance_vector4 (p, q) result (dy)
        type(vector4_t), intent(in) :: p, q
        real(default) :: dy
        dy = rapidity (q) - rapidity (p)
    end function rapidity_distance_vector4

```

The pseudorapidity distance (defined if both $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
    public :: pseudorapidity_distance

<Lorentz: interfaces>+≡
    interface pseudorapidity_distance
        module procedure pseudorapidity_distance_vector4
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function pseudorapidity_distance_vector4 (p, q) result (deta)
        real(default) :: deta
        type(vector4_t), intent(in) :: p, q
    end function pseudorapidity_distance_vector4

<Lorentz: procedures>+≡
    elemental module function pseudorapidity_distance_vector4 (p, q) result (deta)
        real(default) :: deta
        type(vector4_t), intent(in) :: p, q
        deta = pseudorapidity (q) - pseudorapidity (p)
    end function pseudorapidity_distance_vector4

```

The distance on the $\eta - \phi$ cylinder:

```

(Lorentz: public functions)+≡
    public :: eta_phi_distance

(Lorentz: interfaces)+≡
    interface eta_phi_distance
        module procedure eta_phi_distance_vector4
    end interface

(Lorentz: sub interfaces)+≡
    elemental module function eta_phi_distance_vector4 (p, q) result (dr)
        type(vector4_t), intent(in) :: p, q
        real(default) :: dr
    end function eta_phi_distance_vector4

(Lorentz: procedures)+≡
    elemental module function eta_phi_distance_vector4 (p, q) result (dr)
        type(vector4_t), intent(in) :: p, q
        real(default) :: dr
        dr = sqrt ( &
            pseudorapidity_distance (p, q)**2 &
            + azimuthal_distance (p, q)**2)
    end function eta_phi_distance_vector4

```

9.3.7 Lorentz transformations

```

(Lorentz: public)+≡
    public :: lorentz_transformation_t

(Lorentz: types)+≡
    type :: lorentz_transformation_t
        private
        real(default), dimension(0:3, 0:3) :: L
        contains
        (Lorentz: lorentz transformation: TBP)
    end type lorentz_transformation_t

```

Output:

```

(Lorentz: public)+≡
    public :: lorentz_transformation_write

(Lorentz: lorentz transformation: TBP)≡
    procedure :: write => lorentz_transformation_write

(Lorentz: sub interfaces)+≡
    module subroutine lorentz_transformation_write (L, unit, testflag, ultra)
        class(lorentz_transformation_t), intent(in) :: L
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, ultra
    end subroutine lorentz_transformation_write

(Lorentz: procedures)+≡
    module subroutine lorentz_transformation_write (L, unit, testflag, ultra)
        class(lorentz_transformation_t), intent(in) :: L
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, ultra
    end subroutine lorentz_transformation_write

```

```

integer :: u, i
logical :: ult
character(len=7) :: fmt
ult = .false.; if (present (ultra)) ult = ultra
if (ult) then
    call pac_fmt (fmt, FMT_19, FMT_11, ultra)
else
    call pac_fmt (fmt, FMT_19, FMT_13, testflag)
end if
u = given_output_unit (unit); if (u < 0) return
write (u, "(1x,A,3(1x," // fmt // "))" ) "L00 = ", L%L(0,0)
write (u, "(1x,A,3(1x," // fmt // "))" ) "L0j = ", L%L(0,1:3)
do i = 1, 3
    write (u, "(1x,A,I0,A,3(1x," // fmt // "))" ) &
        "L", i, "0 = ", L%L(i,0)
    write (u, "(1x,A,I0,A,3(1x," // fmt // "))" ) &
        "L", i, "j = ", L%L(i,1:3)
end do
end subroutine lorentz_transformation_write

```

Extract all components:

```

<Lorentz: public>+≡
    public :: lorentz_transformation_get_components

<Lorentz: sub interfaces>+≡
    pure module function lorentz_transformation_get_components (L) result (a)
        type(lorentz_transformation_t), intent(in) :: L
        real(default), dimension(0:3,0:3) :: a
    end function lorentz_transformation_get_components

<Lorentz: procedures>+≡
    pure module function lorentz_transformation_get_components (L) result (a)
        type(lorentz_transformation_t), intent(in) :: L
        real(default), dimension(0:3,0:3) :: a
        a = L%L
    end function lorentz_transformation_get_components

```

9.3.8 Functions of Lorentz transformations

For the inverse, we make use of the fact that $\Lambda^{\mu\nu}\Lambda_{\mu\rho} = \delta_{\rho}^{\nu}$. So, lowering the indices and transposing is sufficient.

```

<Lorentz: public functions>+≡
    public :: inverse

<Lorentz: interfaces>+≡
    interface inverse
        module procedure lorentz_transformation_inverse
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function lorentz_transformation_inverse (L) result (IL)
        type(lorentz_transformation_t) :: L
        type(lorentz_transformation_t), intent(in) :: L
    end function lorentz_transformation_inverse

```

```

<Lorentz: procedures>+≡
  elemental module function lorentz_transformation_inverse (L) result (IL)
    type(lorentz_transformation_t) :: IL
    type(lorentz_transformation_t), intent(in) :: L
    IL%L(0,0) = L%L(0,0)
    IL%L(0,1:) = -L%L(1:,0)
    IL%L(1:,0) = -L%L(0,1:)
    IL%L(1:,1:) = transpose(L%L(1:,1:))
  end function lorentz_transformation_inverse

```

9.3.9 Invariants

These are used below. The first array index is varying fastest in FORTRAN; therefore the extra minus in the odd-rank tensor epsilon.

```

<Lorentz: parameters>+≡
  integer, dimension(3,3), parameter :: delta_three = &
    & reshape( source = [ 1,0,0, 0,1,0, 0,0,1 ], &
    &          shape = [3,3] )
  integer, dimension(3,3,3), parameter :: epsilon_three = &
    & reshape( source = [ 0, 0,0, 0,0,-1, 0,1,0, &
    &                    0, 0,1, 0,0, 0, -1,0,0, &
    &                    0,-1,0, 1,0, 0, 0,0,0 ],&
    &          shape = [3,3,3] )

```

This could be of some use:

```

<Lorentz: public>+≡
  public :: identity

<Lorentz: parameters>+≡
  type(lorentz_transformation_t), parameter :: &
    & identity = &
    & lorentz_transformation_t ( &
    & reshape( source = [ one, zero, zero, zero, &
    &                    zero, one, zero, zero, &
    &                    zero, zero, one, zero, &
    &                    zero, zero, zero, one ],&
    &          shape = [4,4] ) )

<Lorentz: public>+≡
  public :: space_reflection

<Lorentz: parameters>+≡
  type(lorentz_transformation_t), parameter :: &
    & space_reflection = &
    & lorentz_transformation_t ( &
    & reshape( source = [ one, zero, zero, zero, &
    &                    zero,-one, zero, zero, &
    &                    zero, zero,-one, zero, &
    &                    zero, zero, zero,-one ],&
    &          shape = [4,4] ) )

```

Builds a unit vector orthogonal to the input vector in the xy-plane.

```

<Lorentz: public functions>+≡
  public :: create_orthogonal

```

```

<Lorentz: sub interfaces>+≡
    module function create_orthogonal (p_in) result (p_out)
        type(vector3_t), intent(in) :: p_in
        type(vector3_t) :: p_out
    end function create_orthogonal

```

```

<Lorentz: procedures>+≡
    module function create_orthogonal (p_in) result (p_out)
        type(vector3_t), intent(in) :: p_in
        type(vector3_t) :: p_out
        real(default) :: ab
        ab = sqrt (p_in%p(1)**2 + p_in%p(2)**2)
        if (abs (ab) < eps0) then
            p_out%p(1) = 1
            p_out%p(2) = 0
            p_out%p(3) = 0
        else
            p_out%p(1) = p_in%p(2)
            p_out%p(2) = -p_in%p(1)
            p_out%p(3) = 0
            p_out = p_out / ab
        end if
    end function create_orthogonal

```

```

<Lorentz: public functions>+≡
    public :: create_unit_vector

```

```

<Lorentz: sub interfaces>+≡
    module function create_unit_vector (p_in) result (p_out)
        type(vector4_t), intent(in) :: p_in
        type(vector3_t) :: p_out
    end function create_unit_vector

```

```

<Lorentz: procedures>+≡
    module function create_unit_vector (p_in) result (p_out)
        type(vector4_t), intent(in) :: p_in
        type(vector3_t) :: p_out
        p_out%p = p_in%p(1:3) / space_part_norm (p_in)
    end function create_unit_vector

```

```

<Lorentz: public functions>+≡
    public :: normalize

```

```

<Lorentz: sub interfaces>+≡
    module function normalize(p) result (p_norm)
        type(vector3_t) :: p_norm
        type(vector3_t), intent(in) :: p
    end function normalize

```

```

<Lorentz: procedures>+≡
    module function normalize(p) result (p_norm)
        type(vector3_t) :: p_norm
        type(vector3_t), intent(in) :: p
        real(default) :: abs
        abs = sqrt (p%p(1)**2 + p%p(2)**2 + p%p(3)**2)
        p_norm = p / abs
    end function normalize

```

```
end function normalize
```

Computes the invariant mass of the momenta sum given by the indices in `i_res_born` and the optional argument `i_emitter`.

```
<Lorentz: public>+≡
```

```
public :: compute_resonance_mass
```

```
<Lorentz: sub interfaces>+≡
```

```
pure module function compute_resonance_mass (p, i_res_born, i_gluon) result (m)
  real(default) :: m
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
end function compute_resonance_mass
```

```
<Lorentz: procedures>+≡
```

```
pure module function compute_resonance_mass (p, i_res_born, i_gluon) result (m)
  real(default) :: m
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
  type(vector4_t) :: p_res
  p_res = get_resonance_momentum (p, i_res_born, i_gluon)
  m = p_res**1
end function compute_resonance_mass
```

```
<Lorentz: public>+≡
```

```
public :: get_resonance_momentum
```

```
<Lorentz: sub interfaces>+≡
```

```
pure module function get_resonance_momentum &
  (p, i_res_born, i_gluon) result (p_res)
  type(vector4_t) :: p_res
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
end function get_resonance_momentum
```

```
<Lorentz: procedures>+≡
```

```
pure module function get_resonance_momentum &
  (p, i_res_born, i_gluon) result (p_res)
  type(vector4_t) :: p_res
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
  integer :: i
  p_res = vector4_null
  do i = 1, size (i_res_born)
    p_res = p_res + p (i_res_born(i))
  end do
  if (present (i_gluon)) p_res = p_res + p (i_gluon)
end function get_resonance_momentum
```

```
<Lorentz: public>+≡
```

```
public :: create_two_particle_decay
```

```

(Lorentz: sub interfaces)+≡
  module function create_two_particle_decay (s, p1, p2) result (p_rest)
    type(vector4_t), dimension(3) :: p_rest
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p1, p2
  end function create_two_particle_decay

(Lorentz: procedures)+≡
  module function create_two_particle_decay (s, p1, p2) result (p_rest)
    type(vector4_t), dimension(3) :: p_rest
    real(default), intent(in) :: s
    type(vector4_t), intent(in) :: p1, p2
    real(default) :: m1_sq, m2_sq
    real(default) :: E1, E2, p
    m1_sq = p1**2; m2_sq = p2**2
    p = sqrt (lambda (s, m1_sq, m2_sq)) / (two * sqrt (s))
    E1 = sqrt (m1_sq + p**2); E2 = sqrt (m2_sq + p**2)
    p_rest(1)%p = [sqrt (s), zero, zero, zero]
    p_rest(2)%p(0) = E1
    p_rest(2)%p(1:3) = p * p1%p(1:3) / space_part_norm (p1)
    p_rest(3)%p(0) = E2; p_rest(3)%p(1:3) = -p_rest(2)%p(1:3)
  end function create_two_particle_decay

```

This function creates a phase-space point for a $1 \rightarrow 3$ decay in the decaying particle's rest frame. There are three rest frames for this system, corresponding to s -, t -, and u -channel momentum exchange, also referred to as Gottfried-Jackson frames. Below, we choose the momentum with index 1 to be aligned along the z -axis. We then have

$$\begin{aligned}
s_1 &= (p_1 + p_2)^2, \\
s_2 &= (p_2 + p_3)^2, \\
s_3 &= (p_1 + p_3)^2, \\
s_1 + s_2 + s_3 &= s + m_1^2 + m_2^2 + m_3^2.
\end{aligned}$$

From these we can construct

$$\begin{aligned}
E_1^{R23} &= \frac{s - s_2 - m_1^2}{2\sqrt{s_2}} & P_1^{R23} &= \frac{\lambda^{1/2}(s, s_2, m_1^2)}{2\sqrt{s_2}}, \\
E_2^{R23} &= \frac{s_2 + m_2^2 - m_3^2}{2\sqrt{s_2}} & P_2^{R23} &= \frac{\lambda^{1/2}(s_2, m_2^2, m_3^2)}{2\sqrt{s_2}}, \\
E_3^{R23} &= \frac{s_2 + m_3^2 - m_2^2}{2\sqrt{s_2}} & P_3^{R23} &= P_2^{R23},
\end{aligned}$$

where $R23$ denotes the Gottfried-Jackson frame of our choice. Finally, the scattering angle θ_{12}^{R23} between momentum 1 and 2 can be determined to be

$$\cos \theta_{12}^{R23} = \frac{(s - s_2 - m_1^2)(s_2 + m_2^2 - m_3^2) + 2s_2(m_1^2 + m_2^2 - s_1)}{\lambda^{1/2}(s, s_2, m_1^2)\lambda^{1/2}(s_2, m_2^2, m_3^2)}$$

```

(Lorentz: public)+≡
  public :: create_three_particle_decay

```


<Lorentz: sub interfaces>+≡

```

module function create_three_particle_decay (p1, p2, p3) result (p_rest)
  type(vector4_t), dimension(4) :: p_rest
  type(vector4_t), intent(in) :: p1, p2, p3
end function create_three_particle_decay

```

<Lorentz: procedures>+≡

```

module function create_three_particle_decay (p1, p2, p3) result (p_rest)
  type(vector4_t), dimension(4) :: p_rest
  type(vector4_t), intent(in) :: p1, p2, p3
  real(default) :: E1, E2, E3
  real(default) :: pr1, pr2, pr3
  real(default) :: s, s1, s2, s3
  real(default) :: m1_sq, m2_sq, m3_sq
  real(default) :: cos_theta_12
  type(vector3_t) :: v3_unit
  type(lorentz_transformation_t) :: rot
  m1_sq = p1**2
  m2_sq = p2**2
  m3_sq = p3**2
  s1 = (p1 + p2)**2
  s2 = (p2 + p3)**2
  s3 = (p3 + p1)**2
  s = s1 + s2 + s3 - m1_sq - m2_sq - m3_sq
  E1 = (s - s2 - m1_sq) / (two * sqrt (s2))
  E2 = (s2 + m2_sq - m3_sq) / (two * sqrt (s2))
  E3 = (s2 + m3_sq - m2_sq) / (two * sqrt (s2))
  pr1 = sqrt (lambda (s, s2, m1_sq)) / (two * sqrt (s2))
  pr2 = sqrt (lambda (s2, m2_sq, m3_sq)) / (two * sqrt(s2))
  pr3 = pr2
  cos_theta_12 = ((s - s2 - m1_sq) * (s2 + m2_sq - m3_sq) + two * s2 * (m1_sq + m2_sq - s1)) / &
    sqrt (lambda (s, s2, m1_sq) * lambda (s2, m2_sq, m3_sq))
  v3_unit%p = [zero, zero, one]
  p_rest(1)%p(0) = E1
  p_rest(1)%p(1:3) = v3_unit%p * pr1
  p_rest(2)%p(0) = E2
  p_rest(2)%p(1:3) = v3_unit%p * pr2
  p_rest(3)%p(0) = E3
  p_rest(3)%p(1:3) = v3_unit%p * pr3
  p_rest(4)%p(0) = (s + s2 - m1_sq) / (2 * sqrt (s2))
  p_rest(4)%p(1:3) = - p_rest(1)%p(1:3)
  rot = rotation (cos_theta_12, sqrt (one - cos_theta_12**2), 2)
  p_rest(2) = rot * p_rest(2)
  p_rest(3)%p(1:3) = - p_rest(2)%p(1:3)
end function create_three_particle_decay

```

<Lorentz: public>+≡

```

public :: evaluate_one_to_two_splitting_special

```

<Lorentz: interfaces>+≡

```

abstract interface
  subroutine evaluate_one_to_two_splitting_special (p_origin, &
    p1_in, p2_in, p1_out, p2_out, msq_in, jac)
    import
    type(vector4_t), intent(in) :: p_origin

```

```

        type(vector4_t), intent(in) :: p1_in, p2_in
        type(vector4_t), intent(inout) :: p1_out, p2_out
        real(default), intent(in), optional :: msq_in
        real(default), intent(inout), optional :: jac
    end subroutine evaluate_one_to_two_splitting_special
end interface

```

<Lorentz: public>+≡

```

    public :: generate_on_shell_decay

```

<Lorentz: sub interfaces>+≡

```

    recursive module subroutine generate_on_shell_decay (p_dec, &
        p_in, p_out, i_real, msq_in, jac, evaluate_special)
        type(vector4_t), intent(in) :: p_dec
        type(vector4_t), intent(in), dimension(:) :: p_in
        type(vector4_t), intent(inout), dimension(:) :: p_out
        integer, intent(in) :: i_real
        real(default), intent(in), optional :: msq_in
        real(default), intent(inout), optional :: jac
        procedure(evaluate_one_to_two_splitting_special), intent(in), &
            pointer, optional :: evaluate_special
    end subroutine generate_on_shell_decay

```

<Lorentz: procedures>+≡

```

    recursive module subroutine generate_on_shell_decay (p_dec, &
        p_in, p_out, i_real, msq_in, jac, evaluate_special)
        type(vector4_t), intent(in) :: p_dec
        type(vector4_t), intent(in), dimension(:) :: p_in
        type(vector4_t), intent(inout), dimension(:) :: p_out
        integer, intent(in) :: i_real
        real(default), intent(in), optional :: msq_in
        real(default), intent(inout), optional :: jac
        procedure(evaluate_one_to_two_splitting_special), intent(in), &
            pointer, optional :: evaluate_special
        type(vector4_t) :: p_dec_new
        integer :: n_recoil
        n_recoil = size (p_in) - 1
        if (n_recoil > 1) then
            if (present (evaluate_special)) then
                call evaluate_special (p_dec, p_in(1), sum (p_in (2 : n_recoil + 1)), &
                    p_out(i_real), p_dec_new)
                call generate_on_shell_decay (p_dec_new, p_in (2 : ), p_out, &
                    i_real + 1, msq_in, jac, evaluate_special)
            else
                call evaluate_one_to_two_splitting (p_dec, p_in(1), &
                    sum (p_in (2 : n_recoil + 1)), p_out(i_real), p_dec_new, msq_in, jac)
                call generate_on_shell_decay (p_dec_new, p_in (2 : ), p_out, &
                    i_real + 1, msq_in, jac)
            end if
        else
            call evaluate_one_to_two_splitting (p_dec, p_in(1), p_in(2), &
                p_out(i_real), p_out(i_real + 1), msq_in, jac)
        end if
    end subroutine generate_on_shell_decay

```

```

subroutine evaluate_one_to_two_splitting (p_origin, &
    p1_in, p2_in, p1_out, p2_out, msq_in, jac)
    type(vector4_t), intent(in) :: p_origin
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(inout) :: p1_out, p2_out
    real(default), intent(in), optional :: msq_in
    real(default), intent(inout), optional :: jac
    type(lorentz_transformation_t) :: L
    type(vector4_t) :: p1_rest, p2_rest
    real(default) :: m, msq, msq1, msq2
    real(default) :: E1, E2, p
    real(default) :: lda, rlda_soft

    call get_rest_frame (p1_in, p2_in, p1_rest, p2_rest)

    msq = p_origin**2; m = sqrt(msq)
    msq1 = p1_in**2; msq2 = p2_in**2

    lda = lambda (msq, msq1, msq2)
    if (lda < zero) then
        print *, 'Encountered lambda < 0 in 1 -> 2 splitting! '
        print *, 'lda: ', lda
        print *, 'm: ', m, 'msq: ', msq
        print *, 'm1: ', sqrt (msq1), 'msq1: ', msq1
        print *, 'm2: ', sqrt (msq2), 'msq2: ', msq2
        stop
    end if
    p = sqrt (lda) / (two * m)

    E1 = sqrt (msq1 + p**2)
    E2 = sqrt (msq2 + p**2)

    p1_out = shift_momentum (p1_rest, E1, p)
    p2_out = shift_momentum (p2_rest, E2, p)

    L = boost (p_origin, p_origin**1)
    p1_out = L * p1_out
    p2_out = L * p2_out

    if (present (jac) .and. present (msq_in)) then
        jac = jac * sqrt(lda) / msq
        rlda_soft = sqrt (lambda (msq_in, msq1, msq2))
        !!! We have to undo the Jacobian which has already been
        !!! supplied by the Born phase space.
        jac = jac * msq_in / rlda_soft
    end if

contains

subroutine get_rest_frame (p1_in, p2_in, p1_out, p2_out)
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(out) :: p1_out, p2_out
    type(lorentz_transformation_t) :: L

```

```

    L = inverse (boost (p1_in + p2_in, (p1_in + p2_in)**1))
    p1_out = L * p1_in; p2_out = L * p2_in
end subroutine get_rest_frame

function shift_momentum (p_in, E, p) result (p_out)
    type(vector4_t) :: p_out
    type(vector4_t), intent(in) :: p_in
    real(default), intent(in) :: E, p
    type(vector3_t) :: vec
    vec%p(1:3) = p_in%p(1:3) / space_part_norm (p_in)
    p_out = vector4_moving (E, p * vec)
end function shift_momentum

end subroutine evaluate_one_to_two_splitting

```

9.3.10 Boosts

We build Lorentz transformations from boosts and rotations. In both cases we can supply a three-vector which defines the axis and (hyperbolic) angle. For a boost, this is the vector $\vec{\beta} = \vec{p}/E$, such that a particle at rest with mass m is boosted to a particle with three-vector \vec{p} . Here, we have

$$\beta = \tanh \chi = p/E, \quad \gamma = \cosh \chi = E/m, \quad \beta\gamma = \sinh \chi = p/m \quad (9.1)$$

<Lorentz: public functions>+≡

```
public :: boost
```

<Lorentz: interfaces>+≡

```
interface boost
    module procedure boost_from_rest_frame
    module procedure boost_from_rest_frame_vector3
    module procedure boost_generic
    module procedure boost_canonical
end interface

```

In the first form, the argument is some four-momentum, the space part of which determines a direction, and the associated mass (which is not checked against the four-momentum). The boost vector $\gamma\vec{\beta}$ is then given by \vec{p}/m . This boosts from the rest frame of a particle to the current frame. To be explicit, if \vec{p} is the momentum of a particle and m its mass, $L(\vec{p}/m)$ is the transformation that turns $(m; \vec{0})$ into $(E; \vec{p})$. Conversely, the inverse transformation boosts a vector *into* the rest frame of a particle, in particular $(E; \vec{p})$ into $(m; \vec{0})$.

<Lorentz: sub interfaces>+≡

```

elemental module function boost_from_rest_frame (p, m) result (L)
    type(lorentz_transformation_t) :: L
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: m
end function boost_from_rest_frame
elemental module function boost_from_rest_frame_vector3 (p, m) result (L)
    type(lorentz_transformation_t) :: L
    type(vector3_t), intent(in) :: p
    real(default), intent(in) :: m
end function boost_from_rest_frame_vector3

```

```

(Lorentz: procedures)+≡
elemental module function boost_from_rest_frame (p, m) result (L)
  type(lorentz_transformation_t) :: L
  type(vector4_t), intent(in) :: p
  real(default), intent(in) :: m
  L = boost_from_rest_frame_vector3 (space_part (p), m)
end function boost_from_rest_frame
elemental module function boost_from_rest_frame_vector3 (p, m) result (L)
  type(lorentz_transformation_t) :: L
  type(vector3_t), intent(in) :: p
  real(default), intent(in) :: m
  type(vector3_t) :: beta_gamma
  real(default) :: bg2, g, c
  integer :: i, j
  if (m > eps0) then
    beta_gamma = p / m
    bg2 = beta_gamma**2
  else
    bg2 = 0
    L = identity
    return
  end if
  if (bg2 > eps0) then
    g = sqrt(1 + bg2); c = (g-1)/bg2
  else
    g = one + bg2 / two
    c = one / two
  end if
  L%L(0,0) = g
  L%L(0,1:) = beta_gamma%p
  L%L(1:,0) = L%L(0,1:)
  do i=1,3
    do j=1,3
      L%L(i,j) = delta_three(i,j) + c*beta_gamma%p(i)*beta_gamma%p(j)
    end do
  end do
end function boost_from_rest_frame_vector3

```

A canonical boost is a boost along one of the coordinate axes, which we may supply as an integer argument. Here, $\gamma\beta$ is scalar.

```

(Lorentz: sub interfaces)+≡
elemental module function boost_canonical (beta_gamma, k) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: beta_gamma
  integer, intent(in) :: k
end function boost_canonical

```

```

(Lorentz: procedures)+≡
elemental module function boost_canonical (beta_gamma, k) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: beta_gamma
  integer, intent(in) :: k
  real(default) :: g
  g = sqrt(1 + beta_gamma**2)
  L = identity

```

```

L%L(0,0) = g
L%L(0,k) = beta_gamma
L%L(k,0) = L%L(0,k)
L%L(k,k) = L%L(0,0)
end function boost_canonical

```

Instead of a canonical axis, we can supply an arbitrary axis which need not be normalized. If it is zero, return the unit matrix.

```

<Lorentz: sub interfaces>+≡
  elemental module function boost_generic (beta_gamma, axis) result (L)
    type(lorentz_transformation_t) :: L
    real(default), intent(in) :: beta_gamma
    type(vector3_t), intent(in) :: axis
  end function boost_generic

<Lorentz: procedures>+≡
  elemental module function boost_generic (beta_gamma, axis) result (L)
    type(lorentz_transformation_t) :: L
    real(default), intent(in) :: beta_gamma
    type(vector3_t), intent(in) :: axis
    if (any (abs (axis%p) > 0)) then
      L = boost_from_rest_frame_vector3 (beta_gamma * axis, axis**1)
    else
      L = identity
    end if
  end function boost_generic

```

9.3.11 Rotations

For a rotation, the vector defines the rotation axis, and its length the rotation angle. All of these rotations rotate counterclockwise in a right-handed coordinate system.

```

<Lorentz: public functions>+≡
  public :: rotation

<Lorentz: interfaces>+≡
  interface rotation
    module procedure rotation_generic
    module procedure rotation_canonical
    module procedure rotation_generic_cs
    module procedure rotation_canonical_cs
  end interface

```

If $\cos \phi$ and $\sin \phi$ is already known, we do not have to calculate them. Of course, the user has to ensure that $\cos^2 \phi + \sin^2 \phi = 1$, and that the given axis \mathbf{n} is normalized to one. In the second form, the length of `axis` is the rotation angle.

```

<Lorentz: sub interfaces>+≡
  elemental module function rotation_generic_cs (cp, sp, axis) result (R)
    type(lorentz_transformation_t) :: R
    real(default), intent(in) :: cp, sp
    type(vector3_t), intent(in) :: axis
  end function rotation_generic_cs

```

```

elemental module function rotation_generic (axis) result (R)
  type(lorentz_transformation_t) :: R
  type(vector3_t), intent(in) :: axis
end function rotation_generic
elemental module function rotation_canonical_cs (cp, sp, k) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: cp, sp
  integer, intent(in) :: k
end function rotation_canonical_cs
elemental module function rotation_canonical (phi, k) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: phi
  integer, intent(in) :: k
end function rotation_canonical

<Lorentz: procedures>+=
elemental module function rotation_generic_cs (cp, sp, axis) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: cp, sp
  type(vector3_t), intent(in) :: axis
  integer :: i,j
  R = identity
  do i=1,3
    do j=1,3
      R%L(i,j) = cp*delta_three(i,j) + (1-cp)*axis%p(i)*axis%p(j) &
        & - sp*dot_product(epsilon_three(i,j,:), axis%p)
    end do
  end do
end function rotation_generic_cs
elemental module function rotation_generic (axis) result (R)
  type(lorentz_transformation_t) :: R
  type(vector3_t), intent(in) :: axis
  real(default) :: phi
  if (any (abs(axis%p) > 0)) then
    phi = abs(axis**1)
    R = rotation_generic_cs (cos(phi), sin(phi), axis/phi)
  else
    R = identity
  end if
end function rotation_generic

```

Alternatively, give just the angle and label the coordinate axis by an integer.

```

<Lorentz: procedures>+=
elemental module function rotation_canonical_cs (cp, sp, k) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: cp, sp
  integer, intent(in) :: k
  integer :: i,j
  R = identity
  do i=1,3
    do j=1,3
      R%L(i,j) = -sp*epsilon_three(i,j,k)
    end do
    R%L(i,i) = cp
  end do

```

```

    R%L(k,k) = 1
end function rotation_canonical_cs
elemental module function rotation_canonical (phi, k) result (R)
    type(lorentz_transformation_t) :: R
    real(default), intent(in) :: phi
    integer, intent(in) :: k
    R = rotation_canonical_cs(cos(phi), sin(phi), k)
end function rotation_canonical

```

This is viewed as a method for the first argument (three-vector): Reconstruct the rotation that rotates it into the second three-vector.

```

<Lorentz: public functions>+≡
    public :: rotation_to_2nd

<Lorentz: interfaces>+≡
    interface rotation_to_2nd
        module procedure rotation_to_2nd_generic
        module procedure rotation_to_2nd_canonical
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function rotation_to_2nd_generic (p, q) result (R)
        type(lorentz_transformation_t) :: R
        type(vector3_t), intent(in) :: p, q
    end function rotation_to_2nd_generic
    elemental module function rotation_to_2nd_canonical (k, p) result (R)
        type(lorentz_transformation_t) :: R
        integer, intent(in) :: k
        type(vector3_t), intent(in) :: p
    end function rotation_to_2nd_canonical

<Lorentz: procedures>+≡
    elemental module function rotation_to_2nd_generic (p, q) result (R)
        type(lorentz_transformation_t) :: R
        type(vector3_t), intent(in) :: p, q
        type(vector3_t) :: a, b, ab
        real(default) :: ct, st
        if (any (abs (p%p) > 0) .and. any (abs (q%p) > 0)) then
            a = direction (p)
            b = direction (q)
            ab = cross_product(a,b)
            ct = a * b; st = ab**1
            if (abs(st) > eps0) then
                R = rotation_generic_cs (ct, st, ab / st)
            else if (ct < 0) then
                R = space_reflection
            else
                R = identity
            end if
        else
            R = identity
        end if
    end function rotation_to_2nd_generic

```

The same for a canonical axis: The function returns the transformation that rotates the k -axis into the direction of p .

```

<Lorentz: procedures>+≡

```



```

elemental module function rotation_to_2nd_canonical (k, p) result (R)
  type(lorentz_transformation_t) :: R
  integer, intent(in) :: k
  type(vector3_t), intent(in) :: p
  type(vector3_t) :: b, ab
  real(default) :: ct, st
  integer :: i, j
  if (any (abs (p%p) > 0)) then
    b = direction (p)
    ab%p = 0
    do i = 1, 3
      do j = 1, 3
        ab%p(j) = ab%p(j) + b%p(i) * epsilon_three(i,j,k)
      end do
    end do
    ct = b%p(k); st = ab**1
    if (abs(st) > eps0) then
      R = rotation_generic_cs (ct, st, ab / st)
    else if (ct < 0) then
      R = space_reflection
    else
      R = identity
    end if
  else
    R = identity
  end if
end function rotation_to_2nd_canonical

```

9.3.12 Composite Lorentz transformations

This function returns the transformation that, given a pair of vectors $p_{1,2}$, (a) boosts from the rest frame of the c.m. system (with invariant mass m) into the lab frame where p_i are defined, and (b) turns the given axis (or the canonical vectors $\pm e_k$) in the rest frame into the directions of $p_{1,2}$ in the lab frame. Note that the energy components are not used; for a consistent result one should have $(p_1 + p_2)^2 = m^2$.

```

<Lorentz: public functions>+≡
  public :: transformation

```

```

<Lorentz: interfaces>+≡
  interface transformation
    module procedure transformation_rec_generic
    module procedure transformation_rec_canonical
  end interface

```

```

<Lorentz: sub interfaces>+≡
  elemental module function transformation_rec_generic (axis, p1, p2, m) result (L)
    type(vector3_t), intent(in) :: axis
    type(vector4_t), intent(in) :: p1, p2
    real(default), intent(in) :: m
    type(lorentz_transformation_t) :: L
  end function transformation_rec_generic
  elemental module function transformation_rec_canonical (k, p1, p2, m) result (L)

```

```

        integer, intent(in) :: k
        type(vector4_t), intent(in) :: p1, p2
        real(default), intent(in) :: m
        type(lorentz_transformation_t) :: L
    end function transformation_rec_canonical

<Lorentz: procedures>+≡
    elemental module function transformation_rec_generic (axis, p1, p2, m) result (L)
        type(vector3_t), intent(in) :: axis
        type(vector4_t), intent(in) :: p1, p2
        real(default), intent(in) :: m
        type(lorentz_transformation_t) :: L
        L = boost (p1 + p2, m)
        L = L * rotation_to_2nd (axis, space_part (inverse (L) * p1))
    end function transformation_rec_generic
    elemental module function transformation_rec_canonical (k, p1, p2, m) result (L)
        integer, intent(in) :: k
        type(vector4_t), intent(in) :: p1, p2
        real(default), intent(in) :: m
        type(lorentz_transformation_t) :: L
        L = boost (p1 + p2, m)
        L = L * rotation_to_2nd (k, space_part (inverse (L) * p1))
    end function transformation_rec_canonical

```

9.3.13 Applying Lorentz transformations

Multiplying vectors and Lorentz transformations is straightforward.

```

<Lorentz: interfaces>+≡
    interface operator(*)
        module procedure prod_LT_vector4
        module procedure prod_LT_LT
        module procedure prod_vector4_LT
    end interface

<Lorentz: sub interfaces>+≡
    elemental module function prod_LT_vector4 (L, p) result (np)
        type(vector4_t) :: np
        type(lorentz_transformation_t), intent(in) :: L
        type(vector4_t), intent(in) :: p
    end function prod_LT_vector4
    elemental module function prod_LT_LT (L1, L2) result (NL)
        type(lorentz_transformation_t) :: NL
        type(lorentz_transformation_t), intent(in) :: L1, L2
    end function prod_LT_LT
    elemental module function prod_vector4_LT (p, L) result (np)
        type(vector4_t) :: np
        type(vector4_t), intent(in) :: p
        type(lorentz_transformation_t), intent(in) :: L
    end function prod_vector4_LT

<Lorentz: procedures>+≡
    elemental module function prod_LT_vector4 (L, p) result (np)
        type(vector4_t) :: np
        type(lorentz_transformation_t), intent(in) :: L
        type(vector4_t), intent(in) :: p

```

```

    np%p = matmul (L%L, p%p)
end function prod_LT_vector4
elemental module function prod_LT_LT (L1, L2) result (NL)
    type(lorentz_transformation_t) :: NL
    type(lorentz_transformation_t), intent(in) :: L1,L2
    NL%L = matmul (L1%L, L2%L)
end function prod_LT_LT
elemental module function prod_vector4_LT (p, L) result (np)
    type(vector4_t) :: np
    type(vector4_t), intent(in) :: p
    type(lorentz_transformation_t), intent(in) :: L
    np%p = matmul (p%p, L%L)
end function prod_vector4_LT

```

9.3.14 Special Lorentz transformations

These routines have their application in the generation and extraction of angles in the phase-space sampling routine. Since this part of the program is time-critical, we calculate the composition of transformations directly instead of multiplying rotations and boosts.

This Lorentz transformation is the composition of a rotation by ϕ around the 3 axis, a rotation by θ around the 2 axis, and a boost along the 3 axis:

$$L = B_3(\beta\gamma) R_2(\theta) R_3(\phi) \quad (9.2)$$

Instead of the angles we provide sine and cosine.

```

<Lorentz: public functions>+≡
    public :: LT_compose_r3_r2_b3

<Lorentz: sub interfaces>+≡
    elemental module function LT_compose_r3_r2_b3 &
        (cp, sp, ct, st, beta_gamma) result (L)
        type(lorentz_transformation_t) :: L
        real(default), intent(in) :: cp, sp, ct, st, beta_gamma
    end function LT_compose_r3_r2_b3

<Lorentz: procedures>+≡
    elemental module function LT_compose_r3_r2_b3 &
        (cp, sp, ct, st, beta_gamma) result (L)
        type(lorentz_transformation_t) :: L
        real(default), intent(in) :: cp, sp, ct, st, beta_gamma
        real(default) :: gamma
        if (abs(beta_gamma) < eps0) then
            L%L(0,0) = 1
            L%L(1:,0) = 0
            L%L(0,1:) = 0
            L%L(1,1:) = [ ct*cp, -ct*sp, st ]
            L%L(2,1:) = [      sp,      cp, zero ]
            L%L(3,1:) = [ -st*cp, st*sp, ct ]
        else
            gamma = sqrt(1 + beta_gamma**2)
            L%L(0,0) = gamma
            L%L(1,0) = 0

```

```

L%L(2,0) = 0
L%L(3,0) = beta_gamma
L%L(0,1:) = beta_gamma * [ -st*cp, st*sp, ct ]
L%L(1,1:) = [ ct*cp, -ct*sp, st ]
L%L(2,1:) = [ sp, cp, zero ]
L%L(3,1:) = gamma * [ -st*cp, st*sp, ct ]
end if
end function LT_compose_r3_r2_b3

```

Different ordering:

$$L = B_3(\beta\gamma) R_3(\phi) R_2(\theta) \quad (9.3)$$

```

(Lorentz: public functions)+≡
public :: LT_compose_r2_r3_b3

(Lorentz: sub interfaces)+≡
elemental module function LT_compose_r2_r3_b3 &
  (ct, st, cp, sp, beta_gamma) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: ct, st, cp, sp, beta_gamma
end function LT_compose_r2_r3_b3

(Lorentz: procedures)+≡
elemental module function LT_compose_r2_r3_b3 &
  (ct, st, cp, sp, beta_gamma) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: ct, st, cp, sp, beta_gamma
  real(default) :: gamma
  if (abs(beta_gamma) < eps0) then
    L%L(0,0) = 1
    L%L(1:,0) = 0
    L%L(0,1:) = 0
    L%L(1,1:) = [ ct*cp, -sp, st*cp ]
    L%L(2,1:) = [ ct*sp, cp, st*sp ]
    L%L(3,1:) = [ -st, zero, ct ]
  else
    gamma = sqrt(1 + beta_gamma**2)
    L%L(0,0) = gamma
    L%L(1,0) = 0
    L%L(2,0) = 0
    L%L(3,0) = beta_gamma
    L%L(0,1:) = beta_gamma * [ -st, zero, ct ]
    L%L(1,1:) = [ ct*cp, -sp, st*cp ]
    L%L(2,1:) = [ ct*sp, cp, st*sp ]
    L%L(3,1:) = gamma * [ -st, zero, ct ]
  end if
end function LT_compose_r2_r3_b3

```

This function returns the previous Lorentz transformation applied to an arbitrary four-momentum and extracts the space part of the result:

$$\vec{n} = [B_3(\beta\gamma) R_2(\theta) R_3(\phi) p]_{\text{space part}} \quad (9.4)$$

The second variant applies if there is no rotation

```

(Lorentz: public functions)+≡
public :: axis_from_p_r3_r2_b3, axis_from_p_b3

```

```

(Lorentz: sub interfaces)+≡
  elemental module function axis_from_p_r3_r2_b3 &
    (p, cp, sp, ct, st, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: cp, sp, ct, st, beta_gamma
  end function axis_from_p_r3_r2_b3
  elemental module function axis_from_p_b3 (p, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: beta_gamma
  end function axis_from_p_b3

(Lorentz: procedures)+≡
  elemental module function axis_from_p_r3_r2_b3 &
    (p, cp, sp, ct, st, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: cp, sp, ct, st, beta_gamma
    real(default) :: gamma, px, py
    px = cp * p%p(1) - sp * p%p(2)
    py = sp * p%p(1) + cp * p%p(2)
    n%p(1) = ct * px + st * p%p(3)
    n%p(2) = py
    n%p(3) = -st * px + ct * p%p(3)
    if (abs(beta_gamma) > eps0) then
      gamma = sqrt(1 + beta_gamma**2)
      n%p(3) = n%p(3) * gamma + p%p(0) * beta_gamma
    end if
  end function axis_from_p_r3_r2_b3

  elemental module function axis_from_p_b3 (p, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: beta_gamma
    real(default) :: gamma
    n%p = p%p(1:3)
    if (abs(beta_gamma) > eps0) then
      gamma = sqrt(1 + beta_gamma**2)
      n%p(3) = n%p(3) * gamma + p%p(0) * beta_gamma
    end if
  end function axis_from_p_b3

```

9.3.15 Special functions

The Källén function, mostly used for the phase space. This is equivalent to $\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$.

```

(Lorentz: public functions)+≡
  public :: lambda

(Lorentz: sub interfaces)+≡
  elemental module function lambda (m1sq, m2sq, m3sq)
    real(default) :: lambda

```

```

        real(default), intent(in) :: m1sq, m2sq, m3sq
    end function lambda

<Lorentz: procedures>+=
    elemental module function lambda (m1sq, m2sq, m3sq)
        real(default) :: lambda
        real(default), intent(in) :: m1sq, m2sq, m3sq
        lambda = (m1sq - m2sq - m3sq)**2 - 4*m2sq*m3sq
    end function lambda

```

Return a pair of head-to-head colliding momenta, given the collider energy, particle masses, and optionally the momentum of the c.m. system.

```

<Lorentz: public functions>+=
    public :: colliding_momenta

<Lorentz: sub interfaces>+=
    module function colliding_momenta (sqrts, m, p_cm) result (p)
        type(vector4_t), dimension(2) :: p
        real(default), intent(in) :: sqrts
        real(default), dimension(2), intent(in), optional :: m
        real(default), intent(in), optional :: p_cm
    end function colliding_momenta

<Lorentz: procedures>+=
    module function colliding_momenta (sqrts, m, p_cm) result (p)
        type(vector4_t), dimension(2) :: p
        real(default), intent(in) :: sqrts
        real(default), dimension(2), intent(in), optional :: m
        real(default), intent(in), optional :: p_cm
        real(default), dimension(2) :: dmsq
        real(default) :: ch, sh
        real(default), dimension(2) :: E0, p0
        integer, dimension(2), parameter :: sgn = [1, -1]
        if (abs(sqrts) < eps0) then
            call msg_fatal (" Colliding beams: sqrts is zero (please set sqrts)")
            p = vector4_null; return
        else if (sqrts <= 0) then
            call msg_fatal (" Colliding beams: sqrts is negative")
            p = vector4_null; return
        end if
        if (present (m)) then
            dmsq = sgn * (m(1)**2-m(2)**2)
            E0 = (sqrts + dmsq/sqrts) / 2
            if (any (E0 < m)) then
                call msg_fatal &
                    (" Colliding beams: beam energy is less than particle mass")
                p = vector4_null; return
            end if
            p0 = sgn * sqrt (E0**2 - m**2)
        else
            E0 = sqrts / 2
            p0 = sgn * E0
        end if
        if (present (p_cm)) then
            sh = p_cm / sqrts

```

```

        ch = sqrt (1 + sh**2)
        p = vector4_moving (E0 * ch + p0 * sh, E0 * sh + p0 * ch, 3)
    else
        p = vector4_moving (E0, p0, 3)
    end if
end function colliding_momenta

```

This subroutine is for the purpose of numerical checks and comparisons. The idea is to set a number to zero if it is numerically equivalent with zero. The equivalence is established by comparing with a `tolerance` argument. We implement this for vectors and transformations.

```

<Lorentz: public functions>+≡
    public :: pacify

<Lorentz: interfaces>+≡
    interface pacify
        module procedure pacify_vector3
        module procedure pacify_vector4
        module procedure pacify_LT
    end interface pacify

<Lorentz: sub interfaces>+≡
    elemental module subroutine pacify_vector3 (p, tolerance)
        type(vector3_t), intent(inout) :: p
        real(default), intent(in) :: tolerance
    end subroutine pacify_vector3
    elemental module subroutine pacify_vector4 (p, tolerance)
        type(vector4_t), intent(inout) :: p
        real(default), intent(in) :: tolerance
    end subroutine pacify_vector4
    elemental module subroutine pacify_LT (LT, tolerance)
        type(lorentz_transformation_t), intent(inout) :: LT
        real(default), intent(in) :: tolerance
    end subroutine pacify_LT

<Lorentz: procedures>+≡
    elemental module subroutine pacify_vector3 (p, tolerance)
        type(vector3_t), intent(inout) :: p
        real(default), intent(in) :: tolerance
        where (abs (p%p) < tolerance)  p%p = zero
    end subroutine pacify_vector3

    elemental module subroutine pacify_vector4 (p, tolerance)
        type(vector4_t), intent(inout) :: p
        real(default), intent(in) :: tolerance
        where (abs (p%p) < tolerance)  p%p = zero
    end subroutine pacify_vector4

    elemental module subroutine pacify_LT (LT, tolerance)
        type(lorentz_transformation_t), intent(inout) :: LT
        real(default), intent(in) :: tolerance
        where (abs (LT%L) < tolerance)  LT%L = zero
    end subroutine pacify_LT

```

```

<Lorentz: public>+≡
    public :: vector_set_reshuffle

<Lorentz: sub interfaces>+≡
    module subroutine vector_set_reshuffle (p1, list, p2)
        type(vector4_t), intent(in), dimension(:), allocatable :: p1
        integer, intent(in), dimension(:), allocatable :: list
        type(vector4_t), intent(out), dimension(:), allocatable :: p2
    end subroutine vector_set_reshuffle

<Lorentz: procedures>+≡
    module subroutine vector_set_reshuffle (p1, list, p2)
        type(vector4_t), intent(in), dimension(:), allocatable :: p1
        integer, intent(in), dimension(:), allocatable :: list
        type(vector4_t), intent(out), dimension(:), allocatable :: p2
        integer :: n, n_p
        n_p = size (p1)
        if (size (list) /= n_p) return
        allocate (p2 (n_p))
        do n = 1, n_p
            p2(n) = p1(list(n))
        end do
    end subroutine vector_set_reshuffle

<Lorentz: public>+≡
    public :: vector_set_is_cms

<Lorentz: sub interfaces>+≡
    module function vector_set_is_cms (p, n_in) result (is_cms)
        logical :: is_cms
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in) :: n_in
    end function vector_set_is_cms

<Lorentz: procedures>+≡
    module function vector_set_is_cms (p, n_in) result (is_cms)
        logical :: is_cms
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in) :: n_in
        integer :: i
        type(vector4_t) :: p_sum
        p_sum%p = 0._default
        do i = 1, n_in
            p_sum = p_sum + p(i)
        end do
        is_cms = all (abs (p_sum%p(1:3)) < tiny_07)
    end function vector_set_is_cms

<Lorentz: public>+≡
    public :: vector4_write_set

<Lorentz: sub interfaces>+≡
    module subroutine vector4_write_set (p, unit, show_mass, testflag, &
        check_conservation, ultra, n_in)
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: unit

```



```

        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
    end subroutine vector4_write_set

<Lorentz: procedures>+≡
    module subroutine vector4_write_set (p, unit, show_mass, testflag, &
        check_conservation, ultra, n_in)
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
        logical :: extreme
        integer :: i, j
        real(default), dimension(0:3) :: p_tot
        character(len=7) :: fmt
        integer :: u
        logical :: yorn, is_test
        integer :: n
        extreme = .false.; if (present (ultra)) extreme = ultra
        is_test = .false.; if (present (testflag)) is_test = testflag
        u = given_output_unit (unit); if (u < 0) return
        n = 2; if (present (n_in)) n = n_in
        p_tot = 0
        yorn = .false.; if (present (check_conservation)) yorn = check_conservation
        do i = 1, size (p)
            if (yorn .and. i > n) then
                forall (j=0:3) p_tot(j) = p_tot(j) - p(i)%p(j)
            else
                forall (j=0:3) p_tot(j) = p_tot(j) + p(i)%p(j)
            end if
            call vector4_write (p(i), u, show_mass=show_mass, &
                testflag=testflag, ultra=ultra)
        end do
        if (extreme) then
            call pac_fmt (fmt, FMT_19, FMT_11, testflag)
        else
            call pac_fmt (fmt, FMT_19, FMT_15, testflag)
        end if
        if (is_test) call pacify (p_tot, 1.E-9_default)
        if (.not. is_test) then
            write (u, "(A5)") 'Total: '
            write (u, "(1x,A,1x," // fmt // ")") "E = ", p_tot(0)
            write (u, "(1x,A,3(1x," // fmt // ")") "P = ", p_tot(1:)
        end if
    end subroutine vector4_write_set

<Lorentz: public>+≡
    public :: vector4_check_momentum_conservation

<Lorentz: sub interfaces>+≡
    module subroutine vector4_check_momentum_conservation (p, n_in, unit, &

```

```

        abs_smallness, rel_smallness, verbose)
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: n_in
    integer, intent(in), optional :: unit
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: verbose
end subroutine vector4_check_momentum_conservation

(Lorentz: procedures)+≡
module subroutine vector4_check_momentum_conservation (p, n_in, unit, &
    abs_smallness, rel_smallness, verbose)
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: n_in
    integer, intent(in), optional :: unit
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: verbose
    integer :: u, i
    type(vector4_t) :: psum_in, psum_out
    logical, dimension(0:3) :: p_diff
    logical :: verb
    u = given_output_unit (unit); if (u < 0) return
    verb = .false.; if (present (verbose)) verb = verbose
    psum_in = vector4_null
    do i = 1, n_in
        psum_in = psum_in + p(i)
    end do
    psum_out = vector4_null
    do i = n_in + 1, size (p)
        psum_out = psum_out + p(i)
    end do
    p_diff = vanishes (psum_in%p - psum_out%p, &
        abs_smallness = abs_smallness, rel_smallness = rel_smallness)
    if (.not. all (p_diff)) then
        call msg_warning ("Momentum conservation: FAIL", unit = u)
        if (verb) then
            write (u, "(A)") "Incoming:"
            call vector4_write (psum_in, u)
            write (u, "(A)") "Outgoing:"
            call vector4_write (psum_out, u)
        end if
    else
        if (verb) then
            write (u, "(A)") "Momentum conservation: CHECK"
        end if
    end if
end subroutine vector4_check_momentum_conservation

```

This computes the quantities

$$\langle ij \rangle = \sqrt{|S_{ij}|} e^{i\phi_{ij}}, [ij] = \sqrt{|S_{ij}|} e^{B\tilde{\phi}_{ij}},$$

with $S_{ij} = (p_i + p_j)^2$. The phase space factor ϕ_{ij} is determined by

$$\cos \phi_{ij} = \frac{p_i^1 p_j^+ - p_j^1 p_i^+}{\sqrt{p_i^+ p_j^+ S_{ij}}}, \sin \phi_{ij} = \frac{p_i^2 p_j^+ - p_j^2 p_i^+}{\sqrt{p_i^+ p_j^+ S_{ij}}}.$$

After $\langle ij \rangle$ has been computed according to these formulae, $[ij]$ can be obtained by using the relation $S_{ij} = \langle ij \rangle [ji]$ and taking into account that $[ij] = -[ji]$. Thus, a minus-sign has to be applied.

```

<Lorentz: public>+≡
    public :: spinor_product

<Lorentz: sub interfaces>+≡
    module subroutine spinor_product (p1, p2, prod1, prod2)
        type(vector4_t), intent(in) :: p1, p2
        complex(default), intent(out) :: prod1, prod2
    end subroutine spinor_product

<Lorentz: procedures>+≡
    module subroutine spinor_product (p1, p2, prod1, prod2)
        type(vector4_t), intent(in) :: p1, p2
        complex(default), intent(out) :: prod1, prod2
        real(default) :: sij
        complex(default) :: phase
        real(default) :: pp_1, pp_2
        pp_1 = p1%p(0) + p1%p(3)
        pp_2 = p2%p(0) + p2%p(3)
        sij = (p1+p2)**2
        phase = cmplx ((p1%p(1)*pp_2 - p2%p(1)*pp_1)/sqrt (sij*pp_1*pp_2), &
            (p1%p(2)*pp_2 - p2%p(2)*pp_1)/sqrt (sij*pp_1*pp_2), &
            default)

        !!! <ij>
        prod1 = sqrt (sij) * phase
        !!! [ij]
        if (abs(prod1) > 0) then
            prod2 = - sij / prod1
        else
            prod2 = 0
        end if
    end subroutine spinor_product

```

9.3.16 Unit tests

Test module, followed by the corresponding implementation module.

```

<lorentz_ut.f90>≡
    <File header>

    module lorentz_ut
        use unit_tests
        use lorentz_util

    <Standard module head>

```

```

    <Lorentz: public test>

contains

    <Lorentz: test driver>

    end module lorentz_ut
<lorentz_uti.f90>≡
    <File header>

    module lorentz_uti

    <Use kinds>
        use constants, only: zero, Pi
        use format_defs, only: FMT_12
        use lorentz

    <Standard module head>

    <Lorentz: test declarations>

contains

    <Lorentz: tests>

    end module lorentz_uti
API: driver for the unit tests below.
<Lorentz: public test>≡
    public :: lorentz_test
<Lorentz: test driver>≡
    subroutine lorentz_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Lorentz: execute tests>
    end subroutine lorentz_test

```

Algebra with 3-vectors

```

<Lorentz: execute tests>≡
    call test (lorentz_1, "lorentz_1", &
        "Test 3-vector functionality", &
        u, results)
<Lorentz: test declarations>≡
    public :: lorentz_1
<Lorentz: tests>≡
    subroutine lorentz_1 (u)
        integer, intent(in) :: u
        type(vector3_t) :: v3_1, v3_2

        write (u, "(A)")  "* Test output: lorentz_1"
    end subroutine lorentz_1

```

```

write (u, "(A)")  "* Purpose: testing vector3_t"
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Null 3-vector"
write (u, "(A)")
call vector3_write (vector3_null, u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Canonical 3-vector"
write (u, "(A)")
call vector3_write (vector3_canonical (1), u, testflag = .true.)
call vector3_write (vector3_canonical (2), u, testflag = .true.)
call vector3_write (vector3_canonical (3), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Canonical moving 3-vector"
write (u, "(A)")
call vector3_write (vector3_moving (42._default, 1), u, testflag = .true.)
call vector3_write (vector3_moving (42._default, 2), u, testflag = .true.)
call vector3_write (vector3_moving (42._default, 3), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Generic moving 3-vector"
write (u, "(A)")
call vector3_write (vector3_moving ([3._default, 4._default, 5._default]), &
    u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Simple algebra with 3-vectors"
write (u, "(A)")
v3_1 = vector3_moving ([3._default, 4._default, 5._default])
v3_2 = vector3_moving ([-2._default, 5._default, -1._default])
write (u, "(1x,A)")  "v3_1:"
call vector3_write (v3_1, u, testflag=.true.)
write (u, "(1x,A)")  "v3_2:"
call vector3_write (v3_2, u, testflag=.true.)
write (u, "(1x,A)")  "-v3_1:"
call vector3_write (-v3_1, u, testflag=.true.)
write (u, "(1x,A)")  "v3_1 / |v3_1|:"
call vector3_write (direction (v3_1), u, testflag=.true.)
write (u, "(1x,A," // FMT_12 // ")")  "v3_1(x): ", vector3_get_component (v3_1, 1)
write (u, "(1x,A," // FMT_12 // ")")  "v3_1(y): ", vector3_get_component (v3_1, 2)
write (u, "(1x,A," // FMT_12 // ")")  "v3_1(z): ", vector3_get_component (v3_1, 3)
write (u, "(1x,A)")  "v3_1 + v3_2:"
call vector3_write (v3_1 + v3_2, u, testflag=.true.)
write (u, "(1x,A)")  "v3_1 - v3_2:"
call vector3_write (v3_1 - v3_2, u, testflag=.true.)
write (u, "(1x,A,L1)")  "v3_1 == v3_2: ", v3_1 == v3_2
write (u, "(1x,A,L1)")  "v3_1 /= v3_2: ", v3_1 /= v3_2
write (u, "(1x,A)")  "2 * v3_1:"
call vector3_write (2._default * v3_1, u, testflag=.true.)
write (u, "(1x,A)")  "v3_2 / 4:"
call vector3_write (v3_2 / 4, u, testflag=.true.)

```

```

write (u, "(1x,A," // FMT_12 // ")") "v3_1, azimuth (radians):", azimuthal_angle (v3_1)
write (u, "(1x,A," // FMT_12 // ")") "v3_1, azimuth (degrees):", &
    azimuthal_angle_deg (v3_1)
write (u, "(1x,A," // FMT_12 // ")") "v3_1, polar (radians) :", polar_angle (v3_1)
write (u, "(1x,A," // FMT_12 // ")") "v3_1, polar (degrees) :", &
    polar_angle_deg (v3_1)
write (u, "(1x,A," // FMT_12 // ")") "v3_1, cosine polar      :", &
    polar_angle_ct (v3_1)
write (u, "(1x,A," // FMT_12 // ")") "v3_1, energy w. mass=1 :", &
    energy (v3_1, 1._default)
write (u, "(1x,A)") "3-vector orthogonal to v3_1:"
call vector3_write (create_orthogonal (v3_1), u, testflag=.true.)
write (u, "(1x,A)") "unit 3-vector from v3_1:"

write (u, "(A)")
write (u, "(A)")  "* Dot and cross product"
write (u, "(A)")
write (u, "(1x,A," // FMT_12 // ")") "v3_1 * v3_2: ", v3_1 * v3_2
write (u, "(1x,A," // FMT_12 // ")") "v3_1**3      : ", v3_1**3
write (u, "(1x,A)") "v3_1 x v3_2:"
call vector3_write (cross_product (v3_1, v3_2), u, testflag=.true.)
write (u, "(1x,A," // FMT_12 // ")") "enclosed angle (radians):", &
    enclosed_angle (v3_1, v3_2)
write (u, "(1x,A," // FMT_12 // ")") "enclosed angle (degrees):", &
    enclosed_angle_deg (v3_1, v3_2)
write (u, "(1x,A," // FMT_12 // ")") "cosine (enclosed angle) :", &
    enclosed_angle_ct (v3_1, v3_2)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lorentz_1"

end subroutine lorentz_1

```

Algebra with 4-vectors

```

<Lorentz: execute tests>+≡
    call test(lorentz_2, "lorentz_2", &
        "Test 4-vector functionality", u, results)

<Lorentz: test declarations>+≡
    public :: lorentz_2

<Lorentz: tests>+≡
    subroutine lorentz_2 (u)
        integer, intent(in) :: u
        type(vector3_t) :: v3_1, v3_2
        type(vector4_t) :: v4_1, v4_2, v4_1_inv

        write (u, "(A)")  "* Test output: lorentz_2"
        write (u, "(A)")  "* Purpose: testing vector4_t"
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)")  "* Null 4-vector"
    end subroutine lorentz_2

```

```

write (u, "(A)")
call vector4_write (vector4_null, u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Canonical 4-vector"
write (u, "(A)")
call vector4_write (vector4_canonical (0), u, testflag = .true.)
call vector4_write (vector4_canonical (1), u, testflag = .true.)
call vector4_write (vector4_canonical (2), u, testflag = .true.)
call vector4_write (vector4_canonical (3), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* 4-vector at rest with mass m = 17"
write (u, "(A)")
call vector4_write (vector4_at_rest (17._default), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Canonical moving 4-vector"
write (u, "(A)")
call vector4_write (vector4_moving (17._default, 42._default, 1), u, testflag = .true.)
call vector4_write (vector4_moving (17._default, 42._default, 2), u, testflag = .true.)
call vector4_write (vector4_moving (17._default, 42._default, 3), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Generic moving 4-vector"
write (u, "(A)")
v3_1 = [3._default, 4._default, 5._default]
call vector4_write (vector4_moving (17._default, v3_1), u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Simple algebra with 4-vectors"
write (u, "(A)")
v3_2 = [-2._default, 5._default, -1._default]
v4_1 = vector4_moving (8._default, v3_1)
v4_2 = vector4_moving (zero, v3_2)
write (u, "(1x,A)")  "v4_1:"
call vector4_write (v4_1, u, testflag=.true.)
write (u, "(1x,A)")  "v4_2:"
call vector4_write (v4_2, u, testflag=.true.)
write (u, "(1x,A)")  "-v4_1:"
call vector4_write (-v4_1, u, testflag=.true.)
v4_1_inv = v4_1
call vector4_invert_direction (v4_1_inv)
write (u, "(1x,A)")  "v4_1, inverted direction:"
call vector4_write (v4_1_inv, u, testflag=.true.)
write (u, "(1x,A)")  "(v4_1)_spatial / |(v4_1)_spatial|:"
call vector3_write (direction (v4_1), u, testflag=.true.)
write (u, "(1x,A," // FMT_12 // ")")  "v4_1(E): ", energy (v4_1)
write (u, "(1x,A," // FMT_12 // ")")  "v4_1(x): ", vector4_get_component (v4_1, 1)
write (u, "(1x,A," // FMT_12 // ")")  "v4_1(y): ", vector4_get_component (v4_1, 2)
write (u, "(1x,A," // FMT_12 // ")")  "v4_1(z): ", vector4_get_component (v4_1, 3)
write (u, "(1x,A)")  "space_part (v4_1):"
call vector3_write (space_part (v4_1), u, testflag=.true.)
write (u, "(1x,A," // FMT_12 // ")")  "norm space_part (v4_1): ", &

```

```

        space_part_norm (v4_1)
write (u, "(1x,A)") "unit vector from v4_1:"
call vector3_write (create_unit_vector (v4_1), u, testflag = .true.)
write (u, "(1x,A)") "v4_1 + v4_2:"
call vector4_write (v4_1 + v4_2, u, testflag=.true.)
write (u, "(1x,A)") "v4_1 - v4_2:"
call vector4_write (v4_1 - v4_2, u, testflag=.true.)
write (u, "(1x,A,L1)") "v4_1 == v4_2: ", v4_1 == v4_2
write (u, "(1x,A,L1)") "v4_1 /= v4_2: ", v4_1 /= v4_2
write (u, "(1x,A)") "2 * v4_1:"
call vector4_write (2._default * v4_1, u, testflag=.true.)
write (u, "(1x,A)") "v4_2 / 4:"
call vector4_write (v4_2 / 4, u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Angles and kinematic properties of 4-vectors"
write (u, "(A)")

write (u, "(1x,A," // FMT_12 // ")") "v4_1, azimuth (radians):", azimuthal_angle (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, azimuth (degrees):", &
    azimuthal_angle_deg (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, polar (radians) :", polar_angle (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, polar (degrees) :", &
    polar_angle_deg (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, cosine polar      :", &
    polar_angle_ct (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, invariant mass  :", &
    invariant_mass (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, invariant mass sq:", &
    invariant_mass_squared (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_2, invariant mass  :", &
    invariant_mass (v4_2)
write (u, "(1x,A," // FMT_12 // ")") "v4_2, invariant mass sq:", &
    invariant_mass_squared (v4_2)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, transverse mass :", &
    transverse_mass (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, rapidity        :", &
    rapidity (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, pseudorapidity  :", &
    pseudorapidity (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, pT              :", &
    transverse_part (v4_1)
write (u, "(1x,A," // FMT_12 // ")") "v4_1, pL              :", &
    longitudinal_part (v4_1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lorentz_2"

end subroutine lorentz_2

```

Bilinear functions of 4-vectors

(Lorentz: execute tests)+≡


```

        call test(lorentz_3, "lorentz_3", &
            "Test 4-vector bilinear functions", u, results)
<Lorentz: test declarations>+≡
    public :: lorentz_3
<Lorentz: tests>+≡
    subroutine lorentz_3 (u)
        integer, intent(in) :: u
        type(vector3_t) :: v3_1, v3_2
        type(vector4_t) :: v4_1, v4_2

        write (u, "(A)")    "* Test output: lorentz_3"
        write (u, "(A)")    "* Purpose: testing bilinear functions of 4-vectors"
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)")    "* Products and distances of 4-vectors"
        write (u, "(A)")
        v3_1 = [3._default, 4._default, 5._default]
        v3_2 = [-2._default, 5._default, -1._default]
        v4_1 = vector4_moving (8._default, v3_1)
        v4_2 = vector4_moving (6._default, v3_2)
        write (u, "(1x,A," // FMT_12 // ")") "v4_1 * v4_2: ", v4_1 * v4_2
        write (u, "(1x,A," // FMT_12 // ")") "rapidity distance      :", &
            rapidity_distance (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "pseudorapidity distance :", &
            pseudorapidity_distance (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "eta phi distance      :", &
            eta_phi_distance (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "enclosed angle (radians):", &
            enclosed_angle (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "enclosed angle (degrees):", &
            enclosed_angle_deg (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "cosine (enclosed angle) :", &
            enclosed_angle_ct (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "rest frame theta (rad)  :", &
            enclosed_angle_rest_frame (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "rest frame theta (deg)  :", &
            enclosed_angle_deg_rest_frame (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "rest frame cosine(theta):", &
            enclosed_angle_ct_rest_frame (v4_1, v4_2)
        write (u, "(1x,A," // FMT_12 // ")") "v4_1_T w.r.t. v4_2      :", &
            transverse_part (v4_1, v4_2)

        write (u, "(A)")
        write (u, "(A)")    "* Test output end: lorentz_3"

    end subroutine lorentz_3

```

Tests for Lorentz transformations

```

<Lorentz: execute tests>+≡
    call test(lorentz_4, "lorentz_4", &

```

```

        "Test Lorentz transformations", u, results)
<Lorentz: test declarations>+=
    public :: lorentz_4
<Lorentz: tests>+=
    subroutine lorentz_4 (u)
        integer, intent(in) :: u
        type(vector3_t) :: v3_1, v3_2
        type(vector4_t) :: v4
        type(lorentz_transformation_t) :: LT
        real(default) :: tol

        write (u, "(A)")  "* Test output: lorentz_4"
        write (u, "(A)")  "* Purpose: testing Lorentz transformations"
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)")  "* Basic Lorentz transformations"
        write (u, "(A)")
        write (u, "(1x,A)")  "LT = 1:"
        call lorentz_transformation_write (identity, u, testflag=.true.)
        write (u, "(A)")
        write (u, "(1x,A)")  "LT = space reflection:"
        call lorentz_transformation_write (space_reflection, u, testflag=.true.)

        write (u, "(A)")
        write (u, "(A)")  "* Lorentz transformations: rotations"
        write (u, "(A)")
        v3_1 = [1._default, 2._default, 3._default]
        v3_2 = [-2._default, 1._default, -5._default]
        tol = 1.e-12_default
        write (u, "(1x,A)")  "Rotation of Pi/4 around 1-axis, def. by cos and sin:"
        LT = rotation (0.707107_default, 0.707107_default, 1)
        call pacify (LT, tol)
        call lorentz_transformation_write (LT, u, testflag=.true.)
        write (u, "(1x,A)")  "Rotation of Pi/4 around 2-axis, def. by cos and sin:"
        LT = rotation (0.707107_default, 0.707107_default, 2)
        call pacify (LT, tol)
        call lorentz_transformation_write (LT, u, testflag=.true.)
        write (u, "(1x,A)")  "Rotation of Pi/4 around 3-axis, def. by cos and sin:"
        LT = rotation (0.707107_default, 0.707107_default, 3)
        call pacify (LT, tol)
        call lorentz_transformation_write (LT, u, testflag=.true.)
        write (u, "(1x,A)")  "Rotation of Pi/4 around 1-axis, def. by angle:"
        LT = rotation (Pi/4._default, 1)
        call pacify (LT, tol)
        call lorentz_transformation_write (LT, u, testflag=.true.)
        write (u, "(1x,A)")  "Rotation of Pi/4 around 2-axis, def. by angle:"
        LT = rotation (Pi/4._default, 2)
        call pacify (LT, tol)
        call lorentz_transformation_write (LT, u, testflag=.true.)
        write (u, "(1x,A)")  "Rotation of Pi/4 around 3-axis, def. by angle:"
        LT = rotation (Pi/4._default, 3)
        call pacify (LT, tol)

```

```

call lorentz_transformation_write (LT, u, testflag=.true.)
write (u, "(1x,A)") "Rotation of Pi/4 around axis = (1,2,3):"
call lorentz_transformation_write (rotation (0.707107_default, 0.707107_default, &
    normalize (v3_1)), u, testflag=.true.)
write (u, "(1x,A)") "Rotation in plane to axis = (1,2,3), angle given by length of axis:"
call lorentz_transformation_write (rotation (v3_1), u, testflag=.true.)
write (u, "(1x,A)") "Rotation from v3_1=(1,2,3) to v3_2=(-2,1,-5):"
call lorentz_transformation_write (rotation_to_2nd (v3_1,v3_2), u, testflag=.true.)
write (u, "(1x,A)") "Rotation from 1-axis to v3_2=(-2,1,-5):"
call lorentz_transformation_write (rotation_to_2nd (1,v3_2), u, testflag=.true.)
write (u, "(1x,A)") "Rotation from 2-axis to v3_2=(-2,1,-5):"
call lorentz_transformation_write (rotation_to_2nd (2,v3_2), u, testflag=.true.)
write (u, "(1x,A)") "Rotation from 3-axis to v3_2=(-2,1,-5):"
call lorentz_transformation_write (rotation_to_2nd (3,v3_2), u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Lorentz transformations: boosts"
write (u, "(A)")
write (u, "(1x,A)") "Boost from rest frame to 3-vector, mass m=10:"
call lorentz_transformation_write (boost (v3_1, 10._default), u, testflag=.true.)
write (u, "(1x,A)") "Boost from rest frame to 4-vector, mass m=10:"
v4 = vector4_moving (42._default, v3_1)
call lorentz_transformation_write (boost (v4, 10._default), u, testflag=.true.)
write (u, "(1x,A)") "Boost along 1-axis, beta*gamma = 12"
call lorentz_transformation_write (boost (12._default, 1), u, testflag=.true.)
write (u, "(1x,A)") "Boost along 2-axis, beta*gamma = 12"
call lorentz_transformation_write (boost (12._default, 2), u, testflag=.true.)
write (u, "(1x,A)") "Boost along 3-axis, beta*gamma = 12"
call lorentz_transformation_write (boost (12._default, 3), u, testflag=.true.)
write (u, "(1x,A)") "Boost along axis=(1,2,3), beta*gamma = 12"
call lorentz_transformation_write (boost (12._default, v3_1), u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lorentz_4"

end subroutine lorentz_4

```

Tests for additional kinematic functions and sets of 4-vectors

```

<Lorentz: execute tests>+≡
    call test(lorentz_5, "lorentz_5", &
        "Test additional kinematics", u, results)

<Lorentz: test declarations>+≡
    public :: lorentz_5

<Lorentz: tests>+≡
    subroutine lorentz_5 (u)
        integer, intent(in) :: u
        type(vector4_t), dimension(2) :: p
        real(default), dimension(2) :: m
        real(default) :: sqrts
        type(vector4_t), dimension(8) :: tt_mom
        type(vector4_t), dimension(:), allocatable :: tin, tout

```

```

integer, dimension(:), allocatable :: shuffle

write (u, "(A)")  "* Test output: lorentz_5"
write (u, "(A)")  "* Purpose: testing additional kinematics and sets of 4-vectors"
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Colliding momenta, 13 TeV, massless"
write (u, "(A)")
sqrts = 13000._default
p = colliding_momenta (sqrts)
call vector4_write (p(1), u, testflag=.true.)
call vector4_write (p(2), u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Colliding momenta, 10 GeV, massive muons"
write (u, "(A)")
sqrts = 10._default
m = [0.1057_default, 0.1057_default]
p = colliding_momenta (sqrts, m)
call vector4_write (p(1), u, testflag=.true.)
call vector4_write (p(2), u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Kinematical function lambda"
write (u, "(A)")

write (u, "(1x,A," // FMT_12 // ")")  "s = 172.3**2, m1 = 4.2, m2 = 80.418:", &
    lambda (172.3_default**2, 4.2_default**2, 80.418_default**2)

write (u, "(A)")
write (u, "(A)")  "* Test vector_set"
write (u, "(A)")

tt_mom(1) = [2.5000000000000000e+02_default, zero, zero, 2.4999999999999999e+02_default]
tt_mom(2) = [2.5000000000000000e+02_default, zero, zero, -2.4999999999999999e+02_default]
tt_mom(3) = [1.1557492413664579e+02_default, 3.9011599241011098e+01_default, &
    -6.4278142734963140e+01_default, 8.7671766153043137e+01_default]
tt_mom(4) = [1.4617918132729235e+02_default, -1.0947970597860679e+02_default, &
    1.5484441802571380e+01_default, -9.5525593923398418e+01_default]
tt_mom(5) = [5.2637589215119526e+01_default, -4.7413198564695762e+01_default, &
    1.0087885417286579e+01_default, 2.0516525153079229e+01_default]
tt_mom(6) = [5.476029292264796e+01_default, 1.5197406985690520e+01_default, &
    5.1527071739328015e+01_default, -1.0615525413924287e+01_default]
tt_mom(7) = [3.2415057664609684e+01_default, 7.5539389341684711e+00_default, &
    -1.5935831743946720e+01_default, -2.7139737100881156e+01_default]
tt_mom(8) = [9.8432954734067863E+01_default, 9.5129959382432399e+01_default, &
    3.1145755197238966e+00_default, 2.5092565132081496e+01_default]
write (u, "(1x,A)")  "Write routine for vector sets, maximal compression:"
call vector4_write_set (tt_mom, u, show_mass=.true., testflag=.true., &
    check_conservation=.true., ultra=.true.)
write (u, "(1x,A,L1)")  "Vector set is CMS frame: ", vector_set_is_cms (tt_mom, 2)
write (u, "(1x,A)")  "Reshuffle vector set, final state inverted:"
allocate (tin (8))

```

```

tin = tt_mom
allocate (shuffle (8), source = [1,2,8,7,6,5,4,3])
call vector_set_reshuffle (tin, shuffle, tout)
call vector4_write_set (tout, u, show_mass=.true., testflag=.true., &
    check_conservation=.true., ultra=.true.)
write (u, "(1x,A)") "Vector set, check momentum conservation:"
call vector4_check_momentum_conservation (tt_mom, 2, u, &
    abs_smallness = 1.e-12_default, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lorentz_5"

end subroutine lorentz_5

```

This is the module file for the M_{T2} calculator based on algorithm by Han and Cheng by Tom James (DESY) August 2013.

```

<kinematics_vars.f90>≡
  <File header>
  module kinematics_vars

    use kinds
    use lorentz
    use format_defs, only: FMT_19
    <Standard module head>

    <Kinematics vars: public>

    <Kinematics vars: parameters>

    <Kinematics vars: types>

    interface
    <Kinematics vars: sub interfaces>
    end interface

  end module kinematics_vars

<kinematics_vars_sub.f90>≡
  <File header>

  submodule (kinematics_vars) kinematics_vars_s

    implicit none

    contains

    <Kinematics vars: procedures>

  end submodule kinematics_vars_s

<Kinematics vars: parameters>≡
  ! Calculation parameters
  real(kind=default), parameter, public :: relative_precision = 0.00001, &

```

```

        absolute_precision=0.0, min_mass=0.1, step=0.1
real(kind=default), public :: prec
! scale and precision
! Define precision=relative_precision*scale where scale=max{Ea, Eb}
! Don't set relative precision <0.00001
! If mass a < min_mass and mass b < min_mass use massless code
! Gives massless particles a very small mass
! scanning step size

<Kinematics vars: procedures>≡
subroutine mt2calcmassive (mt2, mn, mt2_b)
    !!! Code implementation of the massive algorithm for calculating mt2
    type(mt2_t), intent(inout) :: mt2
    real(default), intent(in) :: mn
    real(default) :: Ea, Eb
    real(default) :: masq, mbsq, mnsq
    real(default), intent(out) :: mt2_b
    real(default):: deltasq0, x00, y00, dis, p2x0, p2y0, deltasqmid, &
        deltasqhigh, deltasqhigh1, deltasqhigh2, deltasqhigh21, &
        deltasqhigh22, deltasqlow
    ! Calculation coefficients for the quadratic and quartic curves
    real(default) :: a1, b1, c1, d1, e1, f1, &
        a2, b2, c2, d2, e2, f2
    real(default) :: d20, d11, d21, e11, e20, e21
    real(default) :: f10, f12, f20, f21, f22
    integer:: nsolshigh, nsolslow, findhigh, nsolsmid

    print *, 'using calculation for massive visible particles.'

    !!! Allowed transverse 2-momenta for each invisible particle incloses
    !!! an elliptical region on the px, py plane.
    !!! To satisfy kinematic constraints, the two elliptical regions must
    !!! overlap. MT2 is therefore given by the minimum initial decay mass
    !!! in each branch (mt2_b) which gives overlapping ellipses
    !!! We therefore increase the initial decay mass in each branch (mt2_b)
    !!! until the ellipses overlap - the "balanced configuration".
    !!! In the balanced configuration, the two quadratic equations
    !!! can be combined into one quartic equation.
    !!! We search for the point at which the two ellipses are tangent,
    !!! using the Sturm sequence method and bisection

    !!! When the smaller ellipse is already inside the larger ellipse, this
    !!! is called an "unbalanced configuration", and mt2 is easy to calculate.

    deltasq0 = mt2%ma*(mt2%ma + 2*mt2%mn)

    !!! Find co-efficients at deltasq = deltasq0 for the quadratic
    !!! equations that describe each ellipse

    masq = mt2%ma**2
    mbsq = mt2%mb**2
    mnsq = mt2%mn**2
    Ea = sqrt(mt2%Ea2)

```

```

Eb = sqrt(mt2%Eb2)
a1 = 1 - mt2%pax**2 / mt2% Ea2
b1 = - mt2%pax * mt2%pay / mt2% Ea2
c1 = 1 - mt2%pay**2 / mt2% Ea2
d1 = - (mt2%pax*(deltasq0 - masq))/(2.d0*mt2% Ea2)
e1 = - (mt2%pay * (deltasq0 - masq))/(2.d0*mt2% Ea2)
a2 = 1 - (mt2%pbx * mt2%pbx)/(mt2% Eb2)
b2 = - (mt2%pbx * mt2%pby) / (mt2% Eb2)
c2 = 1 - (mt2%pby * mt2%pby / (mt2% Eb2))
d2 = -mt2%pmx + ((mt2%pbx * (deltasq0 - mbsq))/(2.d0*mt2% Eb2)) + &
      (mt2%pbx*((mt2%pbx*mt2%pmx) + (mt2%pby * mt2%pmy)))/(mt2% Eb2)
e2 = -mt2%pmy + (mt2%pby * (deltasq0 - mbsq))/(2.d0*mt2% Eb2) + &
      (mt2%pby*((mt2%pbx*mt2%pmx) + (mt2%pby * mt2%pmy)))/(mt2% Eb2)
f2 = mt2%pmx*mt2%pmx + mt2%pmy * mt2%pmy - ((deltasq0-mbsq)/(2*Eb) + &
      (mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)/Eb)*((deltasq0-mbsq)/(2*Eb)+ &
      ((mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)/Eb))+ mnsq

!!! find the centre of the small ellipse
x00 = (c1*d1 - b1*e1)/(b1*b1 - a1*c1)
y00 = (a1*e1 - b1*d1)/(b1*b1 - a1*c1)

!!! check if the large ellipse contains the small one -
!!! "unbalanced configuration"
dis = a2*x00*x00 + 2.d0*b2*x00*y00 + c2*y00*y00 + &
      2.d0*d2*x00 + 2.d0*e2*y00 + f2
mt2_b = 0
if (dis<0.01) then
    mt2_b = sqrt(mnsq + deltasq0)
    return
end if

!!! find linear and constant terms in quadratic equations for
!!! delta = (deltasq-msq)/(2Esq) as quadratic terms do not change as we adjust delta

d11 = -mt2%pax
e11 = -mt2%pay
f10 = mnsq
f12 = -mt2% Ea2
d21 = (mt2% Ea2 * mt2%pbx)/(mt2% Eb2)
d20 = ((masq - mbsq)*mt2%pbx)/(2.d0*mt2% Eb2) - mt2%pmx + &
      (mt2%pbx*(mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)) / mt2% Eb2
e21 = (mt2% Ea2 * mt2%pby) / mt2% Eb2
e20 = ((masq - mbsq) * mt2%pby)/(2.d0*mt2% Eb2) - mt2%pmy + &
      (mt2%pby * (mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)) / mt2% Eb2
f22 = -mt2% Ea2*mt2% Ea2 / mt2% Eb2
f21 = (-2.d0*mt2% Ea2*((masq - mbsq)/(2.d0*Eb) + &
      (mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)/Eb))/Eb
f20 = mnsq + mt2%pmx*mt2%pmx + mt2%pmy**2 &
      - ((masq - mbsq)/(2.d0*Eb) + (mt2%pbx*mt2%pmx + &
      mt2%pby * mt2%pmy)/Eb)*((masq - mbsq)/(2.d0*Eb) &
      + (mt2%pbx*mt2%pmx + mt2%pby * mt2%pmy)/Eb)

!!! Estimate upper bound of mT2 if large ellipse contains centre of small ellipse

```

```

p2x0 = mt2%pmx - x00
p2y0 = mt2%pmy - y00
deltasqhigh1 = 2*Eb*sqrt(p2x0*p2x0+p2y0*p2y0+mnsq) - &
    2 * mt2%pbx * p2x0 - 2 * mt2%pby * p2y0 + mbsq

!!! Estimate upper bound of mT2 if both ellipses enclose the origin

deltasqhigh21 = 2.d0*Eb*sqrt(mt2%pmx*mt2%pmx + mt2%pmy * mt2%pmy+mnsq) &
    - 2.d0 * mt2%pbx * mt2%pmx - 2.d0 * mt2%pby * mt2%pmy + mbsq
deltasqhigh22 = 2.d0*Ea*mn + masq

if ( deltasqhigh21 < deltasqhigh22 ) then
    deltasqhigh2 = deltasqhigh22
else
    deltasqhigh2 = deltasqhigh21
end if

! Upper bound on mt2 is the smallest of these two estimates
if (deltasqhigh1 < deltasqhigh2) then
    deltasqhigh = deltasqhigh1
else
    deltasqhigh = deltasqhigh2
end if
deltasqlow=deltasq0
if (nsolutionsmassive(deltasqlow) > 0) then
    mt2_b = sqrt(mnsq + deltasqlow)
    return
end if
nsolslow = nsolutionsmassive (deltasqlow)
nsolshigh = nsolutionsmassive (deltasqhigh)
if (nsolshigh==nsolslow) then
    if (nsolshigh==4) then

        findhigh = findhighfunc(deltasqhigh)

        print *, 'findhigh=', findhigh

        if(findhigh==0) then
            mt2_b = sqrt(deltasqlow + mnsq)
            return
        end if
    end if
end if

do while ((sqrt(deltasqhigh + mnsq) - sqrt(deltasqlow + mnsq)) > prec)
    deltasqmid = (deltasqhigh + deltasqlow)/(2.)
    nsolsmid = nsolutionsmassive(deltasqmid)

    if (nsolsmid==4) then
        deltasqhigh=deltasqmid
        findhigh = findhighfunc(deltasqhigh)
        cycle
    end if
end if

```



```

        if (nsolsmid == nsolslow) then
            deltasqlow=deltasqmid
        else
            deltasqhigh = deltasqmid
        end if

    end do

    mt2_b = sqrt(mnsq + deltasqhigh)
contains
    <Kinematics vars: findhighfunc>
    <Kinematics vars: nsolutionsmassive>
end subroutine mt2calcmassive

subroutine mt2massless (mt2, mn, mt2_b)
    !!! Code implementation of the massless algorithm for calculating mt2
    type(mt2_t), intent(inout) :: mt2
    real(default), intent(in) :: mn
    real(default) :: Ea, Eb
    real(default), intent(out) :: mt2_b
    real(default) :: mnsq, Easq, Ebsq
    real(default) :: pmissxsq, pmissysq
    real(kind=default):: theta, s, c, pxtemp, pytemp, &
        deltasq0, deltasqlow, deltasqhigh, deltasqlow1, deltasqlow2, &
        deltasqhigh1, deltasqhigh2, &
        minmass, maxmass, mass, &
        deltamid, midmass, nsolsmid
    real(default) :: a1, b1, c1, d1, e1, f1, &
        a2, b2, c2, d2, e2, f2
    real(default) :: d20, d21, e20, e21
    real(default) :: f20, f21, f22
    integer :: nsolshigh, nsolslow, findhigh
    print *, 'using calculation for massless visible particles.'
    ! first rotate system so that pay=0
    theta = atan(mt2%pay / mt2%pax)
    s = sin(theta)
    c = cos(theta)
    mnsq = mn*mn
    pmissxsq = mt2%pmx**2
    pmissysq = mt2%pmy**2

    Easq = mt2%pax**2 + mt2%pay**2
    Ebsq = (mt2%pbx * mt2%pbx) + (mt2%pby * mt2%pby)
    Ea = sqrt(Easq)
    Eb = sqrt(Ebsq)

    pxtemp = mt2%pax * c + mt2%pay * s
    mt2%pax = pxtemp
    mt2%pay = 0
    pxtemp = mt2%pbx * c + mt2%pby * s
    pytemp = -s * mt2%pbx + c * mt2%pby
    mt2%pbx= pxtemp
    mt2%pby= pytemp
    pxtemp = mt2%pmx*c + mt2%pmy*s

```

```

pytemp = -s*mt2%pmx + c * mt2%pmy
mt2%pmx = pxtemp
mt2%pmy = pytemp

a2 = 1 - mt2%pbx * mt2%pbx / Ebsq
b2 = - mt2%pbx * mt2%pby / Ebsq
c2 = 1 - mt2%pby * mt2%pby / Ebsq

d21 = (Easq * mt2%pbx)/Ebsq
d20 = - mt2%pmx + (mt2%pbx * (mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy)) / Ebsq
e21 = (Easq * mt2%pby) / Ebsq
e20 = - mt2%pmy + (mt2%pby * (mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy)) / Ebsq
f22 = -(Easq*Easq/Ebsq)
f21 = -2*Easq*(mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy) / Ebsq
f20 = mnsq + pmissxsq + pmissysq - (mt2%pbx * mt2%pmx + &
    mt2%pby * mt2%pmy)*(mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy) / Ebsq

deltasq0 = 0
deltasqlow = deltasq0 + prec
nsolslow = nsolutionsmassless (deltasqlow)

mt2_b = 0
if (nsolslow > 1) then
    mt2_b = sqrt(deltasq0 + mnsq)
    return
end if

deltasqhigh1 = (2*Eb*sqrt((mt2%pmx**2 * mt2%pmy**2) + mnsq)) &
    - (2 * mt2%pbx *mt2%pmx) - (2 * mt2%pby * mt2%pmy)

deltasqhigh2 = 2*Ea*mn

if (deltasqhigh1 < deltasqhigh2) then
    deltasqhigh = deltasqhigh2
else
    deltasqhigh = deltasqhigh1
end if

nsolshigh = nsolutionsmassless(deltasqhigh)

if (nsolshigh==nsolslow) then
    findhigh=0
    minmass = mn
    maxmass = sqrt(mnsq + deltasqhigh)
    mass = minmass + step
    do while (mass < maxmass)
        deltasqhigh = (mass*mass) - mnsq
        nsolshigh = nsolutionsmassless(deltasqhigh)
        if (nsolshigh>0) then
            findhigh=1
            deltasqlow = (mass-step)*(mass-step) - mnsq
        end if
        if(findhigh==0) then
            mt2_b = sqrt (deltasqlow + mnsq)

```

```

        return
    end if
end do
end if

if (nsolslow == nsolshigh) then
    mt2_b = sqrt(mnsq + deltasqlow)
    return
end if

minmass = sqrt (deltasqlow + mnsq)
maxmass = sqrt (deltasqhigh + mnsq)
do while ((maxmass - minmass) > prec)
    midmass = (minmass+maxmass)/2
    nsolsmid = nsolutionsmassless(deltamid)
    if (nsolsmid == nsolslow) then
        minmass = midmass
    else
        maxmass = midmass
    end if
end do
mt2_b = minmass
contains
<Kinematics vars: nsolutionsmassless>
end subroutine mt2massless

<Kinematics vars: public>≡
public :: mt2_t

<Kinematics vars: types>≡
type :: mt2_t
private
real(default) :: mt2 = 0._default
real(default) :: mn = 0._default
real(default) :: ma = 0._default
real(default) :: mb = 0._default
real(default) :: Ea2 = 0._default
real(default) :: Eb2 = 0._default
real(default) :: pax = 0._default
real(default) :: pay = 0._default
real(default) :: pbx = 0._default
real(default) :: pby = 0._default
real(default) :: pmx = 0._default
real(default) :: pmy = 0._default
real(default) :: scale = 0._default
end type mt2_t

<Kinematics vars: public>+≡
public :: mt2_init

<Kinematics vars: sub interfaces>≡
module subroutine mt2_init (mt2, mn, ma, mb, Easq, Ebsq, &
    pax, pay, pbx, pby, pmissx, pmissy, scale)
    type(mt2_t), intent(out) :: mt2

```

```

        real(default), intent(in) :: mn, ma, mb
        real(default), intent(in) :: Easq, Ebsq
        real(default), intent(in) :: pax, pay, pbx, pby
        real(default), intent(in) :: pmissx, pmissy, scale
    end subroutine mt2_init

<Kinematics vars: procedures>+≡
    module subroutine mt2_init (mt2, mn, ma, mb, Easq, Ebsq, &
        pax, pay, pbx, pby, pmissx, pmissy, scale)
        type(mt2_t), intent(out) :: mt2
        real(default), intent(in) :: mn, ma, mb
        real(default), intent(in) :: Easq, Ebsq
        real(default), intent(in) :: pax, pay, pbx, pby
        real(default), intent(in) :: pmissx, pmissy, scale
        mt2%mn = mn
        mt2%ma = ma
        mt2%mb = mb
        mt2%Ea2 = Easq
        mt2%Eb2 = Ebsq
        mt2%pax = pax
        mt2%pay = pay
        mt2%pbx = pbx
        mt2%pby = pby
        mt2%pmx = pmissx
        mt2%pmy = pmissy
        mt2%scale = scale
    end subroutine mt2_init

<Kinematics vars: nsolutionsmassless>≡
    integer function nsolutionsmassless (dsq)
        !!! calculates the number of solutions of quartic function in massless case
        real*16 :: delta, a, b, &
            z0, z1, z2, z3, z4, &
            z0sq, z1sq, z2sq, z3sq, z4sq, &
            y0, y1, y2, y3, &
            x0, x1, x2, &
            w0, w1, &
            v0, &
            t1, t2, t3, t4, t5
        real(kind=default)::deltasqlow, tempmass, maxmass, dsq
        integer:: findhigh, nsolshigh, nsol

        delta = dsq / (2 * mt2%Ea2)

        !!! d1    = d11*delta seems not to be used
        !!! e1    = e11*delta seems not to be used
        !!! f1    = f12*delta*delta+f10    seems not to be used
        d2    = d21*delta+d20
        e2    = e21*delta+e20
        f2    = f22*delta*delta+f21*delta+f20

        if (mt2%pax > 0) then
            a = Ea/Dsq
        else

```

```

        a = -Ea/Dsq
    end if

    if (mt2%pax > 0) then
        b = ((mnsq*Ea)/Dsq)-(Dsq/(4*Ea))
    else
        b = Dsq/(4*Ea) - ((mnsq*Ea)/Dsq)
    end if

    z4 = a*a*a2
    z3 = 2*a*b2/Ea
    z2 = (2*a*a2*b+c2+2*a*d2) / mt2%Ea2
    z1 = (2*b*b2+2*e2) / (mt2%Ea2*Ea)
    z0 = (a2*b*b+2*b*d2+f2)/(mt2%Ea2*mt2%Ea2)

    z0sq = z0*z0
    z1sq = z1*z1
    z2sq = z2*z2
    z3sq = z3*z3
    z4sq = z4*z4

    y3 = 4*z4
    y2 = 3*z3
    y1 = 2*z2
    y0 = z1

    x2 = -(z2/2 - 3*z3sq/(16*z4))
    x1 = -(3*z1/4 - z2*z3/(8*z4))
    x0 = -z0 + z1*z3/(16*z4)

    w1 = -y1 - (y3*x0*x1/x2 - y3*x0 - y2*x1)/x2
    w0 = -y0 - y3 *x0 *x1/(x2*x2)+ y2*x0/x2

    v0 = -x0 - x2*w0*w0/(w1*w1) + x1*w0/w1

    t1 = z4
    t2 = z4
    t3 = x2
    t4 = w1
    t5 = v0

    !!! number of solutions depends on the number of sign changes

    nsol = signchangenegative(t1, t2, t3, t4, t5) - signchangepositive(t1, t2, t3, t4, t5)
    if (nsol<0) then
        nsol=0
    end if
    nsolutionsmassless=nsol
end function nsolutionsmassless

```

(Kinematics vars: nsolutionsmassive)≡

```

integer function nsolutionsmassive ( dsq )
    !!! calculates the number of solutions of quartic function in massive case

```

```

integer:: nsol, nsolsmid
real(kind=default):: deltasqmid, dsq, delta
real*16 :: z0, z1, z2, z3, z4, &
        z0sq, z1sq, z2sq, z3sq, z4sq, &
        y0, y1, y2, y3, &
        x0, x1, x2, &
        w0, w1, &
        v0, &
        t1, t2, t3, t4, t5

delta = (dsq-masq) / (2*mt2%Ea2)

!!! calculate quadratic co-efficients

d1 = d11*delta
e1 = e11*delta
f1 = (f12*delta*delta)+f10
d2 = (d21*delta)+d20
e2 = (e21*delta)+e20
f2 = (f22*delta*delta)+f21*delta+f20

!!! Calculate quartic co-efficients, divided by Ea^n to keep dimensionless

z0 = (-4.d0*a2*d1*d2*f1 + 4.d0*a1*d2*d2*f1 + a2*a2*f1*f1 &
      + 4.d0*a2*d1*d1*f2 - 4.d0*a1*d1*d2*f2 &
      - 2.d0*a1*a2*f1*f2+a1*a1*f2*f2) / (mt2%Ea2 * mt2%Ea2)

z1 = (-8.d0*a2*d1*d2*e1 + 8.d0*a1*d2*d2*e1 + 8.d0*a2*d1*d1*e2 &
      - 8.d0*a1*d1*d2*e2 - 4.d0*a2*b2*d1*f1 - 4.d0*a2*b1*d2*f1 + &
      8.d0*a1*b2*d2*f1 &
      + 4.d0*a2*a2*e1*f1 - 4.d0*a1*a2*e2*f1 + 8.d0*a2*b1*d1*f2 - &
      4.d0*a1*b2*d1*f2 - 4.d0*a1*b1*d2*f2 - 4.d0*a1*a2*e1*f2 + &
      4.d0*a1*a1*e2*f2) / (mt2%Ea2*Ea)

z2 = (4.d0*a2*c2*d1*d1 - 4.d0*a2*c1*d1*d2 - 4.d0*a1*c2*d1*d2 + &
      4.d0*a1*c1*d2*d2 - 8.d0*a2*b2*d1*e1 - 8.d0*a2*b1*d2*e1 + &
      16.d0*a1*b2*d2*e1 &
      + 4.d0*a2*a2*e1*e1 + 16.d0*a2*b1*d1*e2 - 8.d0*a1*b2*d1*e2 - &
      8.d0*a1*b1*d2*e2 - 8.d0*a1*a2*e1*e2 + 4.d0*a1*a1*e2*e2 - &
      4.d0*a2*b1*b2*f1 &
      + 4.d0*a1*b2*b2*f1 + 2.d0*a2*a2*c1*f1 - 2.d0*a1*a2*c2*f1 + &
      4.d0*a2*b1*b1*f2 - 4.d0*a1*b1*b2*f2 - 2.d0*a1*a2*c1*f2 + &
      2.d0*a1*a1*c2*f2) / mt2%Ea2

z3 = (-4*a2*b2*c1*d1 + 8*a2*b1*c2*d1 - 4*a1*b2*c2*d1 - 4*a2*b1*c1*d2 + &
      8*a1*b2*c1*d2 - 4*a1*b1*c2*d2 - 8*a2*b1*b2*e1 + 8*a1*b2*b2*e1 + &
      4*a2*a2*c1*e1 - 4*a1*a2*c2*e1 + 8*a2*b1*b1*e2 - 8*a1*b1*b2*e2 - &
      4*a1*a2*c1*e2 + 4*a1*a1*c2*e2)/Ea

z4 = - (4.d0*a2*b1*b2*c1) + (4.d0*a1*b2*b2*c1) + (a2*a2*c1*c1) + &
      (4.d0*a2*b1*b1*c2) - (4.d0*a1*b1*b2*c2) - (2.d0*a1*a2*c1*c2) + &
      (a1*a1*c2*c2)

```

```

if (z4==0) then
    z4=1e-33
end if

z0sq = z0*z0
z1sq = z1*z1
z2sq = z2*z2
z3sq = z3*z3
z4sq = z4*z4

y0 = z1
y1 = 2.d0*z2
y2 = 3.d0*z3
y3 = 4.d0*z4

x0 = - z0 + (z1*z3)/(16.d0*z4)
x1 = - (3.d0*z1/4.d0) + (z2*z3)/(8.d0*z4)
x2 = - (z2/2.d0) + (3.d0*z3sq)/(16.d0*z4)

w0 = - y0 - ((y3*x0 *x1)/(x2*x2))+ ((y2*x0)/x2)
w1 = - y1 - ((y3*x1*x1/x2) - y3*x0 - y2*x1)/x2

v0 = - x0 - (x2*w0*w0)/(w1*w1) + (x1*w0/w1)

!!! Sturm sequence coefficients of leading order

t1 = z4
t2 = z4
t3 = x2
t4 = w1
t5 = v0

nsol = signchangenegative (t1, t2, t3, t4, t5) - &
        signchangepositive (t1, t2, t3, t4, t5)

!!! correction for roundoff error if it gives a negative result
if (nsol<0) then
    nsol = 0
endif

nsolutionsmassive = nsol
end function nsolutionsmassive

<Kinematics vars: findhighfunc>≡
function findhighfunc (dsq)
    real(kind=default):: x00, y00, deltasqlow, dis, &
        deltasqmid, deltasqhigh, dsq
    integer:: findhighfunc, nsolsmid !!! , nsolutionsmassive

    x00 = (c1*d1 - b1*e1)/(b1*b1 - a1*c1)
    y00 = (a1*e1 - b1*d1)/(b1*b1 - a1*c1)
    deltasqlow = (mn + mt2%ma)*(mn + mt2%ma) - mnsq

    do while ((deltasqhigh - deltasqlow) > 0.001)

```

```

deltasqmid = (deltasqhigh + deltasqlow)/2
nsolsmid = nsolutionsmassive(deltasqmid)
if (nsolsmid==2) then
    deltasqhigh = deltasqmid
end if
if ( nsolsmid==4) then
    deltasqhigh = deltasqmid
end if
if (nsolsmid==0) then
    d1 = -mt2%pax * (deltasqmid - masq) / (2 * mt2%Ea2)
    e1 = -mt2%pay * (deltasqmid - masq) / (2 * mt2%Ea2)
    d2 = -mt2%pmx + mt2%pbx * (deltasqmid - mbsq)/(2*mt2%Eb2) + &
        mt2%pbx * (mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy) / mt2%Eb2
    e2 = - mt2%pmy + mt2%pby * (deltasqmid - mbsq)/(2*mt2%Eb2) &
        + mt2%pby * (mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy) / mt2%Eb2
    f2 = mt2%pmx*mt2%pmx + mt2%pmy**2 - ((deltasqmid - mbsq)/(2*Eb) &
        + (mt2%pbx * mt2%pmx + mt2%pby * mt2%pmy)/Eb) * &
        ((deltasqmid - mbsq)/(2*Eb) + (mt2%pbx * mt2%pmx + &
        mt2%pby * mt2%pmy)/Eb) + mnsq

    dis = a2*x00*x00 + 2*b2*x00*y00 + c2*y00*y00 + 2*d2*x00 + &
        2*e2*y00 + f2

    !!! Check if large ellipse contains small one

    if (dis < 0 ) then
        deltasqhigh = deltasqmid
    else
        deltasqlow = deltasqmid
    end if
end if
end do
findhighfunc=0

end function findhighfunc

```

Print input values.

```

<Kinematics vars: public>+≡
    public :: write_mt2_input

<Kinematics vars: sub interfaces>+≡
    module subroutine write_mt2_input (mt2, u)
        type(mt2_t), intent(in) :: mt2
        integer, intent(in) :: u
    end subroutine write_mt2_input

<Kinematics vars: procedures>+≡
    module subroutine write_mt2_input (mt2, u)
        type(mt2_t), intent(in) :: mt2
        integer, intent(in) :: u

        !!! prints the input variables as a check
        write (u, "(1x,A," // FMT_19 // ")") 'pax =', mt2%pax * mt2%scale
        write (u, "(1x,A," // FMT_19 // ")") 'pay =', mt2%pay * mt2%scale

```



```

write (u, "(1x,A," // FMT_19 // ")") 'ma =', mt2%ma * mt2%scale

write (u, "(1x,A," // FMT_19 // ")") 'pbx =', mt2%pbx * mt2%scale
write (u, "(1x,A," // FMT_19 // ")") 'pby =', mt2%pby * mt2%scale
write (u, "(1x,A," // FMT_19 // ")") 'mb =', mt2%mb * mt2%scale

write (u, "(1x,A," // FMT_19 // ")") 'pmissx =', mt2%pmx * mt2%scale
write (u, "(1x,A," // FMT_19 // ")") 'pmissy =', mt2%pmy * mt2%scale
write (u, "(1x,A," // FMT_19 // ")") 'mn =', mt2%mn * mt2%scale

!!! write (u, *) 'precision = ', prec

end subroutine write_mt2_input

<Kinematics vars: public>+≡
public :: write_mt2_output
<Kinematics vars: sub interfaces>+≡
module subroutine write_mt2_output (mt2, scale, u)
  real(default), intent(in) :: mt2, scale
  integer, intent(in) :: u
end subroutine write_mt2_output
<Kinematics vars: procedures>+≡
module subroutine write_mt2_output (mt2, scale, u)
  real(default), intent(in) :: mt2, scale
  integer, intent(in) :: u
  !!! Prints the output (MT2)
  ! mt2=mt2_b*scale
  write (u, "(1x,A,ES10.4)") 'mt2=', mt2 * scale

end subroutine write_mt2_output

<Kinematics vars: procedures>+≡
function signchangepositive (t1, t2, t3, t4, t5) result (n_sign)
  !!! calculates the number of sign changes in the sturm sequence
  real*16 :: t1, t2, t3, t4, t5
  integer :: n_sign
  integer :: n
  n = 0
  if (t1*t2 < 0) then
    n = n+1
  end if
  if (t2*t3 < 0) then
    n = n+1
  end if
  if (t3*t4 < 0) then
    n = n+1
  end if
  if (t4*t5 < 0) then
    n = n+1
  end if
  n_sign = n
end function signchangepositive

```

```

<Kinematics vars: procedures>+≡
integer function signchangenegative (t1, t2, t3, t4, t5)
  !!! calculates the number of times there is no sign
  !!! change in the sturm sequence
  real*16 :: t1, t2, t3, t4, t5
  integer:: n

  n=0
  if((t1*t2)>0) then
    n=n+1
  endif
  if((t2*t3)>0) then
    n=n+1
  endif
  if((t3*t4)>0) then
    n=n+1
  endif
  if((t4*t5)>0) then
    n=n+1
  endif
  signchangenegative = n
end function signchangenegative

```

It looks like as if this function is not used in the code.

```

<XXX Kinematics vars: procedures>≡
integer function scanhigh (mn, deltasqhigh)
  real(default), intent(in) :: mn
  real(kind=default):: tempmass, maxmass, deltasqlow, deltasqhigh, mass
  integer:: nsolshigh, findhigh
  mnsq = mn*mn
  tempmass = mn+ma
  findhigh = 0
  maxmass = sqrt(mnsq + deltasqhigh)
  mass = tempmass + step
  do while ( mass < maxmass)
    deltasqhigh = mass*mass - mnsq
    nsolshigh = nsolutionsmassive(deltasqhigh)
    if (nsolshigh > 0) then
      deltasqlow = (mass - step)*(mass - step) - mnsq
      findhigh = 1
      exit
    end if
  end do
  scanhigh=findhigh

end function scanhigh

```

All this subroutine does is to decide whether to use the algorithm for massless visible particles, or the algorithm for massive visible particles.

```

<Kinematics vars: public>+≡
public :: mt2calc

<Kinematics vars: sub interfaces>+≡

```

```

module subroutine mt2calc (mt2, mn, mt2_b)
  type(mt2_t), intent(inout) :: mt2
  real(default), intent(in) :: mn
  real(default), intent(out) :: mt2_b
end subroutine mt2calc

```

(Kinematics vars: procedures)+≡

```

module subroutine mt2calc (mt2, mn, mt2_b)
  type(mt2_t), intent(inout) :: mt2
  real(default), intent(in) :: mn
  real(default), intent(out) :: mt2_b
  if (mt2%ma**2 < min_mass .and. mt2%mb**2 < min_mass) then
    call mt2massless (mt2, mn, mt2_b)
  else
    call mt2calcmassive (mt2, mn, mt2_b)
  end if
end subroutine mt2calc

```

This subroutine sets up the event for calculation by defining the input variables, and setting them to a scale that aids calculation. The output variables have been rescaled back.

(Kinematics vars: public)+≡

```

public :: mt2_setevent

```

(Kinematics vars: sub interfaces)+≡

```

module subroutine mt2_setevent (mn, ma, mb, Easq, Ebsq, pax, pay, pbx, pby, &
  pmissx, pmissy, scale, u)
  real(default), intent(out) :: ma, mb ! mass of particles a and b
  real(default), intent(out) :: mn ! invisible particle mass scaled and unscaled
  real(default), intent(out) :: scale
  real(default), intent(out) :: pax, pay, pbx, pby
  real(default), intent(out) :: pmissx, pmissy
  real(default), intent(out) :: Easq, Ebsq
  integer, intent(in) :: u
end subroutine mt2_setevent

```

(Kinematics vars: procedures)+≡

```

module subroutine mt2_setevent (mn, ma, mb, Easq, Ebsq, pax, pay, pbx, pby, &
  pmissx, pmissy, scale, u)
  real(default), intent(out) :: ma, mb ! mass of particles a and b
  real(default), intent(out) :: mn ! invisible particle mass scaled and unscaled
  real(default), intent(out) :: scale
  real(default), intent(out) :: pax, pay, pbx, pby
  ! x and y momentum of particles a and b
  ! missing x and y momentum
  real(default) :: Ea, Eb
  type(vector4_t) :: pmissa, pa, pb
  real(default), intent(out) :: pmissx, pmissy
  real(default) :: masq, mbsq, mnsq, Emiss, pmissz
  real(default), intent(out) :: Easq, Ebsq
  real(default) :: pmissxsq, pmissysq, mn_unscaled
  real*16 :: temp, scalesq, rt, relative_precision100
  integer, intent(in) :: u

```

!!! Here the 8 input variables are entered. This should be read in from

```

!!! the syndarin file - let me know if I can help accomplish this
!!! The units of input are equal to the units of the output e.g GeV
!!! in -> GeV out, MeV in -> MeV out

ma=100 ! total mass of visible particles in branch a
mb=100 ! total mass of visible particles in branch b
!!! 0810.5178
!!! mT2 is invariant under longitudinal boosts => set paz = pbz = 0
! mass = transverse mass here!???

pax=40 ! total x momentum of visible partivles in branch a
pay=40 ! total y momentum of visible partivles in branch a
pbx=40 ! total x momentum of visible partivles in branch b
pby=40 ! total y momentum of visible partivles in branch b

Emiss=0
pmissz=0
pmissx=20 ! Total missing x momentum
pmissy=20 ! Total missing y momentum

pmissa = [ Emiss, pmissx, pmissy, pmissz]

mn=0 ! starting guess for mass of invisible particle
mn_unscaled = 0 ! starting guess for mass of invisible particle

scale=1.d0 ! scale is originally defined as 1
masq = ma*ma
Easq = masq + pax*pax + pay*pay
Ea = sqrt(Easq)
pa = [Ea, pax, pay, 0._default]

mbsq = mb*mb
Ebsq = mbsq + pbx*pbx + pby*pby
Eb = sqrt(Ebsq)

pmissxsq = pmissx*pmissx
pmissysq = pmissy*pmissy

! set ma>=mb to keep consistency

if (masq < mbsq) then

    temp = pax
    pax = pbx
    pbx = temp

    temp = pay
    pay = pby
    pby = temp

    temp = Ea
    Ea = Eb
    Eb = temp

```

```

temp = Easq
Easq = Ebsq
Ebsq = temp

temp = masq
masq = mbsq
mbsq = temp

temp = ma
ma = mb
mb = temp
end if

! normalise to the scale

if (Ea > Eb) then
    scale = Ea/100.d0
else
    scale = Eb/100.d0
end if

rt=(sqrt(pmissxsq+pmissysq))/100.d0
if (rt > scale) then
    scale = (sqrt(pmissxsq+pmissysq))/100.d0
end if

!!! write (u, *) 'scale=', scale
scalesq = scale*scale

ma = ma/scale
mb = mb/scale
masq = masq/scalesq
mbsq = mbsq/scalesq
pax = pax/scale
pay = pay/scale
pbx = pbx/scale
pby = pby/scale
Ea = Ea/scale
Eb = Eb/scale

Easq = Easq/scalesq
Ebsq = Ebsq/scalesq
pmissx = pmissx/scale
pmissy = pmissy/scale
pmissxsq = pmissxsq/scalesq
pmissysq = pmissysq/scalesq
mn = mn_unscaled/scale
mnsq = mn*mn

! calculating precision

relative_precision100 = relative_precision*100.d0
if (absolute_precision > relative_precision100) then
    prec = absolute_precision

```

```

        else
            prec = 100*relative_precision
        end if
    end subroutine mt2_setevent

```

9.3.17 Unit tests

Test module, followed by the corresponding implementation module.

<kinematics_vars_ut.f90>≡
<File header>

```

module kinematics_vars_ut
    use unit_tests
    use kinematics_vars_util

```

<Standard module head>

<Kinematics vars: public test>

contains

<Kinematics vars: test driver>

```

end module kinematics_vars_ut

```

<kinematics_vars_util.f90>≡
<File header>

```

module kinematics_vars_util

```

<Use kinds>

```

    use kinematics_vars

```

<Standard module head>

<Kinematics vars: test declarations>

contains

<Kinematics vars: tests>

```

end module kinematics_vars_util

```

This has been written by Tom James as a DESY summer student in August 2013. It is a self-contained Fortran90 program for calculating M_{T2} using the Cheng-Han algorithm.

<Kinematics vars: public test>≡

```

    public :: kinematics_vars_test

```

<Kinematics vars: test driver>≡

```

    subroutine kinematics_vars_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results

```

```

    <Kinematics vars: execute tests>
end subroutine kinematics_vars_test

```

Testing kinematic variables like MT2

```

<Kinematics vars: execute tests>≡
    call test (kinematics_vars_1, "kinematics_vars_1", "massive mT2 calculation", &
        u, results)

<Kinematics vars: test declarations>≡
    public :: kinematics_vars_1

<Kinematics vars: tests>≡
    subroutine kinematics_vars_1 (u)
        integer, intent(in) :: u
        real(default) :: Easq, Ebsq
        real(default) :: ma, mb, mn
        real(default) :: pmissx, pmissy
        real(default) :: mt2_b, scale
        real(default) :: pax, pay, pbx, pby
        type(mt2_t) :: mt2

        write (u, "(A)")  "* Test output: mt2_1"
        write (u, "(A)")  "* Purpose: calculate MT2 for the massive case"
        write (u, "(A)")

        call mt2_setevent (mn, ma, mb, Easq, Ebsq, pax, pay, pbx, pby, &
            pmissx, pmissy, scale, u)
        call mt2_init (mt2, mn, ma, mb, Easq, Ebsq, pax, pay, pbx, pby, &
            pmissx, pmissy, scale)
        call write_mt2_input (mt2, u)
        call mt2calc (mt2, mn, mt2_b)
        call write_mt2_output (mt2_b, scale, u)
    end subroutine kinematics_vars_1

```

9.4 Collections of Lorentz Vectors

The `phs_point` type is a container for an array of Lorentz vectors. This allows us to transfer Lorentz-vector arrays more freely, and to collect vector arrays of non-uniform size.

```

<phs_points.f90>≡
    <File header>

    module phs_points

    <Use kinds>
        use lorentz, only: vector4_t
        use lorentz, only: lorentz_transformation_t
        use lorentz, only: sum

    <Standard module head>

```

```

    <PHS points: public>

    <PHS points: types>

    <PHS points: interfaces>

    interface
    <PHS points: sub interfaces>
    end interface

end module phs_points
<phs_points_sub.f90>≡
<File header>

submodule (phs_points) phs_points_s

    use lorentz, only: vector4_null
    use lorentz, only: vector4_write_set
    use lorentz, only: operator(==)
    use lorentz, only: operator(*)
    use lorentz, only: operator(**)

    implicit none

contains

    <PHS points: procedures>

end submodule phs_points_s

```

9.4.1 PHS point definition

This is a trivial container for an array of momenta. The main application is to store a non-uniform array of phase-space points.

```

    <PHS points: public>≡
    public :: phs_point_t

    <PHS points: types>≡
    type :: phs_point_t
    private
    type(vector4_t), dimension(:), allocatable :: p
contains
    <PHS points: phs point: TBP>
end type phs_point_t

```

9.4.2 PHS point: basic tools

Output. This is instrumented with options, which have to be provided by the caller.

```

    <PHS points: phs point: TBP>≡

```



```

    procedure :: write => phs_point_write
<PHS points: sub interfaces>≡
    module subroutine phs_point_write (phs_point, unit, show_mass, testflag, &
        check_conservation, ultra, n_in)
        class(phs_point_t), intent(in) :: phs_point
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
    end subroutine phs_point_write
<PHS points: procedures>≡
    module subroutine phs_point_write (phs_point, unit, show_mass, testflag, &
        check_conservation, ultra, n_in)
        class(phs_point_t), intent(in) :: phs_point
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
        if (allocated (phs_point%p)) then
            call vector4_write_set (phs_point%p, &
                unit = unit, &
                show_mass = show_mass, &
                testflag = testflag, &
                check_conservation = check_conservation, &
                ultra = ultra, &
                n_in = n_in)
        end if
    end subroutine phs_point_write

```

Non-intrinsic assignment

```

<PHS points: public>+≡
    public :: assignment(=)
<PHS points: interfaces>≡
    interface assignment(=)
        module procedure phs_point_from_n
        module procedure phs_point_from_vector4
        module procedure vector4_from_phs_point
    end interface

```

Initialize with zero momenta but fixed size

```

<PHS points: sub interfaces>+≡
    pure module subroutine phs_point_from_n (phs_point, n_particles)
        type(phs_point_t), intent(out) :: phs_point
        integer, intent(in) :: n_particles
    end subroutine phs_point_from_n
<PHS points: procedures>+≡
    pure module subroutine phs_point_from_n (phs_point, n_particles)
        type(phs_point_t), intent(out) :: phs_point
        integer, intent(in) :: n_particles
        allocate (phs_point%p (n_particles), source = vector4_null)

```

```
end subroutine phs_point_from_n
```

Transform from/to plain vector array

<PHS points: sub interfaces>+≡

```
pure module subroutine phs_point_from_vector4 (phs_point, p)
  type(phs_point_t), intent(out) :: phs_point
  type(vector4_t), dimension(:), intent(in) :: p
end subroutine phs_point_from_vector4
pure module subroutine vector4_from_phs_point (p, phs_point)
  class(phs_point_t), intent(in) :: phs_point
  type(vector4_t), dimension(:), allocatable, intent(out) :: p
end subroutine vector4_from_phs_point
```

<PHS points: procedures>+≡

```
pure module subroutine phs_point_from_vector4 (phs_point, p)
  type(phs_point_t), intent(out) :: phs_point
  type(vector4_t), dimension(:), intent(in) :: p
  phs_point%p = p
end subroutine phs_point_from_vector4

pure module subroutine vector4_from_phs_point (p, phs_point)
  class(phs_point_t), intent(in) :: phs_point
  type(vector4_t), dimension(:), allocatable, intent(out) :: p
  if (allocated (phs_point%p)) p = phs_point%p
end subroutine vector4_from_phs_point
```

Query the size of the momentum array (assuming it is allocated).

<PHS points: public>+≡

```
public :: size
```

<PHS points: interfaces>+≡

```
interface size
  module procedure phs_point_size
end interface size
```

<PHS points: sub interfaces>+≡

```
pure module function phs_point_size (phs_point) result (s)
  class(phs_point_t), intent(in) :: phs_point
  integer :: s
end function phs_point_size
```

<PHS points: procedures>+≡

```
pure module function phs_point_size (phs_point) result (s)
  class(phs_point_t), intent(in) :: phs_point
  integer :: s
  if (allocated (phs_point%p)) then
    s = size (phs_point%p)
  else
    s = 0
  end if
end function phs_point_size
```

Equality, implemented only for valid points.

<PHS points: public>+≡

```
public :: operator(==)
```

```

<PHS points: interfaces>+≡
  interface operator(==)
    module procedure phs_point_eq
  end interface operator(==)

<PHS points: sub interfaces>+≡
  elemental module function phs_point_eq &
    (phs_point_1, phs_point_2) result (flag)
    class(phs_point_t), intent(in) :: phs_point_1, phs_point_2
    logical :: flag
  end function phs_point_eq

<PHS points: procedures>+≡
  elemental module function phs_point_eq &
    (phs_point_1, phs_point_2) result (flag)
    class(phs_point_t), intent(in) :: phs_point_1, phs_point_2
    logical :: flag
    if (allocated (phs_point_1%p) .and. (allocated (phs_point_2%p))) then
      flag = all (phs_point_1%p == phs_point_2%p)
    else
      flag = .false.
    end if
  end function phs_point_eq

```

Extract all momenta, as a method

```

<PHS points: phs point: TBP>+≡
  procedure :: get => phs_point_get

<PHS points: sub interfaces>+≡
  pure module function phs_point_get (phs_point) result (p)
    class(phs_point_t), intent(in) :: phs_point
    type(vector4_t), dimension(:), allocatable :: p
  end function phs_point_get

<PHS points: procedures>+≡
  pure module function phs_point_get (phs_point) result (p)
    class(phs_point_t), intent(in) :: phs_point
    type(vector4_t), dimension(:), allocatable :: p
    if (allocated (phs_point%p)) then
      p = phs_point%p
    else
      allocate (p (0))
    end if
  end function phs_point_get

```

Extract a subset of all momenta.

```

<PHS points: phs point: TBP>+≡
  procedure :: select => phs_point_select

<PHS points: sub interfaces>+≡
  elemental module function phs_point_select (phs_point, i) result (p)
    class(phs_point_t), intent(in) :: phs_point
    integer, intent(in) :: i
    type(vector4_t) :: p
  end function phs_point_select

```

```

<PHS points: procedures>+≡
  elemental module function phs_point_select (phs_point, i) result (p)
    class(phs_point_t), intent(in) :: phs_point
    integer, intent(in) :: i
    type(vector4_t) :: p
    if (allocated (phs_point%p)) then
      p = phs_point%p(i)
    else
      p = vector4_null
    end if
  end function phs_point_select

```

Return the invariant mass squared for a subset of momenta

```

<PHS points: phs point: TBP>+≡
  procedure :: get_msq => phs_point_get_msq

<PHS points: sub interfaces>+≡
  pure module function phs_point_get_msq (phs_point, iarray) result (msq)
    class(phs_point_t), intent(in) :: phs_point
    integer, dimension(:), intent(in) :: iarray
    real(default) :: msq
  end function phs_point_get_msq

<PHS points: procedures>+≡
  pure module function phs_point_get_msq (phs_point, iarray) result (msq)
    class(phs_point_t), intent(in) :: phs_point
    integer, dimension(:), intent(in) :: iarray
    real(default) :: msq
    if (allocated (phs_point%p)) then
      msq = (sum (phs_point%p(iarray)))*2
    else
      msq = 0
    end if
  end function phs_point_get_msq

```

9.4.3 Lorentz algebra pieces

Lorentz transformation.

```

<PHS points: public>+≡
  public :: operator(*)

<PHS points: interfaces>+≡
  interface operator(*)
    module procedure prod_LT_phs_point
  end interface operator(*)

<PHS points: sub interfaces>+≡
  elemental module function prod_LT_phs_point (L, phs_point) result (phs_point_LT)
    type(lorentz_transformation_t), intent(in) :: L
    type(phs_point_t), intent(in) :: phs_point
    type(phs_point_t) :: phs_point_LT
  end function prod_LT_phs_point

```

```

<PHS points: procedures>+≡
elemental module function prod_LT_phs_point (L, phs_point) result (phs_point_LT)
  type(lorentz_transformation_t), intent(in) :: L
  type(phs_point_t), intent(in) :: phs_point
  type(phs_point_t) :: phs_point_LT
  if (allocated (phs_point%p)) phs_point_LT%p = L * phs_point%p
end function prod_LT_phs_point

```

Compute momentum sum, analogous to the standard `sum` function (`mask`), and additionally using an index array.

```

<PHS points: public>+≡
  public :: sum

<PHS points: interfaces>+≡
  interface sum
    module procedure phs_point_sum
    module procedure phs_point_sum_iarray
  end interface sum

<PHS points: sub interfaces>+≡
  pure module function phs_point_sum (phs_point, mask) result (p)
    class(phs_point_t), intent(in) :: phs_point
    logical, dimension(:), intent(in), optional :: mask
    type(vector4_t) :: p
  end function phs_point_sum
  pure module function phs_point_sum_iarray (phs_point, iarray) result (p)
    class(phs_point_t), intent(in) :: phs_point
    integer, dimension(:), intent(in) :: iarray
    type(vector4_t) :: p
  end function phs_point_sum_iarray

<PHS points: procedures>+≡
  pure module function phs_point_sum (phs_point, mask) result (p)
    class(phs_point_t), intent(in) :: phs_point
    logical, dimension(:), intent(in), optional :: mask
    type(vector4_t) :: p
    if (allocated (phs_point%p)) then
      if (present (mask)) then
        p = sum (phs_point%p, mask)
      else
        p = sum (phs_point%p)
      end if
    else
      p = vector4_null
    end if
  end function phs_point_sum

  pure module function phs_point_sum_iarray (phs_point, iarray) result (p)
    class(phs_point_t), intent(in) :: phs_point
    integer, dimension(:), intent(in) :: iarray
    type(vector4_t) :: p
    logical, dimension(:), allocatable :: mask
    integer :: i
    allocate (mask (size (phs_point)), source = .false.)
    mask(iarray) = .true.

```

```

    p = sum (phs_point, mask)
end function phs_point_sum_iarray

```

9.4.4 Methods for specific applications

Convenience method: compute the pair of energy fractions w.r.t. the specified beam energy. We assume that the momenta represent a scattering process (two incoming particles) in the c.m. frame.

```

<PHS points: phs_point: TBP>+≡
    procedure :: get_x => phs_point_get_x

<PHS points: sub interfaces>+≡
    pure module function phs_point_get_x (phs_point, E_beam) result (x)
        class(phs_point_t), intent(in) :: phs_point
        real(default), dimension(2) :: x
        real(default), intent(in) :: E_beam
    end function phs_point_get_x

<PHS points: procedures>+≡
    pure module function phs_point_get_x (phs_point, E_beam) result (x)
        class(phs_point_t), intent(in) :: phs_point
        real(default), dimension(2) :: x
        real(default), intent(in) :: E_beam
        x = phs_point%p(1:2)%p(0) / E_beam
    end function phs_point_get_x

```

9.4.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_points_ut.f90>≡
    <File header>

    module phs_points_ut
        use unit_tests
        use phs_points_uti

    <Standard module head>

    <PHS points: public test>

    contains

    <PHS points: test driver>

    end module phs_points_ut

<phs_points_uti.f90>≡
    <File header>

    module phs_points_uti

    <Use kinds>

```

```

    use constants, only: zero
    use format_defs, only: FMT_12
    use lorentz
    use phs_points

    <Standard module head>

    <PHS points: test declarations>

contains

    <PHS points: tests>

end module phs_points_util
API: driver for the unit tests below.
<PHS points: public test>≡
    public :: phs_points_test
<PHS points: test driver>≡
    subroutine phs_points_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS points: execute tests>
    end subroutine phs_points_test

```

PHS point unit test implementation

```

<PHS points: execute tests>≡
    call test (phs_points_1, "phs_points_1", &
        "Test PHS point functionality", &
        u, results)
<PHS points: test declarations>≡
    public :: phs_points_1
<PHS points: tests>≡
    subroutine phs_points_1 (u)
        integer, intent(in) :: u
        type(vector4_t), dimension(8) :: tt_mom
        type(phs_point_t) :: phs_p
        type(vector4_t) :: p_sum
        type(vector4_t), dimension(:), allocatable :: p_tau, p_out

        write (u, "(A)")  "*" Test output: phs_points_1"
        write (u, "(A)")  "*" Purpose: handling a 2->6 PSP"
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)")  "*" Setting up a 2->6 off-shell top PSP"
        write (u, "(A)")

        tt_mom(1) = [2.5000000000000000e+02_default, zero, zero, 2.49999999999947775e+02_default]
        tt_mom(2) = [2.5000000000000000e+02_default, zero, zero, -2.49999999999947775e+02_default]
        tt_mom(3) = [1.1557492413664579e+02_default, 3.9011599241011098e+01_default, &

```

```

-6.4278142734963140e+01_default, 8.7671766153043137e+01_default]
tt_mom(4) = [1.4617918132729235e+02_default, -1.0947970597860679e+02_default, &
1.5484441802571380e+01_default, -9.5525593923398418e+01_default]
tt_mom(5) = [5.2637589215119526e+01_default, -4.7413198564695762e+01_default, &
1.0087885417286579e+01_default, 2.0516525153079229e+01_default]
tt_mom(6) = [5.4760292922264796e+01_default, 1.5197406985690520e+01_default, &
5.1527071739328015e+01_default, -1.0615525413924287e+01_default]
tt_mom(7) = [3.2415057664609684e+01_default, 7.5539389341684711e+00_default, &
-1.5935831743946720e+01_default, -2.7139737100881156e+01_default]
tt_mom(8) = [9.8432954734067863e+01_default, 9.5129959382432389e+01_default, &
3.1145755197238953e+00_default, 2.5092565132081493e+01_default]
phs_p = tt_mom

write (u, "(A)")
write (u, "(A)")  "*" Retrieving the size of PSP"
write (u, "(A)")
write (u, "(3x,A,I0)") "Size PSP = ", size (phs_p)

write (u, "(A)")
write (u, "(A)")  "*" Returning the set of 4-momenta from PSP"
write (u, "(A)")
p_out = phs_p%get ()
write (u, "(3x,A)") "set 4-mom. = "
call vector4_write_set (p_out, u, testflag = .true., ultra = .true.)

write (u, "(A)")
write (u, "(A)")  "*" Sum of momenta of PSP"
write (u, "(A)")
p_sum = sum (phs_p)
call pacify (p_sum, tolerance = 1.e-12_default)
write (u, "(3x,A)") "Sum:"
call p_sum%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Reconstructing top/antitop candidate invariant masses from PSP"
write (u, "(A)")
write (u, "(3x,A," // FMT_12 // ")") "m2(top) = ", sqrt (phs_p%get_msq ([3,6,8]))
write (u, "(3x,A," // FMT_12 // ")") "m2(a-top) = ", sqrt (phs_p%get_msq ([4,5,7]))

write (u, "(A)")
write (u, "(A)")  "*" Select a specific 4-vector from PSP, here for a tau"
write (u, "(A)")
p_tau = phs_p%select ([7])
write (u, "(3x,A)") "p(tau):"
call p_tau(1)%write (u, show_mass = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "*" Test output end: phs_points_1"

end subroutine phs_points_1

```


9.5 Special Physics functions

Here, we declare functions that are specific for the Standard Model, including QCD: fixed and running α_s , Catani-Seymour dipole terms, loop functions, etc.

To make maximum use of this, all functions, if possible, are declared elemental (or pure, if this is not possible).

```
<sm_physics.f90>≡  
  <File header>  
  
  module sm_physics  
  
    <Use kinds with double>  
    use constants  
    use physics_defs  
    use lorentz  
  
    <Standard module head>  
  
    <SM physics: public>  
  
    <SM physics: parameters>  
  
    interface  
    <SM physics: sub interfaces>  
    end interface  
  
  end module sm_physics  
  
<sm_physics_sub.f90>≡  
  <File header>  
  
  submodule (sm_physics) sm_physics_s  
  
    use io_units  
    use numeric_utils  
    use diagnostics  
    use permutations, only: factorial  
  
    implicit none  
  
  contains  
  
  <SM physics: procedures>  
  
  end submodule sm_physics_s
```

9.5.1 Constants for Quantum Field Theory calculations

For loop calculations in quantum field theories, one needs the numerical values of the Riemann zeta function:

$$\begin{aligned}\zeta(2) &= 1.64493406684822643647241516665\dots \\ \zeta(3) &= 1.20205690315959428539973816151\dots \\ \zeta(4) &= 1.08232323371113819151600369654\dots \\ \zeta(5) &= 1.03692775514336992633136548646\dots\end{aligned}$$

```
<SM physics: public>≡
  public :: zeta2, zeta3, zeta4, zeta5

<SM physics: parameters>≡
  real(default), parameter :: &
    zeta2 = 1.64493406684822643647241516665_default, &
    zeta3 = 1.20205690315959428539973816151_default, &
    zeta4 = 1.08232323371113819151600369654_default, &
    zeta5 = 1.03692775514336992633136548646_default
```

The Euler-Mascheroni constant is

$$\gamma_E =$$

```
<SM physics: public>+≡
  public :: eulerc

<SM physics: parameters>+≡
  real(default), parameter :: &
    eulerc = 0.5772156649015328606065120900824024310422_default
```

9.5.2 Running α_s

Then we define the coefficients of the beta function of QCD (as a reference cf. the Particle Data Group), where n_f is the number of active flavors in two different schemes:

$$\beta_0 = 11 - \frac{2}{3}n_f \quad (9.5)$$

$$\beta_1 = 51 - \frac{19}{3}n_f \quad (9.6)$$

$$\beta_2 = 2857 - \frac{5033}{9}n_f + \frac{325}{27}n_f^2 \quad (9.7)$$

$$b_0 = \frac{1}{12\pi} (11C_A - 2n_f) \quad (9.8)$$

$$b_1 = \frac{1}{24\pi^2} (17C_A^2 - 5C_A n_f - 3C_F n_f) \quad (9.9)$$

$$b_2 = \frac{1}{(4\pi)^3} \left(\frac{2857}{54} C_A^3 - \frac{1415}{54} C_A^2 n_f - \frac{205}{18} C_A C_F n_f + C_F^2 n_f + \frac{79}{54} C_A n_f^{**2} + \frac{11}{9} C_F n_f^{**2} \right) \quad (9.10)$$

The functions `sumQ2q` and `sumQ4q` provide the sum of the squared and quartic electric charges of a number `nf` of active quark flavors.

```

<SM physics: public>+=
  public :: beta0, beta1, beta2
  public :: coeff_b0, coeff_b1, coeff_b2, coeffqed_b0, coeffqed_b1

<SM physics: sub interfaces>=
  pure module function beta0 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta0
  end function beta0
  pure module function beta1 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta1
  end function beta1
  pure module function beta2 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta2
  end function beta2
  pure module function coeff_b0 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b0
  end function coeff_b0
  pure module function coeff_b1 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b1
  end function coeff_b1
  pure module function coeff_b2 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b2
  end function coeff_b2
  pure module function coeffqed_b0 (nf, nlep)
    integer, intent(in) :: nf, nlep
    real(default) :: n_lep, coeffqed_b0
  end function coeffqed_b0
  pure module function coeffqed_b1 (nf, nlep)
    integer, intent(in) :: nf, nlep
    real(default) :: n_lep, coeffqed_b1
  end function coeffqed_b1

<SM physics: procedures>=
  pure module function beta0 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta0
    beta0 = 11.0_default - two/three * nf
  end function beta0

  pure module function beta1 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta1
    beta1 = 51.0_default - 19.0_default/three * nf
  end function beta1

  pure module function beta2 (nf)
    real(default), intent(in) :: nf

```

```

    real(default) :: beta2
    beta2 = 2857.0_default - 5033.0_default / 9.0_default * &
        nf + 325.0_default/27.0_default * nf**2
end function beta2

pure module function coeff_b0 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b0
    coeff_b0 = (11.0_default * CA - two * nf) / (12.0_default * pi)
end function coeff_b0

pure module function coeff_b1 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b1
    coeff_b1 = (17.0_default * CA**2 - five * CA * nf - three * CF * nf) / &
        (24.0_default * pi**2)
end function coeff_b1

pure module function coeff_b2 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b2
    coeff_b2 = (2857.0_default/54.0_default * CA**3 - &
        1415.0_default/54.0_default * &
        CA**2 * nf - 205.0_default/18.0_default * CA*CF*nf &
        + 79.0_default/54.0_default * CA*nf**2 + &
        11.0_default/9.0_default * CF * nf**2) / (four*pi)**3
end function coeff_b2

pure module function coeffqed_b0 (nf, nlep)
    integer, intent(in) :: nf, nlep
    real(default) :: n_lep, coeffqed_b0
    n_lep = real(nlep, kind=default)
    coeffqed_b0 = - (three * sumQ2q (nf) + n_lep) / (three*pi)
end function coeffqed_b0

pure module function coeffqed_b1 (nf, nlep)
    integer, intent(in) :: nf, nlep
    real(default) :: n_lep, coeffqed_b1
    n_lep = real(nlep, kind=default)
    coeffqed_b1 = - (three * sumQ4q (nf) + n_lep) / (four*pi**2)
end function coeffqed_b1

pure function sumQ2q (nf)
    integer, intent(in) :: nf
    real(default) :: sumQ2q
    select case (nf)
    case (0)
        sumQ2q = zero
    case (1)
        sumQ2q = 1.0_default/9.0_default
    case (2)
        sumQ2q = 5.0_default/9.0_default
    case (3)
        sumQ2q = 2.0_default/3.0_default
    end select
end function sumQ2q

```

```

case (4)
  sumQ2q = 10.0_default/9.0_default
case (5)
  sumQ2q = 11.0_default/9.0_default
case (6:)
  sumQ2q = 5.0_default/3.0_default
end select
end function sumQ2q

pure function sumQ4q (nf)
  integer, intent(in) :: nf
  real(default) :: sumQ4q
  select case (nf)
  case (0)
    sumQ4q = zero
  case (1)
    sumQ4q = 1.0_default/81.0_default
  case (2)
    sumQ4q = 17.0_default/81.0_default
  case (3)
    sumQ4q = 2.0_default/9.0_default
  case (4)
    sumQ4q = 34.0_default/81.0_default
  case (5)
    sumQ4q = 35.0_default/81.0_default
  case (6:)
    sumQ4q = 17.0_default/27.0_default
  end select
end function sumQ4q

```

There should be two versions of running α_s , one which takes the scale and Λ_{QCD} as input, and one which takes the scale and e.g. $\alpha_s(m_Z)$ as input. Here, we take the one which takes the QCD scale and scale as inputs from the PDG book.

```

<SM physics: public>+≡
  public :: running_as, running_as_lam, running_alpha, running_alpha_num

<SM physics: sub interfaces>+≡
  pure module function running_as (scale, al_mz, mz, order, nf) result (ascale)
    real(default), intent(in) :: scale
    real(default), intent(in), optional :: al_mz, nf, mz
    integer, intent(in), optional :: order
    real(default) :: ascale
  end function running_as

  pure module function running_as_lam (nf, scale, lambda, order) result (ascale)
    real(default), intent(in) :: nf, scale
    real(default), intent(in), optional :: lambda
    integer, intent(in), optional :: order
    real(default) :: ascale
  end function running_as_lam

  pure module function running_alpha &
    (scale, al_me, me, order, nf, nlep) result (ascale)
    real(default), intent(in) :: scale
    real(default), intent(in), optional :: al_me, me
    integer, intent(in), optional :: order, nf, nlep

```

```

        real(default) :: ascale
    end function running_alpha
    pure module function running_alpha_num &
        (scale, al_me, me, order, nf, nlep) result (ascale)
        real(default), intent(in) :: scale
        real(default), intent(in), optional :: al_me, me
        integer, intent(in), optional :: order, nf, nlep
        real(default) :: ascale
    end function running_alpha_num

<SM physics: procedures>+≡
    pure module function running_as (scale, al_mz, mz, order, nf) result (ascale)
        real(default), intent(in) :: scale
        real(default), intent(in), optional :: al_mz, nf, mz
        integer, intent(in), optional :: order
        integer :: ord
        real(default) :: az, m_z, as_log, n_f, b0, b1, b2, ascale
        real(default) :: as0, as1
        if (present (mz)) then
            m_z = mz
        else
            m_z = MZ_REF
        end if
        if (present (order)) then
            ord = order
        else
            ord = 0
        end if
        if (present (al_mz)) then
            az = al_mz
        else
            az = ALPHA_QCD_MZ_REF
        end if
        if (present (nf)) then
            n_f = nf
        else
            n_f = 5
        end if
        b0 = coeff_b0 (n_f)
        b1 = coeff_b1 (n_f)
        b2 = coeff_b2 (n_f)
        as_log = one + b0 * az * log(scale**2/m_z**2)
        as0 = az / as_log
        as1 = as0 - as0**2 * b1/b0 * log(as_log)
        select case (ord)
        case (0)
            ascale = as0
        case (1)
            ascale = as1
        case (2)
            ascale = as1 + as0**3 * (b1**2/b0**2 * ((log(as_log))**2 - &
                log(as_log) + as_log - one) - b2/b0 * (as_log - one))
        case default
            ascale = as0
        end select

```

```

end function running_as

pure module function running_as_lam (nf, scale, lambda, order) result (ascale)
  real(default), intent(in) :: nf, scale
  real(default), intent(in), optional :: lambda
  integer, intent(in), optional :: order
  real(default) :: lambda_qcd
  real(default) :: as0, as1, logmul, b0, b1, b2, ascale
  integer :: ord
  if (present (lambda)) then
    lambda_qcd = lambda
  else
    lambda_qcd = LAMBDA_QCD_REF
  end if
  if (present (order)) then
    ord = order
  else
    ord = 0
  end if
  b0 = beta0(nf)
  logmul = log(scale**2/lambda_qcd**2)
  as0 = four*pi / b0 / logmul
  if (ord > 0) then
    b1 = beta1(nf)
    as1 = as0 * (one - two* b1 / b0**2 * log(logmul) / logmul)
  end if
  select case (ord)
  case (0)
    ascale = as0
  case (1)
    ascale = as1
  case (2)
    b2 = beta2(nf)
    ascale = as1 + as0 * four * b1**2/b0**4/logmul**2 * &
      ((log(logmul) - 0.5_default)**2 + &
        b2*b0/8.0_default/b1**2 - five/four)
  case default
    ascale = as0
  end select
end function running_as_lam

pure module function running_alpha &
  (scale, al_me, me, order, nf, nlep) result (ascale)
  real(default), intent(in) :: scale
  real(default), intent(in), optional :: al_me, me
  integer, intent(in), optional :: order, nf, nlep
  integer :: ord, n_f, n_lep
  real(default) :: ae, m_e, a_log, b0, b1, ascale
  real(default) :: a0, a1
  if (present (me)) then
    m_e = me
  else
    m_e = ME_REF
  end if

```

```

    if (present (order)) then
        ord = order
    else
        ord = 0
    end if
    if (present (al_me)) then
        ae = al_me
    else
        ae = ALPHA_QED_ME_REF
    end if
    if (present (nf)) then
        n_f = nf
    else
        n_f = 5
    end if
    if (present (nlep)) then
        n_lep = nlep
    else
        n_lep = 1
    end if
    b0 = coeffqed_b0 (n_f, n_lep)
    b1 = coeffqed_b1 (n_f, n_lep)
    a_log = one + b0 * ae * log(scale**2/m_e**2)
    a0 = ae / a_log
    a1 = ae / (a_log + ae * b1/b0 * &
        log((a_log + ae * b1/b0)/(one + ae * b1/b0)))
    select case (ord)
    case (0)
        ascale = a0
    case (1)
        ascale = a1
    case default
        ascale = a0
    end select
end function running_alpha

pure module function running_alpha_num &
    (scale, al_me, me, order, nf, nlep) result (ascale)
    real(default), intent(in) :: scale
    real(default), intent(in), optional :: al_me, me
    integer, intent(in), optional :: order, nf, nlep
    integer, parameter :: n_steps = 20
    integer :: ord, n_f, n_lep, k1
    real(default), parameter :: sxth = 1._default/6._default
    real(default) :: ae, ascale, m_e, log_q, dlr, &
        b0, b1, xk0, xk1, xk2, xk3
    if (present (order)) then
        ord = order
    else
        ord = 0
    end if
    if (present (al_me)) then
        ae = al_me
    else

```



```

        ae = ALPHA_QED_ME_REF
    end if
    if (present (me)) then
        m_e = me
    else
        m_e = ME_REF
    end if
    if (present (nf)) then
        n_f = nf
    else
        n_f = 5
    end if
    if (present (nlep)) then
        n_lep = nlep
    else
        n_lep = 1
    end if
    ascale = ae
    log_q = log (scale**2/m_e**2)
    dlr = log_q / n_steps
    b0 = coeffqed_b0 (n_f, n_lep)
    b1 = coeffqed_b1 (n_f, n_lep)
    ! ..Solution of the evolution equation depending on ORD
    ! (fourth-order Runge-Kutta beyond the leading order)
    select case (ord)
    case (0)
        ascale = ae / (one + b0 * ae * log_q)
    case (1:)
        do k1 = 1, n_steps
            xk0 = dlr * beta_qed (ascale)
            xk1 = dlr * beta_qed (ascale + 0.5 * xk0)
            xk2 = dlr * beta_qed (ascale + 0.5 * xk1)
            xk3 = dlr * beta_qed (ascale + xk2)
            ascale = ascale + sxth * (xk0 + 2._default * xk1 + &
                2._default * xk2 + xk3)
        end do
    end select
contains
    pure function beta_qed (alpha)
        real(default), intent(in) :: alpha
        real(default) :: beta_qed
        beta_qed = - alpha**2 * (b0 + alpha * b1)
    end function beta_qed
end function running_alpha_num

```

This routine determines the Landau pole $\Lambda_{\overline{MS}}^{(n_f)}$ for given α_s , scale, number of flavors and order.

<SM physics: public>+≡

public :: lambda_qcd

<SM physics: sub interfaces>+≡

```

module function lambda_qcd (as_q, q, nf, order) result (lambda)
    real(default), intent(in) :: as_q, q
    integer, intent(in) :: order, nf

```

```

        real(default) :: lambda
    end function lambda_qcd
<SM physics: procedures>+≡
module function lambda_qcd (as_q, q, nf, order) result (lambda)
    real(default), intent(in) :: as_q, q
    integer, intent(in) :: nf, order
    real(default) :: lambda
    real(default), parameter :: acc = 1e-8_default
    if (order == 0) then
        lambda = lambda_qcd_lo (as_q, q, nf)
    else if (order == 1) then
        lambda = lambda_qcd_nlo (as_q, q, nf)
    else if (order == 2) then
        lambda = lambda_qcd_nnlo (as_q, q, nf)
    else
        call msg_error ("lambda_qcd: order unknown")
    end if
contains
    function lambda_qcd_lo (as_q, q, nf) result (lambda)
        real(default) :: lambda
        real(default), intent(in) :: as_q, q
        integer, intent(in) :: nf
        real(default) :: b0, t0, t1, as0, as1
        b0 = coeff_b0(real(nf, default))
        t1 = one/b0/as_q
        FIND_ROOT: do
            if (signal_is_pending ()) return
            t0 = t1
            as0 = one/b0/t1
            as1 = - one/b0/t1**2
            t1 = (as_q-as0)/as1 + t1
            if (abs(t0-t1)/t0 < acc) exit FIND_ROOT
        end do FIND_ROOT
        lambda = q * exp(-t1/two)
    end function lambda_qcd_lo
    function lambda_qcd_nlo (as_q, q, nf) result (lambda)
        real(default) :: lambda
        real(default), intent(in) :: as_q, q
        integer, intent(in) :: nf
        real(default) :: b0, b1, t0, t1, as0, as1, logt
        b0 = coeff_b0(real(nf, default))
        b1 = coeff_b1(real(nf, default))
        t1 = one/b0/as_q
        FIND_ROOT: do
            if (signal_is_pending ()) return
            logt = log(t1)
            t0 = t1
            as0 = one/b0/t1 - b1/b0 * logt/(b0 * t1)**2
            as1 = - one/b0/t1**2 - b1/b0**3 * (one - two*logt)/t1**3
            t1 = (as_q-as0)/as1 + t1
            if (abs(t0-t1)/t0 < acc) exit FIND_ROOT
        end do FIND_ROOT
        lambda = q * exp(-t1/two)
    end function lambda_qcd_nlo

```

```

function lambda_qcd_nnlo (as_q, q, nf) result (lambda)
  real(default) :: lambda
  real(default), intent(in) :: as_q, q
  integer, intent(in) :: nf
  real(default) :: b0, b1, b2, t0, t1, as0, as1, logt
  b0 = coeff_b0(real(nf, default))
  b1 = coeff_b1(real(nf, default))
  b2 = coeff_b2(real(nf, default))
  t1 = one/b0/as_q
  FIND_ROOT: do
    if (signal_is_pending ()) return
    logt = log(t1)
    t0 = t1
    as0 = one/b0/t1 * (one - b1/b0**2 * logt/t1 + (b1/b0**2 * logt/t1)**2 &
      - (b1**2 * (logt + one) - b0*b2)/b0**4/t1**2)
    as1 = one/b0/t1 * (-two*b1**2 * logt**2/(b0**4 * t1**3) &
      + two*(b1**2 * (logt + one) - b0*b2)/(b0**4 * t1**3) &
      + b1 * logt/(b0**2 * t1**2) + two*b1**2 * logt/(b0**4 * t1**3) &
      - b1/(b0**2 * t1**2) - b1**2/(b0**4 * t1**3)) &
      - (b1**2 * logt**2/(b0**4 * t1**2) - (b1**2 * (logt + one) &
      - b0*b2)/(b0**4 * t1**2) - b1 * logt/(b0**2 * t1) + one)/(b0 * t1**2)
    t1 = (as_q-as0)/as1 + t1
    if (abs(t0-t1)/t0 < acc) exit FIND_ROOT
  end do FIND_ROOT
  lambda = q * exp(-t1/two)
end function lambda_qcd_nnlo
end function lambda_qcd

```

9.5.3 Catani-Seymour Parameters

These are fundamental constants of the Catani-Seymour dipole formalism. Since the corresponding parameters for the gluon case depend on the number of flavors which is treated as an argument, there we do have functions and not parameters.

$$\gamma_q = \gamma_{\bar{q}} = \frac{3}{2}C_F \quad \gamma_g = \frac{11}{6}C_A - \frac{2}{3}T_R N_f \quad (9.11)$$

$$K_q = K_{\bar{q}} = \left(\frac{7}{2} - \frac{\pi^2}{6}\right) C_F \quad K_g = \left(\frac{67}{18} - \frac{\pi^2}{6}\right) C_A - \frac{10}{9}T_R N_f \quad (9.12)$$

<SM physics: parameters>+≡

```

real(default), parameter, public :: gamma_q = three/two * CF, &
  k_q = (7.0_default/two - pi**2/6.0_default) * CF

```

<SM physics: public>+≡

```

public :: gamma_g, k_g

```

<SM physics: sub interfaces>+≡

```

elemental module function gamma_g (nf) result (gg)
  real(default), intent(in) :: nf
  real(default) :: gg
end function gamma_g
elemental module function k_g (nf) result (kg)

```

```

        real(default), intent(in) :: nf
        real(default) :: kg
    end function k_g

<SM physics: procedures>+≡
    elemental module function gamma_g (nf) result (gg)
        real(default), intent(in) :: nf
        real(default) :: gg
        gg = 11.0_default/6.0_default * CA - two/three * TR * nf
    end function gamma_g

    elemental module function k_g (nf) result (kg)
        real(default), intent(in) :: nf
        real(default) :: kg
        kg = (67.0_default/18.0_default - pi**2/6.0_default) * CA - &
            10.0_default/9.0_default * TR * nf
    end function k_g

```

9.5.4 Mathematical Functions

The dilogarithm. This simplified version is bound to double precision, and restricted to argument values less or equal to unity, so we do not need complex algebra. The wrapper converts it to default precision (which is, of course, a no-op if double=default).

The routine calculates the dilogarithm through mapping on the area where there is a quickly convergent series (adapted from an F77 routine by Hans Kuijf, 1988): Map x such that x is not in the neighbourhood of 1. Note that $|z| = -\ln(1-x)$ is always smaller than 1.10, but $\frac{1 \cdot 10^{19}}{19!} \text{Bernoulli}_{19} = 2.7 \times 10^{-15}$.

```

<SM physics: public>+≡
    public :: Li2

<SM physics: sub interfaces>+≡
    elemental module function Li2 (x)
        real(default), intent(in) :: x
        real(default) :: Li2
    end function Li2

<SM physics: procedures>+≡
    elemental module function Li2 (x)
        real(default), intent(in) :: x
        real(default) :: Li2
        Li2 = real( Li2_double (real(x, kind=double)), kind=default)
    end function Li2

<SM physics: procedures>+≡
    elemental function Li2_double (x) result (Li2)
        real(double), intent(in) :: x
        real(double) :: Li2
        real(double), parameter :: pi2_6 = pi**2/6
        if (abs(1-x) < tiny_07) then
            Li2 = pi2_6
        else if (abs(1-x) < 0.5_double) then

```

```

        Li2 = pi2_6 - log(1-x) * log(x) - Li2_restricted (1-x)
    else if (abs(x) > 1.d0) then
        ! Li2 = 0
        ! call msg_bug (" Dilogarithm called outside of defined range.")
        !!! Reactivate Dilogarithm identity
        Li2 = -pi2_6 - 0.5_default * log(-x) * log(-x) - Li2_restricted (1/x)
    else
        Li2 = Li2_restricted (x)
    end if
contains
    elemental function Li2_restricted (x) result (Li2)
        real(double), intent(in) :: x
        real(double) :: Li2
        real(double) :: tmp, z, z2
        z = - log (1-x)
        z2 = z**2
! Horner's rule for the powers z^3 through z^19
        tmp = 43867._double/798._double
        tmp = tmp * z2 /342._double - 3617._double/510._double
        tmp = tmp * z2 /272._double + 7._double/6._double
        tmp = tmp * z2 /210._double - 691._double/2730._double
        tmp = tmp * z2 /156._double + 5._double/66._double
        tmp = tmp * z2 /110._double - 1._double/30._double
        tmp = tmp * z2 / 72._double + 1._double/42._double
        tmp = tmp * z2 / 42._double - 1._double/30._double
        tmp = tmp * z2 / 20._double + 1._double/6._double
! The first three terms of the power series
        Li2 = z2 * z * tmp / 6._double - 0.25_double * z2 + z
    end function Li2_restricted
end function Li2_double

```

Complex digamma function. For this we use the asymptotic formula in Abramowitz/Stegun, Eq. (6.3.18), and the recurrence formula Eq. (6.3.6):

$$\psi^{(0)}(z) := \psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} \quad (9.13)$$

```

<SM physics: public>+≡
    public :: psic
    public :: psir

<SM physics: sub interfaces>+≡
    elemental module function psic (z) result (psi)
        complex(default), intent(in) :: z
        complex(default) :: psi
    end function psic
    elemental module function psir (x) result (psi)
        real(default), intent(in) :: x
        real(default) :: psi
    end function psir

<SM physics: procedures>+≡
    elemental module function psic (z) result (psi)
        complex(default), intent(in) :: z
        complex(default) :: psi

```

```

complex(default) :: shift, zz, zi, zi2
shift = 0
zz = z
if (abs (aimag(zz)) < 10._default) then
  do while (abs (zz) < 10._default)
    shift = shift - 1 / zz
    zz = zz + 1
  end do
end if
zi = 1/zz
zi2 = zi*zi
psi = shift + log(zz) - zi/2 - zi2 / 5040._default * ( 420._default + &
  zi2 * ( -42._default + zi2 * (20._default - 21._default * zi2)))
end function psic

elemental module function psir (x) result (psi)
  real(default), intent(in) :: x
  real(default) :: psi
  psi = real (psic (cmplx (x,0,kind=default)), kind=default)
end function psir

```

Complex polygamma function. For this we use the asymptotic formula in Abramowitz/Stegun, Eq. (6.4.11), and the recurrence formula Eq. (6.4.11):

$$\psi^{(m)}(z) := \frac{d^m}{dz^m} \psi(z) = \frac{d^{m+1}}{dz^{m+1}} \ln \Gamma(z) \quad (9.14)$$

```

<SM physics: public>+≡
  public :: psim
  public :: psimr

<SM physics: sub interfaces>+≡
  elemental module function psim (z, m) result (psi)
    complex(default), intent(in) :: z
    integer, intent(in) :: m
    complex(default) :: psi
  end function psim
  elemental module function psimr (x, m) result (psi)
    real(default), intent(in) :: x
    integer, intent(in) :: m
    real(default) :: psi
  end function psimr

<SM physics: procedures>+≡
  elemental module function psim (z, m) result (psi)
    complex(default), intent(in) :: z
    integer, intent(in) :: m
    complex(default) :: psi
    complex(default) :: shift, rec, zz, zi, zi2
    real(default) :: c1, c2, c3, c4, c5, c6, c7
    integer :: i
    if (m < 1) then
      psi = psic(z)
    else
      shift = 0

```

```

zz = z
if (abs (aimag (zz)) < 10._default) then
  CHECK_ABS: do
    rec = (-1)**m * factorial (m) / zz**(m+1)
    shift = shift - rec
    zz = zz + 1
    if (abs (zz) > 10._default) exit CHECK_ABS
  end do CHECK_ABS
end if
c1 = 1._default
c2 = 1._default / 2._default
c3 = 1._default / 6._default
c4 = - 1._default / 30._default
c5 = 1._default / 42._default
c6 = - 1._default / 30._default
c7 = 5._default / 66._default
do i = 2, m
  c1 = c1 * (i-1)
  c2 = c2 * i
  c3 = c3 * (i+1)
  c4 = c4 * (i+3)
  c5 = c5 * (i+5)
  c6 = c6 * (i+7)
  c7 = c7 * (i+9)
end do
zi = 1/zz
zi2 = zi*zi
psi = shift + (-1)**(m-1) * zi**m * ( c1 + zi * ( c2 + zi * ( &
  c3 + zi2 * ( c4 + zi2 * ( c5 + zi2 * ( c6 + ( c7 * zi2))))))
end if
end function psim

elemental module function psimr (x, m) result (psi)
  real(default), intent(in) :: x
  integer, intent(in) :: m
  real(default) :: psi
  psi = real (psim (cmplx (x,0,kind=default), m), kind=default)
end function psimr

```

Nielsen's generalized polylogarithms,

$$S_{n,m}(x) = \frac{(-1)^{n+m-1}}{(n-1)!m!} \int_0^1 t^{-1} \ln^{n-1} t \ln^m(1-xt) dt ,$$

adapted from the CERNLIB function `wgplg` for real arguments `x` and integer `n` and `m` satisfying $1 \leq n \leq 4$, $1 \leq m \leq 4$, $n + m \leq 5$, i.e. one of the functions $S_{1,1}$, $S_{1,2}$, $S_{2,1}$, $S_{1,3}$, $S_{2,2}$, $S_{3,1}$, $S_{1,4}$, $S_{2,3}$, $S_{3,2}$, $S_{4,1}$. If $x \leq 1$, $S_{n,m}(x)$ is real, and the imaginary part is set to zero.

```

<SM physics: public>+=
  public :: cnielsen
  public :: nielsen

<SM physics: sub interfaces>+=
  module function cnielsen (n, m, x) result (nplog)

```

```

        integer, intent(in) :: n, m
        real(default), intent(in) :: x
        complex(default) :: nplog
    end function cnielsen
module function nielsen (n, m, x) result (nplog)
    integer, intent(in) :: n, m
    real(default), intent(in) :: x
    real(default) :: nplog
end function nielsen
<SM physics: procedures>+≡
module function cnielsen (n, m, x) result (nplog)
    integer, intent(in) :: n, m
    real(default), intent(in) :: x
    complex(default) :: nplog
    real(default), parameter :: c1 = 4._default/3._default, &
        c2 = 1._default/3._default
    real(default), dimension(0:4), parameter :: &
        fct = [1.0_default,1.0_default,2.0_default,6.0_default,24.0_default]
    real(default), dimension(4,4) :: s1, cc
    real(default), dimension(0:30,10) :: aa
    complex(default), dimension(0:5) :: vv
    real(default), dimension(0:5) :: uu
    real(default) :: x1, h, alfa, b0, b1, b2, qq, rr
    complex(default) :: sj, sk
    integer, dimension(10), parameter :: &
        nc = [24,26,28,30,22,24,26,19,22,17]
    integer, dimension(31), parameter :: &
        index = [1,2,3,4,0,0,0,0,0,0,5,6,7,0,0,0,0,0,0, &
            8,9,0,0,0,0,0,0,0,0,10]
    real(default), dimension(0:4), parameter :: &
        sgn = [1._default, -1._default, 1._default, -1._default, 1._default]
    integer :: it, j, k, l, m1, n1
    if ((n<1) .or. (n>4) .or. (m<1) .or. (m>4) .or. (n+m > 5)) then
        call msg_fatal &
            ("The Nielsen dilogarithms cannot be applied for these values.")
    end if
    s1 = 0._default
    s1(1,1) = 1.6449340668482_default
    s1(1,2) = 1.2020569031596_default
    s1(1,3) = 1.0823232337111_default
    s1(1,4) = 1.0369277551434_default
    s1(2,1) = 1.2020569031596_default
    s1(2,2) = 2.7058080842778e-1_default
    s1(2,3) = 9.6551159989444e-2_default
    s1(3,1) = 1.0823232337111_default
    s1(3,2) = 9.6551159989444e-2_default
    s1(4,1) = 1.0369277551434_default
    cc = 0._default
    cc(1,1) = 1.6449340668482_default
    cc(1,2) = 1.2020569031596_default
    cc(1,3) = 1.0823232337111_default
    cc(1,4) = 1.0369277551434_default
    cc(2,2) = -1.8940656589945_default
    cc(2,3) = -3.0142321054407_default

```



```

cc(3,1) = 1.8940656589945_default
cc(3,2) = 3.0142321054407_default
aa = 0._default
aa( 0,1) = 0.96753215043498_default
aa( 1,1) = 0.16607303292785_default
aa( 2,1) = 0.02487932292423_default
aa( 3,1) = 0.00468636195945_default
aa( 4,1) = 0.00100162749616_default
aa( 5,1) = 0.00023200219609_default
aa( 6,1) = 0.00005681782272_default
aa( 7,1) = 0.00001449630056_default
aa( 8,1) = 0.00000381632946_default
aa( 9,1) = 0.00000102990426_default
aa(10,1) = 0.00000028357538_default
aa(11,1) = 0.00000007938705_default
aa(12,1) = 0.00000002253670_default
aa(13,1) = 0.00000000647434_default
aa(14,1) = 0.00000000187912_default
aa(15,1) = 0.00000000055029_default
aa(16,1) = 0.00000000016242_default
aa(17,1) = 0.00000000004827_default
aa(18,1) = 0.00000000001444_default
aa(19,1) = 0.00000000000434_default
aa(20,1) = 0.00000000000131_default
aa(21,1) = 0.00000000000040_default
aa(22,1) = 0.00000000000012_default
aa(23,1) = 0.00000000000004_default
aa(24,1) = 0.00000000000001_default

aa( 0,2) = 0.95180889127832_default
aa( 1,2) = 0.43131131846532_default
aa( 2,2) = 0.10002250714905_default
aa( 3,2) = 0.02442415595220_default
aa( 4,2) = 0.00622512463724_default
aa( 5,2) = 0.00164078831235_default
aa( 6,2) = 0.00044407920265_default
aa( 7,2) = 0.00012277494168_default
aa( 8,2) = 0.00003453981284_default
aa( 9,2) = 0.00000985869565_default
aa(10,2) = 0.00000284856995_default
aa(11,2) = 0.00000083170847_default
aa(12,2) = 0.00000024503950_default
aa(13,2) = 0.00000007276496_default
aa(14,2) = 0.00000002175802_default
aa(15,2) = 0.00000000654616_default
aa(16,2) = 0.00000000198033_default
aa(17,2) = 0.00000000060204_default
aa(18,2) = 0.00000000018385_default
aa(19,2) = 0.00000000005637_default
aa(20,2) = 0.00000000001735_default
aa(21,2) = 0.00000000000536_default
aa(22,2) = 0.00000000000166_default
aa(23,2) = 0.00000000000052_default
aa(24,2) = 0.00000000000016_default

```

```

aa(25,2) = 0.000000000000005_default
aa(26,2) = 0.000000000000002_default

aa( 0,3) = 0.98161027991365_default
aa( 1,3) = 0.72926806320726_default
aa( 2,3) = 0.22774714909321_default
aa( 3,3) = 0.06809083296197_default
aa( 4,3) = 0.02013701183064_default
aa( 5,3) = 0.00595478480197_default
aa( 6,3) = 0.00176769013959_default
aa( 7,3) = 0.00052748218502_default
aa( 8,3) = 0.00015827461460_default
aa( 9,3) = 0.00004774922076_default
aa(10,3) = 0.00001447920408_default
aa(11,3) = 0.00000441154886_default
aa(12,3) = 0.00000135003870_default
aa(13,3) = 0.00000041481779_default
aa(14,3) = 0.00000012793307_default
aa(15,3) = 0.00000003959070_default
aa(16,3) = 0.00000001229055_default
aa(17,3) = 0.00000000382658_default
aa(18,3) = 0.00000000119459_default
aa(19,3) = 0.00000000037386_default
aa(20,3) = 0.00000000011727_default
aa(21,3) = 0.00000000003687_default
aa(22,3) = 0.00000000001161_default
aa(23,3) = 0.00000000000366_default
aa(24,3) = 0.00000000000116_default
aa(25,3) = 0.00000000000037_default
aa(26,3) = 0.00000000000012_default
aa(27,3) = 0.00000000000004_default
aa(28,3) = 0.00000000000001_default

aa( 0,4) = 1.0640521184614_default
aa( 1,4) = 1.0691720744981_default
aa( 2,4) = 0.41527193251768_default
aa( 3,4) = 0.14610332936222_default
aa( 4,4) = 0.04904732648784_default
aa( 5,4) = 0.01606340860396_default
aa( 6,4) = 0.00518889350790_default
aa( 7,4) = 0.00166298717324_default
aa( 8,4) = 0.00053058279969_default
aa( 9,4) = 0.00016887029251_default
aa(10,4) = 0.00005368328059_default
aa(11,4) = 0.00001705923313_default
aa(12,4) = 0.00000542174374_default
aa(13,4) = 0.00000172394082_default
aa(14,4) = 0.00000054853275_default
aa(15,4) = 0.00000017467795_default
aa(16,4) = 0.00000005567550_default
aa(17,4) = 0.00000001776234_default
aa(18,4) = 0.00000000567224_default
aa(19,4) = 0.00000000181313_default
aa(20,4) = 0.00000000058012_default

```

```

aa(21,4) = 0.00000000018579_default
aa(22,4) = 0.00000000005955_default
aa(23,4) = 0.00000000001911_default
aa(24,4) = 0.00000000000614_default
aa(25,4) = 0.00000000000197_default
aa(26,4) = 0.00000000000063_default
aa(27,4) = 0.00000000000020_default
aa(28,4) = 0.00000000000007_default
aa(29,4) = 0.00000000000002_default
aa(30,4) = 0.00000000000001_default

```

```

aa( 0,5) = 0.97920860669175_default
aa( 1,5) = 0.08518813148683_default
aa( 2,5) = 0.00855985222013_default
aa( 3,5) = 0.00121177214413_default
aa( 4,5) = 0.00020722768531_default
aa( 5,5) = 0.00003996958691_default
aa( 6,5) = 0.00000838064065_default
aa( 7,5) = 0.00000186848945_default
aa( 8,5) = 0.00000043666087_default
aa( 9,5) = 0.00000010591733_default
aa(10,5) = 0.00000002647892_default
aa(11,5) = 0.00000000678700_default
aa(12,5) = 0.00000000177654_default
aa(13,5) = 0.00000000047342_default
aa(14,5) = 0.00000000012812_default
aa(15,5) = 0.00000000003514_default
aa(16,5) = 0.00000000000975_default
aa(17,5) = 0.00000000000274_default
aa(18,5) = 0.00000000000077_default
aa(19,5) = 0.00000000000022_default
aa(20,5) = 0.00000000000006_default
aa(21,5) = 0.00000000000002_default
aa(22,5) = 0.00000000000001_default

```

```

aa( 0,6) = 0.95021851963952_default
aa( 1,6) = 0.29052529161433_default
aa( 2,6) = 0.05081774061716_default
aa( 3,6) = 0.00995543767280_default
aa( 4,6) = 0.00211733895031_default
aa( 5,6) = 0.00047859470550_default
aa( 6,6) = 0.00011334321308_default
aa( 7,6) = 0.00002784733104_default
aa( 8,6) = 0.00000704788108_default
aa( 9,6) = 0.00000182788740_default
aa(10,6) = 0.00000048387492_default
aa(11,6) = 0.00000013033842_default
aa(12,6) = 0.00000003563769_default
aa(13,6) = 0.00000000987174_default
aa(14,6) = 0.00000000276586_default
aa(15,6) = 0.00000000078279_default
aa(16,6) = 0.00000000022354_default
aa(17,6) = 0.00000000006435_default
aa(18,6) = 0.00000000001866_default

```

```

aa(19,6) = 0.00000000000545_default
aa(20,6) = 0.00000000000160_default
aa(21,6) = 0.00000000000047_default
aa(22,6) = 0.00000000000014_default
aa(23,6) = 0.00000000000004_default
aa(24,6) = 0.00000000000001_default

aa( 0,7) = 0.95064032186777_default
aa( 1,7) = 0.54138285465171_default
aa( 2,7) = 0.13649979590321_default
aa( 3,7) = 0.03417942328207_default
aa( 4,7) = 0.00869027883583_default
aa( 5,7) = 0.00225284084155_default
aa( 6,7) = 0.00059516089806_default
aa( 7,7) = 0.00015995617766_default
aa( 8,7) = 0.00004365213096_default
aa( 9,7) = 0.00001207474688_default
aa(10,7) = 0.00000338018176_default
aa(11,7) = 0.00000095632476_default
aa(12,7) = 0.00000027313129_default
aa(13,7) = 0.00000007866968_default
aa(14,7) = 0.00000002283195_default
aa(15,7) = 0.00000000667205_default
aa(16,7) = 0.00000000196191_default
aa(17,7) = 0.00000000058018_default
aa(18,7) = 0.00000000017246_default
aa(19,7) = 0.00000000005151_default
aa(20,7) = 0.00000000001545_default
aa(21,7) = 0.00000000000465_default
aa(22,7) = 0.00000000000141_default
aa(23,7) = 0.00000000000043_default
aa(24,7) = 0.00000000000013_default
aa(25,7) = 0.00000000000004_default
aa(26,7) = 0.00000000000001_default

aa( 0,8) = 0.98800011672229_default
aa( 1,8) = 0.04364067609601_default
aa( 2,8) = 0.00295091178278_default
aa( 3,8) = 0.00031477809720_default
aa( 4,8) = 0.00004314846029_default
aa( 5,8) = 0.00000693818230_default
aa( 6,8) = 0.00000124640350_default
aa( 7,8) = 0.00000024293628_default
aa( 8,8) = 0.00000005040827_default
aa( 9,8) = 0.00000001099075_default
aa(10,8) = 0.00000000249467_default
aa(11,8) = 0.00000000058540_default
aa(12,8) = 0.00000000014127_default
aa(13,8) = 0.00000000003492_default
aa(14,8) = 0.00000000000881_default
aa(15,8) = 0.00000000000226_default
aa(16,8) = 0.00000000000059_default
aa(17,8) = 0.00000000000016_default
aa(18,8) = 0.00000000000004_default

```

```

aa(19,8) = 0.00000000000001_default

aa( 0,9) = 0.95768506546350_default
aa( 1,9) = 0.19725249679534_default
aa( 2,9) = 0.02603370313918_default
aa( 3,9) = 0.00409382168261_default
aa( 4,9) = 0.00072681707110_default
aa( 5,9) = 0.00014091879261_default
aa( 6,9) = 0.00002920458914_default
aa( 7,9) = 0.00000637631144_default
aa( 8,9) = 0.00000145167850_default
aa( 9,9) = 0.00000034205281_default
aa(10,9) = 0.00000008294302_default
aa(11,9) = 0.00000002060784_default
aa(12,9) = 0.00000000522823_default
aa(13,9) = 0.00000000135066_default
aa(14,9) = 0.00000000035451_default
aa(15,9) = 0.00000000009436_default
aa(16,9) = 0.00000000002543_default
aa(17,9) = 0.00000000000693_default
aa(18,9) = 0.00000000000191_default
aa(19,9) = 0.00000000000053_default
aa(20,9) = 0.00000000000015_default
aa(21,9) = 0.00000000000004_default
aa(22,9) = 0.00000000000001_default

aa( 0,10) = 0.99343651671347_default
aa( 1,10) = 0.02225770126826_default
aa( 2,10) = 0.00101475574703_default
aa( 3,10) = 0.00008175156250_default
aa( 4,10) = 0.00000899973547_default
aa( 5,10) = 0.00000120823987_default
aa( 6,10) = 0.00000018616913_default
aa( 7,10) = 0.00000003174723_default
aa( 8,10) = 0.00000000585215_default
aa( 9,10) = 0.00000000114739_default
aa(10,10) = 0.00000000023652_default
aa(11,10) = 0.00000000005082_default
aa(12,10) = 0.00000000001131_default
aa(13,10) = 0.00000000000259_default
aa(14,10) = 0.00000000000061_default
aa(15,10) = 0.00000000000015_default
aa(16,10) = 0.00000000000004_default
aa(17,10) = 0.00000000000001_default

if (x == 1._default) then
  nplog = s1(n,m)
else if (x > 2._default .or. x < -1.0_default) then
  x1 = 1._default / x
  h = c1 * x1 + c2
  alfa = h + h
  vv(0) = 1._default
  if (x < -1.0_default) then
    vv(1) = log(-x)

```

```

else if (x > 2._default) then
  vv(1) = log(cmplx(-x,0._default,kind=default))
end if
do l = 2, n+m
  vv(l) = vv(1) * vv(l-1)/l
end do
sk = 0._default
do k = 0, m-1
  m1 = m-k
  rr = x1**m1 / (fct(m1) * fct(n-1))
  sj = 0._default
  do j = 0, k
    n1 = n+k-j
    l = index(10*n1+m1-10)
    b1 = 0._default
    b2 = 0._default
    do it = nc(l), 0, -1
      b0 = aa(it,l) + alfa*b1 - b2
      b2 = b1
      b1 = b0
    end do
    qq = (fct(n1-1) / fct(k-j)) * (b0 - h*b2) * rr / m1**n1
    sj = sj + vv(j) * qq
  end do
  sk = sk + sgn(k) * sj
end do
sj = 0._default
do j = 0, n-1
  sj = sj + vv(j) * cc(n-j,m)
end do
nplog = sgn(n) * sk + sgn(m) * (sj + vv(n+m))
else if (x > 0.5_default) then
  x1 = 1._default - x
  h = c1 * x1 + c2
  alfa = h + h
  vv(0) = 1._default
  uu(0) = 1._default
  vv(1) = log(cmplx(x1,0._default,kind=default))
  uu(1) = log(x)
  do l = 2, m
    vv(l) = vv(1) * vv(l-1) / l
  end do
  do l = 2, n
    uu(l) = uu(1) * uu(l-1) / l
  end do
  sk = 0._default
  do k = 0, n-1
    m1 = n-k
    rr = x1**m1 / fct(m1)
    sj = 0._default
    do j = 0, m-1
      n1 = m-j
      l = index(10*n1 + m1 - 10)
      b1 = 0._default

```

```

        b2 = 0._default
        do it = nc(l), 0, -1
            b0 = aa(it,l) + alfa*b1 - b2
            b2 = b1
            b1 = b0
        end do
        qq = sgn(j) * (b0 - h*b2) * rr / m1**n1
        sj = sj + vv(j) * qq
    end do
    sk = sk + uu(k) * (s1(m1,m) - sj)
end do
nplog = sk + sgn(m) * uu(n) * vv(m)
else
    l = index(10*n + m - 10)
    h = c1 * x + c2
    alfa = h + h
    b1 = 0._default
    b2 = 0._default
    do it = nc(l), 0, -1
        b0 = aa(it,l) + alfa*b1 - b2
        b2 = b1
        b1 = b0
    end do
    nplog = (b0 - h*b2) * x**m / (fct(m) * m**n)
end if
end function cnielsen

module function nielsen (n, m, x) result (nplog)
    integer, intent(in) :: n, m
    real(default), intent(in) :: x
    real(default) :: nplog
    nplog = real (cnielsen (n, m, x))
end function nielsen

```

$$\text{Li}_n(x) = S_{n-1,1}(x).$$

$\langle SM \text{ physics: public} \rangle + \equiv$
 public :: polylog

$\langle SM \text{ physics: sub interfaces} \rangle + \equiv$
 module function polylog (n, x) result (plog)
 integer, intent(in) :: n
 real(default), intent(in) :: x
 real(default) :: plog
 end function polylog

$\langle SM \text{ physics: procedures} \rangle + \equiv$
 module function polylog (n, x) result (plog)
 integer, intent(in) :: n
 real(default), intent(in) :: x
 real(default) :: plog
 plog = nielsen (n-1,1,x)
 end function polylog

$\text{Li}_2(x)$.

```

<SM physics: public>+≡
  public :: dlog

<SM physics: sub interfaces>+≡
  module function dlog (x) result (dlog)
    real(default), intent(in) :: x
    real(default) :: dlog
  end function dlog

<SM physics: procedures>+≡
  module function dlog (x) result (dlog)
    real(default), intent(in) :: x
    real(default) :: dlog
    dlog = polylog (2,x)
  end function dlog

```

$\text{Li}_3(x)$.

```

<SM physics: public>+≡
  public :: trilog

<SM physics: sub interfaces>+≡
  module function trilog (x) result (tlog)
    real(default), intent(in) :: x
    real(default) :: tlog
  end function trilog

<SM physics: procedures>+≡
  module function trilog (x) result (tlog)
    real(default), intent(in) :: x
    real(default) :: tlog
    tlog = polylog (3,x)
  end function trilog

```

9.5.5 Loop Integrals

These functions appear in the calculation of the effective one-loop coupling of a (pseudo)scalar to a vector boson pair.

```

<SM physics: public>+≡
  public :: faux

<SM physics: sub interfaces>+≡
  elemental module function faux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
  end function faux

<SM physics: procedures>+≡
  elemental module function faux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (1 <= x) then
      y = asin(sqrt(1/x))**2
    else
      y = - 1/4.0_default * (log((1 + sqrt(1 - x))/ &

```



```

        (1 - sqrt(1 - x))) - cmplx (0.0_default, pi, kind=default))**2
    end if
end function faux

<SM physics: public>+≡
public :: fonehalf

<SM physics: sub interfaces>+≡
    elemental module function fonehalf (x) result (y)
        real(default), intent(in) :: x
        complex(default) :: y
    end function fonehalf

<SM physics: procedures>+≡
    elemental module function fonehalf (x) result (y)
        real(default), intent(in) :: x
        complex(default) :: y
        if (abs(x) < eps0) then
            y = 0
        else
            y = - 2.0_default * x * (1 + (1 - x) * faux(x))
        end if
    end function fonehalf

<SM physics: public>+≡
public :: fonehalf_pseudo

<SM physics: sub interfaces>+≡
    module function fonehalf_pseudo (x) result (y)
        real(default), intent(in) :: x
        complex(default) :: y
    end function fonehalf_pseudo

<SM physics: procedures>+≡
    module function fonehalf_pseudo (x) result (y)
        real(default), intent(in) :: x
        complex(default) :: y
        if (abs(x) < eps0) then
            y = 0
        else
            y = - 2.0_default * x * faux(x)
        end if
    end function fonehalf_pseudo

<SM physics: public>+≡
public :: fone

<SM physics: sub interfaces>+≡
    elemental module function fone (x) result (y)
        real(default), intent(in) :: x
        complex(default) :: y
    end function fone

```

```

<SM physics: procedures>+≡
  elemental module function fone (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (abs(x) < eps0) then
      y = 2.0_default
    else
      y = 2.0_default + 3.0_default * x + &
        3.0_default * x * (2.0_default - x) * &
        faux(x)
    end if
  end function fone

<SM physics: public>+≡
  public :: gaux

<SM physics: sub interfaces>+≡
  elemental module function gaux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
  end function gaux

<SM physics: procedures>+≡
  elemental module function gaux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (1 <= x) then
      y = sqrt(x - 1) * asin(sqrt(1/x))
    else
      y = sqrt(1 - x) * (log((1 + sqrt(1 - x)) / &
        (1 - sqrt(1 - x)))) - &
        cmplx (0.0_default, pi, kind=default)) / 2.0_default
    end if
  end function gaux

<SM physics: public>+≡
  public :: tri_i1

<SM physics: sub interfaces>+≡
  elemental module function tri_i1 (a,b) result (y)
    real(default), intent(in) :: a,b
    complex(default) :: y
  end function tri_i1

<SM physics: procedures>+≡
  elemental module function tri_i1 (a,b) result (y)
    real(default), intent(in) :: a,b
    complex(default) :: y
    if (a < eps0 .or. b < eps0) then
      y = 0
    else
      y = a*b/2.0_default/(a-b) + a**2 * b**2/2.0_default/(a-b)**2 * &
        (faux(a) - faux(b)) + &
        a**2 * b/(a-b)**2 * (gaux(a) - gaux(b))
    end if

```

```

end function tri_i1

<SM physics: public>+≡
public :: tri_i2

<SM physics: sub interfaces>+≡
elemental module function tri_i2 (a,b) result (y)
  real(default), intent(in) :: a,b
  complex(default) :: y
end function tri_i2

<SM physics: procedures>+≡
elemental module function tri_i2 (a,b) result (y)
  real(default), intent(in) :: a,b
  complex(default) :: y
  if (a < eps0 .or. b < eps0) then
    y = 0
  else
    y = - a * b / 2.0_default / (a-b) * (faux(a) - faux(b))
  end if
end function tri_i2

```

9.5.6 More on α_s

These functions are for the running of the strong coupling constants, α_s .

```

<SM physics: public>+≡
public :: run_b0

<SM physics: sub interfaces>+≡
elemental module function run_b0 (nf) result (bnull)
  integer, intent(in) :: nf
  real(default) :: bnull
end function run_b0

<SM physics: procedures>+≡
elemental module function run_b0 (nf) result (bnull)
  integer, intent(in) :: nf
  real(default) :: bnull
  bnull = 33.0_default - 2.0_default * nf
end function run_b0

<SM physics: public>+≡
public :: run_b1

<SM physics: sub interfaces>+≡
elemental module function run_b1 (nf) result (bone)
  integer, intent(in) :: nf
  real(default) :: bone
end function run_b1

```

```

<SM physics: procedures>+≡
  elemental module function run_b1 (nf) result (bone)
    integer, intent(in) :: nf
    real(default) :: bone
    bone = 6.0_default * (153.0_default - 19.0_default * nf)/run_b0(nf)**2
  end function run_b1

<SM physics: public>+≡
  public :: run_aa

<SM physics: sub interfaces>+≡
  elemental module function run_aa (nf) result (aaa)
    integer, intent(in) :: nf
    real(default) :: aaa
  end function run_aa

<SM physics: procedures>+≡
  elemental module function run_aa (nf) result (aaa)
    integer, intent(in) :: nf
    real(default) :: aaa
    aaa = 12.0_default * PI / run_b0(nf)
  end function run_aa

<SM physics: pubic functions>≡
  public :: run_bb

<SM physics: procedures>+≡
  elemental function run_bb (nf) result (bbb)
    integer, intent(in) :: nf
    real(default) :: bbb
    bbb = run_b1(nf) / run_aa(nf)
  end function run_bb

```

9.5.7 Functions for Catani-Seymour dipoles

For the automated Catani-Seymour dipole subtraction, we need the following functions.

```

<SM physics: public>+≡
  public :: ff_dipole

<SM physics: sub interfaces>+≡
  pure module subroutine ff_dipole (v_ijk, y_ijk, p_ij, pp_k, p_i, p_j, p_k)
    type(vector4_t), intent(in) :: p_i, p_j, p_k
    type(vector4_t), intent(out) :: p_ij, pp_k
    real(default), intent(out) :: y_ijk
    real(default), intent(out) :: v_ijk
  end subroutine ff_dipole

<SM physics: procedures>+≡
  pure module subroutine ff_dipole (v_ijk, y_ijk, p_ij, pp_k, p_i, p_j, p_k)
    type(vector4_t), intent(in) :: p_i, p_j, p_k
    type(vector4_t), intent(out) :: p_ij, pp_k
    real(default), intent(out) :: y_ijk

```

```

real(default) :: z_i
real(default), intent(out) :: v_ijk
z_i = (p_i*p_k) / ((p_k*p_j) + (p_k*p_i))
y_ijk = (p_i*p_j) / ((p_i*p_j) + (p_i*p_k) + (p_j*p_k))
p_ij = p_i + p_j - y_ijk/(1.0_default - y_ijk) * p_k
pp_k = (1.0/(1.0_default - y_ijk)) * p_k
!!! We don't multiply by alpha_s right here:
v_ijk = 8.0_default * PI * CF * &
      (2.0 / (1.0 - z_i*(1.0 - y_ijk)) - (1.0 + z_i))
end subroutine ff_dipole

```

<SM physics: public>+≡
public :: fi_dipole

<SM physics: sub interfaces>+≡
pure module subroutine fi_dipole (v_ija, x_ija, p_ij, pp_a, p_i, p_j, p_a)
type(vector4_t), intent(in) :: p_i, p_j, p_a
type(vector4_t), intent(out) :: p_ij, pp_a
real(default), intent(out) :: x_ija
real(default), intent(out) :: v_ija
end subroutine fi_dipole

<SM physics: procedures>+≡
pure module subroutine fi_dipole (v_ija, x_ija, p_ij, pp_a, p_i, p_j, p_a)
type(vector4_t), intent(in) :: p_i, p_j, p_a
type(vector4_t), intent(out) :: p_ij, pp_a
real(default), intent(out) :: x_ija
real(default) :: z_i
real(default), intent(out) :: v_ija
z_i = (p_i*p_a) / ((p_a*p_j) + (p_a*p_i))
x_ija = ((p_i*p_a) + (p_j*p_a) - (p_i*p_j)) &
 / ((p_i*p_a) + (p_j*p_a))
p_ij = p_i + p_j - (1.0_default - x_ija) * p_a
pp_a = x_ija * p_a
!!! We don't not multiply by alpha_s right here:
v_ija = 8.0_default * PI * CF * &
 (2.0 / (1.0 - z_i + (1.0 - x_ija)) - (1.0 + z_i)) / x_ija
end subroutine fi_dipole

<SM physics: public>+≡
public :: if_dipole

<SM physics: sub interfaces>+≡
pure module subroutine if_dipole (v_kja, u_j, p_aj, pp_k, p_k, p_j, p_a)
type(vector4_t), intent(in) :: p_k, p_j, p_a
type(vector4_t), intent(out) :: p_aj, pp_k
real(default), intent(out) :: u_j
real(default), intent(out) :: v_kja
end subroutine if_dipole

<SM physics: procedures>+≡
pure module subroutine if_dipole (v_kja, u_j, p_aj, pp_k, p_k, p_j, p_a)
type(vector4_t), intent(in) :: p_k, p_j, p_a
type(vector4_t), intent(out) :: p_aj, pp_k
real(default), intent(out) :: u_j

```

real(default) :: x_kja
real(default), intent(out) :: v_kja
u_j = (p_a*p_j) / ((p_a*p_j) + (p_a*p_k))
x_kja = ((p_a*p_k) + (p_a*p_j) - (p_j*p_k)) &
        / ((p_a*p_j) + (p_a*p_k))
p_aj = x_kja * p_a
pp_k = p_k + p_j - (1.0_default - x_kja) * p_a
v_kja = 8.0_default * PI * CF * &
        (2.0 / (1.0 - x_kja + u_j) - (1.0 + x_kja)) / x_kja
end subroutine if_dipole

```

This function depends on a variable number of final state particles whose kinematics all get changed by the initial-initial dipole insertion.

<SM physics: public>+≡

```
public :: ii_dipole
```

<SM physics: sub interfaces>+≡

```

pure module subroutine ii_dipole (v_jab, v_j, p_in, p_out, flag_1or2)
  type(vector4_t), dimension(:), intent(in) :: p_in
  type(vector4_t), dimension(size(p_in)-1), intent(out) :: p_out
  logical, intent(in) :: flag_1or2
  real(default), intent(out) :: v_j
  real(default), intent(out) :: v_jab
end subroutine ii_dipole

```

<SM physics: procedures>+≡

```

pure module subroutine ii_dipole (v_jab, v_j, p_in, p_out, flag_1or2)
  type(vector4_t), dimension(:), intent(in) :: p_in
  type(vector4_t), dimension(size(p_in)-1), intent(out) :: p_out
  logical, intent(in) :: flag_1or2
  real(default), intent(out) :: v_j
  real(default), intent(out) :: v_jab
  type(vector4_t) :: p_a, p_b, p_j
  type(vector4_t) :: k, kk
  type(vector4_t) :: p_aj
  real(default) :: x_jab
  integer :: i
  !!! flag_1or2 decides whether this a 12 or 21 dipole
  if (flag_1or2) then
    p_a = p_in(1)
    p_b = p_in(2)
  else
    p_b = p_in(1)
    p_a = p_in(2)
  end if
  !!! We assume that the unresolved particle has always the last
  !!! momentum
  p_j = p_in(size(p_in))
  x_jab = ((p_a*p_b) - (p_a*p_j) - (p_b*p_j)) / (p_a*p_b)
  v_j = (p_a*p_j) / (p_a * p_b)
  p_aj = x_jab * p_a
  k = p_a + p_b - p_j
  kk = p_aj + p_b
  do i = 3, size(p_in)-1
    p_out(i) = p_in(i) - 2.0*((k+kk)*p_in(i))/((k+kk)*(k+kk)) * (k+kk) + &

```

```

                (2.0 * (k*p_in(i)) / (k*k)) * kk
end do
if (flag_1or2) then
    p_out(1) = p_aj
    p_out(2) = p_b
else
    p_out(1) = p_b
    p_out(2) = p_aj
end if
v_jab = 8.0_default * PI * CF * &
        (2.0 / (1.0 - x_jab) - (1.0 + x_jab)) / x_jab
end subroutine ii_dipole

```

9.5.8 Distributions for integrated dipoles and such

Note that the following formulae are only meaningful for $0 \leq x \leq 1$.

The Dirac delta distribution, modified for Monte-Carlo sampling, centered at $x = 1 - \frac{\epsilon}{2}$:

```

<SM physics: public>+≡
    public :: delta

<SM physics: sub interfaces>+≡
    elemental module function delta (x,eps) result (z)
        real(default), intent(in) :: x, eps
        real(default) :: z
    end function delta

<SM physics: procedures>+≡
    elemental module function delta (x,eps) result (z)
        real(default), intent(in) :: x, eps
        real(default) :: z
        if (x > one - eps) then
            z = one / eps
        else
            z = 0
        end if
    end function delta

```

The $+$ -distribution, $P_+(x) = \left(\frac{1}{1-x}\right)_+$, for the regularization of soft-collinear singularities. The constant part for the Monte-Carlo sampling is the integral over the splitting function divided by the weight for the WHIZARD numerical integration over the interval.

```

<SM physics: public>+≡
    public :: plus_distr

<SM physics: sub interfaces>+≡
    elemental module function plus_distr (x,eps) result (plusr)
        real(default), intent(in) :: x, eps
        real(default) :: plusd
    end function plus_distr

```

```

⟨SM physics: procedures⟩+=
  elemental module function plus_distr (x,eps) result (plusd)
    real(default), intent(in) :: x, eps
    real(default) :: plusd
    if (x > one - eps) then
      plusd = log(eps) / eps
    else
      plusd = one / (one - x)
    end if
  end function plus_distr

```

The splitting function in $D = 4$ dimensions, regularized as +-distributions if necessary:

$$P^{qq}(x) = P^{\bar{q}q}(x) = C_F \cdot \left(\frac{1+x^2}{1-x} \right)_+ \quad (9.15)$$

$$P^{qg}(x) = P^{\bar{q}g}(x) = C_F \cdot \frac{1+(1-x)^2}{x} \quad (9.16)$$

$$P^{gq}(x) = P^{g\bar{q}}(x) = T_R \cdot [x^2 + (1-x)^2] \quad (9.17)$$

$$\begin{aligned}
P^{gg}(x) = 2C_A \left[\left(\frac{1}{1-x} \right)_+ + \frac{1-x}{x} - 1 + x(1-x) \right] \\
+ \delta(1-x) \left(\frac{11}{6}C_A - \frac{2}{3}N_f T_R \right)
\end{aligned} \quad (9.18)$$

Since the number of flavors summed over in the gluon splitting function might depend on the physics case under consideration, it is implemented as an input variable.

```

⟨SM physics: public⟩+=
  public :: pqq

⟨SM physics: sub interfaces⟩+=
  elemental module function pqq (x,eps) result (pqqx)
    real(default), intent(in) :: x, eps
    real(default) :: pqqx
  end function pqq

⟨SM physics: procedures⟩+=
  elemental module function pqq (x,eps) result (pqqx)
    real(default), intent(in) :: x, eps
    real(default) :: pqqx
    if (x > (1.0_default - eps)) then
      pqqx = (eps - one) / two + two * log(eps) / eps - &
        three * (eps - one) / eps / two
    else
      pqqx = (one + x**2) / (one - x)
    end if
    pqqx = CF * pqqx
  end function pqq

⟨SM physics: public⟩+=
  public :: pgq

```



```

⟨SM physics: sub interfaces⟩+≡
    elemental module function pgq (x) result (pgqx)
        real(default), intent(in) :: x
        real(default) :: pgqx
    end function pgq

⟨SM physics: procedures⟩+≡
    elemental module function pgq (x) result (pgqx)
        real(default), intent(in) :: x
        real(default) :: pgqx
        pgqx = TR * (x**2 + (one - x)**2)
    end function pgq

⟨SM physics: public⟩+≡
    public :: pqg

⟨SM physics: sub interfaces⟩+≡
    elemental module function pqg (x) result (pqgx)
        real(default), intent(in) :: x
        real(default) :: pqgx
    end function pqg

⟨SM physics: procedures⟩+≡
    elemental module function pqg (x) result (pqgx)
        real(default), intent(in) :: x
        real(default) :: pqgx
        pqgx = CF * (one + (one - x)**2) / x
    end function pqg

⟨SM physics: public⟩+≡
    public :: pgg

⟨SM physics: sub interfaces⟩+≡
    elemental module function pgg (x, nf, eps) result (pggx)
        real(default), intent(in) :: x, nf, eps
        real(default) :: pggx
    end function pgg

⟨SM physics: procedures⟩+≡
    elemental module function pgg (x, nf, eps) result (pggx)
        real(default), intent(in) :: x, nf, eps
        real(default) :: pggx
        pggx = two * CA * ( plus_distr (x, eps) + (one-x)/x - one + &
            x*(one-x)) + delta (x, eps) * gamma_g(nf)
    end function pgg

```

For the qq and gg cases, there exist “regularized” versions of the splitting functions:

$$P_{\text{reg}}^{qq}(x) = -C_F \cdot (1 + x) \quad (9.19)$$

$$P_{\text{reg}}^{gg}(x) = 2C_A \left[\frac{1-x}{x} - 1 + x(1-x) \right] \quad (9.20)$$

```

⟨SM physics: public⟩+≡
    public :: pqq_reg

```

```

⟨SM physics: sub interfaces⟩+≡
  elemental module function pqq_reg (x) result (pqqregx)
    real(default), intent(in) :: x
    real(default) :: pqqregx
  end function pqq_reg

⟨SM physics: procedures⟩+≡
  elemental module function pqq_reg (x) result (pqqregx)
    real(default), intent(in) :: x
    real(default) :: pqqregx
    pqqregx = - CF * (one + x)
  end function pqq_reg

⟨SM physics: public⟩+≡
  public :: pgg_reg

⟨SM physics: sub interfaces⟩+≡
  elemental module function pgg_reg (x) result (pggregx)
    real(default), intent(in) :: x
    real(default) :: pggregx
  end function pgg_reg

⟨SM physics: procedures⟩+≡
  elemental module function pgg_reg (x) result (pggregx)
    real(default), intent(in) :: x
    real(default) :: pggregx
    pggregx = two * CA * ((one - x)/x - one + x*(one - x))
  end function pgg_reg

```

Here, we collect the expressions needed for integrated Catani-Seymour dipoles, and the so-called flavor kernels. We always distinguish between the “ordinary” Catani-Seymour version, and the one including a phase-space slicing parameter, α .

The standard flavor kernels \overline{K}^{ab} are:

$$\overline{K}^{qq}(x) = \overline{K}^{\bar{q}q}(x) = P^{qq}(x) \log((1-x)/x) + CF \times x \quad (9.21)$$

$$\overline{K}^{gq}(x) = \overline{K}^{g\bar{q}}(x) = P^{gq}(x) \log((1-x)/x) + TR \times 2x(1-x) \quad (9.22)$$

$$\begin{aligned} \overline{K}^{qq} = & C_F \left[\left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ - (1+x) \log((1-x)/x) + (1-x) \right] \\ & - (5 - \pi^2) \cdot C_F \cdot \delta(1-x) \end{aligned} \quad (9.23)$$

$$\begin{aligned} \overline{K}^{gg} = & 2C_A \left[\left(\frac{1}{1-x} \log \frac{1-x}{x} \right)_+ + \left(\frac{1-x}{x} - 1 + x(1-x) \right) \log((1-x)/x) \right] \\ & - \delta(1-x) \left[\left(\frac{50}{9} - \pi^2 \right) C_A - \frac{16}{9} T_R N_f \right] \end{aligned} \quad (9.24)$$

```

⟨SM physics: public⟩+≡
  public :: kbarqg

```

```

⟨SM physics: sub interfaces⟩+≡
  module function kbarqg (x) result (kbarqgx)
    real(default), intent(in) :: x
    real(default) :: kbarqgx
  end function kbarqg

```

```

<SM physics: procedures>+≡
  module function kbarqg (x) result (kbarqgx)
    real(default), intent(in) :: x
    real(default) :: kbarqgx
    kbarqgx = pqg(x) * log((one-x)/x) + CF * x
  end function kbarqg

<SM physics: public>+≡
  public :: kbarqg

<SM physics: sub interfaces>+≡
  module function kbargq (x) result (kbargqx)
    real(default), intent(in) :: x
    real(default) :: kbargqx
  end function kbargq

<SM physics: procedures>+≡
  module function kbargq (x) result (kbargqx)
    real(default), intent(in) :: x
    real(default) :: kbargqx
    kbargqx = pgq(x) * log((one-x)/x) + two * TR * x * (one - x)
  end function kbargq

<SM physics: public>+≡
  public :: kbarqq

<SM physics: sub interfaces>+≡
  module function kbarqq (x,eps) result (kbarqqx)
    real(default), intent(in) :: x, eps
    real(default) :: kbarqqx
  end function kbarqq

<SM physics: procedures>+≡
  module function kbarqq (x,eps) result (kbarqqx)
    real(default), intent(in) :: x, eps
    real(default) :: kbarqqx
    kbarqqx = CF*(log_plus_distr(x,eps) - (one+x) * log((one-x)/x) + (one - &
      x) - (five - pi**2) * delta(x,eps))
  end function kbarqq

<SM physics: public>+≡
  public :: kbargg

<SM physics: sub interfaces>+≡
  module function kbargg (x,eps,nf) result (kbarggx)
    real(default), intent(in) :: x, eps, nf
    real(default) :: kbarggx
  end function kbargg

<SM physics: procedures>+≡
  module function kbargg (x,eps,nf) result (kbarggx)
    real(default), intent(in) :: x, eps, nf
    real(default) :: kbarggx
    kbarggx = CA * (log_plus_distr(x,eps) + two * ((one-x)/x - one + &
      x*(one-x) * log((1-x)/x))) - delta(x,eps) * &
      ((50.0_default/9.0_default - pi**2) * CA - &

```

```

16.0_default/9.0_default * TR * nf)
end function kbargg

```

The \tilde{K} are used when two identified hadrons participate:

$$\tilde{K}^{ab}(x) = P_{\text{reg}}^{ab}(x) \cdot \log(1-x) + \delta^{ab} \mathbf{T}_a^2 \left[\left(\frac{2}{1-x} \log(1-x) \right)_+ - \frac{\pi^2}{3} \delta(1-x) \right] \quad (9.25)$$

```

⟨SM physics: public⟩+≡
  public :: ktildeqq

⟨SM physics: sub interfaces⟩+≡
  module function ktildeqq (x,eps) result (ktildeqqx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeqqx
  end function ktildeqq

⟨SM physics: procedures⟩+≡
  module function ktildeqq (x,eps) result (ktildeqqx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeqqx
    ktildeqqx = pqq_reg (x) * log(one-x) + CF * ( - log2_plus_distr (x,eps) &
      - pi**2/three * delta(x,eps))
  end function ktildeqq

⟨SM physics: public⟩+≡
  public :: ktildeqg

⟨SM physics: sub interfaces⟩+≡
  module function ktildeqg (x,eps) result (ktildeqgx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeqgx
  end function ktildeqg

⟨SM physics: procedures⟩+≡
  module function ktildeqg (x,eps) result (ktildeqgx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeqgx
    ktildeqgx = pqg (x) * log(one-x)
  end function ktildeqg

⟨SM physics: public⟩+≡
  public :: ktildegq

⟨SM physics: sub interfaces⟩+≡
  module function ktildegq (x,eps) result (ktildegqx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildegqx
  end function ktildegq

⟨SM physics: procedures⟩+≡
  module function ktildegq (x,eps) result (ktildegqx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildegqx
    ktildegqx = pgq (x) * log(one-x)
  end function ktildegq

```

```

⟨SM physics: public⟩+≡
  public :: ktildegg

⟨SM physics: sub interfaces⟩+≡
  module function ktildegg (x,eps) result (ktildeggx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeggx
  end function ktildegg

⟨SM physics: procedures⟩+≡
  module function ktildegg (x,eps) result (ktildeggx)
    real(default), intent(in) :: x, eps
    real(default) :: ktildeggx
    ktildeggx = pgg_reg (x) * log(one-x) + CA * ( - &
      log2_plus_distr (x,eps) - pi**2/three * delta(x,eps))
  end function ktildegg

```

The insertion operator might not be necessary for a GOLEM interface but is demanded by the Les Houches NLO accord. It is a three-dimensional array, where the index always gives the inverse power of the DREG expansion parameter, ϵ .

```

⟨SM physics: public⟩+≡
  public :: insert_q

⟨SM physics: sub interfaces⟩+≡
  pure module function insert_q () result (i_q)
    real(default), dimension(0:2) :: i_q
  end function insert_q

⟨SM physics: procedures⟩+≡
  pure module function insert_q () result (i_q)
    real(default), dimension(0:2) :: i_q
    i_q(0) = gamma_q + k_q - pi**2/three * CF
    i_q(1) = gamma_q
    i_q(2) = CF
  end function insert_q

⟨SM physics: public⟩+≡
  public :: insert_g

⟨SM physics: sub interfaces⟩+≡
  pure module function insert_g (nf) result (i_g)
    real(default), intent(in) :: nf
    real(default), dimension(0:2) :: i_g
  end function insert_g

⟨SM physics: procedures⟩+≡
  pure module function insert_g (nf) result (i_g)
    real(default), intent(in) :: nf
    real(default), dimension(0:2) :: i_g
    i_g(0) = gamma_g (nf) + k_g (nf) - pi**2/three * CA
    i_g(1) = gamma_g (nf)
    i_g(2) = CA
  end function insert_g

```

For better convergence, one can exclude regions of phase space with a slicing parameter from the dipole subtraction procedure. First of all, the K functions get modified:

$$K_i(\alpha) = K_i - \mathbf{T}_i^2 \log^2 \alpha + \gamma_i(\alpha - 1 - \log \alpha) \quad (9.26)$$

```

<SM physics: public>+≡
  public :: k_q_al, k_g_al

<SM physics: sub interfaces>+≡
  pure module function k_q_al (alpha)
    real(default), intent(in) :: alpha
    real(default) :: k_q_al
  end function k_q_al
  pure module function k_g_al (alpha, nf)
    real(default), intent(in) :: alpha, nf
    real(default) :: k_g_al
  end function k_g_al

<SM physics: procedures>+≡
  pure module function k_q_al (alpha)
    real(default), intent(in) :: alpha
    real(default) :: k_q_al
    k_q_al = k_q - CF * (log(alpha))**2 + gamma_q * &
      (alpha - one - log(alpha))
  end function k_q_al

  pure module function k_g_al (alpha, nf)
    real(default), intent(in) :: alpha, nf
    real(default) :: k_g_al
    k_g_al = k_g (nf) - CA * (log(alpha))**2 + gamma_g (nf) * &
      (alpha - one - log(alpha))
  end function k_g_al

```

The $+$ -distribution, but with a phase-space slicing parameter, α , $P_{1-\alpha}(x) = \left(\frac{1}{1-x}\right)_{1-x}$. Since we need the fatal error message here, this function cannot be elemental.

```

<SM physics: public>+≡
  public :: plus_distr_al

<SM physics: sub interfaces>+≡
  module function plus_distr_al (x,alpha,eps) result (plusd_al)
    real(default), intent(in) :: x, eps, alpha
    real(default) :: plusd_al
  end function plus_distr_al

<SM physics: procedures>+≡
  module function plus_distr_al (x,alpha,eps) result (plusd_al)
    real(default), intent(in) :: x, eps, alpha
    real(default) :: plusd_al
    if ((one - alpha) >= (one - eps)) then
      plusd_al = zero
      call msg_fatal ('sm_physics, plus_distr_al: alpha and epsilon chosen wrongly')
    elseif (x < (1.0_default - alpha)) then
      plusd_al = 0
    else if (x > (1.0_default - eps)) then

```

```

        plusd_al = log(eps/alpha)/eps
    else
        plusd_al = one/(one-x)
    end if
end function plus_distr_al

```

Introducing phase-space slicing parameters, these standard flavor kernels \overline{K}^{ab} become:

$$\overline{K}_\alpha^{qg}(x) = \overline{K}_\alpha^{\bar{q}g}(x) = P^{qg}(x) \log(\alpha(1-x)/x) + C_F \times x \quad (9.27)$$

$$\overline{K}_\alpha^{gq}(x) = \overline{K}_\alpha^{g\bar{q}}(x) = P^{gq}(x) \log(\alpha(1-x)/x) + T_R \times 2x(1-x) \quad (9.28)$$

$$\begin{aligned} \overline{K}_\alpha^{qq} = & C_F(1-x) + P_{\text{reg}}^{qq}(x) \log \frac{\alpha(1-x)}{x} \\ & + C_F \delta(1-x) \log^2 \alpha + C_F \left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ \\ & - \left(\gamma_q + K_q(\alpha) - \frac{5}{6} \pi^2 C_F \right) \cdot \delta(1-x) C_F \left[+ \frac{2}{1-x} \log \left(\frac{\alpha(2-x)}{1+\alpha-x} \right) - \theta(1-\alpha-x) \cdot \left(\frac{2}{1-x} \right) \right] \end{aligned} \quad (9.29)$$

$$\begin{aligned} \overline{K}_\alpha^{gg} = & P_{\text{reg}}^{gg}(x) \log \frac{\alpha(1-x)}{x} + C_A \delta(1-x) \log^2 \alpha \\ & + C_A \left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ - \left(\gamma_g + K_g(\alpha) - \frac{5}{6} \pi^2 C_A \right) \cdot \delta(1-x) C_A \left[+ \frac{2}{1-x} \log \left(\frac{\alpha(2-x)}{1+\alpha-x} \right) - \theta(1-\alpha-x) \cdot \left(\frac{2}{1-x} \right) \right] \end{aligned} \quad (9.30)$$

```

<SM physics: public>+≡
public :: kbarqg_al

<SM physics: sub interfaces>+≡
module function kbarqg_al (x,alpha,eps) result (kbarqgx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbarqgx
end function kbarqg_al

<SM physics: procedures>+≡
module function kbarqg_al (x,alpha,eps) result (kbarqgx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbarqgx
    kbarqgx = pqg (x) * log(alpha*(one-x)/x) + CF * x
end function kbarqg_al

<SM physics: public>+≡
public :: kbargq_al

<SM physics: sub interfaces>+≡
module function kbargq_al (x,alpha,eps) result (kbargqgx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbargqgx
end function kbargq_al

<SM physics: procedures>+≡
module function kbargq_al (x,alpha,eps) result (kbargqgx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbargqgx

```

```

    kbarqqx = pgq (x) * log(alpha*(one-x)/x) + two * TR * x * (one-x)
end function kbarqq_al

⟨SM physics: public⟩+≡
public :: kbarqq_al

⟨SM physics: sub interfaces⟩+≡
module function kbarqq_al (x,alpha,eps) result (kbarqqx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbarqqx
end function kbarqq_al

⟨SM physics: procedures⟩+≡
module function kbarqq_al (x,alpha,eps) result (kbarqqx)
    real(default), intent(in) :: x, alpha, eps
    real(default) :: kbarqqx
    kbarqqx = CF * (one - x) + pqq_reg(x) * log(alpha*(one-x)/x) &
        + CF * log_plus_distr(x,eps) &
        - (gamma_q + k_q_al(alpha) - CF * &
        five/6.0_default * pi**2 - CF * (log(alpha))**2) * &
        delta(x,eps) + &
        CF * two/(one -x)*log(alpha*(two-x)/(one+alpha-x))
    if (x < (one-alpha)) then
        kbarqqx = kbarqqx - CF * two/(one-x) * log((two-x)/(one-x))
    end if
end function kbarqq_al

⟨SM physics: public⟩+≡
public :: kbargg_al

⟨SM physics: sub interfaces⟩+≡
module function kbargg_al (x,alpha,eps,nf) result (kbarggx)
    real(default), intent(in) :: x, alpha, eps, nf
    real(default) :: kbarggx
end function kbargg_al

⟨SM physics: procedures⟩+≡
module function kbargg_al (x,alpha,eps,nf) result (kbarggx)
    real(default), intent(in) :: x, alpha, eps, nf
    real(default) :: kbarggx
    kbarggx = pgg_reg(x) * log(alpha*(one-x)/x) &
        + CA * log_plus_distr(x,eps) &
        - (gamma_g(nf) + k_g_al(alpha,nf) - CA * &
        five/6.0_default * pi**2 - CA * (log(alpha))**2) * &
        delta(x,eps) + &
        CA * two/(one -x)*log(alpha*(two-x)/(one+alpha-x))
    if (x < (one-alpha)) then
        kbarggx = kbarggx - CA * two/(one-x) * log((two-x)/(one-x))
    end if
end function kbargg_al

```

The \tilde{K} flavor kernels in the presence of a phase-space slicing parameter, are:

$$\tilde{K}^{ab}(x, \alpha) = P^{qq, \text{reg}}(x) \log \frac{1-x}{\alpha} + \dots \quad (9.31)$$

```

⟨SM physics: public⟩+≡
public :: ktildeqq_al

```



```

⟨SM physics: sub interfaces⟩+≡
  module function ktildeqq_al (x,alpha,eps) result (ktildeqqx)
    real(default), intent(in) :: x, eps, alpha
    real(default) :: ktildeqqx
  end function ktildeqq_al

⟨SM physics: procedures⟩+≡
  module function ktildeqq_al (x,alpha,eps) result (ktildeqqx)
    real(default), intent(in) :: x, eps, alpha
    real(default) :: ktildeqqx
    ktildeqqx = pqq_reg(x) * log((one-x)/alpha) + CF*( &
      - log2_plus_distr_al(x,alpha,eps) - Pi**2/three * delta(x,eps) &
      + (one+x**2)/(one-x) * log(min(one,(alpha/(one-x)))) &
      + two/(one-x) * log((one+alpha-x)/alpha))
    if (x > (one-alpha)) then
      ktildeqqx = ktildeqqx - CF*two/(one-x)*log(two-x)
    end if
  end function ktildeqq_al

```

This is a logarithmic +-distribution, $\left(\frac{\log((1-x)/x)}{1-x}\right)_+$. For the sampling, we need the integral over this function over the incomplete sampling interval $[0, 1 - \epsilon]$, which is $\log^2(x) + 2Li_2(x) - \frac{\pi^2}{3}$. As this function is negative definite for $\epsilon > 0.1816$, we take a hard upper limit for that sampling parameter, irrespective of the fact what the user chooses.

```

⟨SM physics: public⟩+≡
  public :: log_plus_distr

⟨SM physics: sub interfaces⟩+≡
  module function log_plus_distr (x,eps) result (lpd)
    real(default), intent(in) :: x, eps
    real(default) :: lpd, eps2
  end function log_plus_distr

⟨SM physics: procedures⟩+≡
  module function log_plus_distr (x,eps) result (lpd)
    real(default), intent(in) :: x, eps
    real(default) :: lpd, eps2
    eps2 = min (eps, 0.1816_default)
    if (x > (1.0_default - eps2)) then
      lpd = ((log(eps2))**2 + two*Li2(eps2) - pi**2/three)/eps2
    else
      lpd = two*log((one-x)/x)/(one-x)
    end if
  end function log_plus_distr

```

Logarithmic +-distribution, $2 \left(\frac{\log(1/(1-x))}{1-x}\right)_+$.

```

⟨SM physics: public⟩+≡
  public :: log2_plus_distr

⟨SM physics: sub interfaces⟩+≡
  module function log2_plus_distr (x,eps) result (lpd)
    real(default), intent(in) :: x, eps
    real(default) :: lpd
  end function log2_plus_distr

```

```

⟨SM physics: procedures⟩+≡
module function log2_plus_distr (x,eps) result (lpd)
  real(default), intent(in) :: x, eps
  real(default) :: lpd
  if (x > (1.0_default - eps)) then
    lpd = - (log(eps))**2/eps
  else
    lpd = two*log(one/(one-x))/(one-x)
  end if
end function log2_plus_distr

```

Logarithmic +-distribution with phase-space slicing parameter, $2 \left(\frac{\log(1/(1-x))}{1-x} \right)_{1-\alpha}$.

```

⟨SM physics: public⟩+≡
  public :: log2_plus_distr_al

⟨SM physics: sub interfaces⟩+≡
  module function log2_plus_distr_al (x,alpha,eps) result (lpd_al)
    real(default), intent(in) :: x, eps, alpha
    real(default) :: lpd_al
  end function log2_plus_distr_al

⟨SM physics: procedures⟩+≡
module function log2_plus_distr_al (x,alpha,eps) result (lpd_al)
  real(default), intent(in) :: x, eps, alpha
  real(default) :: lpd_al
  if ((one - alpha) >= (one - eps)) then
    lpd_al = zero
    call msg_fatal ('alpha and epsilon chosen wrongly')
  elseif (x < (one - alpha)) then
    lpd_al = 0
  elseif (x > (1.0_default - eps)) then
    lpd_al = - ((log(eps))**2 - (log(alpha))**2)/eps
  else
    lpd_al = two*log(one/(one-x))/(one-x)
  end if
end function log2_plus_distr_al

```

9.5.9 Splitting Functions

Analogue to the regularized distributions of the last subsection, we give here the unregularized splitting functions, relevant for the parton shower algorithm. We can use this unregularized version since there will be a cut-off ϵ that ensures that $\{z, 1-z\} > \epsilon(t)$. This cut-off separates resolvable from unresolvable emissions.

p_{xxx} are the kernels that are summed over helicity:

```

⟨SM physics: public⟩+≡
  public :: p_qqg
  public :: p_gqq
  public :: p_ggg

q → qq
⟨SM physics: sub interfaces⟩+≡
  elemental module function p_qqg (z) result (P)

```

```

        real(default), intent(in) :: z
        real(default) :: P
    end function p_qqg
<SM physics: procedures>+≡
    elemental module function p_qqg (z) result (P)
        real(default), intent(in) :: z
        real(default) :: P
        P = CF * (one + z**2) / (one - z)
    end function p_qqg

g → q $\bar{q}$ 
<SM physics: sub interfaces>+≡
    elemental module function p_gqq (z) result (P)
        real(default), intent(in) :: z
        real(default) :: P
    end function p_gqq
<SM physics: procedures>+≡
    elemental module function p_gqq (z) result (P)
        real(default), intent(in) :: z
        real(default) :: P
        P = TR * (z**2 + (one - z)**2)
    end function p_gqq

g → gg
<SM physics: sub interfaces>+≡
    elemental module function p_ggg (z) result (P)
        real(default), intent(in) :: z
        real(default) :: P
    end function p_ggg
<SM physics: procedures>+≡
    elemental module function p_ggg (z) result (P)
        real(default), intent(in) :: z
        real(default) :: P
        P = NC * ((one - z) / z + z / (one - z) + z * (one - z))
    end function p_ggg

Analytically integrated splitting kernels:
<SM physics: public>+≡
    public :: integral_over_p_qqg
    public :: integral_over_p_gqq
    public :: integral_over_p_ggg
<SM physics: sub interfaces>+≡
    pure module function integral_over_p_qqg (zmin, zmax) result (integral)
        real(default), intent(in) :: zmin, zmax
        real(default) :: integral
    end function integral_over_p_qqg
    pure module function integral_over_p_gqq (zmin, zmax) result (integral)
        real(default), intent(in) :: zmin, zmax
        real(default) :: integral
    end function integral_over_p_gqq
    pure module function integral_over_p_ggg (zmin, zmax) result (integral)
        real(default), intent(in) :: zmin, zmax

```

```

        real(default) :: integral
    end function integral_over_p_ggg

<SM physics: procedures>+≡
pure module function integral_over_p_qqg (zmin, zmax) result (integral)
    real(default), intent(in) :: zmin, zmax
    real(default) :: integral
    integral = (two / three) * (- zmax**2 + zmin**2 - &
        two * (zmax - zmin) + four * log((one - zmin) / (one - zmax)))
end function integral_over_p_qqg

pure module function integral_over_p_gqq (zmin, zmax) result (integral)
    real(default), intent(in) :: zmin, zmax
    real(default) :: integral
    integral = 0.5_default * ((two / three) * &
        (zmax**3 - zmin**3) - (zmax**2 - zmin**2) + (zmax - zmin))
end function integral_over_p_gqq

pure module function integral_over_p_ggg (zmin, zmax) result (integral)
    real(default), intent(in) :: zmin, zmax
    real(default) :: integral
    integral = three * ((log(zmax) - two * zmax - &
        log(one - zmax) + zmax**2 / two - zmax**3 / three) - &
        (log(zmin) - zmin - zmin - log(one - zmin) + zmin**2 &
        / two - zmin**3 / three) )
end function integral_over_p_ggg

```

We can also use (massless) helicity dependent splitting functions:

```

<SM physics: public>+≡
    public :: p_qqg_pol

 $q_a \rightarrow q_b g_c$ , the helicity of the quark is not changed by gluon emission and the
gluon is preferably polarized in the branching plane ( $l_c = 1$ ):

<SM physics: sub interfaces>+≡
    elemental module function p_qqg_pol (z, l_a, l_b, l_c) result (P)
        real(default), intent(in) :: z
        integer, intent(in) :: l_a, l_b, l_c
        real(default) :: P
    end function p_qqg_pol

<SM physics: procedures>+≡
    elemental module function p_qqg_pol (z, l_a, l_b, l_c) result (P)
        real(default), intent(in) :: z
        integer, intent(in) :: l_a, l_b, l_c
        real(default) :: P
        if (l_a /= l_b) then
            P = zero
            return
        end if
        if (l_c == -1) then
            P = one - z
        else
            P = (one + z)**2 / (one - z)
        end if
        P = P * CF

```

```
end function p_qqg_pol
```

Mellin transforms of splitting functions

As Mellin transforms necessarily live in the complex plane, all functions are defined as complex functions: Splitting function $P_{qq}(N)$:

```
<SM physics: public>+≡
  public :: pqqm

<SM physics: sub interfaces>+≡
  module function pqqm (n, c_f) result (pqq_m)
    integer, intent(in) :: n
    real(default), intent(in) :: c_f
    complex(default) :: pqq_m
  end function pqqm

<SM physics: procedures>+≡
  module function pqqm (n, c_f) result (pqq_m)
    integer, intent(in) :: n
    real(default), intent(in) :: c_f
    complex(default) :: pqq_m
    pqq_m = three - four * (eulerc + &
      psic(cmplx(N+1,zero,kind=default))) + two/N/(N+1)
  end function pqqm
```

9.5.10 Top width

In order to produce sensible results, the widths have to be recomputed for each parameter and order. We start with the LO-expression for the top width given by the decay $t \rightarrow W^+, b$, cf. doi:10.1016/0550-3213(91)90530-B:

The analytic formula given there is

$$\Gamma = \frac{G_F m_t^2}{16\sqrt{2}\pi} \left[\mathcal{F}_0(\varepsilon, \xi^{-1/2}) - \frac{2\alpha_s}{3\pi} \mathcal{F}_1(\varepsilon, \xi^{-1/2}) \right],$$

with

$$\begin{aligned} \mathcal{F}_0 &= \frac{\sqrt{\lambda}}{2} f_0, \\ f_0 &= 4 \left[(1 - \varepsilon^2)^2 + w^2(1 + \varepsilon^2) - 2w^4 \right], \\ \lambda &= 1 + w^4 + \varepsilon^4 - 2(w^2 + \varepsilon^2 + w^2\varepsilon^2). \end{aligned}$$

Defining

$$u_q = \frac{1 + \varepsilon^2 - w^2 - \lambda^{1/2}}{1 + \varepsilon^2 - w^2 + \lambda^{1/2}}$$

and

$$u_w = \frac{1 - \varepsilon^2 + w^2 - \lambda^{1/2}}{1 - \varepsilon^2 + w^2 + \lambda^{1/2}}$$

the factor \mathcal{F}_1 can be expressed as

$$\begin{aligned}\mathcal{F}_1 = & \frac{1}{2}f_0(1 + \varepsilon^2 - w^2) \left[\pi^2 + 2Li_2(u_w) - 2Li_2(1 - u_w) - 4Li_2(u_q) \right. \\ & - 4Li_2(u_q u_w) + \log\left(\frac{1 - u_q}{w^2}\right) \log(1 - u_q) - \log^2(1 - u_q u_w) \\ & + \frac{1}{4} \log^2\left(\frac{w^2}{u_w}\right) - \log(u_w) \log\left[\frac{(1 - u_q u_w)^2}{1 - u_q}\right] - 2 \log(u_q) \log[(1 - u_q)(1 - u_q u_w)] \Big] \\ & - \sqrt{\lambda} f_0 (2 \log(w) + 3 \log(\varepsilon) - 2 \log \lambda) \\ & + 4(1 - \varepsilon^2) [(1 - \varepsilon^2)^2 + w^2(1 + \varepsilon^2) - 4w^4] \log(u_w) \\ & [(3 - \varepsilon^2 + 11\varepsilon^4 - \varepsilon^6) + w^2(6 - 12\varepsilon^2 + 2\varepsilon^4) - w^4(21 + 5\varepsilon^2) + 12w^6] \log(u_q) \\ & \left. 6\sqrt{\lambda}(1 - \varepsilon^2)(1 + \varepsilon^2 - w^2) \log(\varepsilon) + \sqrt{\lambda} [-5 + 22\varepsilon^2 - 5\varepsilon^4 - 9w^2(1 + \varepsilon^2) + 6w^4] \right].\end{aligned}$$

```

<SM physics: public>+≡
  public :: top_width_sm_lo

<SM physics: sub interfaces>+≡
  elemental module function top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb) &
    result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb
  end function top_width_sm_lo

<SM physics: procedures>+≡
  elemental module function top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb) &
    result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb
    real(default) :: kappa
    kappa = sqrt ((mtop**2 - (mw + mb)**2) * (mtop**2 - (mw - mb)**2))
    gamma = alpha / four * mtop / (two * sinthw**2) * &
      vtb**2 * kappa / mtop**2 * &
      ((mtop**2 + mb**2) / (two * mtop**2) + &
      (mtop**2 - mb**2)**2 / (two * mtop**2 * mw**2) - &
      mw**2 / mtop**2)
  end function top_width_sm_lo

<SM physics: public>+≡
  public :: g_mu_from_alpha

<SM physics: sub interfaces>+≡
  elemental module function g_mu_from_alpha (alpha, mw, sinthw) result (g_mu)
    real(default) :: g_mu
    real(default), intent(in) :: alpha, mw, sinthw
  end function g_mu_from_alpha

<SM physics: procedures>+≡
  elemental module function g_mu_from_alpha (alpha, mw, sinthw) result (g_mu)
    real(default) :: g_mu
    real(default), intent(in) :: alpha, mw, sinthw
    g_mu = pi * alpha / sqrt(two) / mw**2 / sinthw**2
  end function g_mu_from_alpha

```

```

<SM physics: public>+≡
  public :: alpha_from_g_mu

<SM physics: sub interfaces>+≡
  elemental module function alpha_from_g_mu (g_mu, mw, sinhw) result (alpha)
    real(default) :: alpha
    real(default), intent(in) :: g_mu, mw, sinhw
  end function alpha_from_g_mu

<SM physics: procedures>+≡
  elemental module function alpha_from_g_mu (g_mu, mw, sinhw) result (alpha)
    real(default) :: alpha
    real(default), intent(in) :: g_mu, mw, sinhw
    alpha = g_mu * sqrt(two) / pi * mw**2 * sinhw**2
  end function alpha_from_g_mu

```

Cf. (3.3)-(3.7) in 1207.5018.

```

<SM physics: public>+≡
  public :: top_width_sm_qcd_nlo_massless_b

<SM physics: sub interfaces>+≡
  elemental module function top_width_sm_qcd_nlo_massless_b &
    (alpha, sinhw, vtb, mtop, mw, alphas) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinhw, vtb, mtop, mw, alphas
  end function top_width_sm_qcd_nlo_massless_b

<SM physics: procedures>+≡
  elemental module function top_width_sm_qcd_nlo_massless_b &
    (alpha, sinhw, vtb, mtop, mw, alphas) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinhw, vtb, mtop, mw, alphas
    real(default) :: prefac, g_mu, w2
    g_mu = g_mu_from_alpha (alpha, mw, sinhw)
    prefac = g_mu * mtop**3 * vtb**2 / (16 * sqrt(two) * pi)
    w2 = mw**2 / mtop**2
    gamma = prefac * (f0 (w2) - (two * alphas) / (3 * Pi) * f1 (w2))
  end function top_width_sm_qcd_nlo_massless_b

```

```

<SM physics: public>+≡
  public :: f0

<SM physics: sub interfaces>+≡
  elemental module function f0 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
  end function f0

<SM physics: procedures>+≡
  elemental module function f0 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
    f = two * (one - w2)**2 * (1 + 2 * w2)
  end function f0

```

```

<SM physics: public>+≡
  public :: f1

<SM physics: sub interfaces>+≡
  elemental module function f1 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
  end function f1

<SM physics: procedures>+≡
  elemental module function f1 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
    f = f0 (w2) * (pi**2 + two * Li2 (w2) - two * Li2 (one - w2)) &
      + four * w2 * (one - w2 - two * w2**2) * log (w2) &
      + two * (one - w2)**2 * (five + four * w2) * log (one - w2) &
      - (one - w2) * (five + 9 * w2 - 6 * w2**2)
  end function f1

```

Basically, the same as above but with m_b dependence, cf. Jezabek / Kuehn 1989.

```

<SM physics: public>+≡
  public :: top_width_sm_qcd_nlo_jk

<SM physics: sub interfaces>+≡
  elemental module function top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alphas
  end function top_width_sm_qcd_nlo_jk

<SM physics: procedures>+≡
  elemental module function top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alphas
    real(default) :: prefac, g_mu, eps2, i_xi
    g_mu = g_mu_from_alpha (alpha, mw, sinthw)
    prefac = g_mu * mtop**3 * vtb**2 / (16 * sqrt(two) * pi)
    eps2 = (mb / mtop)**2
    i_xi = (mw / mtop)**2
    gamma = prefac * (ff0 (eps2, i_xi) - &
      (two * alphas) / (3 * Pi) * ff1 (eps2, i_xi))
  end function top_width_sm_qcd_nlo_jk

```

Same as above, $m_b > 0$, with the slightly different implementation (2.6) of arXiv:1204.1513v1 by Campbell and Ellis.

```

<SM physics: public>+≡
  public :: top_width_sm_qcd_nlo_ce

<SM physics: sub interfaces>+≡
  elemental module function top_width_sm_qcd_nlo_ce &
    (alpha, sinthw, vtb, mtop, mw, mb, alpha_s) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alpha_s
  end function top_width_sm_qcd_nlo_ce

```


<SM physics: procedures>+≡

```

elemental module function top_width_sm_qcd_nlo_ce &
  (alpha, sinthw, vtb, mtop, mw, mb, alpha_s) result (gamma)
  real(default) :: gamma
  real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alpha_s
  real(default) :: pm, pp, p0, p3
  real(default) :: yw, yp
  real(default) :: W0, Wp, Wm, w2
  real(default) :: beta2
  real(default) :: f
  real(default) :: g_mu, gamma0
  beta2 = (mb / mtop)**2
  w2 = (mw / mtop)**2
  p0 = (one - w2 + beta2) / two
  p3 = sqrt (lambda (one, w2, beta2)) / two
  pp = p0 + p3
  pm = p0 - p3
  W0 = (one + w2 - beta2) / two
  Wp = W0 + p3
  Wm = W0 - p3
  yp = log (pp / pm) / two
  yw = log (Wp / Wm) / two
  f = (one - beta2)**2 + w2 * (one + beta2) - two * w2**2
  g_mu = g_mu_from_alpha (alpha, mw, sinthw)
  gamma0 = g_mu * mtop**3 * vtb**2 / (8 * pi * sqrt(two))
  gamma = gamma0 * alpha_s / twopi * CF * &
    (8 * f * p0 * (Li2(one - pm) - Li2(one - pp) - two * Li2(one - pm / pp) &
      + yp * log((four * p3**2) / (pp**2 * Wp)) + yw * log (pp)) &
      + four * (one - beta2) * ((one - beta2)**2 + w2 * (one + beta2) - four * w2**2) * yw &
      + (3 - beta2 + 11 * beta2**2 - beta2**3 + w2 * (6 - 12 * beta2 + two * beta2**2) &
        - w2**2 * (21 + 5 * beta2) + 12 * w2**3) * yp &
      + 8 * f * p3 * log (sqrt(w2) / (four * p3**2)) &
      + 6 * (one - four * beta2 + 3 * beta2**2 + w2 * (3 + beta2) - four * w2**2) * p3 * log(sq
      + (5 - 22 * beta2 + 5 * beta2**2 + 9 * w2 * (one + beta2) - 6 * w2**2) * p3)
end function top_width_sm_qcd_nlo_ce

```

<SM physics: public>+≡

```

public :: ff0

```

<SM physics: sub interfaces>+≡

```

elemental module function ff0 (eps2, w2) result (f)
  real(default) :: f
  real(default), intent(in) :: eps2, w2
end function ff0

```

<SM physics: procedures>+≡

```

elemental module function ff0 (eps2, w2) result (f)
  real(default) :: f
  real(default), intent(in) :: eps2, w2
  f = one / two * sqrt(ff_lambda (eps2, w2)) * ff_f0 (eps2, w2)
end function ff0

```

<SM physics: public>+≡

```

public :: ff_f0

```

```

<SM physics: sub interfaces>+≡
    elemental module function ff_f0 (eps2, w2) result (f)
        real(default) :: f
        real(default), intent(in) :: eps2, w2
    end function ff_f0

<SM physics: procedures>+≡
    elemental module function ff_f0 (eps2, w2) result (f)
        real(default) :: f
        real(default), intent(in) :: eps2, w2
        f = four * ((1 - eps2)**2 + w2 * (1 + eps2) - 2 * w2**2)
    end function ff_f0

<SM physics: public>+≡
    public :: ff_lambda

<SM physics: sub interfaces>+≡
    elemental module function ff_lambda (eps2, w2) result (l)
        real(default) :: l
        real(default), intent(in) :: eps2, w2
    end function ff_lambda

<SM physics: procedures>+≡
    elemental module function ff_lambda (eps2, w2) result (l)
        real(default) :: l
        real(default), intent(in) :: eps2, w2
        l = one + w2**2 + eps2**2 - two * (w2 + eps2 + w2 * eps2)
    end function ff_lambda

<SM physics: public>+≡
    public :: ff1

<SM physics: sub interfaces>+≡
    elemental module function ff1 (eps2, w2) result (f)
        real(default) :: f
        real(default), intent(in) :: eps2, w2
    end function ff1

<SM physics: procedures>+≡
    elemental module function ff1 (eps2, w2) result (f)
        real(default) :: f
        real(default), intent(in) :: eps2, w2
        real(default) :: uq, uw, sq_lam, fff
        sq_lam = sqrt (ff_lambda (eps2, w2))
        fff = ff_f0 (eps2, w2)
        uw = (one - eps2 + w2 - sq_lam) / &
            (one - eps2 + w2 + sq_lam)
        uq = (one + eps2 - w2 - sq_lam) / &
            (one + eps2 - w2 + sq_lam)
        f = one / two * fff * (one + eps2 - w2) * &
            (pi**2 + two * Li2 (uw) - two * Li2 (one - uw) - four * Li2 (uq) &
            - four * Li2 (uq * uw) + log ((one - uq) / w2) * log (one - uq) &
            - log (one - uq * uw)**2 + one / four * log (w2 / uw)**2 &
            - log (uw) * log ((one - uq * uw)**2 / (one - uq)) &
            - two * log (uq) * log ((one - uq) * (one - uq * uw))) &
            - sq_lam * fff * (two * log (sqrt (w2))) &

```

```

+ three * log (sqrt (eps2)) - two * log (sq_lam**2)) &
+ four * (one - eps2) * ((one - eps2)**2 + w2 * (one + eps2) &
- four * w2**2) * log (uw) &
+ (three - eps2 + 11 * eps2**2 - eps2**3 + w2 * &
(6 - 12 * eps2 + 2 * eps2**2) - w2**2 * (21 + five * eps2) &
+ 12 * w2**3) * log (uq) &
+ 6 * sq_lam * (one - eps2) * &
(one + eps2 - w2) * log (sqrt (eps2)) &
+ sq_lam * (- five + 22 * eps2 - five * eps2**2 - 9 * w2 * &
(one + eps2) + 6 * w2**2)
end function ff1

```

9.5.11 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sm_physics_ut.f90⟩≡
  ⟨File header⟩

  module sm_physics_ut
    use unit_tests
    use sm_physics_uti

    ⟨Standard module head⟩

    ⟨SM physics: public test⟩

    contains

    ⟨SM physics: test driver⟩

  end module sm_physics_ut

⟨sm_physics_uti.f90⟩≡
  ⟨File header⟩

  module sm_physics_uti

    ⟨Use kinds⟩
    use numeric_utils
    use format_defs, only: FMT_15
    use constants

    use sm_physics

    ⟨Standard module head⟩

    ⟨SM physics: test declarations⟩

    contains

    ⟨SM physics: tests⟩

  end module sm_physics_uti

```

API: driver for the unit tests below.

```

<SM physics: public test>≡
  public :: sm_physics_test

<SM physics: test driver>≡
  subroutine sm_physics_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SM physics: execute tests>
  end subroutine sm_physics_test

```

Splitting functions

```

<SM physics: execute tests>≡
  call test (sm_physics_1, "sm_physics_1", &
    "Splitting functions", &
    u, results)

<SM physics: test declarations>≡
  public :: sm_physics_1

<SM physics: tests>≡
  subroutine sm_physics_1 (u)
    integer, intent(in) :: u
    real(default) :: z = 0.75_default

    write (u, "(A)")  "* Test output: sm_physics_1"
    write (u, "(A)")  "* Purpose: check analytic properties"
    write (u, "(A)")

    write (u, "(A)")  "* Splitting functions:"
    write (u, "(A)")

    call assert (u, vanishes (p_qqg_pol (z, +1, -1, +1)), "+-+")
    call assert (u, vanishes (p_qqg_pol (z, +1, -1, -1)), "+-")
    call assert (u, vanishes (p_qqg_pol (z, -1, +1, +1)), "-++")
    call assert (u, vanishes (p_qqg_pol (z, -1, +1, -1)), "-+-")

    !call assert (u, nearly_equal ( &
      !p_qqg_pol (z, +1, +1, -1) + p_qqg_pol (z, +1, +1, +1), &
      !p_qqg (z)), "pol sum")

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sm_physics_1"

  end subroutine sm_physics_1

```

Top width

```

<SM physics: execute tests>+≡
  call test(sm_physics_2, "sm_physics_2", &
    "Top width", u, results)

```

```

<SM physics: test declarations>+≡
    public :: sm_physics_2

<SM physics: tests>+≡
    subroutine sm_physics_2 (u)
        integer, intent(in) :: u
        real(default) :: mtop, mw, mz, mb, g_mu, sinthw, alpha, vtb, gamma0
        real(default) :: w2, alphas, alphas_mz, gamma1
        write (u, "(A)")  "* Test output: sm_physics_2"
        write (u, "(A)")  "* Purpose: Check different top width computations"
        write (u, "(A)")

        write (u, "(A)")  "* Values from [[1207.5018]] (massless b)"
        mtop = 172.0
        mw = 80.399
        mz = 91.1876
        mb = zero
        mb = 0.00001
        g_mu = 1.16637E-5
        sinthw = sqrt(one - mw**2 / mz**2)
        alpha = alpha_from_g_mu (g_mu, mw, sinthw)
        vtb = one
        w2 = mw**2 / mtop**2

        write (u, "(A)")  "* Check Li2 implementation"
        call assert_equal (u, Li2(w2), 0.2317566263959552_default, &
            "Li2(w2)", rel_smallness=1.0E-6_default)
        call assert_equal (u, Li2(one - w2), 1.038200378935867_default, &
            "Li2(one - w2)", rel_smallness=1.0E-6_default)

        write (u, "(A)")  "* Check LO Width"
        gamma0 = top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb)
        call assert_equal (u, gamma0, 1.4655_default, &
            "top_width_sm_lo", rel_smallness=1.0E-5_default)
        alphas = zero
        gamma0 = top_width_sm_qcd_nlo_massless_b &
            (alpha, sinthw, vtb, mtop, mw, alphas)
        call assert_equal (u, gamma0, 1.4655_default, &
            "top_width_sm_qcd_nlo_massless_b", rel_smallness=1.0E-5_default)
        gamma0 = top_width_sm_qcd_nlo_jk &
            (alpha, sinthw, vtb, mtop, mw, mb, alphas)
        call assert_equal (u, gamma0, 1.4655_default, &
            "top_width_sm_qcd_nlo", rel_smallness=1.0E-5_default)

        write (u, "(A)")  "* Check NLO Width"
        alphas_mz = 0.1202      ! MSTW2008 NLO fit
        alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
        gamma1 = top_width_sm_qcd_nlo_massless_b &
            (alpha, sinthw, vtb, mtop, mw, alphas)
        call assert_equal (u, gamma1, 1.3376_default, rel_smallness=1.0E-4_default)
        gamma1 = top_width_sm_qcd_nlo_jk &
            (alpha, sinthw, vtb, mtop, mw, mb, alphas)
        ! It would be nice to get one more significant digit but the
        ! expression is numerically rather unstable for mb -> 0
        call assert_equal (u, gamma1, 1.3376_default, rel_smallness=1.0E-3_default)
    end subroutine sm_physics_2

```

```

write (u, "(A)")  "*"  Values from threshold validation (massive b)"
alpha = one / 125.924
! ee = 0.315901
! cw = 0.881903
! v = 240.024
mtop = 172.0 ! This is the value for M1S !!!
mb = 4.2
sinthw = 0.47143
mz = 91.188
mw = 80.419
call assert_equal (u, sqrt(one - mw**2 / mz**2), sinthw, &
    "sinthw", rel_smallness=1.0E-6_default)

write (u, "(A)")  "*"  Check LO Width"
gamma0 = top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb)
call assert_equal (u, gamma0, 1.5386446_default, &
    "gamma0", rel_smallness=1.0E-7_default)
alphas = zero
gamma0 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
call assert_equal (u, gamma0, 1.5386446_default, &
    "gamma0", rel_smallness=1.0E-7_default)

write (u, "(A)")  "*"  Check NLO Width"
alphas_mz = 0.118 !(Z pole, NLL running to mu_h)
alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
write (u, "(A," // FMT_15 // ")")  "*"  alphas = ", alphas
gamma1 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
write (u, "(A," // FMT_15 // ")")  "*"  Gamma1 = ", gamma1

mb = zero
gamma1 = top_width_sm_qcd_nlo_massless_b &
    (alpha, sinthw, vtb, mtop, mw, alphas)
alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
write (u, "(A," // FMT_15 // ")")  "*"  Gamma1(mb=0) = ", gamma1

write (u, "(A)")
write (u, "(A)")  "*" Test output end: sm_physics_2"
end subroutine sm_physics_2

```

Special functions

```

<SM physics: execute tests>+≡
    call test (sm_physics_3, "sm_physics_3", &
        "Special functions", &
        u, results)

<SM physics: test declarations>+≡
    public :: sm_physics_3

<SM physics: tests>+≡
    subroutine sm_physics_3 (u)

```

```

integer, intent(in) :: u
complex(default) :: z1 = (0.75_default, 1.25_default)
complex(default) :: z2 = (1.33_default, 11.25_default)
complex(default) :: psiz
real(default) :: x1 = 0.045847700_default
real(default) :: psir

write (u, "(A)")  "* Test output: sm_physics_3"
write (u, "(A)")  "* Purpose: check special functions"
write (u, "(A)")

write (u, "(A)")  "* Complex digamma function:"
write (u, "(A)")

psiz = psic (z1)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F7.5,',',F7.5,')')") " psi(z1) = ", &
    real(psiz), aimag(psiz)
psiz = psic (z2)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F7.5,',',F7.5,')')") " psi(z2) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")
write (u, "(A)")  "* Complex polygamma function:"
write (u, "(A)")

psiz = psim (z1,1)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z1,1) = ", &
    real(psiz), aimag(psiz)
psiz = psim (z2,1)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z2,1) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")

psiz = psim (z1,2)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z1,2) = ", &
    real(psiz), aimag(psiz)
psiz = psim (z2,2)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z2,2) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")

```

```

psiz = psim (z1,3)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z1,3) = ", &
    real(psiz), aimag(psiz)
psiz = psim (z2,3)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z2,3) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")

psiz = psim (z1,4)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z1,4) = ", &
    real(psiz), aimag(psiz)
psiz = psim (z2,4)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z2,4) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")

psiz = psim (z1,5)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z1      = ", &
    real(z1), aimag(z1)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z1,5) = ", &
    real(psiz), aimag(psiz)
psiz = psim (z2,5)
write (u, "(1x,A,'(,F5.2,',',F5.2,')')") " z2      = ", &
    real(z2), aimag(z2)
write (u, "(1x,A,'(,F8.5,',',F8.5,')')") " psi(z2,5) = ", &
    real(psiz), aimag(psiz)

write (u, "(A)")
write (u, "(A)")  "* Real polygamma function:"
write (u, "(A)")

psir = psimr (x1,1)
write (u, "(1x,A,'(,F8.5,')')") " x1      = ", x1
write (u, "(1x,A,'(,F8.4,')')") " psir     = ", psir

write (u, "(A)")
write (u, "(A)")  "* Generalized Nielsen polylogarithm:"
write (u, "(A)")

write (u, "(1x,A,F8.5)") " S(1,1,0) = ", &
    nielsen(1,1,0._default)
write (u, "(1x,A,F8.5)") " S(1,1,-1) = ", &
    nielsen(1,1,-1._default)

```



```

write (u, "(1x,A,F8.5)" " S(1,2,-1) = ", &
      nielsen(1,2,-1._default)
write (u, "(1x,A,F8.5)" " S(2,1,-1) = ", &
      nielsen(2,1,-1._default)
write (u, "(1x,A,F8.5)" " S(1,3,-1) = ", &
      nielsen(1,3,-1._default)
write (u, "(1x,A,F8.5)" " S(2,2,-1) = ", &
      nielsen(2,2,-1._default)
write (u, "(1x,A,F8.5)" " S(3,1,-1) = ", &
      nielsen(3,1,-1._default)
write (u, "(1x,A,F8.5)" " S(1,4,-1) = ", &
      nielsen(1,4,-1._default)
write (u, "(1x,A,F8.5)" " S(2,3,-1) = ", &
      nielsen(2,3,-1._default)
write (u, "(1x,A,F8.5)" " S(3,2,-1) = ", &
      nielsen(3,2,-1._default)
write (u, "(1x,A,F8.5)" " S(4,1,-1) = ", &
      nielsen(4,1,-1._default)
write (u, "(1x,A,F8.5)" " S(1,1,0.2) = ", &
      nielsen(1,1,0.2_default)
write (u, "(1x,A,F8.5)" " S(1,2,0.2) = ", &
      nielsen(1,2,0.2_default)
write (u, "(1x,A,F8.5)" " S(2,1,0.2) = ", &
      nielsen(2,1,0.2_default)
write (u, "(1x,A,F8.5)" " S(1,3,0.2) = ", &
      nielsen(1,3,0.2_default)
write (u, "(1x,A,F8.5)" " S(2,2,0.2) = ", &
      nielsen(2,2,0.2_default)
write (u, "(1x,A,F8.5)" " S(3,1,0.2) = ", &
      nielsen(3,1,0.2_default)
write (u, "(1x,A,F8.5)" " S(1,4,0.2) = ", &
      nielsen(1,4,0.2_default)
write (u, "(1x,A,F8.5)" " S(2,3,0.2) = ", &
      nielsen(2,3,0.2_default)
write (u, "(1x,A,F8.5)" " S(3,2,0.2) = ", &
      nielsen(3,2,0.2_default)
write (u, "(1x,A,F8.5)" " S(4,1,0.2) = ", &
      nielsen(4,1,0.2_default)
write (u, "(1x,A,F8.5)" " S(1,1,1) = ", &
      nielsen(1,1,1._default)
write (u, "(1x,A,F8.5)" " S(1,2,1) = ", &
      nielsen(1,2,1._default)
write (u, "(1x,A,F8.5)" " S(2,1,1) = ", &
      nielsen(2,1,1._default)
write (u, "(1x,A,F8.5)" " S(1,3,1) = ", &
      nielsen(1,3,1._default)
write (u, "(1x,A,F8.5)" " S(2,2,1) = ", &
      nielsen(2,2,1._default)
write (u, "(1x,A,F8.5)" " S(3,1,1) = ", &
      nielsen(3,1,1._default)
write (u, "(1x,A,F8.5)" " S(1,4,1) = ", &
      nielsen(1,4,1._default)
write (u, "(1x,A,F8.5)" " S(2,3,1) = ", &
      nielsen(2,3,1._default)

```

```

write (u, "(1x,A,F8.5)") " S(3,2,1) = ", &
    nielsen(3,2,1._default)
write (u, "(1x,A,F8.5)") " S(4,1,1) = ", &
    nielsen(4,1,1._default)
write (u, "(1x,A,F8.5)") " S(1,1,0.75) = ", &
    nielsen(1,1,0.75_default)
write (u, "(1x,A,F8.5)") " S(1,3,0.75) = ", &
    nielsen(1,3,0.75_default)
write (u, "(1x,A,F8.5)") " S(1,4,0.75) = ", &
    nielsen(1,4,0.75_default)
write (u, "(1x,A,F8.5)") " S(2,2,0.75) = ", &
    nielsen(2,2,0.75_default)
write (u, "(1x,A,'(',F8.5,',',F8.5,')')") " S(1,1,2) = ", &
    real(cnielsen(1,1,3._default)), &
    aimag(cnielsen(1,1,3._default))

write (u, "(A)")
write (u, "(A)") "* Dilog, trilog, polylog:"
write (u, "(A)")

write (u, "(1x,A,F8.5)") " Li2(0.66) = ", &
    dilog(0.66_default)
write (u, "(1x,A,F8.5)") " Li3(0.66) = ", &
    trilog(0.66_default)
write (u, "(1x,A,F8.5)") " Poly(4,0.66) = ", &
    polylog(4,0.66_default)

write (u, "(A)")
write (u, "(A)") "* Test output end: sm_physics_3"

end subroutine sm_physics_3

```

9.6 QCD Coupling

We provide various distinct implementations of the QCD coupling. In this module, we define an abstract data type and three implementations: fixed, running with $\alpha_s(M_Z)$ as input, and running with Λ_{QCD} as input. We use the functions defined above in the module `sm_physics` but provide a common interface. Later modules may define additional implementations.

```
<sm_qcd.f90>≡  
  <File header>  
  
  module sm_qcd  
  
    <Use kinds>  
    use physics_defs  
  
    <Standard module head>  
  
    <SM qcd: public>  
  
    <SM qcd: types>  
  
    <SM qcd: interfaces>  
  
    interface  
    <SM qcd: sub interfaces>  
    end interface  
  
  end module sm_qcd  
<sm_qcd_sub.f90>≡  
  <File header>  
  
  submodule (sm_qcd) sm_qcd_s  
  
    use io_units  
    use format_defs, only: FMT_12  
    use numeric_utils  
    use diagnostics  
    use md5  
    use sm_physics  
  
    implicit none  
  
    contains  
  
    <SM qcd: procedures>  
  
  end submodule sm_qcd_s
```

9.6.1 Coupling: Abstract Data Type

This is the abstract version of the QCD coupling implementation.

```
<SM qcd: public>≡
```

```

    public :: alpha_qcd_t
  <SM qcd: types>≡
    type, abstract :: alpha_qcd_t
    contains
    <SM qcd: alpha qcd: TBP>
  end type alpha_qcd_t

```

There must be an output routine.

```

  <SM qcd: alpha qcd: TBP>≡
    procedure (alpha_qcd_write), deferred :: write
  <SM qcd: interfaces>≡
    abstract interface
      subroutine alpha_qcd_write (object, unit)
        import
        class(alpha_qcd_t), intent(in) :: object
        integer, intent(in), optional :: unit
      end subroutine alpha_qcd_write
    end interface

```

This method computes the running coupling, given a certain scale. All parameters (reference value, order of the approximation, etc.) must be set before calling this.

```

  <SM qcd: alpha qcd: TBP>+≡
    procedure (alpha_qcd_get), deferred :: get
  <SM qcd: interfaces>+≡
    abstract interface
      function alpha_qcd_get (alpha_qcd, scale) result (alpha)
        import
        class(alpha_qcd_t), intent(in) :: alpha_qcd
        real(default), intent(in) :: scale
        real(default) :: alpha
      end function alpha_qcd_get
    end interface

```

9.6.2 Fixed Coupling

In this version, the α_s value is fixed, the `scale` argument of the `get` method is ignored. There is only one parameter, the value. By default, this is the value at M_Z .

```

  <SM qcd: public>+≡
    public :: alpha_qcd_fixed_t
  <SM qcd: types>+≡
    type, extends (alpha_qcd_t) :: alpha_qcd_fixed_t
      real(default) :: val = ALPHA_QCD_MZ_REF
    contains
    <SM qcd: alpha qcd fixed: TBP>
  end type alpha_qcd_fixed_t

```

Output.

```

⟨SM qcd: alpha qcd fixed: TBP⟩≡
  procedure :: write => alpha_qcd_fixed_write

⟨SM qcd: sub interfaces⟩≡
  module subroutine alpha_qcd_fixed_write (object, unit)
    class(alpha_qcd_fixed_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine alpha_qcd_fixed_write

⟨SM qcd: procedures⟩≡
  module subroutine alpha_qcd_fixed_write (object, unit)
    class(alpha_qcd_fixed_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (fixed coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "alpha = ", object%val
  end subroutine alpha_qcd_fixed_write

```

Calculation: the scale is ignored in this case.

```

⟨SM qcd: alpha qcd fixed: TBP⟩+≡
  procedure :: get => alpha_qcd_fixed_get

⟨SM qcd: sub interfaces⟩+≡
  module function alpha_qcd_fixed_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_fixed_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
  end function alpha_qcd_fixed_get

⟨SM qcd: procedures⟩+≡
  module function alpha_qcd_fixed_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_fixed_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = alpha_qcd%val
  end function alpha_qcd_fixed_get

```

9.6.3 Running Coupling

In this version, the α_s value runs relative to the value at a given reference scale. There are two parameters: the value of this scale (default: M_Z), the value of α_s at this scale, and the number of effective flavors. Furthermore, we have the order of the approximation.

```

⟨SM qcd: public⟩+≡
  public :: alpha_qcd_from_scale_t

⟨SM qcd: types⟩+≡
  type, extends (alpha_qcd_t) :: alpha_qcd_from_scale_t
    real(default) :: mu_ref = MZ_REF
    real(default) :: ref = ALPHA_QCD_MZ_REF
    integer :: order = 0
    integer :: nf = 5

```

```

contains
  <SM qcd: alpha qcd from scale: TBP>
end type alpha_qcd_from_scale_t

```

Output.

```

<SM qcd: alpha qcd from scale: TBP>≡
  procedure :: write => alpha_qcd_from_scale_write

<SM qcd: sub interfaces>+≡
  module subroutine alpha_qcd_from_scale_write (object, unit)
    class(alpha_qcd_from_scale_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine alpha_qcd_from_scale_write

<SM qcd: procedures>+≡
  module subroutine alpha_qcd_from_scale_write (object, unit)
    class(alpha_qcd_from_scale_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (running coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "Scale mu = ", object%mu_ref
    write (u, "(5x,A," // FMT_12 // ")") "alpha(mu) = ", object%ref
    write (u, "(5x,A,I0)") "LL order = ", object%order
    write (u, "(5x,A,I0)") "N(flav) = ", object%nf
  end subroutine alpha_qcd_from_scale_write

```

Calculation: here, we call the function for running α_s that was defined in `sm_physics` above. The function does not take into account thresholds, so the number of flavors should be the correct one for the chosen scale. Normally, this should be the Z boson mass.

```

<SM qcd: alpha qcd from scale: TBP>+≡
  procedure :: get => alpha_qcd_from_scale_get

<SM qcd: sub interfaces>+≡
  module function alpha_qcd_from_scale_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_from_scale_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
  end function alpha_qcd_from_scale_get

<SM qcd: procedures>+≡
  module function alpha_qcd_from_scale_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_from_scale_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = running_as (scale, alpha_qcd%ref, alpha_qcd%mu_ref, &
      alpha_qcd%order, real (alpha_qcd%nf, kind=default))
  end function alpha_qcd_from_scale_get

```

9.6.4 Running Coupling, determined by Λ_{QCD}

In this version, the inputs are the value Λ_{QCD} and the order of the approximation.

```

⟨SM qcd: public⟩+=
  public :: alpha_qcd_from_lambda_t

⟨SM qcd: types⟩+=
  type, extends (alpha_qcd_t) :: alpha_qcd_from_lambda_t
    real(default) :: lambda = LAMBDA_QCD_REF
    integer :: order = 0
    integer :: nf = 5
  contains
    ⟨SM qcd: alpha qcd from lambda: TBP⟩
  end type alpha_qcd_from_lambda_t

```

Output.

```

⟨SM qcd: alpha qcd from lambda: TBP⟩=
  procedure :: write => alpha_qcd_from_lambda_write

⟨SM qcd: sub interfaces⟩+=
  module subroutine alpha_qcd_from_lambda_write (object, unit)
    class(alpha_qcd_from_lambda_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine alpha_qcd_from_lambda_write

⟨SM qcd: procedures⟩+=
  module subroutine alpha_qcd_from_lambda_write (object, unit)
    class(alpha_qcd_from_lambda_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (Lambda_QCD as input):"
    write (u, "(5x,A," // FMT_12 // ")") "Lambda_QCD = ", object%lambda
    write (u, "(5x,A,I0)") "LL order = ", object%order
    write (u, "(5x,A,I0)") "N(flv) = ", object%nf
  end subroutine alpha_qcd_from_lambda_write

```

Calculation: here, we call the second function for running α_s that was defined in `sm_physics` above. The Λ value should be the one that is appropriate for the chosen number of effective flavors. Again, thresholds are not incorporated.

```

⟨SM qcd: alpha qcd from lambda: TBP⟩+=
  procedure :: get => alpha_qcd_from_lambda_get

⟨SM qcd: sub interfaces⟩+=
  module function alpha_qcd_from_lambda_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_from_lambda_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
  end function alpha_qcd_from_lambda_get

⟨SM qcd: procedures⟩+=
  module function alpha_qcd_from_lambda_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_from_lambda_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = running_as_lam (real (alpha_qcd%nf, kind=default), scale, &
      alpha_qcd%lambda, alpha_qcd%order)
  end function alpha_qcd_from_lambda_get

```

9.6.5 QCD Wrapper type

We could get along with a polymorphic QCD type, but a monomorphic wrapper type with a polymorphic component is easier to handle and probably safer (w.r.t. compiler bugs). However, we keep the object transparent, so we can set the type-specific parameters directly (by a `dispatch` routine).

```

⟨SM qcd: public⟩+≡
    public :: qcd_t

⟨SM qcd: types⟩+≡
    type :: qcd_t
        class(alpha_qcd_t), allocatable :: alpha
        character(32) :: md5sum = ""
        integer :: n_f = -1
    contains
        ⟨SM qcd: qcd: TBP⟩
    end type qcd_t

```

Output. We first print the polymorphic `alpha` which contains a headline, then any extra components.

```

⟨SM qcd: qcd: TBP⟩≡
    procedure :: write => qcd_write

⟨SM qcd: sub interfaces⟩+≡
    module subroutine qcd_write (qcd, unit, show_md5sum)
        class(qcd_t), intent(in) :: qcd
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_md5sum
    end subroutine qcd_write

⟨SM qcd: procedures⟩+≡
    module subroutine qcd_write (qcd, unit, show_md5sum)
        class(qcd_t), intent(in) :: qcd
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_md5sum
        logical :: show_md5
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        show_md5 = .true.; if (present (show_md5sum)) show_md5 = show_md5sum
        if (allocated (qcd%alpha)) then
            call qcd%alpha%write (u)
        else
            write (u, "(3x,A)") "QCD parameters (coupling undefined)"
        end if
        if (show_md5 .and. qcd%md5sum /= "") &
            write (u, "(5x,A,A,A)") "md5sum = '", qcd%md5sum, "'"
    end subroutine qcd_write

```

Compute an MD5 sum for the `alpha_s` setup. This is done by writing them to a temporary file, using a standard format.

```

⟨SM qcd: qcd: TBP⟩+≡
    procedure :: compute_alphas_md5sum => qcd_compute_alphas_md5sum

```



```

⟨SM qcd: sub interfaces⟩+=≡
    module subroutine qcd_compute_alphas_md5sum (qcd)
        class(qcd_t), intent(inout) :: qcd
        integer :: unit
    end subroutine qcd_compute_alphas_md5sum

⟨SM qcd: procedures⟩+=≡
    module subroutine qcd_compute_alphas_md5sum (qcd)
        class(qcd_t), intent(inout) :: qcd
        integer :: unit
        if (allocated (qcd%alpha)) then
            unit = free_unit ()
            open (unit, status="scratch", action="readwrite")
            call qcd%alpha%write (unit)
            rewind (unit)
            qcd%md5sum = md5sum (unit)
            close (unit)
        end if
    end subroutine qcd_compute_alphas_md5sum

```

Retrieve the MD5 sum of the qcd setup.

```

⟨SM qcd: qcd: TBP⟩+=≡
    procedure :: get_md5sum => qcd_get_md5sum

⟨SM qcd: sub interfaces⟩+=≡
    module function qcd_get_md5sum (qcd) result (md5sum)
        character(32) :: md5sum
        class(qcd_t), intent(inout) :: qcd
    end function qcd_get_md5sum

⟨SM qcd: procedures⟩+=≡
    module function qcd_get_md5sum (qcd) result (md5sum)
        character(32) :: md5sum
        class(qcd_t), intent(inout) :: qcd
        md5sum = qcd%md5sum
    end function qcd_get_md5sum

```

9.6.6 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sm_qcd_ut.f90⟩≡
    ⟨File header⟩

    module sm_qcd_ut
        use unit_tests
        use sm_qcd_utl

    ⟨Standard module head⟩

    ⟨SM qcd: public test⟩

    contains

```

```

    <SM qcd: test driver>

end module sm_qcd_ut

<sm_qcd_uti.f90>≡
    <File header>

module sm_qcd_uti

    <Use kinds>
    use physics_defs, only: MZ_REF

    use sm_qcd

    <Standard module head>

    <SM qcd: test declarations>

contains

    <SM qcd: tests>

end module sm_qcd_uti
API: driver for the unit tests below.
<SM qcd: public test>≡
    public :: sm_qcd_test
<SM qcd: test driver>≡
    subroutine sm_qcd_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SM qcd: execute tests>
    end subroutine sm_qcd_test

```

QCD Coupling

We check two different implementations of the abstract QCD coupling.

```

<SM qcd: execute tests>≡
    call test (sm_qcd_1, "sm_qcd_1", &
        "running alpha_s", &
        u, results)
<SM qcd: test declarations>≡
    public :: sm_qcd_1
<SM qcd: tests>≡
    subroutine sm_qcd_1 (u)
        integer, intent(in) :: u
        type(qcd_t) :: qcd

        write (u, "(A)")  "* Test output: sm_qcd_1"
        write (u, "(A)")  "* Purpose: compute running alpha_s"
        write (u, "(A)")

```

```

write (u, "(A)")  "* Fixed:"
write (u, "(A)")

allocate (alpha_qcd_fixed_t :: qcd%alpha)
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)")  "alpha_s (mz)      =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)")  "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)
deallocate (qcd%alpha)

write (u, "(A)")  "* Running from MZ (LO):"
write (u, "(A)")

allocate (alpha_qcd_from_scale_t :: qcd%alpha)
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)")  "alpha_s (mz)      =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)")  "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from MZ (NLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_scale_t)
    alpha%order = 1
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)")  "alpha_s (mz)      =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)")  "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from MZ (NNLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_scale_t)
    alpha%order = 2
end select
call qcd%compute_alphas_md5sum ()

```

```

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz) =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

deallocate (qcd%alpha)
write (u, "(A)")  "* Running from Lambda_QCD (LO):"
write (u, "(A)")

allocate (alpha_qcd_from_lambda_t :: qcd%alpha)
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz) =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from Lambda_QCD (NLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_lambda_t)
    alpha%order = 1
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz) =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from Lambda_QCD (NNLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_lambda_t)
    alpha%order = 2
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz) =", &
    qcd%alpha%get (MZ_REF)

```

```
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &  
    qcd%alpha%get (1000._default)  
  
write (u, "(A)")  
write (u, "(A)")  "* Test output end: sm_qcd_1"  
  
end subroutine sm_qcd_1
```

9.7 QED Coupling

On the surface similar to the QCD coupling module but much simpler. Only a fixed QED coupling α_{em} is allowed. Can be extended later if we want to enable a running of α_{em} as well.

```
<sm_qed.f90>≡  
<File header>  
  
module sm_qed  
  
  <Use kinds>  
  use physics_defs  
  
  <Standard module head>  
  
  <SM qed: public>  
  
  <SM qed: types>  
  
  <SM qed: interfaces>  
  
  interface  
    <SM qed: sub interfaces>  
    end interface  
  
end module sm_qed  
  
<sm_qed_sub.f90>≡  
<File header>  
  
submodule (sm_qed) sm_qed_s  
  
  use io_units  
  use format_defs, only: FMT_12  
  use md5  
  use sm_physics  
  
  implicit none  
  
contains  
  
  <SM qed: procedures>  
  
end submodule sm_qed_s
```

9.7.1 Coupling: Abstract Data Type

This is the abstract version of the QCD coupling implementation.

```
<SM qed: public>≡  
  public :: alpha_qed_t  
  
<SM qed: types>≡  
  type, abstract :: alpha_qed_t
```

```

contains
  <SM qed: alpha qed: TBP>
end type alpha_qed_t

```

There must be an output routine.

```

<SM qed: alpha qed: TBP>≡
  procedure (alpha_qed_write), deferred :: write

<SM qed: interfaces>≡
  abstract interface
    subroutine alpha_qed_write (object, unit)
      import
      class(alpha_qed_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine alpha_qed_write
  end interface

```

This method computes the running coupling, given a certain scale. All parameters (reference value, order of the approximation, etc.) must be set before calling this.

```

<SM qed: alpha qed: TBP>+≡
  procedure (alpha_qed_get), deferred :: get

<SM qed: interfaces>+≡
  abstract interface
    function alpha_qed_get (alpha_qed, scale) result (alpha)
      import
      class(alpha_qed_t), intent(in) :: alpha_qed
      real(default), intent(in) :: scale
      real(default) :: alpha
    end function alpha_qed_get
  end interface

```

9.7.2 Fixed Coupling

In this version, the α value is fixed, the `scale` argument of the `get` method is ignored. There is only one parameter, the value. The default depends on the electroweak scheme chosen in the model.

```

<SM qed: public>+≡
  public :: alpha_qed_fixed_t

<SM qed: types>+≡
  type, extends (alpha_qed_t) :: alpha_qed_fixed_t
    real(default) :: val = ALPHA_QED_ME_REF
  contains
    <SM qed: alpha qed fixed: TBP>
  end type alpha_qed_fixed_t

```

Output.

```

<SM qed: alpha qed fixed: TBP>≡
  procedure :: write => alpha_qed_fixed_write

```

```

⟨SM qed: sub interfaces⟩≡
  module subroutine alpha_qed_fixed_write (object, unit)
    class(alpha_qed_fixed_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine alpha_qed_fixed_write

⟨SM qed: procedures⟩≡
  module subroutine alpha_qed_fixed_write (object, unit)
    class(alpha_qed_fixed_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QED parameters (fixed coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "alpha = ", object%val
  end subroutine alpha_qed_fixed_write

```

Calculation: the scale is ignored in this case.

```

⟨SM qed: alpha qed fixed: TBP⟩+≡
  procedure :: get => alpha_qed_fixed_get

⟨SM qed: sub interfaces⟩+≡
  module function alpha_qed_fixed_get (alpha_qed, scale) result (alpha)
    class(alpha_qed_fixed_t), intent(in) :: alpha_qed
    real(default), intent(in) :: scale
    real(default) :: alpha
  end function alpha_qed_fixed_get

⟨SM qed: procedures⟩+≡
  module function alpha_qed_fixed_get (alpha_qed, scale) result (alpha)
    class(alpha_qed_fixed_t), intent(in) :: alpha_qed
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = alpha_qed%val
  end function alpha_qed_fixed_get

```

9.7.3 Running Coupling

In this version, the α value runs relative to the value at a given reference scale. There are two parameters: the value of this scale (default: M_Z), the value of α at this scale, and the number of effective flavors. Furthermore, we have the order of the approximation.

```

⟨SM qed: public⟩+≡
  public :: alpha_qed_from_scale_t

⟨SM qed: types⟩+≡
  type, extends (alpha_qed_t) :: alpha_qed_from_scale_t
    real(default) :: mu_ref = ME_REF
    real(default) :: ref = ALPHA_QED_ME_REF
    integer :: order = 0
    integer :: nf = 5
    integer :: nlep = 1
    logical :: analytic = .true.
  contains

```



```

    <SM qed: alpha qed from scale: TBP>
end type alpha_qed_from_scale_t

```

Output.

```

<SM qed: alpha qed from scale: TBP>≡
    procedure :: write => alpha_qed_from_scale_write

<SM qed: sub interfaces>+≡
    module subroutine alpha_qed_from_scale_write (object, unit)
        class(alpha_qed_from_scale_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine alpha_qed_from_scale_write

<SM qed: procedures>+≡
    module subroutine alpha_qed_from_scale_write (object, unit)
        class(alpha_qed_from_scale_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(3x,A)") "QED parameters (running coupling):"
        write (u, "(5x,A," // FMT_12 // ")") "Scale mu = ", object%mu_ref
        write (u, "(5x,A," // FMT_12 // ")") "alpha(mu) = ", object%ref
        write (u, "(5x,A,I0)") "LL order = ", object%order
        write (u, "(5x,A,I0)") "N(flν) = ", object%nf
        write (u, "(5x,A,I0)") "N(lep) = ", object%nlep
        write (u, "(5x,A,L1)") "analytic = ", object%analytic
    end subroutine alpha_qed_from_scale_write

```

Calculation: here, we call the function for running α_s that was defined in `sm_physics` above. The function does not take into account thresholds, so the number of flavors should be the correct one for the chosen scale. Normally, this should be the Z boson mass.

```

<SM qed: alpha qed from scale: TBP>+≡
    procedure :: get => alpha_qed_from_scale_get

<SM qed: sub interfaces>+≡
    module function alpha_qed_from_scale_get (alpha_qed, scale) result (alpha)
        class(alpha_qed_from_scale_t), intent(in) :: alpha_qed
        real(default), intent(in) :: scale
        real(default) :: alpha
    end function alpha_qed_from_scale_get

<SM qed: procedures>+≡
    module function alpha_qed_from_scale_get (alpha_qed, scale) result (alpha)
        class(alpha_qed_from_scale_t), intent(in) :: alpha_qed
        real(default), intent(in) :: scale
        real(default) :: alpha
        if (alpha_qed%analytic) then
            alpha = running_alpha (scale, alpha_qed%ref, alpha_qed%mu_ref, &
                alpha_qed%order, alpha_qed%nf, alpha_qed%nlep)
        else
            alpha = running_alpha_num (scale, alpha_qed%ref, alpha_qed%mu_ref, &
                alpha_qed%order, alpha_qed%nf, alpha_qed%nlep)
        end if
    end function alpha_qed_from_scale_get

```

9.7.4 QED type

This module is similar to `qcd_t`, defining the type `qed_t`. It stores the `alpha_qed_t` type which is either constant or a running α with different options.

```

<SM qed: public>+≡
    public :: qed_t

<SM qed: types>+≡
    type :: qed_t
        class(alpha_qed_t), allocatable :: alpha
        character(32) :: md5sum = ""
        integer :: n_f = -1
        integer :: n_lep = -1
    contains
        <SM qed: qed: TBP>
    end type qed_t

```

Output. We first print the polymorphic `alpha` which contains a headline, then any extra components.

```

<SM qed: qed: TBP>≡
    procedure :: write => qed_write

<SM qed: sub interfaces>+≡
    module subroutine qed_write (qed, unit, show_md5sum)
        class(qed_t), intent(in) :: qed
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_md5sum
    end subroutine qed_write

<SM qed: procedures>+≡
    module subroutine qed_write (qed, unit, show_md5sum)
        class(qed_t), intent(in) :: qed
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_md5sum
        logical :: show_md5
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        show_md5 = .true.; if (present (show_md5sum)) show_md5 = show_md5sum
        if (allocated (qed%alpha)) then
            call qed%alpha%write (u)
        else
            write (u, "(3x,A)") "QED parameters (coupling undefined)"
        end if
        if (show_md5 .and. qed%md5sum /= "") &
            write (u, "(5x,A,A,A)") "md5sum = '", qed%md5sum, "'"
    end subroutine qed_write

```

Compute an MD5 sum for the `alpha` setup. This is done by writing them to a temporary file, using a standard format.

```

<SM qed: qed: TBP>+≡
    procedure :: compute_alpha_md5sum => qed_compute_alpha_md5sum

<SM qed: sub interfaces>+≡
    module subroutine qed_compute_alpha_md5sum (qed)
        class(qed_t), intent(inout) :: qed

```

```

        integer :: unit
    end subroutine qed_compute_alpha_md5sum
<SM qed: procedures>+≡
module subroutine qed_compute_alpha_md5sum (qed)
    class(qed_t), intent(inout) :: qed
    integer :: unit
    if (allocated (qed%alpha)) then
        unit = free_unit ()
        open (unit, status="scratch", action="readwrite")
        call qed%alpha%write (unit)
        rewind (unit)
        qed%md5sum = md5sum (unit)
        close (unit)
    end if
end subroutine qed_compute_alpha_md5sum

```

Retrieve the MD5 sum of the qed setup.

```

<SM qed: qed: TBP>+≡
    procedure :: get_md5sum => qed_get_md5sum
<SM qed: sub interfaces>+≡
    module function qed_get_md5sum (qed) result (md5sum)
        character(32) :: md5sum
        class(qed_t), intent(inout) :: qed
    end function qed_get_md5sum
<SM qed: procedures>+≡
    module function qed_get_md5sum (qed) result (md5sum)
        character(32) :: md5sum
        class(qed_t), intent(inout) :: qed
        md5sum = qed%md5sum
    end function qed_get_md5sum

```

9.7.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<sm_qed_ut.f90>≡
    <File header>

    module sm_qed_ut
        use unit_tests
        use sm_qed_util

    <Standard module head>

    <SM qed: public test>

    contains

    <SM qed: test driver>

    end module sm_qed_ut

```

```

⟨sm_qed_uti.f90⟩≡
  ⟨File header⟩

  module sm_qed_uti

    ⟨Use kinds⟩
    use physics_defs, only: ME_REF

    use sm_qed

    ⟨Standard module head⟩

    ⟨SM qed: test declarations⟩

    contains

    ⟨SM qed: tests⟩

  end module sm_qed_uti
API: driver for the unit tests below.
⟨SM qed: public test⟩≡
  public :: sm_qed_test
⟨SM qed: test driver⟩≡
  subroutine sm_qed_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨SM qed: execute tests⟩
  end subroutine sm_qed_test

```

QED Coupling

We check two different implementations of the abstract QED coupling.

```

⟨SM qed: execute tests⟩≡
  call test (sm_qed_1, "sm_qed_1", &
    "running alpha", &
    u, results)
⟨SM qed: test declarations⟩≡
  public :: sm_qed_1
⟨SM qed: tests⟩≡
  subroutine sm_qed_1 (u)
    integer, intent(in) :: u
    type(qed_t) :: qed

    write (u, "(A)")  "* Test output: sm_qed_1"
    write (u, "(A)")  "* Purpose: compute running alpha"
    write (u, "(A)")

    write (u, "(A)")  "* Fixed:"
    write (u, "(A)")

    allocate (alpha_qed_fixed_t :: qed%alpha)

```

```

call qed%compute_alpha_md5sum ()

call qed%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha (me)      =", &
    qed%alpha%get (ME_REF)
write (u, "(1x,A,F10.7)") "alpha (10 GeV) =", &
    qed%alpha%get (10._default)
write (u, "(1x,A,F10.7)") "alpha (1 TeV)  =", &
    qed%alpha%get (1000._default)
write (u, *)
deallocate (qed%alpha)

write (u, "(A)")  "* Running from me (LO):"
write (u, "(A)")

allocate (alpha_qed_from_scale_t :: qed%alpha)
call qed%compute_alpha_md5sum ()

call qed%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha (me)      =", &
    qed%alpha%get (ME_REF)
write (u, "(1x,A,F10.7)") "alpha (10 GeV) =", &
    qed%alpha%get (10._default)
write (u, "(1x,A,F10.7)") "alpha (1 TeV)  =", &
    qed%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from me (NLO, analytic):"
write (u, "(A)")

select type (alpha => qed%alpha)
type is (alpha_qed_from_scale_t)
    alpha%order = 1
end select
call qed%compute_alpha_md5sum ()

call qed%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha (me)      =", &
    qed%alpha%get (ME_REF)
write (u, "(1x,A,F10.7)") "alpha (10 GeV) =", &
    qed%alpha%get (10._default)
write (u, "(1x,A,F10.7)") "alpha (1 TeV)  =", &
    qed%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from me (NLO, numeric):"
write (u, "(A)")

select type (alpha => qed%alpha)
type is (alpha_qed_from_scale_t)
    alpha%order = 1

```

```

        alpha%analytic = .false.
end select
call qed%compute_alpha_md5sum ()

call qed%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha (me)      =", &
    qed%alpha%get (ME_REF)
write (u, "(1x,A,F10.7)") "alpha (10 GeV) =", &
    qed%alpha%get (10._default)
write (u, "(1x,A,F10.7)") "alpha (1 TeV)  =", &
    qed%alpha%get (1000._default)
write (u, *)
deallocate (qed%alpha)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sm_qed_1"

end subroutine sm_qed_1

```

9.8 Shower algorithms

```

⟨shower_algorithms.f90⟩≡
  ⟨File header⟩

  module shower_algorithms

    ⟨Use kinds⟩

    ⟨Standard module head⟩

    ⟨Shower algorithms: public⟩

    ⟨Shower algorithms: interfaces⟩

    interface
    ⟨Shower algorithms: sub interfaces⟩
    end interface

  end module shower_algorithms

⟨shower_algorithms_sub.f90⟩≡
  ⟨File header⟩

  submodule (shower_algorithms) shower_algorithms_s

    use diagnostics
    use constants

    implicit none

  contains

    ⟨Shower algorithms: procedures⟩

    ⟨Shower algorithms: tests⟩

  end submodule shower_algorithms_s

```

We want to generate emission variables $\mathbf{x} \in \mathbb{R}^d$ proportional to

$$f(x) \Delta(f, h(x)) \quad \text{with} \quad (9.32)$$

$$\Delta(f, H) = \exp \left\{ - \int d^d x' f(x') \Theta(h(x') - H) \right\} \quad (9.33)$$

The `true_function` f is however too complicated and we are only able to generate \mathbf{x} according to the `overestimator` F . This algorithm is described in Appendix B of 0709.2092 and is proven e.g. in 1211.7204 and hep-ph/0606275. Intuitively speaking, we overestimate the emission probability and can therefore set `scale_max = scale` if the emission is rejected.

```

⟨Shower algorithms: sub interfaces⟩≡
  module subroutine generate_vetoed (x, overestimator, true_function, &
    sudakov, inverse_sudakov, scale_min)

```

```

    real(default), dimension(:), intent(out) :: x
    !class(rng_t), intent(inout) :: rng
    procedure(XXX_function), pointer, intent(in) :: overestimator, true_function
    procedure(sudakov_p), pointer, intent(in) :: sudakov, inverse_sudakov
    real(default), intent(in) :: scale_min
end subroutine generate_vetoed

(Shower algorithms: procedures)≡
module subroutine generate_vetoed (x, overestimator, true_function, &
    sudakov, inverse_sudakov, scale_min)
    real(default), dimension(:), intent(out) :: x
    !class(rng_t), intent(inout) :: rng
    procedure(XXX_function), pointer, intent(in) :: overestimator, true_function
    procedure(sudakov_p), pointer, intent(in) :: sudakov, inverse_sudakov
    real(default), intent(in) :: scale_min
    real(default) :: random, scale_max, scale
    scale_max = inverse_sudakov (one)
    do while (scale_max > scale_min)
        !call rng%generate (random)
        scale = inverse_sudakov (random * sudakov (scale_max))
        call generate_on_hypersphere (x, overestimator, scale)
        !call rng%generate (random)
        if (random < true_function (x) / overestimator (x)) then
            return !!! accept x
        end if
        scale_max = scale
    end do
end subroutine generate_vetoed

(Shower algorithms: procedures)+≡
subroutine generate_on_hypersphere (x, overestimator, scale)
    real(default), dimension(:), intent(out) :: x
    procedure(XXX_function), pointer, intent(in) :: overestimator
    real(default), intent(in) :: scale
    call msg_bug ("generate_on_hypersphere: not implemented")
end subroutine generate_on_hypersphere

(Shower algorithms: interfaces)≡
interface
    pure function XXX_function (x)
        import
        real(default) :: XXX_function
        real(default), dimension(:), intent(in) :: x
    end function XXX_function
end interface
interface
    pure function sudakov_p (x)
        import
        real(default) :: sudakov_p
        real(default), intent(in) :: x
    end function sudakov_p
end interface

```


9.8.1 Unit tests

(Currently unused.)

```
<XXX Shower algorithms: public>≡
  public :: shower_algorithms_test

<XXX Shower algorithms: tests>≡
  subroutine shower_algorithms_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Shower algorithms: execute tests>
  end subroutine shower_algorithms_test
```

Splitting functions

```
<XXX shower algorithms: execute tests>≡
  call test (shower_algorithms_1, "shower_algorithms_1", &
    "veto technique", &
    u, results)

<XXX shower algorithms: tests>≡
  subroutine shower_algorithms_1 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: shower_algorithms_1"
    write (u, "(A)")  "* Purpose: check veto technique"
    write (u, "(A)")

    write (u, "(A)")  "* Splitting functions:"
    write (u, "(A)")

    !call assert (u, vanishes (p_qqg_pol (z, +1, -1, +1)))
    !call assert (u, nearly_equal ( &
      !p_qqg_pol (z, +1, +1, -1) + p_qqg_pol (z, +1, +1, +1),
      !p_qqg (z))

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: shower_algorithms_1"

  end subroutine shower_algorithms_1
```

Chapter 10

QED Parton Distribution Functions

We start with a module that gives access to the ISR structure function:

`electron_pdfs`

10.1 Electron PDFs

This module contains the formulae for the numerical evaluation of different incarnations of the QED initial-state radiation (ISR) structure functions (a.k.a. electron PDFs).

```
<electron_pdfs.f90>≡  
  <File header>  
  
  module electron_pdfs  
  
    <Use kinds>  
    <electron_pdfs use>
```

No internal dependencies

Figure 10.1: Module dependencies in `src/qed_pdf.f`.

```

    <Standard module head>

    <Electron PDFs: public>

    <Electron PDFs: parameters>

    <Electron PDFs: types>

    interface
    <Electron PDFs: sub interfaces>
    end interface

contains

    <Electron PDFs: main procedures>

end module electron_pdfs

<electron pdfs use>≡
    use io_units
    use sm_qed

<electron_pdfs_sub.f90>≡
    <File header>

    submodule (electron_pdfs) electron_pdfs_s

    <Use strings>
    <electron pdfs use>
    use diagnostics
    use constants
    use format_defs, only: FMT_12
    use numeric_utils
    use physics_defs
    use sm_physics

    implicit none

contains

    <Electron PDFs: procedures>

end submodule electron_pdfs_s

```

10.1.1 The physics for electron beam PDFs (structure functions)

The ISR structure function is in the most crude approximation (LLA without α corrections, i.e. ϵ^0)

$$f_0(x) = \epsilon(1-x)^{-1+\epsilon} \quad \text{with} \quad \epsilon = \frac{\alpha}{\pi} q_e^2 \ln \frac{s}{m^2}, \quad (10.1)$$

where m is the mass of the incoming (and outgoing) particle, which is initially assumed on-shell.

Here, the form of ϵ results from the kinematical bounds for the momentum squared of the outgoing particle, which in the limit $m^2 \ll s$ are given by

$$t_0 = -2\bar{x}E(E + p) + m^2 \approx -\bar{x}s, \quad (10.2)$$

$$t_1 = -2\bar{x}E(E - p) + m^2 \approx xm^2, \quad (10.3)$$

so the integration over the propagator $1/(t - m^2)$ yields

$$\ln \frac{t_0 - m^2}{t_1 - m^2} = \ln \frac{s}{m^2}. \quad (10.4)$$

The structure function has three parameters: α , m_{in} of the incoming particle and s , the hard scale. Internally, we store the exponent ϵ which is the relevant parameter. (In conventional notation, $\epsilon = \beta/2$.) As defaults, we take the actual values of α (which is probably $\alpha(s)$), the actual mass m_{in} and the squared total c.m. energy s .

Including ϵ , ϵ^2 , and ϵ^3 corrections, the successive approximation of the ISR structure function read

$$f_0(x) = \epsilon(1 - x)^{-1+\epsilon} \quad (10.5)$$

$$f_1(x) = g_1(\epsilon) f_0(x) - \frac{\epsilon}{2}(1 + x) \quad (10.6)$$

$$f_2(x) = g_2(\epsilon) f_0(x) - \frac{\epsilon}{2}(1 + x) - \frac{\epsilon^2}{8} \left(\frac{1 + 3x^2}{1 - x} \ln x + 4(1 + x) \ln(1 - x) + 5 + x \right) \quad (10.7)$$

$$f_3(x) = g_3(\epsilon) f_0(x) - \frac{\epsilon}{2}(1 + x) - \frac{\epsilon^2}{8} \left(\frac{1 + 3x^2}{1 - x} \ln x + 4(1 + x) \ln(1 - x) + 5 + x \right) - \frac{\epsilon^3}{48} \left((1 + x) [6 \text{Li}_2(x) + 12 \ln^2(1 - x) - 3\pi^2] + 6(x + 5) \ln(1 - x) + \frac{1}{1 - x} \left[\frac{3}{2}(1 + 8x + 3x^2) \ln x + 12(1 + x^2) \ln x \ln(1 - x) - \frac{1}{2}(1 + 7x^2) \ln^2 x + \frac{1}{4}(39 - 24x - 15x^2) \right] \right) \quad (10.8)$$

where the successive approximations to the prefactor of the leading singularity

$$g(\epsilon) = \frac{\exp(\epsilon(-\gamma_E + \frac{3}{4}))}{\Gamma(1 + \epsilon)}, \quad (10.9)$$

are given by

$$g_0(\epsilon) = 1 \quad (10.10)$$

$$g_1(\epsilon) = 1 + \frac{3}{4}\epsilon \quad (10.11)$$

$$g_2(\epsilon) = 1 + \frac{3}{4}\epsilon + \frac{27 - 8\pi^2}{96}\epsilon^2 \quad (10.12)$$

$$g_3(\epsilon) = 1 + \frac{3}{4}\epsilon + \frac{27 - 8\pi^2}{96}\epsilon^2 + \frac{27 - 24\pi^2 + 128\zeta(3)}{384}\epsilon^3, \quad (10.13)$$

where, numerically

$$\zeta(3) = 1.20205690315959428539973816151 \dots \quad (10.14)$$

Although one could calculate the function $g(\epsilon)$ exactly, truncating its Taylor expansion ensures the exact normalization of the truncated structure function at each given order:

$$\int_0^1 dx f_i(x) = 1 \quad \text{for all } i. \quad (10.15)$$

Effectively, the $O(\epsilon)$ correction reduces the low- x tail of the structure function by 50% while increasing the coefficient of the singularity by $O(\epsilon)$. Relative to this, the $O(\epsilon^2)$ correction slightly enhances $x > \frac{1}{2}$ compared to $x < \frac{1}{2}$. At $x = 0$, $f_2(x)$ introduces a logarithmic singularity which should be cut off at $x_0 = O(e^{-1/\epsilon})$: for lower x the perturbative series breaks down. The f_3 correction is slightly positive for low x values and negative near $x = 1$, where the Li_2 piece slightly softens the singularity at $x = 1$.

Instead of the definition for ϵ given above, it is customary to include a universal nonlogarithmic piece:

$$\epsilon = \frac{\alpha}{\pi} q_e^2 \left(\ln \frac{s}{m^2} - 1 \right) \quad (10.16)$$

10.1.2 Implementation

The basic type for lepton beam (QED) structure functions:

```

<Electron PDFs: public>≡
  public :: qed_pdf_t

<Electron PDFs: types>≡
  type :: qed_pdf_t
    private
    integer :: flv = 0
    class(alpha_qed_t), allocatable :: aqed
    real(default) :: mass = 0
    real(default) :: q_max = 0
    real(default) :: alpha = 0
    real(default) :: eps = 0
    real(default), allocatable :: q_in
    integer :: order
    integer :: log_order
    integer :: n_lep
  contains
    <Electron PDFs: QED PDF: TBP>
  end type qed_pdf_t

<Electron PDFs: parameters>≡
  integer, parameter, public :: EPDF_ELE = 0, EPDF_POS = 1, &
    EPDF_S = 2, EPDF_NS = 3, EPDF_G = 4

<Electron PDFs: QED PDF: TBP>≡
  procedure :: init => qed_pdf_init

```

<Electron PDFs: sub interfaces>≡

```

module subroutine qed_pdf_init &
  (qed_pdf, mass, alpha, charge, q_max, order, log_order, n_lep)
  class(qed_pdf_t), intent(out) :: qed_pdf
  real(default), intent(in) :: mass, alpha, q_max, charge
  integer, intent(in) :: order, log_order, n_lep
end subroutine qed_pdf_init

```

<Electron PDFs: procedures>≡

```

module subroutine qed_pdf_init &
  (qed_pdf, mass, alpha, charge, q_max, order, log_order, n_lep)
  class(qed_pdf_t), intent(out) :: qed_pdf
  real(default), intent(in) :: mass, alpha, q_max, charge
  integer, intent(in) :: order, log_order, n_lep
  qed_pdf%mass = mass
  qed_pdf%q_max = q_max
  qed_pdf%alpha = alpha
  qed_pdf%order = order
  qed_pdf%log_order = log_order
  qed_pdf%n_lep = n_lep
  qed_pdf%eps = alpha/pi * charge**2 &
    * (2 * log (q_max / mass) - 1)
end subroutine qed_pdf_init

```

Write routine.

<Electron PDFs: QED PDF: TBP>+≡

```

procedure :: write => qed_pdf_write

```

<Electron PDFs: sub interfaces>+≡

```

module subroutine qed_pdf_write (qed_pdf, unit, with_qed)
  class(qed_pdf_t), intent(in) :: qed_pdf
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: with_qed
end subroutine qed_pdf_write

```

<Electron PDFs: procedures>+≡

```

module subroutine qed_pdf_write (qed_pdf, unit, with_qed)
  class(qed_pdf_t), intent(in) :: qed_pdf
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: with_qed
  integer :: u
  logical :: show_qed
  u = given_output_unit (unit)
  show_qed = .false.
  if (present (with_qed)) show_qed = with_qed
  write (u, "(3x,A)") "QED structure function (PDF):"
  write (u, "(5x,A,I0)") "Flavor      = ", qed_pdf%flv
  write (u, "(5x,A," // FMT_12 // ")") "Mass      = ", qed_pdf%mass
  write (u, "(5x,A," // FMT_12 // ")") "q_max     = ", qed_pdf%q_max
  write (u, "(5x,A," // FMT_12 // ")") "alpha     = ", qed_pdf%alpha
  write (u, "(5x,A,I0)") "Order     = ", qed_pdf%order
  write (u, "(5x,A,I0)") "Log. ord. = ", qed_pdf%log_order
  write (u, "(5x,A,I0)") "# leptons = ", qed_pdf%n_lep
  write (u, "(5x,A," // FMT_12 // ")") "epsilon   = ", qed_pdf%eps
  if (show_qed) then

```

```

        call qed_pdf%aqed%write (u)
    end if
end subroutine qed_pdf_write

```

For some unit tests, the order has to be set explicitly.

```

<Electron PDFs: QED PDF: TBP>+≡
    procedure :: set_order => qed_pdf_set_order

<Electron PDFs: sub interfaces>+≡
    module subroutine qed_pdf_set_order (qed_pdf, order)
        class(qed_pdf_t), intent(inout) :: qed_pdf
        integer, intent(in) :: order
    end subroutine qed_pdf_set_order

<Electron PDFs: procedures>+≡
    module subroutine qed_pdf_set_order (qed_pdf, order)
        class(qed_pdf_t), intent(inout) :: qed_pdf
        integer, intent(in) :: order
        qed_pdf%order = order
    end subroutine qed_pdf_set_order

```

Calculate the actual value depending on the order and a possible mapping parameter.

```

<Electron PDFs: QED PDF: TBP>+≡
    procedure :: evolve_qed_pdf => qed_pdf_evolve_qed_pdf

<Electron PDFs: sub interfaces>+≡
    module subroutine qed_pdf_evolve_qed_pdf (qed_pdf, x, xb, rb, ff)
        class(qed_pdf_t), intent(inout) :: qed_pdf
        real(default), intent(in) :: x, xb, rb
        real(default), intent(inout) :: ff
    end subroutine qed_pdf_evolve_qed_pdf

<Electron PDFs: procedures>+≡
    module subroutine qed_pdf_evolve_qed_pdf (qed_pdf, x, xb, rb, ff)
        class(qed_pdf_t), intent(inout) :: qed_pdf
        real(default), intent(in) :: x, xb, rb
        real(default), intent(inout) :: ff
        real(default), parameter :: &
            & xmin = 0.00714053329734592839549879772019_default
        real(default), parameter :: &
            g1 = 3._default / 4._default, &
            g2 = (27 - 8 * pi**2) / 96._default, &
            g3 = (27 - 24 * pi**2 + 128 * zeta3) / 384._default
        real(default) :: x_2, log_x, log_xb
        if (ff > 0 .and. qed_pdf%order > 0) then
            ff = ff * (1 + g1 * qed_pdf%eps)
            x_2 = x * x
            if (rb > 0) ff = ff * (1 - (1-x_2) / (2 * rb))
            if (qed_pdf%order > 1) then
                ff = ff * (1 + g2 * qed_pdf%eps**2)
                if (rb > 0 .and. xb > 0 .and. x > xmin) then
                    log_x = log_prec (x, xb)
                    log_xb = log_prec (xb, x)
                    ff = ff * (1 - ((1 + 3 * x_2) * log_x + xb * (4 * (1 + x) * &

```

```

        log_xb + 5 + x)) / (8 * rb) * qed_pdf%eps)
    end if
    if (qed_pdf%order > 2) then
        ff = ff * (1 + g3 * qed_pdf%eps**3)
        if (rb > 0 .and. xb > 0 .and. x > xmin) then
            ff = ff * (1 - ((1 + x) * xb &
                * (6 * Li2(x) + 12 * log_xb**2 - 3 * pi**2) &
                + 1.5_default * (1 + 8 * x + 3 * x_2) * log_x &
                + 6 * (x + 5) * xb * log_xb &
                + 12 * (1 + x_2) * log_x * log_xb &
                - (1 + 7 * x_2) * log_x**2 / 2 &
                + (39 - 24 * x - 15 * x_2) / 4) &
                / (48 * rb) * qed_pdf%eps**2)
        end if
    end if
end if
end if
end if
end subroutine qed_pdf_evolve_qed_pdf

```

Gfortran 7/8/9 bug, has to remain in the main module:

```

<Electron PDFs: QED PDF: TBP>+≡
    procedure :: allocate_aqed => qed_pdf_allocate_aqed

<Electron PDFs: main procedures>≡
    subroutine qed_pdf_allocate_aqed (qed, order, n_f, n_lep, running)
        class(qed_pdf_t), intent(inout) :: qed
        integer, intent(in) :: order, n_f, n_lep
        logical, intent(in) :: running
        if (running) then
            allocate (alpha_qed_from_scale_t :: qed%aqed)
            select type (aqed => qed%aqed)
            type is (alpha_qed_from_scale_t)
                aqed%order = order
                aqed%nf = n_f
                aqed%nlep = n_lep
            end select
        else
            allocate (alpha_qed_fixed_t :: qed%aqed)
        end if
    end subroutine qed_pdf_allocate_aqed

```

Part for the singlet- and non-singlet contributions of the PDF.

```

<Electron PDFs: public>+≡
    public :: elec_asym

<Electron PDFs: sub interfaces>+≡
    module function elec_asym (epdf, x, scale, alpha, running) result (elec_as)
        type(qed_pdf_t), intent(in) :: epdf
        real(default) :: elec_as
        real(default), intent(in) :: x
        real(default), intent(in) :: scale
        real(default), intent(in) :: alpha
        logical, intent(in) :: running
    end function elec_asym

```


(Electron PDFs: procedures)+≡

```

module function elec_asym (epdf, x, scale, alpha, running) result (elec_as)
  type(qed_pdf_t), intent(in) :: epdf
  real(default) :: elec_as
  real(default), intent(in) :: x
  real(default), intent(in) :: scale
  real(default), intent(in) :: alpha
  logical, intent(in) :: running
  real(default) :: lambda0, lambda1, xi1, xihat1, fac
  real(default) :: al0_2pi, al2pi, ca, cb, psixi1
  real(default) :: ln0, eta0, t, xi0, b0, b1
  integer :: nf, nlep
  lambda0 = 3._default/4._default
  al0_2pi = alpha / two / Pi
  if (allocated (epdf%q_in)) then
    ln0 = log(epdf%q_in**2/epdf%mass**2)
    eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
  else
    ln0 = zero
    eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
  end if
  if (running) then
    t = t_alpha (epdf, scale)
    xi0 = two*t
  else
    xi0 = eta0
  end if
  select case (epdf%log_order)
  case (EPDF_LL)
    elec_as = exp((lambda0 - eulerc) * xi0) / gamma (one + xi0) * &
      xi0 * (1 - x)**(-one + xi0)
  case (EPDF_NLL)
    lambda1 = 3._default/8._default - Pi2/two + 6._default*zeta3 - &
      epdf%n_lep/18._default * (three + four*Pi2)
    if (running) then
      select type (aqed => epdf%aqed)
      type is (alpha_qed_from_scale_t)
        nf = aqed%nf
        nlep = aqed%nlep
        al2pi = aqed%get (scale) / two / Pi
      type is (alpha_qed_fixed_t)
        call msg_fatal &
          ("elec_asym: has to be called with running alpha.")
    end select
    b0 = coeffqed_b0(nf,nlep)
    b1 = coeffqed_b1(nf,nlep)
    xi1 = xi0 + al2pi / two / Pi / b0 * (one - exp (Pi * b0 * xi0)) * &
      (20._default/9._default * epdf%n_lep + four * Pi * b1 / b0)
    xihat1 = xi0 * lambda0 - al2pi / two / Pi / b0 * &
      (one - exp (Pi * b0 * xi0)) * (lambda1 - three * Pi * b1 / b0)
  else
    al2pi = al0_2pi
    xi1 = xi0 * ( one - 10._default/9._default * al2pi * epdf%n_lep)
    xihat1 = xi0 * ( lambda0 + al2pi/two * lambda1 )
  end if
end function

```

```

end if
fac = exp( xihat1 - eulerc * xi1 ) / gamma (1 + xi1) * &
    xi1 * (1 - x)**(-one + xi1)
psixi1 = psir(xi1)
ca = - eulerc - psixi1
cb = 0.5_default * eulerc**2 + Pi2/12. + eulerc*psixi1 + &
    0.5_default * psixi1**2 - 0.5_default * psimr(xi1,1)
elec_as = fac * (one + two*al0_2pi * &
    ( (ln0 - one)*( ca + 3._default/4._default ) - &
    2*cb + 7._default/4._default + &
    (ln0 - one - two*ca)*log(1-x) - log(1-x)**2 ))
case default
    elec_as = 0
end select
end function elec_asym

```

Photon component of the PDF.

```

<Electron PDFs: public>+≡
public :: phot_asym

<Electron PDFs: sub interfaces>+≡
module function phot_asym &
    (epdf, x, scale, alpha, nlep, running) result (phot_as)
    type(qed_pdf_t), intent(in) :: epdf
    real(default) :: phot_as
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    integer, intent(in) :: nlep
    logical, intent(in) :: running
end function phot_asym

<Electron PDFs: procedures>+≡
module function phot_asym &
    (epdf, x, scale, alpha, nlep, running) result (phot_as)
    type(qed_pdf_t), intent(in) :: epdf
    real(default) :: phot_as
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    integer, intent(in) :: nlep
    logical, intent(in) :: running
    real(default) :: ln0, eta0, t, xi0, xihat0, den
    real(default) :: al0_2pi, c_b0, c_b1ob0
    real(default) :: lambda1, xi10, xihat10
    real(default) :: chi10, mf1k, mf10
    real(default) :: gam1, gam2, gam3, gam4, gam5
    real(default) :: d11, d21, d12, d22, d13, d23, d14, d24
    real(default) :: c11, c21, c31, c12, c22, c32, c13, c23, c33, &
        c14, c24, c34, k1, k2, k3, k4
    al0_2pi = alpha / two / Pi
    if (allocated (epdf%q_in)) then
        ln0 = log(epdf%q_in**2/epdf%mass**2)
        eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
    else

```

```

ln0 = zero
eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
end if
if (running) then
  c_b0 = - coeffqed_b0 (0, nlep)
  c_blob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
  t = t_alpha (epdf, scale)
  chi10 = zero
else
  c_b0 = zero
  c_blob0 = zero
  t = eta0 / two
  chi10 = al0_2pi * nlep
end if
select case (epdf%log_order)
case (EPDF_LL)
  xi0 = two * t
  xihat0 = three * t / two
  den = -two/three * nlep - three/two - two * log(1-x)
  mf1k = exp(-eulerc * xi0) * (1-x)**xi0 / gamma(1+xi0) * &
    (one / den - (Pi2*xi0 - 6._default * zeta3 * xi0**2) / &
    three / den**2 - (30._default * Pi2 - 360._default * &
    zeta3 * xi0 + Pi**4 * xi0**2) / 45._default / den**3)
  mf10 = one / den - 2._default * Pi2 / three / den**3
  phot_as = - exp(xihat0) * mf1k + &
    exp(-two/three * nlep * t) * mf10
case (EPDF_NLL)
  lambda1 = three/8._default - Pi2/two + 6._default*zeta3 - &
    nlep/18._default * (three + four*Pi2)
  xi10 = two - four*al0_2pi * (5._default/9._default * nlep + Pi*c_blob0)
  xihat10 = three/two * ( one + al0_2pi * two * &
    (lambda1/three - Pi * c_blob0))
  d11 = xi10
  d21 = - (two/three * nlep + two * Pi * c_b0 + xihat10 + chi10)
  c11 = al0_2pi * exp(-D21*t)
  c21 = - al0_2pi * (five + four/three * nlep) * exp(-d21*t)
  c31 = al0_2pi * (6._default + Pi2/6._default + 32._default/9._default * &
    nlep + two * Pi * c_blob0) * exp(-d21*t)
  d12 = d11
  d22 = d21
  c12 = - al0_2pi
  c22 = al0_2pi * (5._default + four/three * nlep)
  c32 = - al0_2pi * (6._default + Pi2/6._default + &
    32._default/9._default * nlep + two *Pi *c_blob0)
  d13 = d11
  d23 = - (two/three * nlep + xihat10 + chi10)
  c13 = zero
  c23 = zero
  c33 = - exp(-d23*t)
  d14 = d13
  d24 = d23
  c14 = zero
  c24 = zero
  c34 = one

```

```

k1 = xi10 * t
k2 = zero
k3 = xi10 * t
k4 = zero
gam1 = sum_rm (x, al0_2pi, ln0, &
  c11, c21, c31, d21/d11, d11, k1, d11, d21)
gam2 = sum_rm (x, al0_2pi, ln0, &
  c12, c22, c32, d22/d12, d12, k2, d12, d22)
gam3 = sum_rm (x, al0_2pi, ln0, &
  c13, c23, c33, d23/d13, d13, k3, d13, d23)
gam4 = sum_rm (x, al0_2pi, ln0, &
  c14, c24, c34, d24/d14, d14, k4, d14, d24)
gam5 = al0_2pi * (one + (1-x)**2)/x * (ln0 - two*log(x) - one)
phot_as = exp( - ( two/three * nlep + chi10 ) * t ) * &
  (gam1 + gam2 + gam3 + gam4 + gam5)
end select
end function phot_asym

```

(Electron PDFs: public)+≡

```
public :: bar_asym
```

(Electron PDFs: sub interfaces)+≡

```

module function bar_asym &
  (epdf, flv, x, scale, alpha, running) result (bar_as)
  type(qed_pdf_t), intent(in) :: epdf
  integer, intent(in) :: flv
  real(default) :: bar_as
  real(default), intent(in) :: x
  real(default), intent(in) :: scale
  real(default), intent(in) :: alpha
  logical, intent(in) :: running
end function bar_asym

```

(Electron PDFs: procedures)+≡

```

module function bar_asym &
  (epdf, flv, x, scale, alpha, running) result (bar_as)
  type(qed_pdf_t), intent(in) :: epdf
  integer, intent(in) :: flv
  real(default) :: bar_as
  real(default), intent(in) :: x
  real(default), intent(in) :: scale
  real(default), intent(in) :: alpha
  logical, intent(in) :: running
  logical, dimension(6) :: order
  integer :: nlep
  real(default) :: ln0, eta0, al_2pi, p
  real(default), dimension(6) :: jll_nll
  if (allocated (epdf%q_in)) then
    ln0 = log(epdf%q_in**2/epdf%mass**2)
    eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
  else
    ln0 = zero
    eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
  end if
  if (running) then

```

```

        p = t_alpha (epdf, scale)
    else
        p = eta0 / two
    end if
    order = .false.
    order(1:3) = .true.
    select case (epdf%log_order)
    case (EPDF_LL)
        nlep = epdf%n_lep
        al_2pi = zero
    case (EPDF_NLL)
        if (running) then
            select type (aqed => epdf%aqed)
            type is (alpha_qed_from_scale_t)
                nlep = aqed%nlep
                al_2pi = aqed%get (scale) / two / Pi
            type is (alpha_qed_fixed_t)
                call msg_fatal &
                    ("bar_asym: has to be called with running alpha.")
            end select
        else
            nlep = epdf%n_lep
            al_2pi = alpha / two / Pi
        end if
        order(4:6) = .true.
    end select
    select case (flv)
    case (EPDF_ELE,EPDF_POS,EPDF_S,EPDF_NS)
        call elecbar_asym_p (x, jll_nll, nlep, ln0, order, running)
    case (EPDF_G)
        call photbar_asym_p (x, jll_nll, nlep, ln0, order, running)
    case default
        call msg_fatal &
            ("bar_asym: wrong lepton flavor.")
    end select
    bar_as = rec_series (p, al_2pi, jll_nll)
end function bar_asym

```

(Electron PDFs: public)+≡

```
public :: rec_num
```

(Electron PDFs: sub interfaces)+≡

```

module function rec_num &
    (epdf, flv, x, scale, alpha, running) result (recnum)
    type(qed_pdf_t), intent(in) :: epdf
    integer, intent(in) :: flv
    real(default) :: recnum
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    logical, intent(in) :: running
end function rec_num

```

(Electron PDFs: procedures)+≡

```
module function rec_num &
```

```

      (epdf, flv, x, scale, alpha, running) result (recnum)
type(qed_pdf_t), intent(in) :: epdf
integer, intent(in) :: flv
real(default) :: recnum
real(default), intent(in) :: x
real(default), intent(in) :: scale
real(default), intent(in) :: alpha
logical, intent(in) :: running
integer :: nlep
real(default) :: ln0, eta0, al_2pi, p, prefac
if (allocated (epdf%q_in)) then
  ln0 = log(epdf%q_in**2/epdf%mass**2)
  eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
else
  ln0 = zero
  eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
end if
if (running) then
  p = t_alpha (epdf, scale)
else
  p = eta0 / two
end if
select case (epdf%log_order)
case (EPDF_LL)
  recnum = 0
  return
case (EPDF_NLL)
  if (running) then
    select type (aqed => epdf%aqed)
    type is (alpha_qed_from_scale_t)
      nlep = aqed%nlep
      al_2pi = aqed%get (scale) / two / Pi
    type is (alpha_qed_fixed_t)
      call msg_fatal &
        ("bar_asym: has to be called with running alpha.")
    end select
  else
    nlep = epdf%n_lep
    al_2pi = alpha / two / Pi
  end if
  prefac = al_2pi * p**2 / two
end select
select case (flv)
case (EPDF_S)
  recnum = prefac * endpoint_func_S (x, nlep)
case (EPDF_NS)
  recnum = prefac * endpoint_func_NS (x)
case (EPDF_G)
  recnum = prefac * endpoint_func_GAM (x)
case default
  call msg_fatal &
    ("rec_num: wrong lepton flavor.")
end select
end function rec_num

```

```

<Electron PDFs: public>+≡
public :: recbar

<Electron PDFs: sub interfaces>+≡
module function recbar &
    (epdf, flv, x, scale, alpha, running) result (bar)
    type(qed_pdf_t), intent(in) :: epdf
    integer, intent(in) :: flv
    real(default) :: bar
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    logical, intent(in) :: running
end function recbar

<Electron PDFs: procedures>+≡
module function recbar &
    (epdf, flv, x, scale, alpha, running) result (bar)
    type(qed_pdf_t), intent(in) :: epdf
    integer, intent(in) :: flv
    real(default) :: bar
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    logical, intent(in) :: running
    logical, dimension(6) :: order
    integer :: nlep
    real(default) :: ln0, eta0, al_2pi, p
    real(default), dimension(6) :: jll_nll
    if (allocated (epdf%q_in)) then
        ln0 = log(epdf%q_in**2/epdf%mass**2)
        eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
    else
        ln0 = zero
        eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
    end if
    if (running) then
        p = t_alpha (epdf, scale)
    else
        p = eta0 / two
    end if
    order = .false.
    order(1:3) = .true.
    select case (epdf%log_order)
    case (EPDF_LL)
        nlep = epdf%n_lep
        al_2pi = zero
    case (EPDF_NLL)
        if (running) then
            select type (aqed => epdf%aqed)
            type is (alpha_qed_from_scale_t)
                nlep = aqed%nlep
                al_2pi = aqed%get (scale) / two / Pi
            type is (alpha_qed_fixed_t)

```

```

        call msg_fatal &
            ("recbar: has to be called with running alpha.")
    end select
else
    nlep = epdf%n_lep
    al_2pi = alpha / two / Pi
    end if
    order(4:6) = .true.
end select
select case (flv)
case (EPDF_S)
    call recbar_singlet (x, jll_nll, nlep, ln0, order, running)
case (EPDF_G)
    call recbar_photon (x, jll_nll, nlep, ln0, order, running)
case (EPDF_NS)
    call recbar_nonsinglet (x, jll_nll, nlep, ln0, order, running)
case default
    call msg_fatal &
        ("recbar: wrong lepton flavor.")
    end select
bar = rec_series (p, al_2pi, jll_nll)
end function recbar

```

(Electron PDFs: public)+≡
 public :: rechat

(Electron PDFs: sub interfaces)+≡
 module function rechat &
 (epdf, flv, x, scale, alpha, running) result (hat)
 type(qed_pdf_t), intent(in) :: epdf
 integer, intent(in) :: flv
 real(default) :: hat
 real(default), intent(in) :: x
 real(default), intent(in) :: scale
 real(default), intent(in) :: alpha
 logical, intent(in) :: running
 end function rechat

(Electron PDFs: procedures)+≡
 module function rechat &
 (epdf, flv, x, scale, alpha, running) result (hat)
 type(qed_pdf_t), intent(in) :: epdf
 integer, intent(in) :: flv
 real(default) :: hat
 real(default), intent(in) :: x
 real(default), intent(in) :: scale
 real(default), intent(in) :: alpha
 logical, intent(in) :: running
 logical, dimension(6) :: order
 integer :: nlep
 real(default) :: ln0, eta0, al_2pi, p
 real(default), dimension(6) :: jll_nll
 if (allocated (epdf%q_in)) then
 ln0 = log(epdf%q_in**2/epdf%mass**2)
 eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)


```

else
  ln0 = zero
  eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
end if
if (running) then
  p = t_alpha (epdf, scale)
else
  p = eta0 / two
end if
order = .false.
order(1:3) = .true.
select case (epdf%log_order)
case (EPDF_LL)
  nlep = epdf%n_lep
  al_2pi = zero
case (EPDF_NLL)
  if (running) then
    select type (aqed => epdf%aqed)
    type is (alpha_qed_from_scale_t)
      nlep = aqed%nlep
      al_2pi = aqed%get (scale) / two / Pi
    type is (alpha_qed_fixed_t)
      call msg_fatal &
        ("rechat: has to be called with running alpha.")
    end select
  else
    nlep = epdf%n_lep
    al_2pi = alpha / two / Pi
  end if
  order(4:6) = .true.
end select
select case (flv)
case (EPDF_S)
  call rechat_singlet (x, jll_nll, nlep, ln0, order, running)
case (EPDF_G)
  call rechat_photon (x, jll_nll, nlep, ln0, order, running)
case (EPDF_NS)
  call rechat_nonsinglet (x, jll_nll, nlep, ln0, order, running)
case default
  call msg_fatal &
    ("rechat: wrong lepton flavor.")
end select
hat = rec_series (p, al_2pi, jll_nll)
end function rechat

```

The logical array `order` allows to individually switch the expansion terms on and off. For LL, the first three are taken, for NLL all of them.

(Electron PDFs: public)+≡

public :: elecbar_asym_p

(Electron PDFs: sub interfaces)+≡

```

module subroutine elecbar_asym_p (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll

```

```

    real(default), intent(in) :: ln0
    integer, intent(in) :: nlep
    logical, dimension(6), intent(in) :: order
    logical, intent(in) :: running
end subroutine elecbar_asym_p

```

(Electron PDFs: procedures)+≡

```

module subroutine elecbar_asym_p (x, jll_nll, nlep, ln0, order, running)
    real(default), intent(in) :: x
    real(default), dimension(6), intent(out) :: jll_nll
    real(default), intent(in) :: ln0
    integer, intent(in) :: nlep
    logical, dimension(6), intent(in) :: order
    logical, intent(in) :: running
    real(default) :: c_b0, c_b1
    jll_nll = 0._default
    c_b0 = - coeffqed_b0 (0, nlep)
    c_b1 = - coeffqed_b1 (0, nlep)
    if (order(1)) then
        jll_nll(1) = two/(one - x)
    end if
    if (order(2)) then
        jll_nll(2) = (two*(-three - four*log(1-x))) / (-one + x)
    end if
    if (order(3)) then
        jll_nll(3) = (-27._default + 8._default*Pi2 - 72._default*log(1-x) &
            - 48*log(1-x)**2) / (two*(-one + x))
    end if
    if (order(4)) then
        jll_nll(4) = (two*(-one + ln0)) / (one-x) - &
            (four*log(1-x))/(one-x)
    end if
    if (order(5)) then
        if (running) then
            jll_nll(5) = (one - 20._default * nlep/9._default + four*c_b0*Pi &
                - (four*c_b1*Pi)/c_b0 + (four*Pi2)/three + &
                ln0*(6._default-four*c_b0*Pi))/(one-x) - (two*(7._default - &
                four*ln0 - four*c_b0*Pi)*log(1-x))/(one-x) - &
                (12._default*log(1-x)**2)/(one-x)
        else
            jll_nll(5) = (one + 6._default*ln0 - (20._default * nlep)/9._default &
                + (four*Pi2)/three)/(one-x) - (two*(7._default-four*ln0) * &
                log(1-x))/(one-x) - (12._default*log(1-x)**2)/(one-x);
        end if
    end if
    if (order(6)) then
        if (running) then
            jll_nll(6) = two * (-((8.5_default + (80._default*nlep)/9._default - &
                28._default*c_b0*Pi + (16._default*c_b1*Pi)/c_b0 &
                - (20._default*Pi2)/three + 8._default*c_b0**2*Pi2 - &
                two*ln0*(9._default - 8._default*c_b0*Pi))*log(1-x))/(one-x)) - &
                (6._default*(five - two*ln0 - four*c_b0*Pi) * log(1-x)**2) / &
                (one-x) - (16._default*log(1-x)**3) / (one-x) + (4.5_default - &
                (12._default*c_b1*Pi)/c_b0 - four*c_b0**2*Pi2 + (three + &
                four*c_b1)*Pi2 - nlep*(11._default/3._default - &

```

```

(20._default*c_b0*Pi)/9._default + (four*Pi2)/9._default) - &
(two*c_b0*Pi*(three + four*Pi2))/three + ln0*(6.75_default - &
12._default*c_b0*Pi - two*Pi2 + four*c_b0**2*Pi2) - &
20._default*zeta3) / (one-x))
else
  jll_nll(6) = two * (-((8.5_default - 18._default*ln0 + (80._default &
    * nlep)/9._default - (20._default*Pi2)/three) * log(1-x))/(one-x)) - &
    (6._default*(five-two*ln0) * log(1-x)**2)/(one-x) - &
    (16._default*log(1-x)**3)/(one-x) + (4.5_default + three*Pi2 + &
    ln0*(6.75_default - two*Pi2) - nlep*(11._default/3._default + &
    (four*Pi2)/9._default) - 20._default*zeta3) / (one-x))
end if
end if
end subroutine elecbar_asym_p

```

(Electron PDFs: public)+≡

```
public :: photbar_asym_p
```

(Electron PDFs: sub interfaces)+≡

```

module subroutine photbar_asym_p (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
end subroutine photbar_asym_p

```

(Electron PDFs: procedures)+≡

```

module subroutine photbar_asym_p (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
  real(default) :: c_b0, c_b1ob0
  jll_nll = 0._default
  if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)
    c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
  else
    c_b0 = zero
    c_b1ob0 = zero
  end if
  if (order(1)) then
    jll_nll(1) = one
  end if
  if (order(2)) then
    jll_nll(2) = 1.5_default - (two * nlep)/three +two*log(1-x)
  end if
  if (order(3)) then
    jll_nll(3) = 2.25_default - nlep + four * nlep**2 / 9._default - &
      (two*Pi2)/three + (6._default - (four*nlep)/three)*log(1-x) + &
      four*log(1-x)**2
  end if

```

```

end if
if (order(4)) then
  jll_nll(4) = -one + ln0
end if
if (order(5)) then
  jll_nll(5) = -four + (three*ln0)/two - (two*(13._default + &
    three*ln0)*nlep)/9._default - two*c_b1ob0*Pi - 2*c_b0*(-one + &
    ln0)*Pi + (-7._default + two*ln0 - (four*nlep)/three)*log(1-x) &
    - three*log(1-x)**2
end if
if (order(6)) then
  jll_nll(6) = -5.625_default - (23._default * nlep)/6._default + &
    (52._default * nlep**2)/27._default + four*c_b0*Pi - &
    6._default*c_b1ob0*Pi + (40._default*c_b0*nlep*Pi)/9._default + &
    (8._default*c_b1ob0*nlep*Pi)/three + (11._default*Pi2)/6._default &
    - four*c_b0**2*Pi2 + four*c_b0*c_b1ob0*Pi2 + &
    (two*nlep*Pi2)/9._default + ln0*(2.25_default + &
    (four*nlep**2)/9._default - 6._default*c_b0*Pi - (two*Pi2)/three + &
    four*c_b0**2*Pi2 + nlep*(-one + (8._default*c_b0*Pi)/three)) + &
    (-18.5_default + (8._default*nlep**2)/9._default + &
    18._default*c_b0*Pi - 8._default*c_b1ob0*Pi + two*Pi2 + &
    ln0*(6._default - (four*nlep)/three - 8._default*c_b0*Pi) + &
    (four*nlep*(-5._default + two*c_b0*Pi))/three)*log(1-x) + &
    (-18.5_default + four*ln0 - (two*nlep)/three + &
    10._default*c_b0*Pi)*log(1-x)**2 - 6._default*log(1-x)**3 - &
    6._default*zeta3
end if
end subroutine photbar_asym_p

```

(Electron PDFs: public)+≡

```
public :: recbar_singlet
```

(Electron PDFs: sub interfaces)+≡

```

module subroutine recbar_singlet (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
end subroutine recbar_singlet

```

(Electron PDFs: procedures)+≡

```

module subroutine recbar_singlet (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
  real(default) :: c_b0, c_b1ob0
  jll_nll = 0._default
  if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)
    c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
  end if
end subroutine recbar_singlet

```

```

else
  c_b0 = zero
  c_b1ob0 = zero
end if
if (order(1)) then
  jll_nll(1) = -two + two/(one-x)
end if
if (order(2)) then
  jll_nll(2) = -two + 6._default/(one-x) - &
    8._default*log(1-x) + (8._default*log(1-x))/(one-x)
end if
if (order(3)) then
  jll_nll(3) = 4.5_default + four*Pi2 + (13.5_default - &
    four*Pi2)/(one-x) - 12._default*log(1-x) + &
    (36._default*log(1-x))/(one-x) - 24._default*log(1-x)**2 + &
    (24._default*log(1-x)**2)/(one-x)
end if
if (order(4)) then
  jll_nll(4) = two - two*ln0 + (-two+two*ln0)/(one-x) + &
    four*log(1-x) - (four*log(1-x))/(one-x)
end if
if (order(5)) then
  jll_nll(5) = (9._default - 12._default*nlep - 18._default*x &
    + 32._default*nlep*x - 36._default*c_b0*Pi*x + &
    36._default*c_b1ob0*Pi*x - 12._default*Pi2*x + &
    18._default*ln0*(-two-x+two*c_b0*Pi*x) - &
    18._default*(-two+(-five + four*ln0 + four*c_b0*Pi)*x)*log(1-x) &
    + 108._default*x*log(1-x)**2)/(9._default*(-one+x))
end if
if (order(6)) then
  jll_nll(6) = (-9._default*ln0*(36._default + 16._default*c_b0**2*Pi2*x - &
    (9._default + 8._default*Pi2)*x - 16._default*c_b0*Pi*(two+x)) + &
    two*nlep*(44._default + (22._default + 8._default*Pi2)*x - &
    8._default*c_b0*Pi*(-three + 8._default*x)) + &
    two*(16._default*nlep*(-three + 13._default*x) + 36._default*ln0* &
    (-6._default + (-three + 8._default*c_b0*Pi)*x) + three*(72._default + &
    48._default*c_b0**2*Pi2*x + (-21._default + 96._default*c_b1ob0*Pi - &
    40._default*Pi2)*x - 24._default*c_b0*Pi*(three + four*x))*log(1-x) - &
    216._default*(-two + (-three + two*ln0 + four*c_b0*Pi)*x)*log(1-x)**2 + &
    576._default*x*log(1-x)**3 + &
    6._default*(-15._default - 8._default*Pi2 - 12._default*x - &
    10._default*Pi2*x + 24._default*c_b0**2*Pi2*x + &
    24._default*c_b1ob0*Pi*(two+x) + two*c_b0*Pi*(-15._default + &
    (21._default - 12._default*c_b1ob0*Pi + 8._default*Pi2)*x) + &
    120._default*x*zeta3)) / (18.*(-one+x))
end if
end subroutine recbar_singlet

```

(Electron PDFs: public)+≡
 public :: recbar_nonsinglet

(Electron PDFs: sub interfaces)+≡
 module subroutine recbar_nonsinglet (x, jll_nll, nlep, ln0, order, running)
 real(default), intent(in) :: x

```

    real(default), dimension(6), intent(out) :: jll_nll
    real(default), intent(in) :: ln0
    integer, intent(in) :: nlep
    logical, dimension(6), intent(in) :: order
    logical, intent(in) :: running
end subroutine recbar_nonsinglet

```

(*Electron PDFs: procedures*) + ≡

```

module subroutine recbar_nonsinglet (x, jll_nll, nlep, ln0, order, running)
    real(default), intent(in) :: x
    real(default), dimension(6), intent(out) :: jll_nll
    real(default), intent(in) :: ln0
    integer, intent(in) :: nlep
    logical, dimension(6), intent(in) :: order
    logical, intent(in) :: running
    real(default) :: c_b0, c_b1ob0
    jll_nll = 0._default
    if (running) then
        c_b0 = - coeffqed_b0 (0, nlep)
        c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
    else
        c_b0 = zero
        c_b1ob0 = zero
    end if
    if (order(1)) then
        jll_nll(1) = -two + two/(one - x)
    end if
    if (order(2)) then
        jll_nll(2) = -two + 6._default/(one - x) &
            - 8._default*log(1-x) + (8._default*log(1-x))/(one - x)
    end if
    if (order(3)) then
        jll_nll(3) = 4.5_default + 4._default*Pi2 + (13.5_default &
            - four*Pi2)/(one - x) - 12._default*log(1-x) + &
            (36._default*log(1-x))/(one - x) - 24._default*log(1-x)**2 + &
            (24._default*log(1-x)**2)/(one - x)
    end if
    if (order(4)) then
        jll_nll(4) = two - two*ln0 + (-two + two*ln0)/(one-x) + &
            four*log(1-x) - (four*log(1-x))/(one-x)
    end if
    if (order(5)) then
        jll_nll(5) = -two - two*ln0+(32._default*nlep)/9._default + &
            four*c_b1ob0*Pi - (four*Pi2)/three + one/(one-x) + &
            (6._default*ln0)/(one-x) - (20._default*nlep)/(9._default*(one-x)) - &
            (four*c_b1ob0*Pi)/(one-x) + (four*Pi2)/(three*(one-x)) + &
            10._default*log(1-x) - 8._default*ln0*log(1-x) - &
            (14._default*log(1-x))/(one-x) + (8._default*ln0*log(1-x))/(one-x) + &
            12._default*log(1-x)**2 - (12._default*log(1-x)**2)/(one-x) + &
            c_b0*(-four*Pi + four*ln0*Pi + (four*Pi))/(one-x) - &
            (four*ln0*Pi)/(one-x) - 8._default*Pi*log(1-x) + &
            (8._default*Pi*log(1-x))/(one-x)
    end if
    if (order(6)) then
        jll_nll(6) = -four + (9._default * ln0)/two + (22._default*nlep)/9._default + &

```

```

8._default*c_b1ob0*Pi - (10._default*Pi2)/three + four*ln0*Pi2 + &
(8._default*nlep*Pi2)/9._default + 9._default/(one-x) + &
(27._default*ln0)/(two*(one-x)) - (22._default*nlep)/(three*(one-x)) - &
(24._default*c_b1ob0*Pi)/(one-x) + (6._default*Pi2)/(one-x) - &
(four*ln0*Pi2)/(one-x) - (8._default*nlep*Pi2)/(9._default*(one-x)) - &
7._default*log(1-x) - 12._default*ln0*log(1-x) + (208._default* &
nlep*log(1-x))/9._default + 32._default*c_b1ob0*Pi*log(1-x) - &
(40._default*Pi2*log(1-x))/three - (17._default*log(1-x))/(one-x) + &
(36._default*ln0*log(1-x))/(one-x) - (160._default*nlep*log(1-x))/ &
(9._default*(one-x)) - (32._default*c_b1ob0*Pi*log(1-x))/(one-x) + &
(40._default*Pi2*log(1-x))/(three*(one-x)) + 36._default*log(1-x)**2 - &
24._default*ln0*log(1-x)**2 - (60._default*log(1-x)**2)/(one-x) + &
(24._default*ln0*log(1-x)**2)/(one-x) + 32._default*log(1-x)**3 - &
(32*log(1-x)**3)/(one-x) + c_b0**2*(8._default*Pi2 - &
8._default*ln0*Pi2 - (8._default*Pi2)/(one-x) + &
(8._default*ln0*Pi2)/(one-x) + 16._default*Pi2*log(1-x) - &
(16._default*Pi2*log(1-x))/(one-x)) + c_b0*(14._default*Pi + &
8._default*ln0*Pi - (64._default*nlep*Pi)/9._default - &
8._default*c_b1ob0*Pi2 + (16._default*Pi**3)/three - &
(24._default*ln0*Pi)/(one-x) + (40._default*nlep*Pi)/(9._default*(one-x)) + &
(8._default*c_b1ob0*Pi2)/(one-x) + (-four*Pi - &
(16._default*Pi**3)/three)/(one-x) - 32._default*Pi*log(1-x) + &
32._default*ln0*Pi*log(1-x) + (56._default*Pi*log(1-x))/(one-x) - &
(32._default*ln0*Pi*log(1-x))/(one-x) - 48._default*Pi*log(1-x)**2 + &
(48*Pi*log(1-x)**2)/(1-x)) + 40._default*zeta3 - (40._default*zeta3)/(one-x)
end if
end subroutine recbar_nonsinglet

```

(Electron PDFs: public)+≡

```
public :: recbar_photon
```

(Electron PDFs: sub interfaces)+≡

```

module subroutine recbar_photon (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
end subroutine recbar_photon

```

(Electron PDFs: procedures)+≡

```

module subroutine recbar_photon (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
  real(default) :: c_b0, c_b1ob0
  jll_nll = 0._default
  if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)
    c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
  else

```

```

        c_b0 = zero
        c_b1ob0 = zero
    end if
    if (order(1)) then
        jll_nll(1) = one
    end if
    if (order(2)) then
        jll_nll(2) = 1.5_default - (two*nlep)/three + two*log(1-x)
    end if
    if (order(3)) then
        jll_nll(3) = 2.25_default - nlep + (four*nlep**2)/9._default - &
            (two*Pi2)/three + (6._default - (four*nlep)/three)*log(1-x) + &
            four*log(1-x)**2
    end if
    if (order(4)) then
        jll_nll(4) = -one + ln0
    end if
    if (order(5)) then
        jll_nll(5) = -four + (three*ln0)/two - (two*(13._default + &
            three*ln0)*nlep)/9._default - two*c_b1ob0*Pi - &
            two*c_b0*(-one+ln0)*Pi + (-7._default + two*ln0 - &
            (four*nlep)/three)*log(1-x) - three*log(1-x)**2
    end if
    if (order(6)) then
        jll_nll(6) = -5.625_default - (23._default*nlep)/6._default + &
            (52._default*nlep**2)/27._default + four*c_b0*Pi - &
            6._default*c_b1ob0*Pi + (40._default*c_b0*nlep*Pi)/9._default + &
            (8._default*c_b1ob0*nlep*Pi)/three + (11._default*Pi2)/6._default - &
            four*c_b0**2*Pi2 + four*c_b0*c_b1ob0*Pi2 + (two*nlep*Pi2)/9._default + &
            ln0*(2.25_default + (four*nlep**2)/9._default - 6._default*c_b0*Pi - &
            (two*Pi2)/three + four*c_b0**2*Pi2 + nlep*(-one + &
            (8._default*c_b0*Pi)/three)) + (-18.5_default + &
            (8._default*nlep**2)/9._default + 18._default*c_b0*Pi - &
            8._default*c_b1ob0*Pi + two*Pi2 + ln0*(6._default - (four*nlep)/three - &
            8._default*c_b0*Pi) + (four*nlep*(-five + two*c_b0*Pi))/three)*log(1-x) + &
            (-18.5_default + four*ln0 - (two*nlep)/three + 10._default*c_b0*Pi) * &
            log(1-x)**2 - 6._default*log(1-x)**3 - 6._default*zeta3
    end if
end subroutine rechat_photon

```

(Electron PDFs: public)+≡

```
public :: rechat_singlet
```

(Electron PDFs: sub interfaces)+≡

```

module subroutine rechat_singlet (x, jll_nll, nlep, ln0, order, running)
    real(default), intent(in) :: x
    real(default), dimension(6), intent(out) :: jll_nll
    real(default), intent(in) :: ln0
    integer, intent(in) :: nlep
    logical, dimension(6), intent(in) :: order
    logical, intent(in) :: running
end subroutine rechat_singlet

```

(Electron PDFs: procedures)+≡

```
module subroutine rechat_singlet (x, jll_nll, nlep, ln0, order, running)
```



```

real(default), intent(in) :: x
real(default), dimension(6), intent(out) :: jll_nll
real(default), intent(in) :: ln0
integer, intent(in) :: nlep
logical, dimension(6), intent(in) :: order
logical, intent(in) :: running
real(default) :: c_b0, c_blob0
real(default) :: j6_1, j6_2, j6_3
jll_nll = 0._default
if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)
    c_blob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
else
    c_b0 = zero
    c_blob0 = zero
end if
if (order(1)) then
    jll_nll(1) = 1-x
end if
if (order(2)) then
    jll_nll(2) = -three-x - (two*nlep*(-one+x)*(four+x*(7+4*x)))/(three*x) - &
        four*(-one+x)*log(1-x) + ((one-four*nlep+(three+four*nlep)*x**2)*log(x))/(-one+x)
end if
if (order(3)) then
    jll_nll(3) = -(-64*nlep**2 - 513*x -552*nlep*x + 16*nlep**2*x - 36*Pi2*x + &
        96*nlep*Pi2*x + 378*x**2 + 1104*nlep*x**2 + 96*nlep**2*x**2 + 144*Pi2*x**2 + &
        135*x**3 - 552*nlep*x**3 + 16*nlep**2*x**3 - 108*Pi2*x**3 -96*nlep*Pi2*x**3 - &
        64*nlep**2*x**4 + 432*(-1+x)**2*x*log(1-x)**2 -54*x*log(x) - &
        96*nlep**2*x*log(x) - 432*x**2*log(x) + 288*nlep*x**2*log(x) - &
        162*x**3*log(x) +96*nlep*x**3*log(x) + 96*nlep**2*x**3*log(x) - &
        384*nlep*x**4*log(x) + 18*x*log(x)**2 - 144*nlep*x*log(x)**2 + &
        126*x**3*log(x)**2 + 144*nlep*x**3*log(x)**2 + 24*log(1-x)*((-1+x) * &
        (9*x*(3+x) + 4*nlep*(-4-3*x+3*x**2+4*x**3)) - 18*(x+x**3)*log(x)) + &
        72*(3+8*nlep)*x*(-1+x**2)*polylog(2,x)) / (36._default*(-1+x)*x)
end if
if (order(4)) then
    jll_nll(4) = -one + ln0*(1-x) + x - 2*(1-x)*log(1-x)
end if
if (order(5)) then
    jll_nll(5) = -(-72*nlep + 48*ln0*nlep+9*x - 54*ln0*x - 176*nlep*x + 36*ln0*nlep*x + &
        36*c_b0*Pi*x - 36*c_blob0*Pi*x - 36*c_b0*ln0*Pi*x + 42*Pi2*x + 9*x**2 - &
        18*ln0*x**2 + 368*nlep*x**2 -84*ln0*nlep*x**2 - 36*c_b0*Pi*x**2 + &
        36*c_blob0*Pi*x**2 + 36*c_b0*ln0*Pi*x**2 - 42*Pi2*x**2 - 9*x**3 + 54*ln0*x**3 + &
        104*nlep*x**3 - 84*ln0*nlep*x**3 - 36*c_b0*Pi*x**3 + 36*c_blob0*Pi*x**3 + &
        36*c_b0*ln0*Pi*x**3 - 18*Pi2*x**3 - 9*x**4 + 18*ln0*x**4 - 296*nlep*x**4 + &
        36*ln0*nlep*x**4 + 36*c_b0*Pi*x**4 - 36*c_blob0*Pi*x**4 - 36*c_b0*ln0*Pi*x**4 + &
        18*Pi2*x**4 + 72*nlep*x**5 + 48*ln0*nlep*x**5 + 18*x*log(1-x) + &
        72*ln0*x*log(1-x) + 72*c_b0*Pi*x*log(1-x) + 54*x**2*log(1-x) - &
        72*ln0*x**2*log(1-x) - 72*c_b0*Pi*x**2*log(1-x) - 18*x**3*log(1-x) - &
        72*ln0*x**3*log(1-x) - 72*c_b0*Pi*x**3*log(1-x) - 54*x**4*log(1-x) + &
        72*ln0*x**4*log(1-x) + 72*c_b0*Pi*x**4*log(1-x) - 108*x*log(1-x)**2 + &
        108*x**2*log(1-x)**2 + 108*x**3*log(1-x)**2 - 108*x**4*log(1-x)**2 - &
        96*nlep*log(x) - 18*ln0*x*log(x) - 192*nlep*x*log(x) + 72*ln0*nlep*x*log(x) - &
        18*ln0*x**2*log(x) + 120*nlep*x**2*log(x) + 72*ln0*nlep*x**2*log(x) + &

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18*x**3*log(x) - 54*ln0*x**3*log(x) + 264*nlep*x**3*log(x) - &
72*ln0*nlep*x**3*log(x) + 18*x**4*log(x) - 54*ln0*x**4*log(x) - &
48*nlep*x**4*log(x) - 72*ln0*nlep*x**4*log(x) - 96*nlep*x**5*log(x) + &
72*x**3*log(1-x)*log(x) + 72*x**4*log(1-x)*log(x) + 9*x*log(x)**2 - &
108*nlep*x*log(x)**2 - 27*x**2*log(x)**2 - 108*nlep*x**2*log(x)**2 + &
27*x**3*log(x)**2 + 108*nlep*x**3*log(x)**2 - 9*x**4*log(x)**2 + &
108*nlep*x**4*log(x)**2 + 144*x*log(x)*log(1+x) - 144*x**2*log(x)*log(1+x) - &
72*x**3*log(x)*log(1+x) + 72*x**4*log(x)*log(1+x) - 108*x*log(1+x)**2 + &
108*x**2*log(1+x)**2 + 36*(-one+x)*x*(1+x)**2*polylog(2,1-x) + &
72*x*(2-2*x-x**2+x**3)*polylog(2,-x) - 216*x*polylog(2,1/(1+x)) + &
216*x**2*polylog(2,1/(1+x))) / (18.*x*(-one+x**2))
end if
if (order(6)) then
  j6_1 = -1152*nlep + 32*nlep**2 + 192*ln0*nlep**2 + 1152*c_b1ob0*nlep*Pi + 96*nlep*Pi2 - &
1350*x + 1539*ln0*x - 3660*nlep*x + 1656*ln0*nlep*x + 720*nlep**2*x + 144*ln0*nlep**2*x &
1296*c_b1ob0*Pi*x + 864*c_b1ob0*nlep*Pi*x + 72*Pi2*x + 216*ln0*Pi2*x + 120*nlep*Pi2*x &
486*x**2 + 405*ln0*x**2 + 5004*nlep*x**2 - 1656*ln0*nlep*x**2 - 176*nlep**2*x**2 - &
336*ln0*nlep**2*x**2 - 432*c_b1ob0*Pi*x**2 - 2016*c_b1ob0*nlep*Pi*x**2 + 108*Pi2*x**2 &
216*ln0*Pi2*x**2 - 216*nlep*Pi2*x**2 + 1350*x**3 - 1539*ln0*x**3 + 4092*nlep*x**3 - &
1656*ln0*nlep*x**3 - 1328*nlep**2*x**3 - 336*ln0*nlep**2*x**3 + 1296*c_b1ob0*Pi*x**3 - &
2016*c_b1ob0*nlep*Pi*x**3 - 504*Pi2*x**3 - 216*ln0*Pi2*x**3 - 216*nlep*Pi2*x**3 - &
486*x**4 - 405*ln0*x**4 - 3852*nlep*x**4 + 1656*ln0*nlep*x**4 + 144*nlep**2*x**4 + &
144*ln0*nlep**2*x**4 + 432*c_b1ob0*Pi*x**4 + 864*c_b1ob0*nlep*Pi*x**4 + &
324*Pi2*x**4 + 216*ln0*Pi2*x**4 + 120*nlep*Pi2*x**4 - 432*nlep*x**5 + &
608*nlep**2*x**5 + 192*ln0*nlep**2*x**5 + 1152*c_b1ob0*nlep*Pi*x**5 + &
96*nlep*Pi2*x**5 + 288*Pi2*x*(-1+2*x+x**3)*log(2._default) - &
216*(-1+x)*(1+x)*(3+x*(7+9*x))*log(2._default)**2 - &
144*x*(-11+x*(16+x+4*x**2))*log(2._default)**3 - &
432*c_b0**2*Pi2*(-1+x)**2*x*(1+x)*(-1+ln0-2*log(1-x)) + &
1728*c_b1ob0*Pi*(-1+x)**2*x*(1+x)*log(1-x) + 6*(16*nlep**2*(-3+x)*x*(1+x)*(-1+3*x) + &
4*nlep*(8+12*ln0*(-4+x*(-3+7*x*(1+x)))) + x*(181+x*(-237+x*(-117+229*x)))) - &
3*(-1+x)*x*(36*ln0*(1+x)*(3+x)+Pi2*(-56-4*x+44*x**2) + 3*(-37+(-36+x)*x - &
40*log(2._default)**2))*log(1-x)
  j6_2 = 1512*(-1+x)*x*(1+x)*log(1-x)**2 + 1296*ln0*(-1+x)*x*(1+x)*log(1-x)**2 + &
1080*(-1+x)*x**2*(1+x)*log(1-x)**2 - 1296*ln0*(-1+x)*x**2*(1+x)*log(1-x)**2 + &
144*nlep*(-1+x)**2*(1+x)*(4+7*x+4*x**2)*log(1-x)**2 + &
1728*(-1+x)**2*x*(1+x)*log(1-x)**3 + &
96*nlep*(4*nlep-9*ln0*x**4+4*(-4-3*ln0+nlep)*x**5)*(log(1-x)-log(x)) - &
432*c_b1ob0*Pi*x*(1+x)*(1-4*nlep+(3+4*nlep)*x**2)*log(x) - &
6*(3*ln0*x*(16*nlep**2*(-1+x)*(1+x)**2 + 16*nlep*x*(3+4*x) - 9*(1+x)*(1+x*(8+3*x))) - &
216*log(2._default) + 2*x*(8*nlep**2*(1+x)*(-7+x*(-13+16*x)) + &
3*Pi2*(-13+x*(9+(5-9*x)*x)) + 2*nlep*(238 + 18*Pi2*(-1+x)*(1+x)*(2+x) + &
x*(-83+x*(-152+105*x))) + 144*x*log(2._default) + &
9*(1+x)*(3-x**2+8*(-1+x)*log(2._default) + 4*(-1+x)**2*log(2._default)**2))*log(x) + &
216*x*log(1-x)*log(x) - 576*nlep**2*(-1+x)*x*(1+x)**2*log(1-x)*log(x) - &
216*x**2*(7+10*x)*log(1-x)*log(x) + 648*ln0*x*(1+x)*(1+3*x**2)*log(1-x)*log(x) + &
144*nlep*(1+x)*(8+x*(15+8*x**3-9*x*(2+x)+12*ln0*(-1+x**2)))*log(1-x)*log(x) - &
216*(1+x)*(x-4*nlep*x+(11+4*nlep)*x**3)*log(1-x)**2*log(x) + 648*log(x)**2 + &
432*x*log(x)**2 - 504*nlep*x*(1+x)*log(x)**2 - 1440*nlep*x**4*(1+x)*log(x)**2 + &
288*nlep**2*(-1+x)*x*(1+x)**2*log(x)**2 + 72*nlep*x**2*(1+x)*(15+8*x)*log(x)**2 - &
54*ln0*x*(1+x)*(1-8*nlep+(7+8*nlep)*x**2)*log(x)**2 + &
108*x**2*(-13+x*(-8+7*x))*log(x)**2 - 216*(-1+x)*x*(-5-x*(5+2*x) + &
2*nlep*(-1+x+2*x**2))*log(1-x)*log(x)**2 + &
36*x*(-1+x**2)*(-1+5*x+12*nlep*(2+x))*log(x)**3 + 72*x*(Pi2*(-1+x)*(1+x**2) + &

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(-x**3+2*(-1+x)*(4+x**2)*log(2._default))*log(64._default))*log(1+x) + &
1728*(-1+x)*x*log(1-x)*log(x/four)*log(1+x) - 1296*(-1+x)*x*log(x)*log(1+x) - &
1728*(-1+x)*x**2*log(x)*log(1+x) + 432*x*(1+x)*(2+x*(-3+2*x))*log(x)**2*log(1+x) + &
432*(-3+2*x*(-1+x*(2+x)))+ 2*(-1+x)*x**3*log(2._default) - &
2*(-1+x)*x*log(2-2*x))*log(2*x)*log(1+x) - 1296*(-1+x)*log(1+x)**2 - &
2484*(-1+x)*x*log(1+x)**2 + 108*(-1+x)*x**2*(29+14*x)*log(1+x)**2 - &
1728*x**4*log(2._default)*log(1+x)**2 + 432*x*(-13+15*x)*log(x)*log(1+x)**2 + &
864*x**3*log(4*x)*log(1+x)**2 - 432*x**4*log(x)*(log((1-x)/2.))+log(1+x)) + &
288*(-1+x)*x*log(1+x)**2*(3*(log(4-4*x)+log(x)) + (-16+x**2)*log(1+x)) + &
864*(-1+x)*x*(-((-1+x**2)*log(1-x)) + x**2*log(1+x) -log(32*(1+x)))*polylog(2,(1-x)/2.
j6_3 = 648*x*(1+x)*polylog(2,1-x) + 648*ln0*x*(1+x)*(-1+x**2)*polylog(2,1-x) - &
576*nlep**2*x*(1+x)*(-1+x**2)*polylog(2,1-x) + 288*nlep*(-1+x)*(1+x)*(-2 + &
6*ln0*x*(1+x)+(-3+x)*x*(3+2*x))*polylog(2,1-x) - 432*(-1+x)*x*(1+x)*(4*(2 + &
nlep+x+nlep*x)*log(1-x)+(-1+2*nlep*(-2+x)-x)*log(x)+2*(-1+x)*log(1+x))*polylog(2,1-x)
432*(-1+x**2)*(3+x*(2+x*(-1+log(4._default)))-log(4._default)) - &
2*(-1+x)*x*log(1-x))*polylog(2,(-1+x)/(2.*x)) -1296*(-1+x)*polylog(2,-x) - &
4320*(-1+x)*x*polylog(2,-x) + 216*(-1+x)*x**2*(-1+15*x)*polylog(2,-x) + &
864*x*((-1+x)*log(1-x) + (1+x**3)*log(x) + (-5+6*x+x**2)*log(1+x))*polylog(2,-x) + &
1296*(-1+x)*x*polylog(2,1/(1+x)) + 864*(-1+x)*x**2*polylog(2,1/(1+x)) - &
1728*(-1+x)*x**3*polylog(2,1/(1+x)) - 2592*(-1+x)*x*log(1-x)*polylog(2,1/(1+x)) - &
864*x*(-4+5*x+x**3)*log(1+x)*polylog(2,1/(1+x)) + 12*c_b0*Pi*(-224*nlep+96*ln0*nlep +
90*x-108*ln0*x - 212*nlep*x+72*ln0*nlep*x - 36*c_b1ob0*Pi*x+54*Pi2*x - 36*ln0*x**2 + &
556*nlep*x**2-168*ln0*nlep*x**2 + 36*c_b1ob0*Pi*x**2 - 54*Pi2*x**2 - 90*x**3 + &
108*ln0*x**3+292*nlep*x**3 - 168*ln0*nlep*x**3 + 36*c_b1ob0*Pi*x**3 - 30*Pi2*x**3 + &
36*ln0*x**4 - 332*nlep*x**4 + 72*ln0*nlep*x**4 - 36*c_b1ob0*Pi*x**4 + &
30*Pi2*x**4 - 80*nlep*x**5 + 96*ln0*nlep*x**5 + 36*x*(-1+x**2)*(4*ln0*(-1+x) - &
3*(1+x))*log(1-x) + 216*(-1+x)*x*(1+x)*log(1-x)**2 - 216*(-1+x)*x**2*(1+x)*log(1-x)**2
6*(1+x)*(3*x*(-1-2*x*(1+x)+ln0*(2+6*x**2)) + 4*nlep*(8+x*(9+4*(-3+x)*x*(1+x) + &
6*ln0*(-1+x**2))))*log(x) + 36*x*(1+x)*(1+5*x**2)*log(1-x)*log(x) - &
9*(-1+x)**3*x*log(x)**2 + 180*nlep*x*(1+x)*(-1+x**2)*log(x)**2 + &
72*(-1+x)*x*(-2+x**2)*log(x)*log(1+x) + 108*(-1+x)*x*log(1+x)**2 + &
72*x*(1+x)*(-1+x**2)*polylog(2,1-x) + 72*(-1+x)*x*(-2+x**2)*polylog(2,-x) + &
216*(-1+x)*x*polylog(2,1/(1+x))) + &
216*(-1+x**2)*(-6+x*(-8+5*x)+10*(-1+x)*x*log(1+x))*polylog(2,x/(1+x)) + &
432*(-1+x)*(1+x)*(-3+x*(-2+x+log(4._default)-x*log(4._default)))+2*(-1+x)*x*log(1+x)) *
polylog(2,-1+2/(1+x)) + 864*(-1+x)**2*x*(1+x)*polylog(3,(1-x)/2.) + &
432*x*(-1+x**2)*(8+3*x+4*nlep*(1+x))*polylog(3,1-x) - &
864*(-1+x)**2*x*(1+x)*polylog(3,(-1+x)/(2.*x)) - &
432*x*(6*nlep+x)*(-1+x**2)*polylog(3,(-1+x)/x) + &
432*x*(1+x)*(7+x*(-16+7*x))*polylog(3,-x) + &
216*x*(9+20*nlep+3*x+8*nlep*x)*(-1+x**2)*polylog(3,x) + &
864*x*(1+x)*(3+x*(-4+3*x))*polylog(3,1/(1+x)) + &
3024*(-1+x)**2*x*(1+x)*polylog(3,x/(1+x)) - &
864*(-1+x)**2*x*(1+x)*polylog(3,(2*x)/(1+x)) + &
864*(-1+x)*x*(4+x**2)*polylog(3,(1+x)/2.) - &
54*x*(-107+16*nlep*(-1+x)*(1+x)*(5+2*x)+x*(99+x*(67+21*x)))*zeta3
jll_nll(6) = (j6_1 + j6_2 + j6_3) / (108._default*x*(-one+x**2))
end if
end subroutine rechat_singlet

```

(Electron PDFs: public)+≡
public :: rechat_nonsinglet
(Electron PDFs: sub interfaces)+≡

```

module subroutine rechat_nonsinglet (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
end subroutine rechat_nonsinglet

```

(*Electron PDFs: procedures*)+≡

```

module subroutine rechat_nonsinglet (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
  real(default) :: c_b0, c_b1ob0
  real(default) :: j6_1, j6_2, j6_3
  jll_nll = 0._default
  if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)
    c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
  else
    c_b0 = zero
    c_b1ob0 = zero
  end if
  if (order(1)) then
    jll_nll(1) = 1-x
  end if
  if (order(2)) then
    jll_nll(2) = ((1 - x)*(3 + x) - 4*(-1 + x)**2*log(1-x) + log(x) + 3*x**2*log(x)) / (-1 + x)
  end if
  if (order(3)) then
    jll_nll(3) = ((-1 + x)*(4*Pi2*(-1 + 3*x) - 3*(19 + 5*x)) - 48*(-1 + x)**2*log(1-x)**2 - &
      2*log(x)*(-3 - 9*x**2 + log(x) + 7*x**2*log(x)) + 24*log(1-x)*(3 - x**2 + &
      2*(1 + x**2)*log(x)) - 48*x*(log(2 - 2*x) - log(2*x)) - 24*(-1 + x**2)*polylog(2,x)) / &
      (four*(-1 + x))
  end if
  if (order(4)) then
    jll_nll(4) = (1-x)*(-1+ln0-2*log(1-x))
  end if
  if (order(5)) then
    jll_nll(5) = (135 + 54*ln0 + 68*nlep - 36*c_b0*Pi + 36*c_b1ob0*Pi + 36*c_b0*ln0*Pi + &
      18*Pi2 - 153*x + 18*ln0*x - 44*nlep*x + 36*c_b0*Pi*x - 36*c_b1ob0*Pi*x - &
      36*c_b0*ln0*Pi*x - 18*Pi2*x - 135*x**2 - 54*ln0*x**2 - 68*nlep*x**2 + 36*c_b0*Pi*x**2 &
      36*c_b1ob0*Pi*x**2 - 36*c_b0*ln0*Pi*x**2 + 6*Pi2*x**2 + 153*x**3 - 18*ln0*x**3 + &
      44*nlep*x**3 - 36*c_b0*Pi*x**3 + 36*c_b1ob0*Pi*x**3 + 36*c_b0*ln0*Pi*x**3 - &
      6*Pi2*x**3 - 18*log(1-x) - 72*ln0*log(1-x) - 72*c_b0*Pi*log(1-x) - 54*x*log(1-x) + &
      72*ln0*x*log(1-x) + 72*c_b0*Pi*x*log(1-x) + 18*x**2*log(1-x) + 72*ln0*x**2*log(1-x) + &
      72*c_b0*Pi*x**2*log(1-x) + 54*x**3*log(1-x) - 72*ln0*x**3*log(1-x) - &
      72*c_b0*Pi*x**3*log(1-x) + 108*log(1-x)**2 - 108*x*log(1-x)**2 - 108*x**2*log(1-x)**2 &
      108*x**3*log(1-x)**2 + 72*log(x) + 18*ln0*log(x) + 12*nlep*log(x) + 72*x*log(x) + &
      18*ln0*x*log(x) + 12*nlep*x*log(x) - 90*x**2*log(x) + 54*ln0*x**2*log(x) + &
      12*nlep*x**2*log(x) - 90*x**3*log(x) + 54*ln0*x**3*log(x) + 12*nlep*x**3*log(x) - &

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72*x**2*log(1-x)*log(x) - 72*x**3*log(1-x)*log(x) + 27*log(x)**2 - 9*x*log(x)**2 + &
9*x**2*log(x)**2 - 27*x**3*log(x)**2 + 144*log(x)*log(1+x) - 144*x*log(x)*log(1+x) - &
72*x**2*log(x)*log(1+x) + 72*x**3*log(x)*log(1+x) - 108*log(1+x)**2 + 108*x*log(1+x)**
36*(-1+x)*(1+x)**2*polylog(2,1-x) + 72*(2-2*x-x**2+x**3)*polylog(2,-x) - &
216*polylog(2,1/(1+x)) + 216*x*polylog(2,1/(1+x))) / (18._default*(-1+x**2))
end if
if (order(6)) then
j6_1 = 24*Pi2*(-1+x)*x + 4*nlep*(63+4*Pi2*(-1+x)-19*x)*(-1+x)*x*(1+x) + &
144*c_blob0*Pi*(-1+x)*x*(1+x)*(3+x) - 12*Pi2*(-1+x)*x**2*(3+17*x) - &
18*(-1+x)*x*(1+x)*(-73+57*x) + 9*ln0*(-1+x)*x*(1+x)*(8*Pi2*(-1+x)-3*(19+5*x)) + &
24*log(2._default)*(-4*Pi2*x*(-1+2*x+x**3)+2*x*(-11+x*(16+x+4*x**2))*log(2._default)**
(-1+x)*(1+x)*(3+x*(7+9*x))*log(8._default)) - &
144*c_b0**2*Pi2*(-1+x)**2*x*(1+x)*(-1+ln0-2*log(1-x)) + &
576*c_blob0*Pi*(-1+x)**2*x*(1+x)*log(1-x) - &
2*(-1+x)*x*(108*ln0*(1+x)*(3+x)+32*nlep*(11+(3-8*x)*x)+3*(81-27*x*(4+7*x) + &
4*Pi2*(-6+x+9*x**2)+120*log(2._default)**2))*log(1-x) + &
504*(-1+x)*x*(1+x)*log(1-x)**2 - 432*ln0*(-1+x)**2*x*(1+x)*log(1-x)**2 + &
360*(-1+x)*x**2*(1+x)*log(1-x)**2 + 576*(-1+x)**2*x*(1+x)*log(1-x)**3 - &
540*x*log(x) + 54*ln0*x*log(x) - 152*nlep*x*log(x) - 144*c_blob0*Pi*x*log(x) - &
84*Pi2*x*log(x) + 612*x**2*log(x) + 486*ln0*x**2*log(x) + 136*nlep*x**2*log(x) - &
144*c_blob0*Pi*x**2*log(x) + 132*Pi2*x**2*log(x) + 468*x**3*log(x) + &
594*ln0*x**3*log(x)-24*nlep*x**3*log(x) - 432*c_b1ob0*Pi*x**3*log(x) + &
84*Pi2*x**3*log(x) - 684*x**4*log(x)+162*ln0*x**4*log(x) - &
312*nlep*x**4*log(x) - 432*c_b1ob0*Pi*x**4*log(x) - 36*Pi2*x**4*log(x) - &
432*log(2._default)*log(x) - 288*x*log(2._default)*log(x) + &
576*x**2*log(2._default)*log(x)+288*x**3*log(2._default)*log(x) - &
144*x**4*log(2._default)*log(x)
j6_2 = 144*x*log(2._default)**2*log(x) - 144*x**2*log(2._default)**2*log(x) - &
144*x**3*log(2._default)**2*log(x) + 144*x**4*log(2._default)**2*log(x) + &
648*x*(1+x)*log(1-x)*log(x) + 216*ln0*x*(1+x)*log(1-x)*log(x) + &
96*nlep*x*(1+x)*log(1-x)*log(x) - 576*x**2*(1+x)*log(1-x)*log(x) - &
720*x**3*(1+x)*log(1-x)*log(x) + 648*ln0*x**3*(1+x)*log(1-x)*log(x) + &
96*nlep*x**3*(1+x)*log(1-x)*log(x) - 72*x*(1+x)*(1+11*x**2)*log(1-x)**2*log(x) - &
216*log(x)**2-288*x*log(x)**2 - 18*ln0*x*log(x)**2-24*nlep*x*log(x)**2 + &
108*x**2*log(x)**2 - 18*ln0*x**2*log(x)**2-24*nlep*x**2*log(x)**2 + &
288*x**3*log(x)**2 - 126*ln0*x**3*log(x)**2 - 72*nlep*x**3*log(x)**2 - &
36*x**4*log(x)**2 - 126*ln0*x**4*log(x)**2 - 72*nlep*x**4*log(x)**2 + &
72*(-1+x)*x*(1+x*(5+2*x))*log(1-x)*log(x)**2 - 36*x*log(x)**3 - &
12*x**2*log(x)**3+36*x**3*log(x)**3 + 12*x**4*log(x)**3 - &
576*(-1+x)*x*log(1-x)*log(x/four)*log(1+x) + 432*(-1+x)*x*log(x)*log(1+x) + &
576*(-1+x)*x**2*log(x)*log(1+x) - 144*x*(1+x)*(2+x*(-3+2*x))*log(x)**2*log(1+x) - &
24*(-1+x)*(Pi2*(x+x**3)+12*x*(4+x**2)*log(2._default)**2 + &
6*(3+x*(5+x+x**2*(-1+log(4._default))))-2*x*log(2-2*x))*log(2*x))*log(1+x) + &
432*(-1+x)*log(1+x)**2+828*(-1+x)*x*log(1+x)**2 - 36*(-1+x)*x**2*(29+14*x)*log(1+x)**2
j6_3 = 576*x**4*log(2._default)*log(1+x)**2 - 144*x*(-13+15*x)*log(x)*log(1+x)**2 - &
288*(-1+x)*x*(log(4-4*x)+log(x))*log(1+x)**2 - 288*x**3*log(4*x)*log(1+x)**2 - &
96*(-4+x)*(-1+x)*x*(4+x)*log(1+x)**3 + &
288*(-1+x)*x*(log(32._default)+(-1+x**2)*log(1-x)-(-1+x**2)*log(1+x))*polylog(2,(1-x)/
792*x*(1+x)*polylog(2,1-x) - 216*ln0*x*(1+x)*polylog(2,1-x) - &
576*x**3*(1+x)*polylog(2,1-x) + 216*ln0*x**3*(1+x)*polylog(2,1-x) + &
72*x*(1+x)*log((-1+x)**8)*polylog(2,1-x) - 144*x*(1+x)*log(x)*polylog(2,1-x) + &
288*x*(1+x)*log(1+x)*polylog(2,1-x) + &
144*x**2*(1+x)*((4-8*x)*log(1-x)+x*log(x)+2*(-2+x)*log(1+x))*polylog(2,1-x) + &
144*(-1+x**2)*(3+x*(2+x*(-1+log(4._default)))-log(4._default)) - &

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2*(-1+x)*x*log(1-x))*polylog(2,(-1+x)/(two*x)) + 432*(-1+x)*polylog(2,-x) + &
1440*(-1+x)*x*polylog(2,-x) - 72*(-1+x)*x**2*(-1+15*x)*polylog(2,-x) - &
288*x*(-1+x)*log(1-x)+(1+x**3)*log(x)+(-5+6*x+x**2)*log(1+x))*polylog(2,-x) - &
432*(-1+x)*x*polylog(2,1/(1+x)) - 288*(-1+x)*x**2*polylog(2,1/(1+x)) + &
576*(-1+x)*x**3*polylog(2,1/(1+x)) + 864*(-1+x)*x*log(1-x)*polylog(2,1/(1+x)) + &
288*x*(-4+5*x+x**3)*log(1+x)*polylog(2,1/(1+x)) + &
4*c_b0*Pi*x*(-36*c_b1ob0*Pi*(-1+x)*(-1+x**2)-2*(1-x)*(18*ln0*(1+x)*(3+x) - &
2*nlep*(1+x)*(-17+11*x)+3*(9+Pi2-15*x+3*(-8+Pi2)*x**2))+36*(3-3*(-1+x)*x + &
4*ln0*(-1+x)**2*(1+x))*log(1-x)-216*(-1+x)**2*(1+x)*log(1-x)**2 - &
108*x**3*(log(1-x)-log(x))-54*log(x)-36*ln0*log(x) - &
12*nlep*log(x)-18*x*log(x)-36*ln0*x*log(x)-12*nlep*x*log(x)+144*x**2*log(x) - &
108*ln0*x**2*log(x)-12*nlep*x**2*log(x)-108*ln0*x**3*log(x)-12*nlep*x**3*log(x) + &
36*(1+x)*log(1-x)*log(x) + &
180*x**2*(1+x)*log(1-x)*log(x)-27*log(x)**2+9*x*log(x)**2-9*x**2*log(x)**2 + &
27*x**3*log(x)**2 - 72*(-1+x)*(-2+x**2)*log(x)*log(1+x)-108*(-1+x)*log(1+x)**2 - &
72*(1+x)*polylog(2,1-x) + 72*x**2*(1+x)*polylog(2,1-x)-72*(-1+x)*(-2+x**2)*polylog(2,-
216*(-1+x)*polylog(2,one/(1+x))) - &
72*(-1+x**2)*(-6+x*(-8+5*x)+10*(-1+x)*x*log(1+x))*polylog(2,x/(1+x)) + &
144*(-1+x**2)*(3+x*(2+x*(-1+log(4._default)))-log(4._default)) - &
2*(-1+x)*x*log(1+x))*polylog(2,-one+two/(1+x)) - 288*(-1+x)**2*x*(1+x)*polylog(3,(1-x)
144*(-1+x)*x*(1+x)*(4+7*x)*polylog(3,1-x) + 288*(-1+x)**2*x*(1+x)*polylog(3,(-1+x)/(tw
144*x**2*(-1+x**2)*polylog(3,(-1+x)/x) - 144*x*(1+x)*(7+x*(-16+7*x))*polylog(3,-x) + &
72*(-1+x)*x*(1+x)*(5+7*x)*polylog(3,x) + 288*x*(-3+x+x**2-3*x**3)*polylog(3,one/(1+x))
1008*(-1+x)**2*x*(1+x)*polylog(3,x/(1+x)) + 288*(-1+x)**2*x*(1+x)*polylog(3,(2*x)/(1+x)
288*(-1+x)*x*(4+x**2)*polylog(3,(1+x)/two) + 18*x*(29+x*(59+x*(-69+61*x)))*zeta3
jll_nll(6) = (j6_1 + j6_2 + j6_3) / (36._default*x*(-1+x**2))
end if
end subroutine rechat_nonsinglet

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<Electron PDFs: public>+≡
public :: rechat_photon

<Electron PDFs: sub interfaces>+≡
module subroutine rechat_photon (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
end subroutine rechat_photon

<Electron PDFs: procedures>+≡
module subroutine rechat_photon (x, jll_nll, nlep, ln0, order, running)
  real(default), intent(in) :: x
  real(default), dimension(6), intent(out) :: jll_nll
  real(default), intent(in) :: ln0
  integer, intent(in) :: nlep
  logical, dimension(6), intent(in) :: order
  logical, intent(in) :: running
  real(default) :: c_b0, c_b1ob0
  real(default) :: j6_1, j6_2, j6_3
  jll_nll = 0._default
  if (running) then
    c_b0 = - coeffqed_b0 (0, nlep)

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c_b1ob0 = coeffqed_b1 (0, nlep) / coeffqed_b0 (0, nlep)
else
  c_b0 = zero
  c_b1ob0 = zero
end if
if (order(1)) then
  jll_nll(1) = -3 + 2/x + x
end if
if (order(2)) then
  jll_nll(2) = -((-1+x)*(4*nlep*(-2+x)+3*x)-12*(2-3*x+x**2)*log(1-x) + 6*(-2+x)*x*log(x)) / &
    (6._default*x)
end if
if (order(3)) then
  jll_nll(3) = (-99 + 1068*nlep - 48*nlep**2 + 72*Pi2 - (496*nlep)/x + (32*nlep**2)/x + &
    99*x - 636*nlep*x + 16*nlep**2*x - 24*Pi2*x + 64*nlep*x**2 + &
    (144*(2-3*x+x**2)*log(1-x)**2)/x - 180*log(x) - 48*nlep*log(x) - (192*nlep*log(x))/x + &
    72*x*log(x) + 240*nlep*x*log(x) - 36*log(x)**2 + 144*nlep*log(x)**2 + 18*x*log(x)**2 - &
    72*nlep*x*log(x)**2 - (24*log(1-x)*((-1+x)*(2*nlep*(-2+x)+3*x) + &
    6*(2-2*x+x**2)*log(x))) / x - (288*polylog(2,x))/x) / 36._default
end if
if (order(4)) then
  jll_nll(4) = ((-1+ln0)*(2-3*x+x**2) - 2*(2-2*x+x**2)*log(x)) / x
end if
if (order(5)) then
  jll_nll(5) = (45 + 9*ln0 + 108*nlep + 36*ln0*nlep + 108*c_b1ob0*Pi - (56*nlep)/x - &
    (24*ln0*nlep)/x - (72*c_b1ob0*Pi)/x - 45*x - 9*ln0*x - 52*nlep*x - 12*ln0*nlep*x - &
    36*c_b1ob0*Pi*x - (54*(2-3*x+x**2)*log(1-x)**2)/x + 36*ln0*log(x) - 48*nlep*log(x) + &
    (48*nlep*log(x))/x + 45*x*log(x) - 18*ln0*x*log(x) + 24*nlep*x*log(x) - 18*log(x)**2 + &
    9*x*log(x)**2 + (6*log(1-x)*((-1+x)*(12+8*nlep+6*ln0*(-2+x)-9*x-4*nlep*x) + &
    6*(-2+x)*x*log(x)))/x - (36*c_b0*Pi*((-1+ln0)*(2-3*x+x**2) - 2*(2-2*x+x**2)*log(x))) / &
    36*(-2+x)*polylog(2,1-x))/18._default
end if
if (order(6)) then
  j6_1 = -2808+2176*nlep + 2976*ln0*nlep - 448*nlep**2 - 192*ln0*nlep**2 - 768*c_b0*nlep*Pi - &
    1152*c_b1ob0*nlep*Pi - 1152*c_b0*ln0*nlep*Pi + 144*Pi2 + 1728*c_b0**2*Pi2 - &
    1728*c_b0*c_b1ob0*Pi2 + 288*ln0*Pi2 - 1728*c_b0**2*ln0*Pi2 - 96*nlep*Pi2 + &
    3645*x+594*ln0*x + 12420*nlep*x - 6408*ln0*nlep*x + 864*nlep**2*x + 288*ln0*nlep**2*x &
    648*c_b0*Pi*x + 432*c_b1ob0*Pi*x + 432*c_b0*ln0*Pi*x + 1728*c_b0*nlep*Pi*x + &
    1728*c_b1ob0*nlep*Pi*x + 1728*c_b0*ln0*nlep*Pi*x + 324*Pi2*x - 2592*c_b0**2*Pi2*x + &
    2592*c_b0*c_b1ob0*Pi2*x - 432*ln0*Pi2*x + 2592*c_b0**2*ln0*Pi2*x + 144*nlep*Pi2*x + &
    1971*x**2 - 594*ln0*x**2 - 16324*nlep*x**2 + 840*ln0*nlep*x**2 + 32*nlep**2*x**2 + &
    96*ln0*nlep**2*x**2 - 648*c_b0*Pi*x**2 - 432*c_b1ob0*Pi*x**2 - 432*c_b0*ln0*Pi*x**2 - &
    192*c_b0*nlep*Pi*x**2 + 576*c_b1ob0*nlep*Pi*x**2 + 576*c_b0*ln0*nlep*Pi*x**2 - &
    180*Pi2*x**2-864*c_b0**2*Pi2*x**2 + 864*c_b0*c_b1ob0*Pi2*x**2 - 144*ln0*Pi2*x**2 + &
    864*c_b0**2*ln0*Pi2*x**2 + 48*nlep*Pi2*x**2 - 3645*x**3-594*ln0*x**3 - &
    12868*nlep*x**3+6024*ln0*nlep*x**3 - 864*nlep**2*x**3 - 288*ln0*nlep**2*x**3 - &
    648*c_b0*Pi*x**3 - 432*c_b1ob0*Pi*x**3 - 432*c_b0*ln0*Pi*x**3 - 1728*c_b0*nlep*Pi*x**3 &
    1728*c_b1ob0*nlep*Pi*x**3 - 1728*c_b0*ln0*nlep*Pi*x**3 - 468*Pi2*x**3 + &
    2592*c_b0**2*Pi2*x**3 - 2592*c_b0*c_b1ob0*Pi2*x**3 + 432*ln0*Pi2*x**3 - &
    2592*c_b0**2*ln0*Pi2*x**3 - 144*nlep*Pi2*x**3 + 837*x**4 + 594*ln0*x**4 + 14148*nlep*x &
    3816*ln0*nlep*x**4 + 416*nlep**2*x**4 + 96*ln0*nlep**2*x**4 + 648*c_b0*Pi*x**4 + &
    432*c_b1ob0*Pi*x**4 + 432*c_b0*ln0*Pi*x**4 + 960*c_b0*nlep*Pi*x**4 + &
    576*c_b1ob0*nlep*Pi*x**4 + 576*c_b0*ln0*nlep*Pi*x**4 + 180*Pi2*x**4 - 864*c_b0**2*Pi2* &
    864*c_b0*c_b1ob0*Pi2*x**4 - 144*ln0*Pi2*x**4 + 864*c_b0**2*ln0*Pi2*x**4 + 48*nlep*Pi2*

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$$\begin{aligned}
& 448*\text{nlep}*x^{**5} + 384*\ln0*\text{nlep}*x^{**5} - 864*\text{Pi}2*x*\log(2._\text{default}) + \& \\
& 864*\text{Pi}2*x^{**3}*\log(2._\text{default}) + 2016*x*\log(2._\text{default})^{**3} - 2016*x^{**3}*\log(2._\text{default})^{**3} \\
& 384*\text{nlep}^{**2}*\log(2-2*x) + 432*\ln0*x^{**2}*\log(2-2*x) + 192*\text{nlep}^{**2}*x^{**2}*\log(2-2*x) - \& \\
& 432*\ln0*x^{**4}*\log(2-2*x) + 192*\text{nlep}^{**2}*x^{**4}*\log(2-2*x) + 1080*\log(1-x) + 2304*\text{nlep}*\log(1-x) \\
& 576*\ln0*\text{nlep}*\log(1-x) - 864*c_b0*\text{Pi}*\log(1-x) + 3456*c_b1ob0*\text{Pi}*\log(1-x) + \& \\
& 3456*c_b0*\ln0*\text{Pi}*\log(1-x) - 1152*c_b0*\text{nlep}*\text{Pi}*\log(1-x) - 576*\text{Pi}2*\log(1-x) - 3564*x*\log(1-x) \\
& 432*\ln0*x*\log(1-x) - 3744*\text{nlep}*x*\log(1-x) - 864*\ln0*\text{nlep}*x*\log(1-x) + \& \\
& 576*\text{nlep}^{**2}*x*\log(1-x) + 1296*c_b0*\text{Pi}*x*\log(1-x) - 5184*c_b1ob0*\text{Pi}*x*\log(1-x) - \& \\
& 5184*c_b0*\ln0*\text{Pi}*x*\log(1-x) + 1728*c_b0*\text{nlep}*\text{Pi}*x*\log(1-x) + 1008*\text{Pi}2*x*\log(1-x) \\
j6_2 = & 1404*x^{**2}*\log(1-x) - 864*\text{nlep}*x^{**2}*\log(1-x) - 288*\ln0*\text{nlep}*x^{**2}*\log(1-x) + \& \\
& 432*c_b0*\text{Pi}*x^{**2}*\log(1-x) - 1728*c_b1ob0*\text{Pi}*x^{**2}*\log(1-x) - 1728*c_b0*\ln0*\text{Pi}*x^{**2}*\log(1-x) \\
& 576*c_b0*\text{nlep}*\text{Pi}*x^{**2}*\log(1-x) + 144*\text{Pi}2*x^{**2}*\log(1-x) + 3564*x^{**3}*\log(1-x) + \& \\
& 432*\ln0*x^{**3}*\log(1-x) + 3744*\text{nlep}*x^{**3}*\log(1-x) + 864*\ln0*\text{nlep}*x^{**3}*\log(1-x) - \& \\
& 576*\text{nlep}^{**2}*x^{**3}*\log(1-x) - 1296*c_b0*\text{Pi}*x^{**3}*\log(1-x) + 5184*c_b1ob0*\text{Pi}*x^{**3}*\log(1-x) \\
& 5184*c_b0*\ln0*\text{Pi}*x^{**3}*\log(1-x) - 1728*c_b0*\text{nlep}*\text{Pi}*x^{**3}*\log(1-x) - 1008*\text{Pi}2*x^{**3}*\log(1-x) \\
& 2484*x^{**4}*\log(1-x) - 1440*\text{nlep}*x^{**4}*\log(1-x) - 288*\ln0*\text{nlep}*x^{**4}*\log(1-x) + \& \\
& 432*c_b0*\text{Pi}*x^{**4}*\log(1-x) - 1728*c_b1ob0*\text{Pi}*x^{**4}*\log(1-x) - 1728*c_b0*\ln0*\text{Pi}*x^{**4}*\log(1-x) \\
& 576*c_b0*\text{nlep}*\text{Pi}*x^{**4}*\log(1-x) + 432*\text{Pi}2*x^{**4}*\log(1-x) + 1728*\log(1-x)^{**2} - \& \\
& 1728*\ln0*\log(1-x)^{**2} + 288*\text{nlep}*\log(1-x)^{**2} - 4320*c_b0*\text{Pi}*\log(1-x)^{**2} - \& \\
& 2700*x*\log(1-x)^{**2} + 2592*\ln0*x*\log(1-x)^{**2} - 432*\text{nlep}*x*\log(1-x)^{**2} + \& \\
& 6480*c_b0*\text{Pi}*x*\log(1-x)^{**2} - 756*x^{**2}*\log(1-x)^{**2} + 864*\ln0*x^{**2}*\log(1-x)^{**2} - \& \\
& 144*\text{nlep}*x^{**2}*\log(1-x)^{**2} + 2160*c_b0*\text{Pi}*x^{**2}*\log(1-x)^{**2} + 2700*x^{**3}*\log(1-x)^{**2} - \& \\
& 2592*\ln0*x^{**3}*\log(1-x)^{**2} + 432*\text{nlep}*x^{**3}*\log(1-x)^{**2} - 6480*c_b0*\text{Pi}*x^{**3}*\log(1-x)^{**2} \\
& 972*x^{**4}*\log(1-x)^{**2} + 864*\ln0*x^{**4}*\log(1-x)^{**2} - 144*\text{nlep}*x^{**4}*\log(1-x)^{**2} + \& \\
& 2160*c_b0*\text{Pi}*x^{**4}*\log(1-x)^{**2} + 1728*\log(1-x)^{**3} - 3024*x*\log(1-x)^{**3} - \& \\
& 432*x^{**2}*\log(1-x)^{**3} + 3024*x^{**3}*\log(1-x)^{**3} - 1296*x^{**4}*\log(1-x)^{**3} - 2880*\text{nlep}*\log(x) \\
& 1152*\ln0*\text{nlep}*\log(x) + 2304*c_b0*\text{nlep}*\text{Pi}*\log(x) + 3456*c_b0^{**2}*\text{Pi}2*\log(x) - \& \\
& 2916*x*\log(x) + 1080*\ln0*x*\log(x) + 18288*\text{nlep}*x*\log(x) + 288*\ln0*\text{nlep}*x*\log(x) - \& \\
& 384*\text{nlep}^{**2}*x*\log(x) - 864*c_b0*\text{Pi}*x*\log(x) + 1728*c_b1ob0*\text{Pi}*x*\log(x) + \& \\
& 1728*c_b0*\ln0*\text{Pi}*x*\log(x) - 2304*c_b0*\text{nlep}*\text{Pi}*x*\log(x) + 288*\text{Pi}2*x*\log(x) - \& \\
& 3456*c_b0^{**2}*\text{Pi}2*x*\log(x) - 702*x^{**2}*\log(x) + 3960*\text{nlep}*x^{**2}*\log(x) - \& \\
& 2592*\ln0*\text{nlep}*x^{**2}*\log(x) + 648*c_b0*\text{Pi}*x^{**2}*\log(x) - 864*c_b1ob0*\text{Pi}*x^{**2}*\log(x) - \& \\
& 864*c_b0*\ln0*\text{Pi}*x^{**2}*\log(x) - 1152*c_b0*\text{nlep}*\text{Pi}*x^{**2}*\log(x) - 864*\text{Pi}2*x^{**2}*\log(x) - \& \\
& 1728*c_b0^{**2}*\text{Pi}2*x^{**2}*\log(x) + 2916*x^{**3}*\log(x) - 1080*\ln0*x^{**3}*\log(x) - \& \\
& 17520*\text{nlep}*x^{**3}*\log(x) - 288*\ln0*\text{nlep}*x^{**3}*\log(x) + 384*\text{nlep}^{**2}*x^{**3}*\log(x) + \& \\
& 864*c_b0*\text{Pi}*x^{**3}*\log(x) - 1728*c_b1ob0*\text{Pi}*x^{**3}*\log(x) - 1728*c_b0*\ln0*\text{Pi}*x^{**3}*\log(x) + \& \\
& 2304*c_b0*\text{nlep}*\text{Pi}*x^{**3}*\log(x) - 864*\text{Pi}2*x^{**3}*\log(x) + 3456*c_b0^{**2}*\text{Pi}2*x^{**3}*\log(x) + \& \\
& 702*x^{**4}*\log(x) - 1080*\text{nlep}*x^{**4}*\log(x) + 1440*\ln0*\text{nlep}*x^{**4}*\log(1-x) - \& \\
& 648*c_b0*\text{Pi}*x^{**4}*\log(x) + 864*c_b1ob0*\text{Pi}*x^{**4}*\log(x) + 864*c_b0*\ln0*\text{Pi}*x^{**4}*\log(x) - \& \\
& 1152*c_b0*\text{nlep}*\text{Pi}*x^{**4}*\log(x) + 288*\text{Pi}2*x^{**4}*\log(x) - 1728*c_b0^{**2}*\text{Pi}2*x^{**4}*\log(x) - \& \\
& 768*\text{nlep}*x^{**5}*\log(x) - 1296*x*\log(1-x)*\log(x) - 1728*\ln0*x*\log(1-x)*\log(x) - \& \\
& 3456*c_b0*\text{Pi}*x*\log(1-x)*\log(x) - 648*x^{**2}*\log(1-x)*\log(x) + \& \\
& 864*\ln0*x^{**2}*\log(1-x)*\log(x) + 1728*c_b0*\text{Pi}*x^{**2}*\log(1-x)*\log(x) + \& \\
& 1296*x^{**3}*\log(1-x)*\log(x) + 1728*\ln0*x^{**3}*\log(1-x)*\log(x) \\
j6_3 = & 3456*c_b0*\text{Pi}*x^{**3}*\log(1-x)*\log(x) + 648*x^{**4}*\log(1-x)*\log(x) - \& \\
& 864*\ln0*x^{**4}*\log(1-x)*\log(x) - 1728*c_b0*\text{Pi}*x^{**4}*\log(1-x)*\log(x) + \& \\
& 3024*x*\log(1-x)^{**2}*\log(x) - 1512*x^{**2}*\log(1-x)^{**2}*\log(x) - \& \\
& 3024*x^{**3}*\log(1-x)^{**2}*\log(x) + 1512*x^{**4}*\log(1-x)^{**2}*\log(x) - 1152*\text{nlep}*\log(x)^{**2} - \& \\
& 432*x*\log(x)^{**2} + 216*\ln0*x*\log(x)^{**2} + 1728*\text{nlep}*x*\log(x)^{**2} - \& \\
& 864*\ln0*\text{nlep}*x*\log(x)^{**2} - 432*c_b0*\text{Pi}*x*\log(x)^{**2} - 432*x^{**2}*\log(x)^{**2} - \& \\
& 108*\ln0*x^{**2}*\log(x)^{**2} + 2016*\text{nlep}*x^{**2}*\log(x)^{**2} + 432*\ln0*\text{nlep}*x^{**2}*\log(x)^{**2} + \& \\
& 216*c_b0*\text{Pi}*x^{**2}*\log(x)^{**2} + 432*x^{**3}*\log(x)^{**2} - 216*\ln0*x^{**3}*\log(x)^{**2} - \& \\
& 1728*\text{nlep}*x^{**3}*\log(x)^{**2} + 864*\ln0*\text{nlep}*x^{**3}*\log(x)^{**2} + 432*c_b0*\text{Pi}*x^{**3}*\log(x)^{**2} + \& \\
& 432*x^{**4}*\log(x)^{**2} + 108*\ln0*x^{**4}*\log(x)^{**2} - 864*\text{nlep}*x^{**4}*\log(x)^{**2} - \&
\end{aligned}$$


```

432*ln0*nlep*x**4*log(x)**2 - 216*c_b0*Pi*x**4*log(x)**2 - 2592*x*log(1-x)*log(x)**2 +
3024*x**2*log(1-x)*log(x)**2 + 4320*x**3*log(1-x)*log(x)**2 - &
1296*x**4*log(1-x)*log(x)**2 - 144*x*log(x)**3 + 1152*nlep*x*log(x)**3 - &
936*x**2*log(x)**3 - 576*nlep*x**2*log(x)**3 - 432*x**3*log(x)**3 - &
1152*nlep*x**3*log(x)**3 + 360*x**4*log(x)**3 + 576*nlep*x**4*log(x)**3 + &
384*nlep**2*log(2*x) - 432*ln0*x**2*log(2*x) - 192*nlep**2*x**2*log(2*x) + &
432*ln0*x**4*log(2*x) - 192*nlep**2*x**4*log(2*x) + 576*Pi2*log(1+x) + &
2016*Pi2*x*log(1+x) - 2016*Pi2*x**2*log(1+x) - 576*Pi2*x**3*log(1+x) + &
2592*log(x)*log(1+x) + 2592*x*log(x)*log(1+x) - 864*x**2*log(x)*log(1+x) - &
3456*x**3*log(x)*log(1+x) - 864*x**4*log(x)*log(1+x) + 864*log(x)**2*log(1+x) + &
864*x*log(x)**2*log(1+x) - 432*x**2*log(x)**2*log(1+x) - 864*x**3*log(x)**2*log(1+x) - &
432*x**4*log(x)**2*log(1+x)+1296*log(1+x)**2+3456*x*log(1+x)**2 - &
648*x**2*log(1+x)**2-3456*x**3*log(1+x)**2 - 648*x**4*log(1+x)**2+864*log(x)*log(1+x)*
10368*x*log(x)*log(1+x)**2 - 9504*x**2*log(x)*log(1+x)**2 - &
1728*x**3*log(x)*log(1+x)**2 - 1440*log(1+x)**3 - 4608*x*log(1+x)**3 + &
3888*x**2*log(1+x)**3 + 288*x**3*log(1+x)**3 + 1872*x**4*log(1+x)**3 - &
144*(-1+x**2)*(12-12*ln0+4*nlep-15*x-4*nlep*x-24*c_b0*Pi*x+6*x**2+2*nlep*x**2 + &
12*c_b0*Pi*x**2 + (12+18*x-9*x**2)*log(1-x)+3*(-6+x)*x*log(x))*polylog(2,1-x) + &
432*(-1+x)*(-12-30*x-25*x**2-3*x**3-8*(1+x)**2*log(x) + &
2*x*(-12+x+3*x**2)*log(1+x))*polylog(2,-x) + 1728*x*polylog(2,1/(1+x)) - &
864*x**3*polylog(2,1/(1+x)) - 864*x**4*polylog(2,1/(1+x)) - &
10368*x*log(1+x)*polylog(2,1/(1+x)) + 7776*x**2*log(1+x)*polylog(2,1/(1+x)) + &
1728*x**3*log(1+x)*polylog(2,1/(1+x)) + 864*x**4*log(1+x)*polylog(2,1/(1+x)) + &
2592*polylog(2,x/(1+x)) + 5184*x*polylog(2,x/(1+x)) - 1296*x**2*polylog(2,x/(1+x)) - &
6048*x**3*polylog(2,x/(1+x)) - 432*x**4*polylog(2,x/(1+x)) + &
1728*log(x)*polylog(2,x/(1+x)) - 1728*x**2*log(x)*polylog(2,x/(1+x)) + &
3456*x*log(1+x)*polylog(2,x/(1+x)) - 3456*x**2*log(1+x)*polylog(2,x/(1+x)) - &
3456*x**3*log(1+x)*polylog(2,x/(1+x)) + 3456*x**4*log(1+x)*polylog(2,x/(1+x)) - &
4320*x*polylog(3,1-x) + 6480*x**2*polylog(3,1-x) + 7776*x**3*polylog(3,1-x) - &
3024*x**4*polylog(3,1-x) + 5184*x**2*polylog(3,(-1+x)/x) + 3456*x**3*polylog(3,(-1+x)/
1728*x**4*polylog(3,(-1+x)/x) + 1728*polylog(3,x) - 4320*x*polylog(3,x) + &
5616*x**2*polylog(3,x) + 7776*x**3*polylog(3,x) - 3888*x**4*polylog(3,x) - &
432*polylog(3,x**2) - 432*x*polylog(3,x**2) + 216*x**2*polylog(3,x**2) + &
432*x**3*polylog(3,x**2) + 216*x**4*polylog(3,x**2) + 3456*x*polylog(3,x/(1+x)) - &
1728*x**2*polylog(3,x/(1+x)) - 3456*x**3*polylog(3,x/(1+x)) + 1728*x**4*polylog(3,x/(1
3456*zeta3 + 2592*x*zeta3 - 864*x**2*zeta3 - 6048*x**3*zeta3 + 864*x**4*zeta3
jll_nll(6) = (j6_1 + j6_2 + j6_3) / (216.*default*x*(-1+x**2))
end if
end subroutine rechat_photon

```

(*Electron PDFs: procedures*)+≡

```

function sum_rm (x, al0_2pi, ln0, cc1, cc2, cc3, cc4, cc5, &
k, m1, m2) result (s_rm)
real(default) :: s_rm
real(default), intent(in) :: x, k, al0_2pi, ln0, m1, m2
real(default), intent(in) :: cc1, cc2, cc3, cc4, cc5
real(default) :: f0, f1, f2, fac, den
real(default) :: mf1, mf2, mf3, mf4, mf5
real(default) :: rr1, rr2, rr3, rr4, rr5
f0 = two - Pi2/three + three/two * ln0
f1 = two*(one - ln0)
f2 = - two
den = m2 - m1 * log(1-x)
fac = exp(-eulerc*k) * (1-x)**k / gamma(1+k)

```

```

mf1 = one/den - (Pi2*k - 6._default*zeta3 * k**2)*m1/6._default / den**2 &
      - (30._default*Pi2 - 360._default*zeta3*k + &
        Pi**4 * k**2)*m1**2/180._default / den**3
mf2 = one
mf3 = - log(1-x) + Pi2*k/6._default - zeta3 * k**2
mf4 = log(1-x)**2 - Pi2/6._default + k*(-Pi2/three*log(1-x) + two*zeta3) + &
      k**2 * (two*zeta3*log(1-x) - Pi**4/180._default)
mf5 = - log(1-x)**3 + Pi2/two*log(1-x) - two*zeta3 + &
      k*(Pi2/two*log(1-x)**2 - 6._default*zeta3*log(1-x) - &
        Pi**4/60._default) + k**2 * (-three*zeta3*log(1-x)**2 + &
        Pi**4/60._default*log(1-x) + three/two*Pi2*zeta3 - 12._default*zeta5)
rr1 = (cc3 - cc4*cc2 + cc4**2 * cc1) * &
      (one + al0_2pi * (f0 - cc4*f1 + cc4**2 * f2))
rr2 = (cc2 - cc4*cc1) / cc5 + al0_2pi/cc5 * (cc2*f0 + cc3*f1 - &
      cc4*(cc1*f0 + cc2*f1 + cc3*f2) + cc4**2 * (cc1*f1 + cc2*f2) - &
      cc4**3 * cc1 * f2)
rr3 = cc1/cc5 + al0_2pi/cc5 * (cc1*f0 + cc2*f1 + cc3*f2 - &
      cc4*(cc1*f1 + cc2*f2) + cc4**2 * cc1 * f2)
rr4 = al0_2pi * 1/cc5 * (cc1*f1 + cc2*f2 - cc4*cc1*f2)
rr5 = al0_2pi * cc1/cc5 * f2
s_rm = fac * (rr1*mf1 + rr2*mf2 + rr3*mf3 + rr4*mf4 + rr5*mf5)
end function sum_rm

```

For the moment, the number of quark flavors in the running of α is set equal to zero.

(Electron PDFs: public)+≡
 public :: t_alpha

(Electron PDFs: sub interfaces)+≡
 module function t_alpha (epdf, scale) result (t)
 real(default) :: t
 type(qed_pdf_t), intent(in) :: epdf
 real(default), intent(in) :: scale
 end function t_alpha

(Electron PDFs: procedures)+≡
 module function t_alpha (epdf, scale) result (t)
 real(default) :: t
 type(qed_pdf_t), intent(in) :: epdf
 real(default), intent(in) :: scale
 real(default) :: alphamu, alpharef
 select type (alpha => epdf%aqed)
 type is (alpha_qed_from_scale_t)
 alpharef = alpha%ref
 alphamu = alpha%get (scale)
 type is (alpha_qed_fixed_t)
 call msg_fatal &
 ("t integrator: has to be called with running alpha.")
 end select
 t = - log (alphamu/alpharef) / two / Pi / coeffqed_b0 (0, epdf%n_lep)
 end function t_alpha

(Electron PDFs: procedures)+≡
 function rec_series (p, al_2pi, expansion) result (rec)

```

real(default) :: rec
real(default), intent(in) :: p, al_2pi
real(default), dimension(6) :: expansion
rec = expansion(1) * p + expansion(2) * p**2 / two + &
      expansion(3) * p**3/6._default + al_2pi * (expansion(4) + &
      expansion(5) * p + expansion(6) * p**2 / two)
end function rec_series

```

(Electron PDFs: procedures)+≡

```

function f_lim_1 (x) result (f)
  real(default), intent(in) :: x
  real(default) :: xb, f
  xb = one - x
  f = two * log(xb)**2 + (two/three)*Pi2 * log(xb) + &
      (two/three)*Pi2 - four * zeta3
end function f_lim_1

```

(Electron PDFs: procedures)+≡

```

function f_lim_2 (x) result (f)
  real(default), intent(in) :: x
  real(default) :: xb, f
  xb = one - x
  f = -two*log(xb)**2 + (two - two/three*Pi2) * log(xb) + &
      (Pi2/three) + four*zeta3
end function f_lim_2

```

The functions for the numeric integrations are of the form $f_N(x) = \int_0^1 dy \tilde{f}_N(y, x)$.

(Electron PDFs: procedures)+≡

```

function func_1 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((2 + (-1 + x)*y*(2 + (-1 + x)*y)) * &
      ((1 + (-1 + x)*y)*log(1 - x)* &
      ((-1 + x)*log(1 - x) + 2*x*log(x)) - &
      2*x*log(x/(1 + (-1 + x)*y))* &
      log(1 - x/(1 + (-1 + x)*y)) + &
      (-1 + x)*(-1 + y)* &
      log(1 - x/(1 + (-1 + x)*y)**2))/ &
      ((-1 + x)*x*y*(1 + (-1 + x)*y)) + &
      2*(1 + (-1 + x)*y)* &
      (log(1 - x)**2*log(x) - &
      log(x/(1 + (-1 + x)*y))* &
      log(one - x/(one + (-one + x)*y)**2) - &
      f_lim_1 (x)
end function func_1

```

(Electron PDFs: procedures)+≡

```

function func_2 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x

```

```

f = -(((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2) * &
      ((-1 + x)*((1 + y*(-1 + x))*log(1 - x)**2 + &
      (-1 + y)*log(((1 + y)*(-1 + x))/(1 + y*(-1 + x)))**2) &
      - (x + y*(-1 + x)*x)*polylog(2,x) + &
      x*polylog(2,x/(1 + y*(-1 + x)))))/(y*(1 + &
      y*(-1 + x))*(-1 + x)*x) + 2*(1 + y*(-1 + x)) * &
      (log(1 - x)*polylog(2,x) - log(((1 + y)*(-1 + x)) / &
      (1 + y*(-1 + x)))*polylog(2,x/(1 + y*(-1 + x)))) - &
      f_lim_2(x)
end function func_2

```

(Electron PDFs: procedures)+≡

```

function func_3 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2) * &
      ((1 + y*(-1 + x))*polylog(2,1 - x) - &
      polylog(2,((-1 + y)*(-1 + x))/(1 + y*(-1 + x)))) / &
      (y*(1 + y*(-1 + x))*(-1 + x)) + 2*(1 + y*(-1 + x)) * &
      (polylog(3,1 - x) - polylog(3,((-1 + y)*(-1 + x)) / &
      (1 + y*(-1 + x)))) + two
end function func_3

```

(Electron PDFs: procedures)+≡

```

function func_4 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = two*(1 + y*(-1 + x))*(log(x)**2*log(1 + x) - &
      log(x/(1 + y*(-1 + x)))*log(1 + x/(1 + y*(-1 + x)))) - &
      ((1 + (1 + y*(-1 + x))**2) * (-log(x)**2/(1 + x)) - &
      (2*log(x)*log(1 + x))/x - ((-1 + y)*log(x/(1 + y*(-1 + x)))) * &
      (x*log(x/(1 + y*(-1 + x)))) + 2*(1 + y*(-1 + x) + x) * &
      log(1 + x/(1 + y*(-1 + x)))) / ((1 + y*(-1 + x)) * x * &
      (1 + y*(-1 + x) + x)))/y
end function func_4

```

(Electron PDFs: procedures)+≡

```

function func_5 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((1 + (1 + y*(-1 + x))**2) * ((-2*log(x)*log(1 + x)) / &
      (1 + x) - log(1 + x)**2/x - (2*(-1 + y)*log(x/(1 + &
      y*(-1 + x)))*log(1 + x/(1 + y*(-1 + x)))) / ((1 + &
      y*(-1 + x))*(1 + y*(-1 + x) + x)) - ((-1 + y) * &
      log(1 + x/(1 + y*(-1 + x)))*log(1 + x/(1 + y*(-1 + x)))/y) + &
      2*(1 + y*(-1 + x))*(log(x)*log(1 + x)**2 - log(x/(1 + &
      y*(-1 + x))) * log(1 + x/(1 + y*(-1 + x)))*log(1 + x/(1 + &
      y*(-1 + x))**2) - &
      two*log(two)**2
end function func_5

```

(Electron PDFs: procedures)+≡

```
function func_8 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2)*(log(x)*log(1 + x) - &
    y*log(x)*log(1 + x) + y*x*log(x)*log(1 + x) - log(x)/(1 + &
    y*(-1 + x))*log(1 + x/(1 + y*(-1 + x))) + y*log(x)/(1 + &
    y*(-1 + x))*log(1 + x/(1 + y*(-1 + x))) + (-1 + y - y*x) * &
    polylog(2,-x) - (-1 + y)*polylog(2,-(x/(1 + y*(-1 + x))))) / &
    (y*(1 + y*(-1 + x)*x)) + 2*(1 + y*(-1 + x))*(log(x) * &
    polylog(2,-x) - log(x)/(1 + y*(-1 + x))) * &
    polylog(2,-(x/(1 + y*(-1 + x))))) + Pi2/6._default
end function func_8
```

(Electron PDFs: procedures)+≡

```
function func_9 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((1 + (1 + y*(-1 + x))**2) * (log(1 + x)**2 / x + &
    ((-1 + y)*log(1 + x/(1 + y*(-1 + x))**2) / (x + &
    y*(-1 + x)*x) - polylog(2,-x)/(1 + x) - ((-1 + y) * &
    polylog(2,-(x/(1 + y*(-1 + x))))) / ((1 + y*(-1 + x)) * &
    (1 + y*(-1 + x) + x)))/y) + 2*(1 + y*(-1 + x)) * &
    (log(1 + x)*polylog(2,-x) - log(1 + x/(1 + y*(-1 + x))) * &
    polylog(2,-(x/(1 + y*(-1 + x))))) + Pi2/12._default + &
    two*log(two)**2
end function func_9
```

(Electron PDFs: procedures)+≡

```
function func_10 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((1 + (1 + y*(-1 + x))**2) * (-((log(x)/(1 + x)) * &
    log(1 + x))/(1 + x)) - ((-1 + y) * &
    log(x/(1 + y*(-1 + x) + x))*log(1 + x/(1 + y*(-1 + x)))) / &
    ((1 + y*(-1 + x))*(1 + y*(-1 + x) + x)) - &
    polylog(2,1/(1 + x))/(1 + x) - ((-1 + y) * &
    polylog(2,1/(1 + x/(1 + y*(-1 + x))))) / &
    ((1 + y*(-1 + x))*(1 + y*(-1 + x) + x)))/y) + &
    2*(1 + y*(-1 + x))*(log(1 + x)*polylog(2,one/(1 + x)) - &
    log(1 + x/(1 + y*(-1 + x))) * polylog(2,one/(1 + x/(1 + y*(-1 + x))))) - &
    Pi2/12._default + three/two*log(two)**2
end function func_10
```

(Electron PDFs: procedures)+≡

```
function func_11 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2)*((1 + &
```

```

y*(-1 + x))*polylog(2,-x) + (-1 + y) * &
polylog(2,-(x/(1 + y*(-1 + x))))) / (y*(1 + &
y*(-1 + x))*x) + 2*(1 + y*(-1 + x))*(polylog(3,-x) - &
polylog(3,-(x/(1 + y*(-1 + x))))) + Pi2/6._default
end function func_11

```

(Electron PDFs: procedures)+≡

```

function func_12 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((1 + (1 + y*(-1 + x))**2)*(polylog(2,1/(1 + x))/(1 + x) + &
  ((-1 + y)*polylog(2,1/(1 + x/(1 + y*(-1 + x))))) / &
  ((1 + y*(-1 + x))*(1 + y*(-1 + x) + x)))/y) + 2*(1 + &
  y*(-1 + x))*(polylog(3,1/(1 + x)) - &
  polylog(3,1/(1 + x/(1 + y*(-1 + x))))) + Pi2/12._default - &
  0.5_default*log(two)**2
end function func_12

```

(Electron PDFs: procedures)+≡

```

function func_13 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = -(((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2)*log((1 - y) / &
  (1 + y*(-1 + x)))*log(1 + y*(-1 + x)))/(y*(-1 + x)) - &
  ((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2)*log((1 - y) / &
  (1 + y*(-1 + x)))*log(y - y*x))/(1 + y*(-1 + x)) + &
  ((2 + 2*y*(-1 + x) + y**2*(-1 + x)**2)*log(1 + &
  y*(-1 + x))*log(y - y*x))/(1 + y*(-1 + x)) - 2*(1 + &
  y*(-1 + x))*log((1 - y)/(1 + y*(-1 + x)))*log(1 + &
  y*(-1 + x))*log(y - y*x) - two*log(1-x) + two - Pi2/three
end function func_13

```

(Electron PDFs: procedures)+≡

```

function func_14 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (log(1 + y*(-1 + x)) * (((2 + y*(-1 + x))*(2 + &
  2*y*(-1 + x) + y**2*(-1 + x)**2)*log(1 + &
  y*(-1 + x)))/(1 + y*(-1 + x)) + (2*y*(2 + &
  y*(-1 + x))*(2 + 2*y*(-1 + x) + y**2*(-1 + x)**2) * &
  (-1 + x) * log(((1 + y)*(-1 + x))/(1 + &
  y*(-1 + x)))) / (1 + y*(-1 + x)) + (1 + (1 + &
  y*(-1 + x))**2)*(2 + y*(-1 + x)) * log(1 + y*(-1 + x)) * &
  log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) + &
  y*(1 + (1 + y*(-1 + x))**2)*(1 - x)* log(1 + y*(-1 + x)) * &
  log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) + &
  2*y*(1 + y*(-1 + x))*(2 + y*(-1 + x))*(-1 + x) * &
  log(1 + y*(-1 + x)) * log(((1 + y)*(-1 + x)) / &
  (1 + y*(-1 + x)))) / (2 + y*(-1 + x)**2
end function func_14

```

(Electron PDFs: procedures)+≡

```
function func_15 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (((2 + y*(-1 + x))*(2 + 2*y*(-1 + x) + &
    y**2*(-1 + x)**2)*log(1 + y*(-1 + x))*log(2 + &
    y*(-1 + x)))/(1 + y*(-1 + x)) - y*(1 + (1 + &
    y*(-1 + x))**2)*(1 - x)*log(1 + y*(-1 + x)) * &
    log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) + &
    (y*(2 + y*(-1 + x))*(2 + 2*y*(-1 + x) + &
    y**2*(-1 + x)**2)*(-1 + x)*log(2 + y*(-1 + x)) * &
    log(((1 + y)*(-1 + x))/(1 + y*(-1 + x)))) / &
    (1 + y*(-1 + x)) + (1 + (1 + y*(-1 + x))**2) * &
    (2 + y*(-1 + x))*log(1 + y*(-1 + x))*log(2 + &
    y*(-1 + x))*log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) + &
    y*(1 + (1 + y*(-1 + x))**2)*(1 - x)*log(1 + &
    y*(-1 + x))*log(2 + y*(-1 + x))*log(((1 + y) * &
    (-1 + x))/(1 + y*(-1 + x))) + 2*y*(1 + y*(-1 + &
    x))*(2 + y*(-1 + x))*(-1 + x)*log(1 + y*(-1 + x)) * &
    log(2 + y*(-1 + x))*log(((1 + y)*(-1 + x)) / &
    (1 + y*(-1 + x)))) / (2 + y*(-1 + x))**2
end function func_15
```

(Electron PDFs: procedures)+≡

```
function func_16 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (-(y*(2 + y*(-1 + x))*(2 + 2*y*(-1 + x) + y**2*(-1 + x)**2) * &
    (-1 + x)*log(2 + y*(-1 + x))*log(((1 + y)*(-1 + x))/(1 + &
    y*(-1 + x))))/(1 + y*(-1 + x)) + ((2 + y*(-1 + x))*(2 + &
    2*y*(-1 + x) + y**2*(-1 + x)**2)*polylog(2, -1 + y - y*x)) / &
    (1 + y*(-1 + x)) + (1 + (1 + y*(-1 + x))**2)*(2 + y*(-1 + &
    x))*log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) * &
    polylog(2, -1 + y - y*x) + y*(1 + (1 + y*(-1 + x))**2) * &
    (1 - x)*log(((1 + y)*(-1 + x))/(1 + y*(-1 + x))) * &
    polylog(2, -1 + y - y*x) + 2*y*(1 + y*(-1 + x))*(2 + &
    y*(-1 + x))*(-1 + x)*log(((1 + y)*(-1 + x))/(1 + &
    y*(-1 + x)))*polylog(2, -1 + y - y*x))/(2 + y*(-1 + x))**2 + &
    Pi2/12._default*log(xb)
end function func_16
```

(Electron PDFs: procedures)+≡

```
function func_20 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = polylog(2, ((1 + y)*(-1 + x))/(1 + y*(-1 + x))) / (1 + y*(-1 + x)) + &
    polylog(3, ((1 + y)*(-1 + x))/(1 + y*(-1 + x)))
end function func_20
```

(Electron PDFs: procedures)+≡

```
function func_24 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (log(1 + x/(1 + y*(-1 + x)))*(-((-1 + y)*(-1 + x)*(1 + y*(-1 + x) + x) * &
    log(1 + x/(1 + y*(-1 + x)))) + x*log(x/(1 + y*(-1 + x)))*(2*(-1 + y + &
    x - y*x) + (1 + y*(-1 + x) + x)*log(1 + x/(1 + y*(-1 + x))))) / &
    ((1 + y*(-1 + x))**2*x*(1 + y*(-1 + x) + x))
end function func_24
```

(Electron PDFs: procedures)+≡

```
function func_25 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (((-1 + y)*(-1 + x)*log(1 + x/(1 + y*(-1 + x))**2)/x + ((-1 + y + x - &
    y*x + (1 + y*(-1 + x) + x)*log(1 + x/(1 + y*(-1 + x))))) * &
    polylog(2, -x/(1 + y*(-1 + x)))) / (1 + y*(-1 + x) + x)) / &
    (1 + y*(-1 + x))**2 + Pi2/12._default * log(two)
end function func_25
```

(Electron PDFs: procedures)+≡

```
function func_30 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((-1 + y + x - y*x)*log(x/(1 + y*(-1 + x) + x)) * log(1 + x/(1 + &
    y*(-1 + x))) + (-1 + y + x - y*x + (1 + y*(-1 + x) + x)*log(1 + &
    x/(1 + y*(-1 + x))))*polylog(2, 1/(1 + x/(1 + y*(-1 + x))))) / &
    ((1 + y*(-1 + x))**2*(1 + y*(-1 + x) + x)) - Pi2/12._default*log(two) + &
    0.5*log(two)**3
end function func_30
```

(Electron PDFs: procedures)+≡

```
function func_32 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (polylog(2, ((-1 + y)*(-1 + x))/(1 + y*(-1 + x))) + &
    polylog(3, ((-1 + y)*(-1 + x))/(1 + y*(-1 + x)))) / &
    (1 + y*(-1 + x))**2
end function func_32
```

(Electron PDFs: procedures)+≡

```
function func_34 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((-1 + y)*(-1 + x)*polylog(2, 1/(1 + x/(1 + y*(-1 + x))))) / &
    ((1 + y*(-1 + x))*(1 + y*(-1 + x) + x)) + polylog(3, 1/(1 + &
    x/(1 + y*(-1 + x)))) - one/6._default*log(two)**3 + &
```



```

      Pi2/12._default*log(two) - 7._default/8._default*zeta3
end function func_34

```

(Electron PDFs: procedures)+≡

```

function func_35 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = ((-1 + y)*(-1 + x)*polylog(2,1/(1 + x/(1 + y*(-1 + x)))) + &
      (1 + y*(-1 + x) + x)*polylog(3,1/(1 + x/(1 + y*(-1 + x)))) / &
      ((1 + y*(-1 + x))*2*(1 + y*(-1 + x) + x)) - &
      one/6._default*log(two)**3 + Pi2/12._default*log(two) - &
      7._default/8._default*zeta3
end function func_35

```

(Electron PDFs: procedures)+≡

```

function func_37 (y, x) result (f)
  real(default), intent(in) :: x, y
  real(default) :: xb, f
  xb = one - x
  f = (log(y - y*x)*(log(y - y*x) + log((-1 + y)*(-1 + x)) / &
      (1 + y*(-1 + x)))*(2 + 2*y*(-1 + x) + log(y - y*x))) / &
      (1 + y*(-1 + x))**2 - log(xb)**3 + Pi2/three*log(xb) - two*zeta3
end function func_37

```

(Electron PDFs: public)+≡

```

public :: endpoint_func_S

```

(Electron PDFs: sub interfaces)+≡

```

module function endpoint_func_S (x, nlep) result (f)
  real(default), intent(in) :: x
  integer, intent(in) :: nlep
  real(default) :: f
end function endpoint_func_S

```

(Electron PDFs: procedures)+≡

```

module function endpoint_func_S (x, nlep) result (f)
  real(default), intent(in) :: x
  integer, intent(in) :: nlep
  real(default) :: f
  real(default) :: result, abserr
  real(default), parameter :: epsabs = 0.001_default, &
    epsrel = 0.001_default
  real(default), parameter :: a = 0._default, b = 1._default
  integer, parameter :: limit = 10000
  call gauss_kronrod (GAUSS_KRONROD_41, int_fun, a, b, &
    limit, result, abserr, epsabs, epsrel)
  f = result
contains
  function int_fun (y) result (d_f)
    real(default) :: d_f
    real(default), intent(in) :: y
    d_f = four*func_1(y,x) + four*func_2(y,x) + four*func_3(y,x) - &
      two*func_4(y,x) - four*func_5(y,x) - four*func_8(y,x) - &

```

```

        four*func_9(y,x) + four*func_10(y,x) + 4.*func_11(y,x) - &
        8._default*func_12(y,x) - four*func_13(y,x) + two*func_14(y,x) - &
        8._default*func_15(y,x) - 8._default*func_16(y,x) - &
        24._default*real(nlep,kind=default)*func_20(y,x);
    end function int_fun
end function endpoint_func_S

```

```

<Electron PDFs: public>+≡
    public :: endpoint_func_NS

```

```

<Electron PDFs: sub interfaces>+≡
    module function endpoint_func_NS (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
    end function endpoint_func_NS

```

```

<Electron PDFs: procedures>+≡
    module function endpoint_func_NS (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
        real(default) :: result, abserr
        real(default), parameter :: epsabs = 0.001_default, &
            epsrel = 0.001_default
        real(default), parameter :: a = 0._default, b = 1._default
        integer, parameter :: limit = 10000
        call gauss_kronrod (GAUSS_KRONROD_41, int_fun, a, b, &
            limit, result, abserr, epsabs, epsrel)
        f = result
    contains
        function int_fun (y) result (d_f)
            real(default) :: d_f
            real(default), intent(in) :: y
            d_f = four*func_1(y,x) + four*func_2(y,x) + four*func_3(y,x) + &
                two*func_4(y,x) + four*func_5(y,x) + four*func_8(y,x) + &
                four*func_9(y,x) - four*func_10(y,x) - four*func_11(y,x) + &
                8._default*func_12(y,x) - four*func_13(y,x) - two*func_14(y,x) + &
                8._default*func_15(y,x) + 8._default*func_16(y,x)
        end function int_fun
    end function endpoint_func_NS

```

```

<Electron PDFs: public>+≡
    public :: endpoint_func_GAM

```

```

<Electron PDFs: sub interfaces>+≡
    module function endpoint_func_GAM (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
    end function endpoint_func_GAM

```

```

<Electron PDFs: procedures>+≡
    module function endpoint_func_GAM (x) result (f)
        real(default), intent(in) :: x
        real(default) :: f
        real(default) :: result, abserr
        real(default), parameter :: epsabs = 0.001_default, &

```

```

        epsrel = 0.001_default
real(default), parameter :: a = 0._default, b = 1._default
integer, parameter :: limit = 10000
call gauss_kronrod (GAUSS_KRONROD_41, int_fun, a, b, &
        limit, result, abserr, epsabs, epsrel)
f = result
contains
function int_fun (y) result (d_f)
    real(default) :: d_f
    real(default), intent(in) :: y
    d_f = -8._default*func_24(y,x) - 8._default*func_25(y,x) + &
        8._default*func_30(y,x) + 8._default*func_32(y,x) + 16._default* &
        func_34(y,x) - 16._default*func_35(y,x) - four*func_37(y,x)
end function int_fun
end function endpoint_func_GAM

```

(Electron PDFs: procedures)+≡

```

function photon_matching (x, x0, x1, p) result (p_match)
    real(default) :: p_match
    real(default), intent(in) :: x, x0, x1, p
    real(default) :: xm, logx
    logx = - log10(1-x)
    if (logx < x0) then
        p_match = zero
    else if (logx > x1) then
        p_match = one
    else
        xm = (logx - x0) / (x1 - x0)
        p_match = xm**p / (xm**p + (1-xm)**p)
    end if
end function photon_matching

```

(Electron PDFs: public)+≡

```

public :: elec_pdf

```

(Electron PDFs: sub interfaces)+≡

```

module function elec_pdf (epdf, flv, x, scale, alpha, &
    running, w_num) result (e_pdf)
    type(qed_pdf_t), intent(in) :: epdf
    integer, intent(in) :: flv
    real(default) :: e_pdf
    real(default), intent(in) :: x
    real(default), intent(in) :: scale
    real(default), intent(in) :: alpha
    logical, intent(in) :: running, w_num
end function elec_pdf

```

(Electron PDFs: procedures)+≡

```

module function elec_pdf (epdf, flv, x, scale, alpha, &
    running, w_num) result (e_pdf)
    type(qed_pdf_t), intent(in) :: epdf
    integer, intent(in) :: flv
    real(default) :: e_pdf
    real(default), intent(in) :: x
    real(default), intent(in) :: scale

```

```

real(default), intent(in) :: alpha
logical, intent(in) :: running, w_num
integer :: nlep
real(default) :: ln0, eta0, al_2pi, p
real(default), parameter :: x0gam = 2.0_default, x1gam = &
    6._default, pgam = 2._default
if (allocated (epdf%q_in)) then
    ln0 = log(epdf%q_in**2/epdf%mass**2)
    eta0 = alpha/Pi * log(scale**2/epdf%q_in**2)
else
    ln0 = zero
    eta0 = alpha/Pi * log(scale**2/epdf%mass**2)
end if
if (running) then
    p = t_alpha (epdf, scale)
else
    p = eta0 / two
end if
select case (epdf%log_order)
case (EPDF_LL)
    nlep = epdf%n_lep
    al_2pi = zero
case (EPDF_NLL)
    if (running) then
        select type (aqed => epdf%aqed)
        type is (alpha_qed_from_scale_t)
            nlep = aqed%nlep
            al_2pi = aqed%get (scale) / two / Pi
        type is (alpha_qed_fixed_t)
            call msg_fatal &
                ("elec_pdf: has to be called with running alpha.")
        end select
    else
        nlep = epdf%n_lep
        al_2pi = alpha / two / Pi
    end if
end select
select case (flv)
case (EPDF_S)
    e_pdf = elec_asym (epdf, x, scale, alpha, running) + &
        recbar (epdf, flv, x, scale, alpha, running) + &
        rechat (epdf, flv, x, scale, alpha, running) - &
        bar_asym (epdf, flv, x, scale, alpha, running)
    if (w_num) then
        e_pdf = e_pdf + &
            rec_num (epdf, flv, x, scale, alpha, running)
    end if
case (EPDF_NS)
    e_pdf = elec_asym (epdf, x, scale, alpha, running) + &
        recbar (epdf, flv, x, scale, alpha, running) + &
        rechat (epdf, flv, x, scale, alpha, running) - &
        bar_asym (epdf, flv, x, scale, alpha, running)
    if (w_num) then
        e_pdf = e_pdf + &

```

```

        rec_num (epdf, flv, x, scale, alpha, running)
    end if
case (EPDF_G)
    e_pdf = recbar (epdf, flv, x, scale, alpha, running) + &
        rechat (epdf, flv, x, scale, alpha, running) + &
        photon_matching (x, x0gam, x1gam, pgam) * &
        (phot_asym (epdf, x, scale, alpha, nlep, running) - &
        recbar (epdf, flv, x, scale, alpha, running))
    if (w_num) then
        e_pdf = e_pdf + &
            rec_num (epdf, flv, x, scale, alpha, running)
    end if
case (EPDF_ELE)
    e_pdf = elec_asym (epdf, x, scale, alpha, running) - &
        bar_asym (epdf, EPDF_S, x, scale, alpha, running) + &
        0.5_default * (recbar (epdf, EPDF_S, x, scale, alpha, running) + &
        recbar (epdf, EPDF_NS, x, scale, alpha, running) + &
        rechat (epdf, EPDF_S, x, scale, alpha, running) + &
        rechat (epdf, EPDF_NS, x, scale, alpha, running))
    if (w_num) then
        e_pdf = e_pdf + 0.5_default * ( &
            rec_num (epdf, EPDF_S, x, scale, alpha, running) + &
            rec_num (epdf, EPDF_NS, x, scale, alpha, running))
    end if
case (EPDF_POS)
    e_pdf = 0.5_default * (recbar (epdf, EPDF_S, x, scale, alpha, running) - &
        recbar (epdf, EPDF_NS, x, scale, alpha, running) + &
        rechat (epdf, EPDF_S, x, scale, alpha, running) - &
        rechat (epdf, EPDF_NS, x, scale, alpha, running))
    if (w_num) then
        e_pdf = e_pdf + 0.5_default * ( &
            rec_num (epdf, EPDF_S, x, scale, alpha, running) - &
            rec_num (epdf, EPDF_NS, x, scale, alpha, running))
    end if
case default
    call msg_fatal &
        ("elec_pdf: wrong lepton flavor.")
end select
end function elec_pdf

```

10.1.3 Unit tests

Test module, followed by the corresponding implementation module.

`<electron_pdfs_ut.f90>`≡
<File header>

```

module electron_pdfs_ut
    use unit_tests
    use electron_pdfs_uti

```

<Standard module head>

```

    <Electron PDFs: public test>

contains

    <Electron PDFs: test driver>

end module electron_pdfs_ut
<electron_pdfs_util.f90>≡
    <File header>

module electron_pdfs_util

    <Use kinds>
    use numeric_utils
    use format_defs, only: FMT_15
    use constants
    use physics_defs, only: ME_REF, ALPHA_QED_ME_REF
    use electron_pdfs

    <Standard module head>

    <Electron PDFs: test declarations>

contains

    <Electron PDFs: tests>

end module electron_pdfs_util
API: driver for the unit tests below.
<Electron PDFs: public test>≡
    public :: electron_pdfs_test
<Electron PDFs: test driver>≡
    subroutine electron_pdfs_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Electron PDFs: execute tests>
    end subroutine electron_pdfs_test

```

Electron PDF tests

```

<Electron PDFs: execute tests>≡
    call test (electron_pdfs_1, "electron_pdfs_1", &
        "Electron PDFs: auxiliary functions", &
        u, results)
<Electron PDFs: test declarations>≡
    public :: electron_pdfs_1
<Electron PDFs: tests>≡
    subroutine electron_pdfs_1 (u)
        integer, intent(in) :: u
        type(qed_pdf_t) :: pdf

```

```

real(default) :: Q, alpha
real(default) :: x1, x2, x3, x4
integer :: n_lep
Q = 10._default
x1 = 0.1_default
x2 = 0.5_default
x3 = 0.9_default
x4 = 0.999_default
alpha = ALPHA_QED_ME_REF
n_lep = 1

write (u, "(A)")  "* Test output: electron_pdfs_1"
write (u, "(A)")  "* Purpose: check analytic properties"
write (u, "(A)")

write (u, "(A)")  "* Auxiliary functions I:"
write (u, "(A)")

write (u, "(A)")  "* Q = 10 GeV, elec_asym, LL+NLL, alpha fixed:"
write (u, "(A)")

call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
  3000._default, 3, 0, 1)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.1) = ", &
  elec_asym (pdf, x1, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.5) = ", &
  elec_asym (pdf, x2, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.9) = ", &
  elec_asym (pdf, x3, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.999) = ", &
  elec_asym (pdf, x4, Q, alpha, .false.)
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
  3000._default, 3, 1, 1)
write (u, "(A)")
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.1) = ", &
  elec_asym (pdf, x1, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.5) = ", &
  elec_asym (pdf, x2, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.9) = ", &
  elec_asym (pdf, x3, Q, alpha, .false.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.999) = ", &
  elec_asym (pdf, x4, Q, alpha, .false.)

call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
  3000._default, 3, 0, 1)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(A)")
call pdf%write (u, with_qed = .true.)
write (u, "(A)")

write (u, "(A)")  "* Q = 10 GeV, elec_asym, LL+NLL, alpha running:"
write (u, "(A)")

write (u, "(1x,A,F9.6)") " Integrator t (10 GeV) = ", &

```

```

t_alpha (pdf, Q)
write (u, "(A)")

write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.1) = ", &
elec_asym (pdf, x1, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.5) = ", &
elec_asym (pdf, x2, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.9) = ", &
elec_asym (pdf, x3, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (LL,x=0.999) = ", &
elec_asym (pdf, x4, Q, alpha, .true.)
write (u, "(A)")

call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, 1)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.1) = ", &
elec_asym (pdf, x1, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.5) = ", &
elec_asym (pdf, x2, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.9) = ", &
elec_asym (pdf, x3, Q, alpha, .true.)
write (u, "(1x,A,F9.6)") " elec_asym (NLL,x=0.999) = ", &
elec_asym (pdf, x4, Q, alpha, .true.)

write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, phot_asym, LL+NLL, alpha fixed:"
write (u, "(A)")

call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, 1)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.1) = ", &
phot_asym (pdf, x1, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.5) = ", &
phot_asym (pdf, x2, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.9) = ", &
phot_asym (pdf, x3, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.999) = ", &
phot_asym (pdf, x4, Q, alpha, n_lep, .false.)
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, 1)
write (u, "(A)")
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.1) = ", &
phot_asym (pdf, x1, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.5) = ", &
phot_asym (pdf, x2, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.9) = ", &
phot_asym (pdf, x3, Q, alpha, n_lep, .false.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.999) = ", &
phot_asym (pdf, x4, Q, alpha, n_lep, .false.)

write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, phot_asym, LL+NLL, alpha running:"
write (u, "(A)")

```



```

call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, 1)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.1) = ", &
phot_asym (pdf, x1, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.5) = ", &
phot_asym (pdf, x2, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.9) = ", &
phot_asym (pdf, x3, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (LL,x=0.999) = ", &
phot_asym (pdf, x4, Q, alpha, n_lep, .true.)
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, 1)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(A)")
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.1) = ", &
phot_asym (pdf, x1, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.5) = ", &
phot_asym (pdf, x2, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.9) = ", &
phot_asym (pdf, x3, Q, alpha, n_lep, .true.)
write (u, "(1x,A,F9.6)") " phot_asym (NLL,x=0.999) = ", &
phot_asym (pdf, x4, Q, alpha, n_lep, .true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: electron_pdfs_1"

```

end subroutine electron_pdfs_1

(Electron PDFs: execute tests)+≡

```

call test (electron_pdfs_2, "electron_pdfs_2", &
"Electron PDFs: auxiliary functions (2)", &
u, results)

```

(Electron PDFs: test declarations)+≡

```

public :: electron_pdfs_2

```

(Electron PDFs: tests)+≡

```

subroutine electron_pdfs_2 (u)
integer, intent(in) :: u
real(default) :: Q, alpha
real(default) :: x1, x2, x3, x4, ln0
real(default), dimension(6):: jll_nll
logical, dimension(6) :: order
integer :: n_lep
Q = 10._default
x1 = 0.1_default
x2 = 0.5_default
x3 = 0.9_default
x4 = 0.999_default
ln0 = 0._default
n_lep = 1
order = .true.

```

```

write (u, "(A)")  "* Test output: electron_pdfs_2"
write (u, "(A)")  "* Purpose: check analytic properties"
write (u, "(A)")

write (u, "(A)")  "* Auxiliary functions II:"
write (u, "(A)")

write (u, "(A)")  "* Q = 10 GeV, elecbar_asym_p, LL+NLL, alpha fixed:"
write (u, "(A)")
call elecbar_asym_p (x1, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.100)  = ", jll_nll
call elecbar_asym_p (x2, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.500)  = ", jll_nll
call elecbar_asym_p (x3, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.900)  = ", jll_nll
call elecbar_asym_p (x4, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.999)  = ", jll_nll
write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, elecbar_asym_p, LL+NLL, alpha running:"
write (u, "(A)")
call elecbar_asym_p (x1, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.100)  = ", jll_nll
call elecbar_asym_p (x2, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.500)  = ", jll_nll
call elecbar_asym_p (x3, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.900)  = ", jll_nll
call elecbar_asym_p (x4, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " elecbar_asym_p (x=0.999)  = ", jll_nll

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, photbar_asym_p, LL+NLL, alpha fixed:"
write (u, "(A)")
call photbar_asym_p (x1, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.100)  = ", jll_nll
call photbar_asym_p (x2, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.500)  = ", jll_nll
call photbar_asym_p (x3, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.900)  = ", jll_nll
call photbar_asym_p (x4, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.999)  = ", jll_nll
write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, photbar_asym_p, LL+NLL, alpha running:"
write (u, "(A)")
call photbar_asym_p (x1, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.100)  = ", jll_nll
call photbar_asym_p (x2, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.500)  = ", jll_nll
call photbar_asym_p (x3, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.900)  = ", jll_nll
call photbar_asym_p (x4, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " photbar_asym_p (x=0.999)  = ", jll_nll

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, rechat_s, LL+NLL, alpha fixed:"

```

```

write (u, "(A)")
call rechat_singlet (x1, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.100) = ", jll_nll
call rechat_singlet (x2, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.500) = ", jll_nll
call rechat_singlet (x3, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.900) = ", jll_nll
call rechat_singlet (x4, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.999) = ", jll_nll
write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat_s, LL+NLL, alpha running:"
write (u, "(A)")
call rechat_singlet (x1, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.100) = ", jll_nll
call rechat_singlet (x2, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.500) = ", jll_nll
call rechat_singlet (x3, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.900) = ", jll_nll
call rechat_singlet (x4, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_singlet (x=0.999) = ", jll_nll

write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat_ns, LL+NLL, alpha fixed:"
write (u, "(A)")
call rechat_nonsinglet (x1, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.100) = ", jll_nll
call rechat_nonsinglet (x2, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.500) = ", jll_nll
call rechat_nonsinglet (x3, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.900) = ", jll_nll
call rechat_nonsinglet (x4, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.999) = ", jll_nll
write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat_ns, LL+NLL, alpha running:"
write (u, "(A)")
call rechat_nonsinglet (x1, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.100) = ", jll_nll
call rechat_nonsinglet (x2, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.500) = ", jll_nll
call rechat_nonsinglet (x3, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.900) = ", jll_nll
call rechat_nonsinglet (x4, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_nonsinglet (x=0.999) = ", jll_nll

write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat_photon, LL+NLL, alpha fixed:"
write (u, "(A)")
call rechat_photon (x1, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.100) = ", jll_nll
call rechat_photon (x2, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.500) = ", jll_nll
call rechat_photon (x3, jll_nll, n_lep, ln0, order, running=.false.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.900) = ", jll_nll
call rechat_photon (x4, jll_nll, n_lep, ln0, order, running=.false.)

```

```

write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.999) = ", jll_nll
write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat_photon, LL+NLL, alpha running:"
write (u, "(A)")
call rechat_photon (x1, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.100) = ", jll_nll
call rechat_photon (x2, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.500) = ", jll_nll
call rechat_photon (x3, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.900) = ", jll_nll
call rechat_photon (x4, jll_nll, n_lep, ln0, order, running=.true.)
write (u, "(1x,A,6(1x,ES11.4))") " rechat_photon (x=0.999) = ", jll_nll

write (u, "(A)")
write (u, "(A)") "* Test output end: electron_pdfs_2"

end subroutine electron_pdfs_2

```

<Electron PDFs: execute tests>+≡

```

call test (electron_pdfs_3, "electron_pdfs_3", &
  "Electron PDFs: auxiliary functions (3)", &
  u, results)

```

<Electron PDFs: test declarations>+≡

```

public :: electron_pdfs_3

```

<Electron PDFs: tests>+≡

```

subroutine electron_pdfs_3 (u)
  integer, intent(in) :: u
  type(qed_pdf_t) :: pdf
  real(default) :: Q, alpha
  real(default) :: x1, x2, x3, x4
  integer :: n_lep
  Q = 10._default
  x1 = 0.1_default
  x2 = 0.5_default
  x3 = 0.9_default
  x4 = 0.999_default
  alpha = ALPHA_QED_ME_REF
  n_lep = 1

  write (u, "(A)") "* Test output: electron_pdfs_3"
  write (u, "(A)") "* Purpose: check analytic properties"
  write (u, "(A)")

  write (u, "(A)") "* Auxiliary functions III:"
  write (u, "(A)")

```

```

  write (u, "(A)") "* Q = 10 GeV, bar_asym, e+-, LL+NLL, alpha fixed:"
  write (u, "(A)")
  call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 0, n_lep)
  write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.100) = ", &
    bar_asym (pdf, EPDF_ELE, x1, Q, alpha, running=.false.)
  write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.500) = ", &

```

```

        bar_asym (pdf, EPDF_ELE, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.900) = ", &
        bar_asym (pdf, EPDF_ELE, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.999) = ", &
        bar_asym (pdf, EPDF_ELE, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.100) = ", &
        bar_asym (pdf, EPDF_ELE, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.500) = ", &
        bar_asym (pdf, EPDF_ELE, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.900) = ", &
        bar_asym (pdf, EPDF_ELE, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.999) = ", &
        bar_asym (pdf, EPDF_ELE, x4, Q, alpha, running=.false.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, bar_asym, e+-, LL+NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, n_lep)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.100) = ", &
        bar_asym (pdf, EPDF_ELE, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.500) = ", &
        bar_asym (pdf, EPDF_ELE, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.900) = ", &
        bar_asym (pdf, EPDF_ELE, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,LL,x=0.999) = ", &
        bar_asym (pdf, EPDF_ELE, x4, Q, alpha, running=.true.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.100) = ", &
        bar_asym (pdf, EPDF_ELE, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.500) = ", &
        bar_asym (pdf, EPDF_ELE, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.900) = ", &
        bar_asym (pdf, EPDF_ELE, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (ELE,NLL,x=0.999) = ", &
        bar_asym (pdf, EPDF_ELE, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, bar_asym, gam, LL+NLL, alpha fixed:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, n_lep)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.100) = ", &
        bar_asym (pdf, EPDF_G, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.500) = ", &
        bar_asym (pdf, EPDF_G, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.900) = ", &

```

```

        bar_asym (pdf, EPDF_G, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.999) = ", &
        bar_asym (pdf, EPDF_G, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
        3000._default, 3, 1, n_lep)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.100) = ", &
        bar_asym (pdf, EPDF_G, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.500) = ", &
        bar_asym (pdf, EPDF_G, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.900) = ", &
        bar_asym (pdf, EPDF_G, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.999) = ", &
        bar_asym (pdf, EPDF_G, x4, Q, alpha, running=.false.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, bar_asym, gam, LL+NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
        3000._default, 3, 0, n_lep)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.100) = ", &
        bar_asym (pdf, EPDF_G, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.500) = ", &
        bar_asym (pdf, EPDF_G, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.900) = ", &
        bar_asym (pdf, EPDF_G, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,LL,x=0.999) = ", &
        bar_asym (pdf, EPDF_G, x4, Q, alpha, running=.true.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
        3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.100) = ", &
        bar_asym (pdf, EPDF_G, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " bar_asym (GAM,NLL,x=0.500) = ", &
        bar_asym (pdf, EPDF_G, x2, Q, alpha, running=.true.)
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        bar_asym (pdf, EPDF_G, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recbar, S, LL+NLL, alpha fixed:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
        3000._default, 3, 0, n_lep)
write (u, "(1x,A,F11.6)") " recbar (S,LL,x=0.100) = ", &
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        recbar (pdf, EPDF_S, x3, Q, alpha, running=.false.)
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```

        recbar (pdf, EPDF_S, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
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call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
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write (u, "(A)") "* Q = 10 GeV, recbar, NS, LL+NLL, alpha fixed:"
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3000._default, 3, 0, n_lep)
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write (u, "(1x,A,F11.6)") " recbar (NS,LL,x=0.999) = ", &
recbar (pdf, EPDF_NS, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &

```

```

3000._default, 3, 1, n_lep)
write (u, "(1x,A,F11.6)") " recbar (NS,NLL,x=0.100) = ", &
    recbar (pdf, EPDF_NS, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (NS,NLL,x=0.500) = ", &
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    recbar (pdf, EPDF_NS, x4, Q, alpha, running=.false.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recbar, NS, LL+NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 0, n_lep)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " recbar (NS,LL,x=0.100) = ", &
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    recbar (pdf, EPDF_NS, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (NS,LL,x=0.900) = ", &
    recbar (pdf, EPDF_NS, x3, Q, alpha, running=.true.)
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call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 1, n_lep)
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write (u, "(1x,A,F11.6)") " recbar (NS,NLL,x=0.100) = ", &
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    recbar (pdf, EPDF_NS, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (NS,NLL,x=0.900) = ", &
    recbar (pdf, EPDF_NS, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (NS,NLL,x=0.999) = ", &
    recbar (pdf, EPDF_NS, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recbar, GAM, LL+NLL, alpha fixed:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 0, n_lep)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.100) = ", &
    recbar (pdf, EPDF_G, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.500) = ", &
    recbar (pdf, EPDF_G, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.900) = ", &
    recbar (pdf, EPDF_G, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.999) = ", &
    recbar (pdf, EPDF_G, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 1, n_lep)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.100) = ", &

```



```

        recbar (pdf, EPDF_G, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.500) = ", &
        recbar (pdf, EPDF_G, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.900) = ", &
        recbar (pdf, EPDF_G, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.999) = ", &
        recbar (pdf, EPDF_G, x4, Q, alpha, running=.false.)
write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recbar, GAM, LL+NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, n_lep)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.100) = ", &
        recbar (pdf, EPDF_G, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.500) = ", &
        recbar (pdf, EPDF_G, x2, Q, alpha, running=.true.)
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        recbar (pdf, EPDF_G, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,LL,x=0.999) = ", &
        recbar (pdf, EPDF_G, x4, Q, alpha, running=.true.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.100) = ", &
        recbar (pdf, EPDF_G, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.500) = ", &
        recbar (pdf, EPDF_G, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.900) = ", &
        recbar (pdf, EPDF_G, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " recbar (GAM,NLL,x=0.999) = ", &
        recbar (pdf, EPDF_G, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: electron_pdfs_3"

end subroutine electron_pdfs_3

```

<Electron PDFs: execute tests>+≡

```

call test (electron_pdfs_4, "electron_pdfs_4", &
"Electron PDFs: auxiliary functions (4)", &
u, results)

```

<Electron PDFs: test declarations>+≡

```

public :: electron_pdfs_4

```

<Electron PDFs: tests>+≡

```

subroutine electron_pdfs_4 (u)
integer, intent(in) :: u
type(qed_pdf_t) :: pdf
real(default) :: Q, alpha
real(default) :: x1, x2, x3, x4
integer :: n_lep
Q = 10._default

```

```

x1 = 0.1_default
x2 = 0.5_default
x3 = 0.9_default
x4 = 0.999_default
alpha = ALPHA_QED_ME_REF
n_lep = 1

write (u, "(A)")  "* Test output: electron_pdfs_4"
write (u, "(A)")  "* Purpose: check analytic properties"
write (u, "(A)")

write (u, "(A)")  "* Auxiliary functions IV:"
write (u, "(A)")

write (u, "(A)")  "* Q = 10 GeV, rechat, S, LL+NLL, alpha fixed:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 0, n_lep)
write (u, "(1x,A,F11.6)")  " rechat (S,LL,x=0.100) = ", &
rechat (pdf, EPDF_S, x1, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)")  " rechat (S,LL,x=0.500) = ", &
rechat (pdf, EPDF_S, x2, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)")  " rechat (S,LL,x=0.900) = ", &
rechat (pdf, EPDF_S, x3, Q, alpha, running=.false.)
write (u, "(1x,A,F11.6)")  " rechat (S,LL,x=0.999) = ", &
rechat (pdf, EPDF_S, x4, Q, alpha, running=.false.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
write (u, "(1x,A,F11.6)")  " rechat (S,NLL,x=0.100) = ", &
rechat (pdf, EPDF_S, x1, Q, alpha, running=.false.)
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rechat (pdf, EPDF_S, x2, Q, alpha, running=.false.)
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write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, rechat, S, LL+NLL, alpha running:"
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rechat (pdf, EPDF_S, x4, Q, alpha, running=.true.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &

```

```

3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " rechat (S,NLL,x=0.100) = ", &
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write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat, NS, LL+NLL, alpha fixed:"
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```

```

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    rechat (pdf, EPDF_NS, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)") "* Q = 10 GeV, rechat, GAM, LL+NLL, alpha fixed:"
write (u, "(A)")
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    3000._default, 3, 0, n_lep)
write (u, "(1x,A,F11.6)") " rechat (GAM,LL,x=0.100) = ", &
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write (u, "(A)") "* Q = 10 GeV, rechat, GAM, LL+NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 0, n_lep)
call pdf%allocate_aqed (order = 0, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,LL,x=0.100) = ", &
    rechat (pdf, EPDF_G, x1, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,LL,x=0.500) = ", &
    rechat (pdf, EPDF_G, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,LL,x=0.900) = ", &
    rechat (pdf, EPDF_G, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,LL,x=0.999) = ", &
    rechat (pdf, EPDF_G, x4, Q, alpha, running=.true.)
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,NLL,x=0.100) = ", &
    rechat (pdf, EPDF_G, x1, Q, alpha, running=.true.)

```

```

write (u, "(1x,A,F11.6)") " rechat (GAM,NLL,x=0.500) = ", &
    rechat (pdf, EPDF_G, x2, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,NLL,x=0.900) = ", &
    rechat (pdf, EPDF_G, x3, Q, alpha, running=.true.)
write (u, "(1x,A,F11.6)") " rechat (GAM,NLL,x=0.999) = ", &
    rechat (pdf, EPDF_G, x4, Q, alpha, running=.true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: electron_pdfs_4"

end subroutine electron_pdfs_4

```

<Electron PDFs: execute tests>+≡

```

call test (electron_pdfs_5, "electron_pdfs_5", &
    "Electron PDFs: auxiliary functions (5)", &
    u, results)

```

<Electron PDFs: test declarations>+≡

```

public :: electron_pdfs_5

```

<Electron PDFs: tests>+≡

```

subroutine electron_pdfs_5 (u)
    integer, intent(in) :: u
    type(qed_pdf_t) :: pdf
    real(default) :: Q, alpha
    real(default) :: x1, x2, x3, x4
    integer :: n_lep
    Q = 10._default
    x1 = 0.1_default
    x2 = 0.5_default
    x3 = 0.9_default
    x4 = 0.999_default
    alpha = ALPHA_QED_ME_REF
    n_lep = 1

    write (u, "(A)")  "* Test output: electron_pdfs_5"
    write (u, "(A)")  "* Purpose: check analytic properties"
    write (u, "(A)")

    write (u, "(A)")  "* Auxiliary functions V:"
    write (u, "(A)")

    write (u, "(A)")  "* Integrals over endpoint_func_NS, interval [0,1]:"
    write (u, "(A)")
    write (u, "(1x,A,F11.6)") " endpoint_func_NS (0.100) = ", &
        endpoint_func_NS (x1)
    write (u, "(1x,A,F11.6)") " endpoint_func_NS (0.500) = ", &
        endpoint_func_NS (x2)
    write (u, "(1x,A,F11.6)") " endpoint_func_NS (0.900) = ", &
        endpoint_func_NS (x3)
    write (u, "(1x,A,F11.6)") " endpoint_func_NS (0.999) = ", &
        endpoint_func_NS (x4)

    write (u, "(A)")
    write (u, "(A)")  "* Integrals over endpoint_func_S, interval [0,1]:"

```

```

write (u, "(A)")
write (u, "(1x,A,F11.6)") " endpoint_func_S (0.100) = ", &
    endpoint_func_S (x1, n_lep)
write (u, "(1x,A,F11.6)") " endpoint_func_S (0.500) = ", &
    endpoint_func_S (x2, n_lep)
write (u, "(1x,A,F11.6)") " endpoint_func_S (0.900) = ", &
    endpoint_func_S (x3, n_lep)
write (u, "(1x,A,F11.6)") " endpoint_func_S (0.999) = ", &
    endpoint_func_S (x4, n_lep)

write (u, "(A)")
write (u, "(A)")  "* Integrals over endpoint_func_GAM, interval [0,1]:"
write (u, "(A)")
write (u, "(1x,A,F11.6)") " endpoint_func_GAM (0.100) = ", &
    endpoint_func_GAM (x1)
write (u, "(1x,A,F11.6)") " endpoint_func_GAM (0.500) = ", &
    endpoint_func_GAM (x2)
write (u, "(1x,A,F11.6)") " endpoint_func_GAM (0.900) = ", &
    endpoint_func_GAM (x3)
write (u, "(1x,A,F11.6)") " endpoint_func_GAM (0.999) = ", &
    endpoint_func_GAM (x4)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recnum, alpha fixed:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
    3000._default, 3, 1, n_lep)
write (u, "(1x,A,ES11.4)") " recnum (S, 0.100) = ", &
    rec_num (pdf, EPDF_S, x1, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (S, 0.500) = ", &
    rec_num (pdf, EPDF_S, x2, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (S, 0.900) = ", &
    rec_num (pdf, EPDF_S, x3, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (S, 0.999) = ", &
    rec_num (pdf, EPDF_S, x4, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (NS, 0.100) = ", &
    rec_num (pdf, EPDF_NS, x1, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (NS, 0.500) = ", &
    rec_num (pdf, EPDF_NS, x2, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (NS, 0.900) = ", &
    rec_num (pdf, EPDF_NS, x3, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (NS, 0.999) = ", &
    rec_num (pdf, EPDF_NS, x4, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (GAM, 0.100) = ", &
    rec_num (pdf, EPDF_G, x1, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (GAM, 0.500) = ", &
    rec_num (pdf, EPDF_G, x2, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (GAM, 0.900) = ", &
    rec_num (pdf, EPDF_G, x3, Q, alpha, .false.)
write (u, "(1x,A,ES11.4)") " recnum (GAM, 0.999) = ", &
    rec_num (pdf, EPDF_G, x4, Q, alpha, .false.)

write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, recnum, alpha running:"

```

```

write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,ES11.4)" " recnum (S, 0.100) = ", &
rec_num (pdf, EPDF_S, x1, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (S, 0.500) = ", &
rec_num (pdf, EPDF_S, x2, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (S, 0.900) = ", &
rec_num (pdf, EPDF_S, x3, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (S, 0.999) = ", &
rec_num (pdf, EPDF_S, x4, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (NS, 0.100) = ", &
rec_num (pdf, EPDF_NS, x1, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (NS, 0.500) = ", &
rec_num (pdf, EPDF_NS, x2, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (NS, 0.900) = ", &
rec_num (pdf, EPDF_NS, x3, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (NS, 0.999) = ", &
rec_num (pdf, EPDF_NS, x4, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (GAM, 0.100) = ", &
rec_num (pdf, EPDF_G, x1, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (GAM, 0.500) = ", &
rec_num (pdf, EPDF_G, x2, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (GAM, 0.900) = ", &
rec_num (pdf, EPDF_G, x3, Q, alpha, .true.)
write (u, "(1x,A,ES11.4)" " recnum (GAM, 0.999) = ", &
rec_num (pdf, EPDF_G, x4, Q, alpha, .true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: electron_pdfs_5"

```

```

end subroutine electron_pdfs_5

```

<Electron PDFs: execute tests>+≡

```

call test (electron_pdfs_6, "electron_pdfs_6", &
"Electron PDFs: full electron PDFs", &
u, results)

```

<Electron PDFs: test declarations>+≡

```

public :: electron_pdfs_6

```

<Electron PDFs: tests>+≡

```

subroutine electron_pdfs_6 (u)
integer, intent(in) :: u
type(qed_pdf_t) :: pdf
real(default) :: Q, alpha
real(default), dimension(12) :: x
integer :: n_lep
Q = 10._default
x( 1) = 0.1_default
x( 2) = 0.2_default
x( 3) = 0.3_default
x( 4) = 0.4_default
x( 5) = 0.5_default

```

```

x( 6) = 0.6_default
x( 7) = 0.7_default
x( 8) = 0.8_default
x( 9) = 0.9_default
x(10) = 0.95_default
x(11) = 0.99_default
x(12) = 0.999_default
alpha = ALPHA_QED_ME_REF
n_lep = 1

write (u, "(A)")  "* Test output: electron_pdfs_6"
write (u, "(A)")  "* Purpose: full electron PDFs"
write (u, "(A)")

write (u, "(A)")  "* Full NLL electron PDFs:"
write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, NLL, alpha fixed:"
write (u, "(A)")
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.100, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(1), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(1), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(1), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.200, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(2), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(2), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(2), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.300, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(3), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(3), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(3), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.400, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(4), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(4), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(4), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.500, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(5), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(5), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(5), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.600, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(6), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(6), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(6), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.700, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(7), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(7), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(7), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.800, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(8), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(8), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(8), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.900, S/GAM/NS) = ", &

```



```

elec_pdf (pdf, EPDF_S, x(9), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(9), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(9), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.950, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(10), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(10), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(10), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.990, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(11), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(11), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(11), Q, alpha, .false., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.999, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(12), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_G, x(12), Q, alpha, .false., .true.), &
elec_pdf (pdf, EPDF_NS, x(12), Q, alpha, .false., .true.)
write (u, "(A)")
write (u, "(A)")  "* Q = 10 GeV, NLL, alpha running:"
write (u, "(A)")
call pdf%init (ME_REF, ALPHA_QED_ME_REF, -1._default, &
3000._default, 3, 1, n_lep)
call pdf%allocate_aqed (order = 1, n_f = 0, n_lep = 1, running = .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.100, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(1), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(1), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(1), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.200, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(2), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(2), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(2), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.300, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(3), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(3), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(3), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.400, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(4), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(4), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(4), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.500, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(5), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(5), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(5), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.600, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(6), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(6), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(6), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.700, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(7), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(7), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(7), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.800, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(8), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(8), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(8), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.900, S/GAM/NS) = ", &

```

```

elec_pdf (pdf, EPDF_S, x(9), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(9), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(9), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.950, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(10), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(10), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(10), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.990, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(11), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(11), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(11), Q, alpha, .true., .true.)
write (u, "(1x,A,3(1x,F11.6))") " ePDF (x = 0.999, S/GAM/NS) = ", &
elec_pdf (pdf, EPDF_S, x(12), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_G, x(12), Q, alpha, .true., .true.), &
elec_pdf (pdf, EPDF_NS, x(12), Q, alpha, .true., .true.)
write (u, "(A)")
write (u, "(A)")  "* Check singlet-nonsinglet linear combination"
write (u, "(A)")
write (u, "(1x,A,F11.6)") " ePDF (x = 0.950, e- - [S + NS]/2) = ", &
abs(elec_pdf (pdf, EPDF_ELE, x(10), Q, alpha, .true., .true.) - &
(elec_pdf (pdf, EPDF_S, x(10), Q, alpha, .true., .true.) + &
elec_pdf (pdf, EPDF_NS, x(10), Q, alpha, .true., .true.))/two)
write (u, "(1x,A,F11.6)") " ePDF (x = 0.950, e+ - [S - NS]/2) = ", &
abs(elec_pdf (pdf, EPDF_POS, x(10), Q, alpha, .true., .true.) - &
(elec_pdf (pdf, EPDF_S, x(10), Q, alpha, .true., .true.) - &
elec_pdf (pdf, EPDF_NS, x(10), Q, alpha, .true., .true.))/two)

write (u, "(A)")
write (u, "(A)")  "* Test output end: electron_pdfs_6"

end subroutine electron_pdfs_6

```

Chapter 11

Quantum Field Theory Concepts

The objects and methods defined here implement concepts and data for the underlying quantum field theory that we use for computing matrix elements and processes.

model_data Fields and coupling parameters, operators as vertex structures, for a specific model.

model_testbed Provide hooks to deal with a **model_data** extension without referencing it explicitly.

helicities Types and methods for spin density matrices.

colors Dealing with colored particles, using the color-flow representation.

flavors PDG codes and particle properties, depends on the model.

quantum_numbers Quantum numbers and density matrices for entangled particle systems.

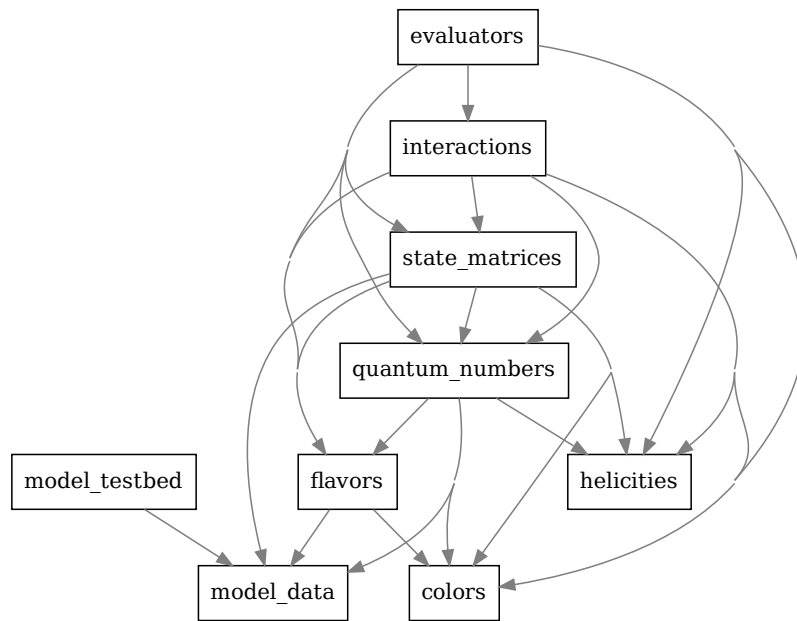


Figure 11.1: Module dependencies in `src/qft`.

11.1 Model Data

These data represent a specific Lagrangian in numeric terms. That is, we have the fields with their quantum numbers, the masses, widths and couplings as numerical values, and the vertices as arrays of fields.

We do not store the relations between coupling parameters. They should be represented by expressions for evaluation, implemented as Sindarin objects in a distinct data structure. Neither do we need the algebraic structure of vertices. The field content of vertices is required for the sole purpose of setting up phase space.

```
<model_data.f90>≡
  <File header>

  module model_data

    use, intrinsic :: iso_c_binding !NODEP!

    <Use kinds>
    use kinds, only: i8, i32
    use kinds, only: c_default_float
    <Use strings>
    use physics_defs, only: UNDEFINED, SCALAR

    <Standard module head>

    <Model data: public>

    <Model data: types>

    interface
    <Model data: sub interfaces>
    end interface

  end module model_data

<model_data_sub.f90>≡
  <File header>

  submodule (model_data) model_data_s

    use format_defs, only: FMT_19
    use io_units
    use diagnostics
    use md5
    use hashes, only: hash

    implicit none

    <Model data: parameters>

    contains

    <Model data: procedures>
```

```
end submodule model_data_s
```

11.1.1 Physics Parameters

Couplings, masses, and widths are physics parameters. Each parameter has a unique name (used, essentially, for diagnostics output and debugging) and a value. The value may be a real or a complex number, so we provide to implementations of an abstract type.

```
<Model data: public>≡
  public :: modelpar_data_t

<Model data: types>≡
  type, abstract :: modelpar_data_t
    private
    type(string_t) :: name
    contains
    <Model data: par data: TBP>
  end type modelpar_data_t

  type, extends (modelpar_data_t) :: modelpar_real_t
    private
    real(default) :: value
  end type modelpar_real_t

  type, extends (modelpar_data_t) :: modelpar_complex_t
    private
    complex(default) :: value
  end type modelpar_complex_t
```

Output for diagnostics. Non-advancing.

```
<Model data: par data: TBP>≡
  procedure :: write => par_write

<Model data: sub interfaces>≡
  module subroutine par_write (par, unit)
    class(modelpar_data_t), intent(in) :: par
    integer, intent(in), optional :: unit
  end subroutine

<Model data: procedures>≡
  module subroutine par_write (par, unit)
    class(modelpar_data_t), intent(in) :: par
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,1x,A)", advance="no") char (par%name), "= "
    select type (par)
    type is (modelpar_real_t)
      write (u, "(" // FMT_19 // ")", advance="no") par%value
    type is (modelpar_complex_t)
      write (u, "(" // FMT_19 // ",1x,'+',1x," // FMT_19 // ",1x,'I')", &
        advance="no") par%value
    end select
```

```
end subroutine par_write
```

Pretty-printed on separate line, with fixed line length

<Model data: par data: TBP>+≡

```
procedure :: show => par_show
```

<Model data: sub interfaces>+≡

```
module subroutine par_show (par, l, u)
  class(modelpar_data_t), intent(in) :: par
  integer, intent(in) :: l, u
end subroutine par_show
```

<Model data: procedures>+≡

```
module subroutine par_show (par, l, u)
  class(modelpar_data_t), intent(in) :: par
  integer, intent(in) :: l, u
  character(len=1) :: buffer
  buffer = par%name
  select type (par)
    type is (modelpar_real_t)
      write (u, "(4x,A,1x,'=',1x," // FMT_19 // ")") buffer, par%value
    type is (modelpar_complex_t)
      write (u, "(4x,A,1x,'=',1x," // FMT_19 // ",1x,'+',1x," &
        // FMT_19 // ",1x,'I')") buffer, par%value
  end select
end subroutine par_show
```

Initialize with name and value. The type depends on the argument type. If the type does not match, the value is converted following Fortran rules.

<Model data: par data: TBP>+≡

```
generic :: init => modelpar_data_init_real, modelpar_data_init_complex
procedure, private :: modelpar_data_init_real
procedure, private :: modelpar_data_init_complex
```

<Model data: sub interfaces>+≡

```
module subroutine modelpar_data_init_real (par, name, value)
  class(modelpar_data_t), intent(out) :: par
  type(string_t), intent(in) :: name
  real(default), intent(in) :: value
end subroutine modelpar_data_init_real
module subroutine modelpar_data_init_complex (par, name, value)
  class(modelpar_data_t), intent(out) :: par
  type(string_t), intent(in) :: name
  complex(default), intent(in) :: value
end subroutine modelpar_data_init_complex
```

<Model data: procedures>+≡

```
module subroutine modelpar_data_init_real (par, name, value)
  class(modelpar_data_t), intent(out) :: par
  type(string_t), intent(in) :: name
  real(default), intent(in) :: value
  par%name = name
  par = value
end subroutine modelpar_data_init_real
```

```

module subroutine modelpar_data_init_complex (par, name, value)
  class(modelpar_data_t), intent(out) :: par
  type(string_t), intent(in) :: name
  complex(default), intent(in) :: value
  par%name = name
  par = value
end subroutine modelpar_data_init_complex

```

Modify the value. We assume that the parameter has been initialized. The type (real or complex) must not be changed, and the name is also fixed.

```

<Model data: par data: TBP>+≡
  generic :: assignment(=) => modelpar_data_set_real, modelpar_data_set_complex
  procedure, private :: modelpar_data_set_real
  procedure, private :: modelpar_data_set_complex

```

```

<Model data: sub interfaces>+≡
  elemental module subroutine modelpar_data_set_real (par, value)
    class(modelpar_data_t), intent(inout) :: par
    real(default), intent(in) :: value
  end subroutine modelpar_data_set_real
  elemental module subroutine modelpar_data_set_complex (par, value)
    class(modelpar_data_t), intent(inout) :: par
    complex(default), intent(in) :: value
  end subroutine modelpar_data_set_complex

```

```

<Model data: procedures>+≡
  elemental module subroutine modelpar_data_set_real (par, value)
    class(modelpar_data_t), intent(inout) :: par
    real(default), intent(in) :: value
    select type (par)
      type is (modelpar_real_t)
        par%value = value
      type is (modelpar_complex_t)
        par%value = value
    end select
  end subroutine modelpar_data_set_real

  elemental module subroutine modelpar_data_set_complex (par, value)
    class(modelpar_data_t), intent(inout) :: par
    complex(default), intent(in) :: value
    select type (par)
      type is (modelpar_real_t)
        par%value = value
      type is (modelpar_complex_t)
        par%value = value
    end select
  end subroutine modelpar_data_set_complex

```

Return the parameter name.

```

<Model data: par data: TBP>+≡
  procedure :: get_name => modelpar_data_get_name

<Model data: sub interfaces>+≡
  module function modelpar_data_get_name (par) result (name)

```



```

        class(modelpar_data_t), intent(in) :: par
        type(string_t) :: name
    end function modelpar_data_get_name
<Model data: procedures>+≡
    module function modelpar_data_get_name (par) result (name)
        class(modelpar_data_t), intent(in) :: par
        type(string_t) :: name
        name = par%name
    end function modelpar_data_get_name

Return the value. In case of a type mismatch, follow Fortran conventions.
<Model data: par data: TBP>+≡
    procedure, pass :: get_real => modelpar_data_get_real
    procedure, pass :: get_complex => modelpar_data_get_complex
<Model data: sub interfaces>+≡
    elemental module function modelpar_data_get_real (par) result (value)
        class(modelpar_data_t), intent(in), target :: par
        real(default) :: value
    end function modelpar_data_get_real
    elemental module function modelpar_data_get_complex (par) result (value)
        class(modelpar_data_t), intent(in), target :: par
        complex(default) :: value
    end function modelpar_data_get_complex
<Model data: procedures>+≡
    elemental module function modelpar_data_get_real (par) result (value)
        class(modelpar_data_t), intent(in), target :: par
        real(default) :: value
        select type (par)
            type is (modelpar_real_t)
                value = par%value
            type is (modelpar_complex_t)
                value = par%value
        end select
    end function modelpar_data_get_real

    elemental module function modelpar_data_get_complex (par) result (value)
        class(modelpar_data_t), intent(in), target :: par
        complex(default) :: value
        select type (par)
            type is (modelpar_real_t)
                value = par%value
            type is (modelpar_complex_t)
                value = par%value
        end select
    end function modelpar_data_get_complex

```

Return a pointer to the value. This makes sense only for matching types.

```

<Model data: par data: TBP>+≡
    procedure :: get_real_ptr => modelpar_data_get_real_ptr
    procedure :: get_complex_ptr => modelpar_data_get_complex_ptr

```

```

<Model data: sub interfaces>+≡
    module function modelpar_data_get_real_ptr (par) result (ptr)
        class(modelpar_data_t), intent(in), target :: par
        real(default), pointer :: ptr
    end function modelpar_data_get_real_ptr
    module function modelpar_data_get_complex_ptr (par) result (ptr)
        class(modelpar_data_t), intent(in), target :: par
        complex(default), pointer :: ptr
    end function modelpar_data_get_complex_ptr

<Model data: procedures>+≡
    module function modelpar_data_get_real_ptr (par) result (ptr)
        class(modelpar_data_t), intent(in), target :: par
        real(default), pointer :: ptr
        select type (par)
        type is (modelpar_real_t)
            ptr => par%value
        class default
            ptr => null ()
        end select
    end function modelpar_data_get_real_ptr

    module function modelpar_data_get_complex_ptr (par) result (ptr)
        class(modelpar_data_t), intent(in), target :: par
        complex(default), pointer :: ptr
        select type (par)
        type is (modelpar_complex_t)
            ptr => par%value
        class default
            ptr => null ()
        end select
    end function modelpar_data_get_complex_ptr

```

11.1.2 Field Data

The field-data type holds all information that pertains to a particular field (or particle) within a particular model. Information such as spin type, particle code etc. is stored within the object itself, while mass and width are associated to parameters, otherwise assumed zero.

```

<Model data: public>+≡
    public :: field_data_t

<Model data: types>+≡
    type :: field_data_t
        private
        type(string_t) :: longname
        integer :: pdg = UNDEFINED
        logical :: visible = .true.
        logical :: parton = .false.
        logical :: gauge = .false.
        logical :: left_handed = .false.
        logical :: right_handed = .false.
        logical :: has_anti = .false.

```

```

logical :: p_is_stable = .true.
logical :: p_decays_isotropically = .false.
logical :: p_decays_diagonal = .false.
logical :: p_has_decay_helicity = .false.
integer :: p_decay_helicity = 0
logical :: a_is_stable = .true.
logical :: a_decays_isotropically = .false.
logical :: a_decays_diagonal = .false.
logical :: a_has_decay_helicity = .false.
integer :: a_decay_helicity = 0
logical :: p_polarized = .false.
logical :: a_polarized = .false.
type(string_t), dimension(:), allocatable :: name, anti
type(string_t) :: tex_name, tex_anti
integer :: spin_type = UNDEFINED
integer :: isospin_type = 1
integer :: charge_type = 1
integer :: color_type = 1
real(default), pointer :: mass_val => null ()
class(modelpar_data_t), pointer :: mass_data => null ()
real(default), pointer :: width_val => null ()
class(modelpar_data_t), pointer :: width_data => null ()
integer :: multiplicity = 1
type(string_t), dimension(:), allocatable :: p_decay
type(string_t), dimension(:), allocatable :: a_decay
contains
  <Model data: field data: TBP>
end type field_data_t

```

Initialize field data with PDG long name and PDG code. T_EX names should be initialized to avoid issues with accessing unallocated string contents.

```

<Model data: field data: TBP>≡
  procedure :: init => field_data_init

<Model data: sub interfaces>+≡
  module subroutine field_data_init (prt, longname, pdg)
    class(field_data_t), intent(out) :: prt
    type(string_t), intent(in) :: longname
    integer, intent(in) :: pdg
  end subroutine field_data_init

<Model data: procedures>+≡
  module subroutine field_data_init (prt, longname, pdg)
    class(field_data_t), intent(out) :: prt
    type(string_t), intent(in) :: longname
    integer, intent(in) :: pdg
    prt%longname = longname
    prt%pdg = pdg
    prt%tex_name = ""
    prt%tex_anti = ""
  end subroutine field_data_init

```

Copy quantum numbers from another particle. Do not compute the multiplicity yet, because this depends on the association of the `mass_data` pointer.

```

<Model data: field data: TBP>+≡
  procedure :: copy_from => field_data_copy_from

<Model data: sub interfaces>+≡
  module subroutine field_data_copy_from (prt, prt_src)
    class(field_data_t), intent(inout) :: prt
    class(field_data_t), intent(in) :: prt_src
  end subroutine field_data_copy_from

<Model data: procedures>+≡
  module subroutine field_data_copy_from (prt, prt_src)
    class(field_data_t), intent(inout) :: prt
    class(field_data_t), intent(in) :: prt_src
    prt%visible = prt_src%visible
    prt%parton = prt_src%parton
    prt%gauge = prt_src%gauge
    prt%left_handed = prt_src%left_handed
    prt%right_handed = prt_src%right_handed
    prt%p_is_stable = prt_src%p_is_stable
    prt%p_decays_isotropically = prt_src%p_decays_isotropically
    prt%p_decays_diagonal = prt_src%p_decays_diagonal
    prt%p_has_decay_helicity = prt_src%p_has_decay_helicity
    prt%p_decay_helicity = prt_src%p_decay_helicity
    prt%p_decays_diagonal = prt_src%p_decays_diagonal
    prt%a_is_stable = prt_src%a_is_stable
    prt%a_decays_isotropically = prt_src%a_decays_isotropically
    prt%a_decays_diagonal = prt_src%a_decays_diagonal
    prt%a_has_decay_helicity = prt_src%a_has_decay_helicity
    prt%a_decay_helicity = prt_src%a_decay_helicity
    prt%p_polarized = prt_src%p_polarized
    prt%a_polarized = prt_src%a_polarized
    prt%spin_type = prt_src%spin_type
    prt%isospin_type = prt_src%isospin_type
    prt%charge_type = prt_src%charge_type
    prt%color_type = prt_src%color_type
    prt%has_anti = prt_src%has_anti
    if (allocated (prt_src%name)) then
      if (allocated (prt%name)) deallocate (prt%name)
      allocate (prt%name (size (prt_src%name)), source = prt_src%name)
    end if
    if (allocated (prt_src%anti)) then
      if (allocated (prt%anti)) deallocate (prt%anti)
      allocate (prt%anti (size (prt_src%anti)), source = prt_src%anti)
    end if
    prt%tex_name = prt_src%tex_name
    prt%tex_anti = prt_src%tex_anti
    if (allocated (prt_src%p_decay)) then
      if (allocated (prt%p_decay)) deallocate (prt%p_decay)
      allocate (prt%p_decay (size (prt_src%p_decay)), source = prt_src%p_decay)
    end if
    if (allocated (prt_src%a_decay)) then
      if (allocated (prt%a_decay)) deallocate (prt%a_decay)
      allocate (prt%a_decay (size (prt_src%a_decay)), source = prt_src%a_decay)
    end if
  end subroutine field_data_copy_from

```

Set particle quantum numbers.

(Model data: field data: TBP)+≡

```
procedure :: set => field_data_set
```

(Model data: sub interfaces)+≡

```
module subroutine field_data_set (prt, &
    is_visible, is_parton, is_gauge, is_left_handed, is_right_handed, &
    p_is_stable, p_decays_isotropically, p_decays_diagonal, &
    p_decay_helicity, &
    a_is_stable, a_decays_isotropically, a_decays_diagonal, &
    a_decay_helicity, &
    p_polarized, a_polarized, &
    name, anti, tex_name, tex_anti, &
    spin_type, isospin_type, charge_type, color_type, &
    mass_data, width_data, &
    p_decay, a_decay)
class(field_data_t), intent(inout) :: prt
logical, intent(in), optional :: is_visible, is_parton, is_gauge
logical, intent(in), optional :: is_left_handed, is_right_handed
logical, intent(in), optional :: p_is_stable
logical, intent(in), optional :: p_decays_isotropically, p_decays_diagonal
integer, intent(in), optional :: p_decay_helicity
logical, intent(in), optional :: a_is_stable
logical, intent(in), optional :: a_decays_isotropically, a_decays_diagonal
integer, intent(in), optional :: a_decay_helicity
logical, intent(in), optional :: p_polarized, a_polarized
type(string_t), dimension(:), intent(in), optional :: name, anti
type(string_t), intent(in), optional :: tex_name, tex_anti
integer, intent(in), optional :: spin_type, isospin_type
integer, intent(in), optional :: charge_type, color_type
class(modelpar_data_t), intent(in), pointer, optional :: mass_data, width_data
type(string_t), dimension(:), intent(in), optional :: p_decay, a_decay
end subroutine field_data_set
```

(Model data: procedures)+≡

```
module subroutine field_data_set (prt, &
    is_visible, is_parton, is_gauge, is_left_handed, is_right_handed, &
    p_is_stable, p_decays_isotropically, p_decays_diagonal, &
    p_decay_helicity, &
    a_is_stable, a_decays_isotropically, a_decays_diagonal, &
    a_decay_helicity, &
    p_polarized, a_polarized, &
    name, anti, tex_name, tex_anti, &
    spin_type, isospin_type, charge_type, color_type, &
    mass_data, width_data, &
    p_decay, a_decay)
class(field_data_t), intent(inout) :: prt
logical, intent(in), optional :: is_visible, is_parton, is_gauge
logical, intent(in), optional :: is_left_handed, is_right_handed
logical, intent(in), optional :: p_is_stable
logical, intent(in), optional :: p_decays_isotropically, p_decays_diagonal
integer, intent(in), optional :: p_decay_helicity
logical, intent(in), optional :: a_is_stable
logical, intent(in), optional :: a_decays_isotropically, a_decays_diagonal
```

```

integer, intent(in), optional :: a_decay_helicity
logical, intent(in), optional :: p_polarized, a_polarized
type(string_t), dimension(:), intent(in), optional :: name, anti
type(string_t), intent(in), optional :: tex_name, tex_anti
integer, intent(in), optional :: spin_type, isospin_type
integer, intent(in), optional :: charge_type, color_type
class(modelpar_data_t), intent(in), pointer, optional :: mass_data, width_data
type(string_t), dimension(:), intent(in), optional :: p_decay, a_decay
if (present (is_visible)) prt%visible = is_visible
if (present (is_parton)) prt%parton = is_parton
if (present (is_gauge)) prt%gauge = is_gauge
if (present (is_left_handed)) prt%left_handed = is_left_handed
if (present (is_right_handed)) prt%right_handed = is_right_handed
if (present (p_is_stable)) prt%p_is_stable = p_is_stable
if (present (p_decays_isotropically)) &
    prt%p_decays_isotropically = p_decays_isotropically
if (present (p_decays_diagonal)) &
    prt%p_decays_diagonal = p_decays_diagonal
if (present (p_decay_helicity)) then
    prt%p_has_decay_helicity = .true.
    prt%p_decay_helicity = p_decay_helicity
end if
if (present (a_is_stable)) prt%a_is_stable = a_is_stable
if (present (a_decays_isotropically)) &
    prt%a_decays_isotropically = a_decays_isotropically
if (present (a_decays_diagonal)) &
    prt%a_decays_diagonal = a_decays_diagonal
if (present (a_decay_helicity)) then
    prt%a_has_decay_helicity = .true.
    prt%a_decay_helicity = a_decay_helicity
end if
if (present (p_polarized)) prt%p_polarized = p_polarized
if (present (a_polarized)) prt%a_polarized = a_polarized
if (present (name)) then
    if (allocated (prt%name)) deallocate (prt%name)
    allocate (prt%name (size (name)), source = name)
end if
if (present (anti)) then
    if (allocated (prt%anti)) deallocate (prt%anti)
    allocate (prt%anti (size (anti)), source = anti)
    prt%has_anti = .true.
end if
if (present (tex_name)) prt%tex_name = tex_name
if (present (tex_anti)) prt%tex_anti = tex_anti
if (present (spin_type)) prt%spin_type = spin_type
if (present (isospin_type)) prt%isospin_type = isospin_type
if (present (charge_type)) prt%charge_type = charge_type
if (present (color_type)) prt%color_type = color_type
if (present (mass_data)) then
    prt%mass_data => mass_data
    if (associated (mass_data)) then
        prt%mass_val => mass_data%get_real_ptr ()
    else
        prt%mass_val => null ()
    end if
end if

```

```

        end if
    end if
    if (present (width_data)) then
        prt%width_data => width_data
        if (associated (width_data)) then
            prt%width_val => width_data%get_real_ptr ()
        else
            prt%width_val => null ()
        end if
    end if
    if (present (spin_type) .or. present (mass_data)) then
        call prt%set_multiplicity ()
    end if
    if (present (p_decay)) then
        if (allocated (prt%p_decay)) deallocate (prt%p_decay)
        if (size (p_decay) > 0) &
            allocate (prt%p_decay (size (p_decay)), source = p_decay)
    end if
    if (present (a_decay)) then
        if (allocated (prt%a_decay)) deallocate (prt%a_decay)
        if (size (a_decay) > 0) &
            allocate (prt%a_decay (size (a_decay)), source = a_decay)
    end if
end subroutine field_data_set

```

Calculate the multiplicity given spin type and mass.

```

<Model data: field data: TBP>+≡
    procedure, private :: &
        set_multiplicity => field_data_set_multiplicity

<Model data: sub interfaces>+≡
    module subroutine field_data_set_multiplicity (prt)
        class(field_data_t), intent(inout) :: prt
    end subroutine field_data_set_multiplicity

<Model data: procedures>+≡
    module subroutine field_data_set_multiplicity (prt)
        class(field_data_t), intent(inout) :: prt
        if (prt%spin_type /= SCALAR) then
            if (associated (prt%mass_data)) then
                prt%multiplicity = prt%spin_type
            else if (prt%left_handed .or. prt%right_handed) then
                prt%multiplicity = 1
            else
                prt%multiplicity = 2
            end if
        end if
    end subroutine field_data_set_multiplicity

```

Set the mass/width value (not the pointer). The mass/width pointer must be allocated.

```

<Model data: field data: TBP>+≡
    procedure, private :: set_mass => field_data_set_mass
    procedure, private :: set_width => field_data_set_width

```

```

<Model data: sub interfaces>+≡
    module subroutine field_data_set_mass (prt, mass)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: mass
    end subroutine field_data_set_mass
    module subroutine field_data_set_width (prt, width)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: width
    end subroutine field_data_set_width

<Model data: procedures>+≡
    module subroutine field_data_set_mass (prt, mass)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: mass
        if (associated (prt%mass_val)) prt%mass_val = mass
    end subroutine field_data_set_mass

    module subroutine field_data_set_width (prt, width)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: width
        if (associated (prt%width_val)) prt%width_val = width
    end subroutine field_data_set_width

```

Loose ends: name arrays should be allocated.

```

<Model data: field data: TBP>+≡
    procedure :: freeze => field_data_freeze

<Model data: sub interfaces>+≡
    elemental module subroutine field_data_freeze (prt)
        class(field_data_t), intent(inout) :: prt
    end subroutine field_data_freeze

<Model data: procedures>+≡
    elemental module subroutine field_data_freeze (prt)
        class(field_data_t), intent(inout) :: prt
        if (.not. allocated (prt%name)) allocate (prt%name (0))
        if (.not. allocated (prt%anti)) allocate (prt%anti (0))
    end subroutine field_data_freeze

```

Output

```

<Model data: field data: TBP>+≡
    procedure :: write => field_data_write

<Model data: sub interfaces>+≡
    module subroutine field_data_write (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
    end subroutine field_data_write

<Model data: procedures>+≡
    module subroutine field_data_write (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return

```



```

write (u, "(3x,A,1x,A)", advance="no") "particle", char (prt%longname)
write (u, "(1x,I0)", advance="no") prt%pdg
if (.not. prt%visible) write (u, "(2x,A)", advance="no") "invisible"
if (prt%parton) write (u, "(2x,A)", advance="no") "parton"
if (prt%gauge) write (u, "(2x,A)", advance="no") "gauge"
if (prt%left_handed) write (u, "(2x,A)", advance="no") "left"
if (prt%right_handed) write (u, "(2x,A)", advance="no") "right"
write (u, *)
write (u, "(5x,A)", advance="no") "name"
if (allocated (prt%name)) then
  do i = 1, size (prt%name)
    write (u, "(1x,A)", advance="no") ' ' // char (prt%name(i)) // ' '
  end do
  write (u, *)
  if (prt%has_anti) then
    write (u, "(5x,A)", advance="no") "anti"
    do i = 1, size (prt%anti)
      write (u, "(1x,A)", advance="no") ' ' // char (prt%anti(i)) // ' '
    end do
    write (u, *)
  end if
  if (prt%tex_name /= "") then
    write (u, "(5x,A)") &
      "tex_name " // ' ' // char (prt%tex_name) // ' '
  end if
  if (prt%has_anti .and. prt%tex_anti /= "") then
    write (u, "(5x,A)") &
      "tex_anti " // ' ' // char (prt%tex_anti) // ' '
  end if
else
  write (u, "(A)") "???"
end if
write (u, "(5x,A)", advance="no") "spin "
select case (mod (prt%spin_type - 1, 2))
case (0); write (u, "(I0)", advance="no") (prt%spin_type-1) / 2
case default; write (u, "(I0,A)", advance="no") prt%spin_type-1, "/2"
end select
! write (u, "(2x,A,I1,A)") "! [multiplicity = ", prt%multiplicity, "]"
if (abs (prt%isospin_type) /= 1) then
  write (u, "(2x,A)", advance="no") "isospin "
  select case (mod (abs (prt%isospin_type) - 1, 2))
  case (0); write (u, "(I0)", advance="no") &
    sign (abs (prt%isospin_type) - 1, prt%isospin_type) / 2
  case default; write (u, "(I0,A)", advance="no") &
    sign (abs (prt%isospin_type) - 1, prt%isospin_type), "/2"
  end select
end if
if (abs (prt%charge_type) /= 1) then
  write (u, "(2x,A)", advance="no") "charge "
  select case (mod (abs (prt%charge_type) - 1, 3))
  case (0); write (u, "(I0)", advance="no") &
    sign (abs (prt%charge_type) - 1, prt%charge_type) / 3
  case default; write (u, "(I0,A)", advance="no") &
    sign (abs (prt%charge_type) - 1, prt%charge_type), "/3"

```

```

        end select
    end if
    if (prt%color_type /= 1) then
        write (u, "(2x,A,I0)", advance="no") "color ", prt%color_type
    end if
    write (u, *)
    if (associated (prt%mass_data)) then
        write (u, "(5x,A)", advance="no") &
            "mass " // char (prt%mass_data%get_name ())
        if (associated (prt%width_data)) then
            write (u, "(2x,A)") &
                "width " // char (prt%width_data%get_name ())
        else
            write (u, *)
        end if
    end if
    call prt%write_decays (u)
end subroutine field_data_write

```

Write decay and polarization data.

```

<Model data: field data: TBP>+≡
    procedure :: write_decays => field_data_write_decays

<Model data: sub interfaces>+≡
    module subroutine field_data_write_decays (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
    end subroutine field_data_write_decays

<Model data: procedures>+≡
    module subroutine field_data_write_decays (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        if (.not. prt%p_is_stable) then
            if (allocated (prt%p_decay)) then
                write (u, "(5x,A)", advance="no") "p_decay"
                do i = 1, size (prt%p_decay)
                    write (u, "(1x,A)", advance="no") char (prt%p_decay(i))
                end do
                if (prt%p_decays_isotropically) then
                    write (u, "(1x,A)", advance="no") "isotropic"
                else if (prt%p_decays_diagonal) then
                    write (u, "(1x,A)", advance="no") "diagonal"
                else if (prt%p_has_decay_helicity) then
                    write (u, "(1x,A,I0)", advance="no") "helicity = ", &
                        prt%p_decay_helicity
                end if
                write (u, *)
            end if
        else if (prt%p_polarized) then
            write (u, "(5x,A)") "p_polarized"
        end if
        if (.not. prt%a_is_stable) then

```

```

    if (allocated (prt%a_decay)) then
      write (u, "(5x,A)", advance="no") "a_decay"
      do i = 1, size (prt%a_decay)
        write (u, "(1x,A)", advance="no") char (prt%a_decay(i))
      end do
      if (prt%a_decays_isotropically) then
        write (u, "(1x,A)", advance="no") "isotropic"
      else if (prt%a_decays_diagonal) then
        write (u, "(1x,A)", advance="no") "diagonal"
      else if (prt%a_has_decay_helicity) then
        write (u, "(1x,A,I0)", advance="no") "helicity = ", &
          prt%a_decay_helicity
      end if
      write (u, *)
    end if
  else if (prt%a_polarized) then
    write (u, "(5x,A)") "a_polarized"
  end if
end subroutine field_data_write_decays

```

Screen version of output.

<Model data: field data: TBP>+≡

```

  procedure :: show => field_data_show

```

<Model data: sub interfaces>+≡

```

  module subroutine field_data_show (prt, l, u)
    class(field_data_t), intent(in) :: prt
    integer, intent(in) :: l, u
  end subroutine field_data_show

```

<Model data: procedures>+≡

```

  module subroutine field_data_show (prt, l, u)
    class(field_data_t), intent(in) :: prt
    integer, intent(in) :: l, u
    character(len=1) :: buffer
    integer :: i
    type(string_t), dimension(:), allocatable :: decay
    buffer = prt%get_name (.false.)
    write (u, "(4x,A,1x,I8)", advance="no") buffer, &
      prt%get_pdg ()
    if (prt%is_polarized ()) then
      write (u, "(3x,A)") "polarized"
    else if (.not. prt%is_stable ()) then
      write (u, "(3x,A)", advance="no") "decays:"
      call prt%get_decays (decay)
      do i = 1, size (decay)
        write (u, "(1x,A)", advance="no") char (decay(i))
      end do
      write (u, *)
    else
      write (u, *)
    end if
    if (prt%has_antiparticle ()) then
      buffer = prt%get_name (.true.)
      write (u, "(4x,A,1x,I8)", advance="no") buffer, &

```

```

        prt%get_pdg_anti ()
    if (prt%is_polarized (.true.)) then
        write (u, "(3x,A)") "polarized"
    else if (.not. prt%is_stable (.true.)) then
        write (u, "(3x,A)", advance="no") "decays:"
        call prt%get_decays (decay, .true.)
        do i = 1, size (decay)
            write (u, "(1x,A)", advance="no") char (decay(i))
        end do
        write (u, *)
    else
        write (u, *)
    end if
end if
end subroutine field_data_show

```

Retrieve data:

```

<Model data: field data: TBP>+=
    procedure :: get_pdg => field_data_get_pdg
    procedure :: get_pdg_anti => field_data_get_pdg_anti

<Model data: sub interfaces>+=
    elemental module function field_data_get_pdg (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
    end function field_data_get_pdg
    elemental module function field_data_get_pdg_anti (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
    end function field_data_get_pdg_anti

<Model data: procedures>+=
    elemental module function field_data_get_pdg (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
        pdg = prt%pdg
    end function field_data_get_pdg

    elemental module function field_data_get_pdg_anti (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
        if (prt%has_anti) then
            pdg = - prt%pdg
        else
            pdg = prt%pdg
        end if
    end function field_data_get_pdg_anti

```

Predicates:

```

<Model data: field data: TBP>+=
    procedure :: is_visible => field_data_is_visible
    procedure :: is_parton => field_data_is_parton
    procedure :: is_gauge => field_data_is_gauge
    procedure :: is_left_handed => field_data_is_left_handed

```

```

procedure :: is_right_handed => field_data_is_right_handed
procedure :: has_antiparticle => field_data_has_antiparticle
procedure :: is_stable => field_data_is_stable
procedure :: get_decays => field_data_get_decays
procedure :: decays_isotropically => field_data_decays_isotropically
procedure :: decays_diagonal => field_data_decays_diagonal
procedure :: has_decay_helicity => field_data_has_decay_helicity
procedure :: decay_helicity => field_data_decay_helicity
procedure :: is_polarized => field_data_is_polarized

```

(Model data: sub interfaces)+≡

```

elemental module function field_data_is_visible (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_is_visible
elemental module function field_data_is_parton (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_is_parton
elemental module function field_data_is_gauge (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_is_gauge
elemental module function field_data_is_left_handed (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_is_left_handed
elemental module function field_data_is_right_handed (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_is_right_handed
elemental module function field_data_has_antiparticle (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
end function field_data_has_antiparticle
elemental module function field_data_is_stable (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
end function field_data_is_stable
module subroutine field_data_get_decays (prt, decay, anti)
    class(field_data_t), intent(in) :: prt
    type(string_t), dimension(:), intent(out), allocatable :: decay
    logical, intent(in), optional :: anti
end subroutine field_data_get_decays
elemental module function field_data_decays_isotropically &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
end function field_data_decays_isotropically
elemental module function field_data_decays_diagonal &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt

```

```

        logical, intent(in), optional :: anti
    end function field_data_decays_diagonal
    elemental module function field_data_has_decay_helicity &
        (prt, anti) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        logical, intent(in), optional :: anti
    end function field_data_has_decay_helicity
    elemental module function field_data_decay_helicity &
        (prt, anti) result (hel)
        integer :: hel
        class(field_data_t), intent(in) :: prt
        logical, intent(in), optional :: anti
    end function field_data_decay_helicity
    elemental module function field_data_is_polarized (prt, anti) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        logical, intent(in), optional :: anti
    end function field_data_is_polarized
<Model data: procedures>+≡
    elemental module function field_data_is_visible (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%visible
    end function field_data_is_visible

    elemental module function field_data_is_parton (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%parton
    end function field_data_is_parton

    elemental module function field_data_is_gauge (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%gauge
    end function field_data_is_gauge

    elemental module function field_data_is_left_handed (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%left_handed
    end function field_data_is_left_handed

    elemental module function field_data_is_right_handed (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%right_handed
    end function field_data_is_right_handed

    elemental module function field_data_has_antiparticle (prt) result (flag)
        logical :: flag
        class(field_data_t), intent(in) :: prt
        flag = prt%has_anti

```

```

end function field_data_has_antiparticle

elemental module function field_data_is_stable (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            flag = prt%a_is_stable
        else
            flag = prt%p_is_stable
        end if
    else
        flag = prt%p_is_stable
    end if
end function field_data_is_stable

module subroutine field_data_get_decays (prt, decay, anti)
    class(field_data_t), intent(in) :: prt
    type(string_t), dimension(:), intent(out), allocatable :: decay
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            allocate (decay (size (prt%a_decay)), source = prt%a_decay)
        else
            allocate (decay (size (prt%p_decay)), source = prt%p_decay)
        end if
    else
        allocate (decay (size (prt%p_decay)), source = prt%p_decay)
    end if
end subroutine field_data_get_decays

elemental module function field_data_decays_isotropically &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            flag = prt%a_decays_isotropically
        else
            flag = prt%p_decays_isotropically
        end if
    else
        flag = prt%p_decays_isotropically
    end if
end function field_data_decays_isotropically

elemental module function field_data_decays_diagonal &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then

```

```

        if (anti) then
            flag = prt%a_decays_diagonal
        else
            flag = prt%p_decays_diagonal
        end if
    else
        flag = prt%p_decays_diagonal
    end if
end function field_data_decays_diagonal

elemental module function field_data_has_decay_helicity &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            flag = prt%a_has_decay_helicity
        else
            flag = prt%p_has_decay_helicity
        end if
    else
        flag = prt%p_has_decay_helicity
    end if
end function field_data_has_decay_helicity

elemental module function field_data_decay_helicity &
    (prt, anti) result (hel)
    integer :: hel
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            hel = prt%a_decay_helicity
        else
            hel = prt%p_decay_helicity
        end if
    else
        hel = prt%p_decay_helicity
    end if
end function field_data_decay_helicity

elemental module function field_data_is_polarized (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    logical :: a
    if (present (anti)) then
        a = anti
    else
        a = .false.
    end if
    if (a) then
        flag = prt%a_polarized
    end if
end function field_data_is_polarized

```



```

    else
        flag = prt%p_polarized
    end if
end function field_data_is_polarized

```

Names. Return the first name in the list (or the first antiparticle name)

```

<Model data: field data: TBP>+≡
    procedure :: get_longname => field_data_get_longname
    procedure :: get_name => field_data_get_name
    procedure :: get_name_array => field_data_get_name_array

<Model data: sub interfaces>+≡
    pure module function field_data_get_longname (prt) result (name)
        type(string_t) :: name
        class(field_data_t), intent(in) :: prt
    end function field_data_get_longname
    pure module function field_data_get_name &
        (prt, is_antiparticle) result (name)
        type(string_t) :: name
        class(field_data_t), intent(in) :: prt
        logical, intent(in) :: is_antiparticle
    end function field_data_get_name
    module subroutine field_data_get_name_array (prt, is_antiparticle, name)
        class(field_data_t), intent(in) :: prt
        logical, intent(in) :: is_antiparticle
        type(string_t), dimension(:), allocatable, intent(inout) :: name
    end subroutine field_data_get_name_array

<Model data: procedures>+≡
    pure module function field_data_get_longname (prt) result (name)
        type(string_t) :: name
        class(field_data_t), intent(in) :: prt
        name = prt%longname
    end function field_data_get_longname

    pure module function field_data_get_name (prt, is_antiparticle) result (name)
        type(string_t) :: name
        class(field_data_t), intent(in) :: prt
        logical, intent(in) :: is_antiparticle
        name = prt%longname
        if (is_antiparticle) then
            if (prt%has_anti) then
                if (allocated (prt%anti)) then
                    if (size(prt%anti) > 0) name = prt%anti(1)
                end if
            else
                if (allocated (prt%name)) then
                    if (size (prt%name) > 0) name = prt%name(1)
                end if
            end if
        else
            if (allocated (prt%name)) then
                if (size (prt%name) > 0) name = prt%name(1)
            end if
        end if
    end function field_data_get_name

```

```

end function field_data_get_name

module subroutine field_data_get_name_array (prt, is_antiparticle, name)
  class(field_data_t), intent(in) :: prt
  logical, intent(in) :: is_antiparticle
  type(string_t), dimension(:), allocatable, intent(inout) :: name
  if (allocated (name)) deallocate (name)
  if (is_antiparticle) then
    if (prt%has_anti) then
      allocate (name (size (prt%anti)))
      name = prt%anti
    else
      allocate (name (0))
    end if
  else
    allocate (name (size (prt%name)))
    name = prt%name
  end if
end subroutine field_data_get_name_array

```

Same for the T_EX name.

```

<Model data: field data: TBP>+≡
  procedure :: get_tex_name => field_data_get_tex_name

<Model data: sub interfaces>+≡
  elemental module function field_data_get_tex_name &
    (prt, is_antiparticle) result (name)
    type(string_t) :: name
    class(field_data_t), intent(in) :: prt
    logical, intent(in) :: is_antiparticle
  end function field_data_get_tex_name

<Model data: procedures>+≡
  elemental module function field_data_get_tex_name &
    (prt, is_antiparticle) result (name)
    type(string_t) :: name
    class(field_data_t), intent(in) :: prt
    logical, intent(in) :: is_antiparticle
    if (is_antiparticle) then
      if (prt%has_anti) then
        name = prt%tex_anti
      else
        name = prt%tex_name
      end if
    else
      name = prt%tex_name
    end if
    if (name == "") name = prt%get_name (is_antiparticle)
  end function field_data_get_tex_name

```

Check if any of the field names matches the given string.

```

<Model data: field data: TBP>+≡
  procedure, private :: matches_name => field_data_matches_name

```

<Model data: sub interfaces>+≡

```

module function field_data_matches_name &
    (field, name, is_antiparticle) result (flag)
    class(field_data_t), intent(in) :: field
    type(string_t), intent(in) :: name
    logical, intent(in) :: is_antiparticle
    logical :: flag
end function field_data_matches_name

```

<Model data: procedures>+≡

```

module function field_data_matches_name &
    (field, name, is_antiparticle) result (flag)
    class(field_data_t), intent(in) :: field
    type(string_t), intent(in) :: name
    logical, intent(in) :: is_antiparticle
    logical :: flag
    if (is_antiparticle) then
        if (field%has_anti) then
            flag = any (name == field%anti)
        else
            flag = .false.
        end if
    else
        flag = name == field%longname .or. any (name == field%name)
    end if
end function field_data_matches_name

```

Quantum numbers

<Model data: field data: TBP>+≡

```

procedure :: get_spin_type => field_data_get_spin_type
procedure :: get_multiplicity => field_data_get_multiplicity
procedure :: get_isospin_type => field_data_get_isospin_type
procedure :: get_charge_type => field_data_get_charge_type
procedure :: get_color_type => field_data_get_color_type

```

<Model data: sub interfaces>+≡

```

elemental module function field_data_get_spin_type (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt
end function field_data_get_spin_type
elemental module function field_data_get_multiplicity (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt
end function field_data_get_multiplicity
elemental module function field_data_get_isospin_type (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt
end function field_data_get_isospin_type
elemental module function field_data_get_charge_type (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt
end function field_data_get_charge_type
elemental module function field_data_get_color_type (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt

```

```

        end function field_data_get_color_type

<Model data: procedures>+≡
    elemental module function field_data_get_spin_type (prt) result (type)
        integer :: type
        class(field_data_t), intent(in) :: prt
        type = prt%spin_type
    end function field_data_get_spin_type

    elemental module function field_data_get_multiplicity (prt) result (type)
        integer :: type
        class(field_data_t), intent(in) :: prt
        type = prt%multiplicity
    end function field_data_get_multiplicity

    elemental module function field_data_get_isospin_type (prt) result (type)
        integer :: type
        class(field_data_t), intent(in) :: prt
        type = prt%isospin_type
    end function field_data_get_isospin_type

    elemental module function field_data_get_charge_type (prt) result (type)
        integer :: type
        class(field_data_t), intent(in) :: prt
        type = prt%charge_type
    end function field_data_get_charge_type

    elemental module function field_data_get_color_type (prt) result (type)
        integer :: type
        class(field_data_t), intent(in) :: prt
        type = prt%color_type
    end function field_data_get_color_type

```

In the MSSM, neutralinos can have a negative mass. This is relevant for computing matrix elements. However, within the `WHIZARD` main program we are interested only in kinematics, therefore we return the absolute value of the particle mass. If desired, we can extract the sign separately.

```

<Model data: field data: TBP>+≡
    procedure :: get_charge => field_data_get_charge
    procedure :: get_isospin => field_data_get_isospin
    procedure :: get_mass => field_data_get_mass
    procedure :: get_mass_sign => field_data_get_mass_sign
    procedure :: get_width => field_data_get_width

<Model data: sub interfaces>+≡
    elemental module function field_data_get_charge (prt) result (charge)
        real(default) :: charge
        class(field_data_t), intent(in) :: prt
    end function field_data_get_charge
    elemental module function field_data_get_isospin (prt) result (isospin)
        real(default) :: isospin
        class(field_data_t), intent(in) :: prt
    end function field_data_get_isospin
    elemental module function field_data_get_mass (prt) result (mass)

```

```

        real(default) :: mass
        class(field_data_t), intent(in) :: prt
    end function field_data_get_mass
    elemental module function field_data_get_mass_sign (prt) result (sgn)
        integer :: sgn
        class(field_data_t), intent(in) :: prt
    end function field_data_get_mass_sign
    elemental module function field_data_get_width (prt) result (width)
        real(default) :: width
        class(field_data_t), intent(in) :: prt
    end function field_data_get_width

<Model data: procedures>+≡
    elemental module function field_data_get_charge (prt) result (charge)
        real(default) :: charge
        class(field_data_t), intent(in) :: prt
        if (prt%charge_type /= 0) then
            charge = real (sign ((abs(prt%charge_type) - 1), &
                prt%charge_type), default) / 3
        else
            charge = 0
        end if
    end function field_data_get_charge

    elemental module function field_data_get_isospin (prt) result (isospin)
        real(default) :: isospin
        class(field_data_t), intent(in) :: prt
        if (prt%isospin_type /= 0) then
            isospin = real (sign (abs(prt%isospin_type) - 1, &
                prt%isospin_type), default) / 2
        else
            isospin = 0
        end if
    end function field_data_get_isospin

    elemental module function field_data_get_mass (prt) result (mass)
        real(default) :: mass
        class(field_data_t), intent(in) :: prt
        if (associated (prt%mass_val)) then
            mass = abs (prt%mass_val)
        else
            mass = 0
        end if
    end function field_data_get_mass

    elemental module function field_data_get_mass_sign (prt) result (sgn)
        integer :: sgn
        class(field_data_t), intent(in) :: prt
        if (associated (prt%mass_val)) then
            sgn = sign (1._default, prt%mass_val)
        else
            sgn = 0
        end if
    end function field_data_get_mass_sign

```

```

elemental module function field_data_get_width (prt) result (width)
  real(default) :: width
  class(field_data_t), intent(in) :: prt
  if (associated (prt%width_val)) then
    width = prt%width_val
  else
    width = 0
  end if
end function field_data_get_width

```

Find the model containing the PDG given two model files.

<Model data: public>+≡

```
public :: find_model
```

<Model data: sub interfaces>+≡

```

module subroutine find_model (model, PDG, model_A, model_B)
  class(model_data_t), pointer, intent(out) :: model
  integer, intent(in) :: PDG
  class(model_data_t), intent(in), target :: model_A, model_B
end subroutine find_model

```

<Model data: procedures>+≡

```

module subroutine find_model (model, PDG, model_A, model_B)
  class(model_data_t), pointer, intent(out) :: model
  integer, intent(in) :: PDG
  class(model_data_t), intent(in), target :: model_A, model_B
  character(len=10) :: buffer
  if (model_A%test_field (PDG)) then
    model => model_A
  else if (model_B%test_field (PDG)) then
    model => model_B
  else
    call model_A%write ()
    call model_B%write ()
    write (buffer, "(I10)") PDG
    call msg_fatal ("Parton " // buffer // &
      " not found in the given model files")
  end if
end subroutine find_model

```

11.1.3 Vertex data

The vertex object contains an array of particle-data pointers, for which we need a separate type. (We could use the flavor type defined in another module.)

The program does not (yet?) make use of vertex definitions, so they are not stored here.

<Model data: types>+≡

```

type :: field_data_p
  type(field_data_t), pointer :: p => null ()
end type field_data_p

```

```

<Model data: types>+≡
  type :: vertex_t
    private
    logical :: trilinear
    integer, dimension(:), allocatable :: pdg
    type(field_data_p), dimension(:), allocatable :: prt
    contains
    <Model data: vertex: TBP>
  end type vertex_t

<Model data: vertex: TBP>≡
  procedure :: write => vertex_write

<Model data: sub interfaces>+≡
  module subroutine vertex_write (vtx, unit)
    class(vertex_t), intent(in) :: vtx
    integer, intent(in), optional :: unit
  end subroutine vertex_write

<Model data: procedures>+≡
  module subroutine vertex_write (vtx, unit)
    class(vertex_t), intent(in) :: vtx
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(3x,A)", advance="no") "vertex"
    do i = 1, size (vtx%prt)
      if (associated (vtx%prt(i)%p)) then
        write (u, "(1x,A)", advance="no") &
          '"" // char (vtx%prt(i)%p%get_name (vtx%pdg(i) < 0)) &
          // '""
      else
        write (u, "(1x,I7)", advance="no") vtx%pdg(i)
      end if
    end do
    write (u, *)
  end subroutine vertex_write

```

Initialize using PDG codes. The model is used for finding particle data pointers associated with the pdg codes.

```

<Model data: vertex: TBP>+≡
  procedure :: init => vertex_init

<Model data: sub interfaces>+≡
  module subroutine vertex_init (vtx, pdg, model)
    class(vertex_t), intent(out) :: vtx
    integer, dimension(:), intent(in) :: pdg
    type(model_data_t), intent(in), target, optional :: model
  end subroutine vertex_init

<Model data: procedures>+≡
  module subroutine vertex_init (vtx, pdg, model)
    class(vertex_t), intent(out) :: vtx
    integer, dimension(:), intent(in) :: pdg
    type(model_data_t), intent(in), target, optional :: model

```

```

integer :: i
allocate (vtx%pdg (size (pdg)))
allocate (vtx%prt (size (pdg)))
vtx%trilinear = size (pdg) == 3
vtx%pdg = pdg
if (present (model)) then
  do i = 1, size (pdg)
    vtx%prt(i)%p => model%get_field_ptr (pdg(i))
  end do
end if
end subroutine vertex_init

```

Copy vertex: we must reassign the field-data pointer to a new model.

<Model data: vertex: TBP>+≡

```

procedure :: copy_from => vertex_copy_from

```

<Model data: sub interfaces>+≡

```

module subroutine vertex_copy_from (vtx, old_vtx, new_model)
  class(vertex_t), intent(out) :: vtx
  class(vertex_t), intent(in) :: old_vtx
  type(model_data_t), intent(in), target, optional :: new_model
end subroutine vertex_copy_from

```

<Model data: procedures>+≡

```

module subroutine vertex_copy_from (vtx, old_vtx, new_model)
  class(vertex_t), intent(out) :: vtx
  class(vertex_t), intent(in) :: old_vtx
  type(model_data_t), intent(in), target, optional :: new_model
  call vtx%init (old_vtx%pdg, new_model)
end subroutine vertex_copy_from

```

Single-particle lookup: Given a particle code, we return matching codes if present, otherwise zero. Actually, we return the antiparticles of the matching codes, as appropriate for computing splittings.

<Model data: vertex: TBP>+≡

```

procedure :: get_match => vertex_get_match

```

<Model data: sub interfaces>+≡

```

module subroutine vertex_get_match (vtx, pdg1, pdg2)
  class(vertex_t), intent(in) :: vtx
  integer, intent(in) :: pdg1
  integer, dimension(:), allocatable, intent(out) :: pdg2
end subroutine vertex_get_match

```

<Model data: procedures>+≡

```

module subroutine vertex_get_match (vtx, pdg1, pdg2)
  class(vertex_t), intent(in) :: vtx
  integer, intent(in) :: pdg1
  integer, dimension(:), allocatable, intent(out) :: pdg2
  integer :: i, j
  do i = 1, size (vtx%pdg)
    if (vtx%pdg(i) == pdg1) then
      allocate (pdg2 (size (vtx%pdg) - 1))
      do j = 1, i-1
        pdg2(j) = anti (j)
      end do
    end if
  end do

```



```

        end do
        do j = i, size (pdg2)
            pdg2(j) = anti (j+1)
        end do
        exit
    end if
end do
contains
function anti (i) result (pdg)
    integer, intent(in) :: i
    integer :: pdg
    if (vtx%prt(i)%p%has_antiparticle ()) then
        pdg = - vtx%pdg(i)
    else
        pdg = vtx%pdg(i)
    end if
end function anti
end subroutine vertex_get_match

```

To access this from the outside, we create an iterator. The iterator has the sole purpose of returning the matching particles for a given array of PDG codes.

```

<Model data: public>+≡
    public :: vertex_iterator_t
<Model data: types>+≡
    type :: vertex_iterator_t
        private
        class(model_data_t), pointer :: model => null ()
        integer, dimension(:), allocatable :: pdg
        integer :: vertex_index = 0
        integer :: pdg_index = 0
        logical :: save_pdg_index
    contains
        procedure :: init => vertex_iterator_init
        procedure :: get_next_match => vertex_iterator_get_next_match
    end type vertex_iterator_t

```

We initialize the iterator for a particular model with the pdg index of the particle we are looking at.

```

<Model data: sub interfaces>+≡
    module subroutine vertex_iterator_init (it, model, pdg, save_pdg_index)
        class(vertex_iterator_t), intent(out) :: it
        class(model_data_t), intent(in), target :: model
        integer, dimension(:), intent(in) :: pdg
        logical, intent(in) :: save_pdg_index
    end subroutine vertex_iterator_init
    module subroutine vertex_iterator_get_next_match (it, pdg_match)
        class(vertex_iterator_t), intent(inout) :: it
        integer, dimension(:), allocatable, intent(out) :: pdg_match
    end subroutine vertex_iterator_get_next_match
<Model data: procedures>+≡
    module subroutine vertex_iterator_init (it, model, pdg, save_pdg_index)
        class(vertex_iterator_t), intent(out) :: it

```

```

class(model_data_t), intent(in), target :: model
integer, dimension(:), intent(in) :: pdg
logical, intent(in) :: save_pdg_index
it%model => model
allocate (it%pdg (size (pdg)), source = pdg)
it%save_pdg_index = save_pdg_index
end subroutine vertex_iterator_init

module subroutine vertex_iterator_get_next_match (it, pdg_match)
class(vertex_iterator_t), intent(inout) :: it
integer, dimension(:), allocatable, intent(out) :: pdg_match
integer :: i, j
do i = it%vertex_index + 1, size (it%model%vtx)
do j = it%pdg_index + 1, size (it%pdg)
call it%model%vtx(i)%get_match (it%pdg(j), pdg_match)
if (it%save_pdg_index) then
if (allocated (pdg_match) .and. j < size (it%pdg)) then
it%pdg_index = j
return
else if (allocated (pdg_match) .and. j == size (it%pdg)) then
it%vertex_index = i
it%pdg_index = 0
return
end if
else if (allocated (pdg_match)) then
it%vertex_index = i
return
end if
end do
end do
it%vertex_index = 0
it%pdg_index = 0
end subroutine vertex_iterator_get_next_match

```

11.1.4 Vertex lookup table

The vertex lookup table is a hash table: given two particle codes, we check which codes are allowed for the third one.

The size of the hash table should be large enough that collisions are rare. We first select a size based on the number of vertices (multiplied by six because all permutations count), with some margin, and then choose the smallest integer power of two larger than this.

```

<Model data: parameters>≡
integer, parameter :: VERTEX_TABLE_SCALE_FACTOR = 60

<Model data: procedures>+≡
function vertex_table_size (n_vtx) result (n)
integer(i32) :: n
integer, intent(in) :: n_vtx
integer :: i, s
s = VERTEX_TABLE_SCALE_FACTOR * n_vtx
n = 1

```

```

do i = 1, 31
  n = ishft (n, 1)
  s = ishft (s,-1)
  if (s == 0) exit
end do
end function vertex_table_size

```

The specific hash function takes two particle codes (arbitrary integers) and returns a 32-bit integer. It makes use of the universal function `hash` which operates on a byte array.

```

<Model data: procedures>+≡
function hash2 (pdg1, pdg2)
  integer(i32) :: hash2
  integer, intent(in) :: pdg1, pdg2
  integer(i8), dimension(1) :: mold
  hash2 = hash (transfer ([pdg1, pdg2], mold))
end function hash2

```

Each entry in the vertex table stores the two particle codes and an array of possibilities for the third code.

```

<Model data: types>+≡
type :: vertex_table_entry_t
  private
  integer :: pdg1 = 0, pdg2 = 0
  integer :: n = 0
  integer, dimension(:), allocatable :: pdg3
end type vertex_table_entry_t

```

The vertex table:

```

<Model data: types>+≡
type :: vertex_table_t
  type(vertex_table_entry_t), dimension(:), allocatable :: entry
  integer :: n_collisions = 0
  integer(i32) :: mask
  contains
  <Model data: vertex table: TBP>
end type vertex_table_t

```

Output.

```

<Model data: vertex table: TBP>≡
procedure :: write => vertex_table_write

<Model data: sub interfaces>+≡
module subroutine vertex_table_write (vt, unit)
  class(vertex_table_t), intent(in) :: vt
  integer, intent(in), optional :: unit
end subroutine vertex_table_write

<Model data: procedures>+≡
module subroutine vertex_table_write (vt, unit)
  class(vertex_table_t), intent(in) :: vt
  integer, intent(in), optional :: unit

```

```

integer :: u, i
character(9) :: size_pdg3
u = given_output_unit (unit)
write (u, "(A)") "vertex hash table:"
write (u, "(A,I7)") " size = ", size (vt%entry)
write (u, "(A,I7)") " used = ", count (vt%entry%  
n /= 0)
write (u, "(A,I7)") " coll = ", vt%n_collisions
do i = lbound (vt%entry, 1), ubound (vt%entry, 1)
  if (vt%entry(i)%  
n /= 0) then
    write (size_pdg3, "(I7)") size (vt%entry(i)%  
pdg3)
    write (u, "(A,1x,I7,1x,A,2(1x,I7),A," // &
      size_pdg3 // "(1x,I7))") &
      " ", i, ":", vt%entry(i)%  
pdg1, &
      vt%entry(i)%  
pdg2, "->", vt%entry(i)%  
pdg3
  end if
end do
end subroutine vertex_table_write

```

Initializing the vertex table: This is done in two passes. First, we scan all permutations for all vertices and count the number of entries in each bucket of the hashtable. Then, the buckets are allocated accordingly and filled.

Collision resolution is done by just incrementing the hash value until an empty bucket is found. The vertex table size is fixed, since we know from the beginning the number of entries.

```

<Model data: vertex table: TBP>+≡
  procedure :: init => vertex_table_init

<Model data: sub interfaces>+≡
  module subroutine vertex_table_init (vt, prt, vtx)
    class(vertex_table_t), intent(out) :: vt
    type(field_data_t), dimension(:), intent(in) :: prt
    type(vertex_t), dimension(:), intent(in) :: vtx
  end subroutine vertex_table_init

<Model data: procedures>+≡
  module subroutine vertex_table_init (vt, prt, vtx)
    class(vertex_table_t), intent(out) :: vt
    type(field_data_t), dimension(:), intent(in) :: prt
    type(vertex_t), dimension(:), intent(in) :: vtx
    integer :: n_vtx, vt_size, i, p1, p2, p3
    integer, dimension(3) :: p
    n_vtx = size (vtx)
    vt_size = vertex_table_size (count (vtx%trilinear))
    vt%mask = vt_size - 1
    allocate (vt%entry (0:vt_size-1))
    do i = 1, n_vtx
      if (vtx(i)%trilinear) then
        p = vtx(i)%pdg
        p1 = p(1); p2 = p(2)
        call create (hash2 (p1, p2))
        if (p(2) /= p(3)) then
          p2 = p(3)
          call create (hash2 (p1, p2))
        end if
      end if
    end do
  end subroutine vertex_table_init

```

```

        if (p(1) /= p(2)) then
            p1 = p(2); p2 = p(1)
            call create (hash2 (p1, p2))
            if (p(1) /= p(3)) then
                p2 = p(3)
                call create (hash2 (p1, p2))
            end if
        end if
        if (p(1) /= p(3)) then
            p1 = p(3); p2 = p(1)
            call create (hash2 (p1, p2))
            if (p(1) /= p(2)) then
                p2 = p(2)
                call create (hash2 (p1, p2))
            end if
        end if
    end if
end do
do i = 0, vt_size - 1
    allocate (vt%entry(i)%pdg3 (vt%entry(i)%n))
end do
vt%entry%n = 0
do i = 1, n_vtx
    if (vtx(i)%trilinear) then
        p = vtx(i)%pdg
        p1 = p(1); p2 = p(2); p3 = p(3)
        call register (hash2 (p1, p2))
        if (p(2) /= p(3)) then
            p2 = p(3); p3 = p(2)
            call register (hash2 (p1, p2))
        end if
        if (p(1) /= p(2)) then
            p1 = p(2); p2 = p(1); p3 = p(3)
            call register (hash2 (p1, p2))
            if (p(1) /= p(3)) then
                p2 = p(3); p3 = p(1)
                call register (hash2 (p1, p2))
            end if
        end if
        if (p(1) /= p(3)) then
            p1 = p(3); p2 = p(1); p3 = p(2)
            call register (hash2 (p1, p2))
            if (p(1) /= p(2)) then
                p2 = p(2); p3 = p(1)
                call register (hash2 (p1, p2))
            end if
        end if
    end if
end do
contains
recursive subroutine create (hashval)
    integer(i32), intent(in) :: hashval
    integer :: h
    h = iand (hashval, vt%mask)

```

```

    if (vt%entry(h)%n == 0) then
        vt%entry(h)%pdg1 = p1
        vt%entry(h)%pdg2 = p2
        vt%entry(h)%n = 1
    else if (vt%entry(h)%pdg1 == p1 .and. vt%entry(h)%pdg2 == p2) then
        vt%entry(h)%n = vt%entry(h)%n + 1
    else
        vt%n_collisions = vt%n_collisions + 1
        call create (hashval + 1)
    end if
end subroutine create
recursive subroutine register (hashval)
    integer(i32), intent(in) :: hashval
    integer :: h
    h = iand (hashval, vt%mask)
    if (vt%entry(h)%pdg1 == p1 .and. vt%entry(h)%pdg2 == p2) then
        vt%entry(h)%n = vt%entry(h)%n + 1
        vt%entry(h)%pdg3(vt%entry(h)%n) = p3
    else
        call register (hashval + 1)
    end if
end subroutine register
end subroutine vertex_table_init

```

Return the array of particle codes that match the given pair.

<Model data: vertex table: TBP>+≡

```
procedure :: match => vertex_table_match
```

<Model data: sub interfaces>+≡

```

module subroutine vertex_table_match (vt, pdg1, pdg2, pdg3)
    class(vertex_table_t), intent(in) :: vt
    integer, intent(in) :: pdg1, pdg2
    integer, dimension(:), allocatable, intent(out) :: pdg3
end subroutine vertex_table_match

```

<Model data: procedures>+≡

```

module subroutine vertex_table_match (vt, pdg1, pdg2, pdg3)
    class(vertex_table_t), intent(in) :: vt
    integer, intent(in) :: pdg1, pdg2
    integer, dimension(:), allocatable, intent(out) :: pdg3
    call match (hash2 (pdg1, pdg2))
contains
    recursive subroutine match (hashval)
        integer(i32), intent(in) :: hashval
        integer :: h
        h = iand (hashval, vt%mask)
        if (vt%entry(h)%n == 0) then
            allocate (pdg3 (0))
        else if (vt%entry(h)%pdg1 == pdg1 .and. vt%entry(h)%pdg2 == pdg2) then
            allocate (pdg3 (size (vt%entry(h)%pdg3)))
            pdg3 = vt%entry(h)%pdg3
        else
            call match (hashval + 1)
        end if
    end subroutine match
end subroutine match

```

```
end subroutine vertex_table_match
```

Return true if the triplet is represented as a vertex.

<Model data: vertex table: TBP>+≡

```
procedure :: check => vertex_table_check
```

<Model data: sub interfaces>+≡

```
module function vertex_table_check (vt, pdg1, pdg2, pdg3) result (flag)
  class(vertex_table_t), intent(in) :: vt
  integer, intent(in) :: pdg1, pdg2, pdg3
  logical :: flag
end function vertex_table_check
```

<Model data: procedures>+≡

```
module function vertex_table_check (vt, pdg1, pdg2, pdg3) result (flag)
  class(vertex_table_t), intent(in) :: vt
  integer, intent(in) :: pdg1, pdg2, pdg3
  logical :: flag
  flag = check (hash2 (pdg1, pdg2))
contains
  recursive function check (hashval) result (flag)
    integer(i32), intent(in) :: hashval
    integer :: h
    logical :: flag
    h = iand (hashval, vt%mask)
    if (vt%entry(h)%n == 0) then
      flag = .false.
    else if (vt%entry(h)%pdg1 == pdg1 .and. vt%entry(h)%pdg2 == pdg2) then
      flag = any (vt%entry(h)%pdg3 == pdg3)
    else
      flag = check (hashval + 1)
    end if
  end function check
end function vertex_table_check
```

11.1.5 Model Data Record

This type collects the model data as defined above.

We deliberately implement the parameter arrays as pointer arrays. We thus avoid keeping track of TARGET attributes.

The `scheme` identifier provides meta information. It doesn't give the client code an extra parameter, but it tells something about the interpretation of the parameters. If the scheme ID is left as default (zero), it is ignored.

<Model data: public>+≡

```
public :: model_data_t
```

<Model data: types>+≡

```
type :: model_data_t
  private
  type(string_t) :: name
  integer :: scheme = 0
  type(modelpar_real_t), dimension(:), pointer :: par_real => null ()
  type(modelpar_complex_t), dimension(:), pointer :: par_complex => null ()
```

```

        type(field_data_t), dimension(:), allocatable :: field
        type(vertex_t), dimension(:), allocatable :: vtx
        type(vertex_table_t) :: vt
contains
    <Model data: model data: TBP>
end type model_data_t

```

Finalizer, deallocate pointer arrays.

```

<Model data: model data: TBP>≡
    procedure :: final => model_data_final

<Model data: sub interfaces>+≡
    module subroutine model_data_final (model)
        class(model_data_t), intent(inout) :: model
    end subroutine model_data_final

<Model data: procedures>+≡
    module subroutine model_data_final (model)
        class(model_data_t), intent(inout) :: model
        if (associated (model%par_real)) then
            deallocate (model%par_real)
        end if
        if (associated (model%par_complex)) then
            deallocate (model%par_complex)
        end if
    end subroutine model_data_final

```

Output. The signature matches the signature of the high-level `model_write` procedure, so some of the options don't actually apply.

```

<Model data: model data: TBP>+≡
    procedure :: write => model_data_write

<Model data: sub interfaces>+≡
    module subroutine model_data_write (model, unit, verbose, &
        show_md5sum, show_variables, show_parameters, &
        show_particles, show_vertices, show_scheme)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: show_md5sum
        logical, intent(in), optional :: show_variables
        logical, intent(in), optional :: show_parameters
        logical, intent(in), optional :: show_particles
        logical, intent(in), optional :: show_vertices
        logical, intent(in), optional :: show_scheme
    end subroutine model_data_write

<Model data: procedures>+≡
    module subroutine model_data_write (model, unit, verbose, &
        show_md5sum, show_variables, show_parameters, &
        show_particles, show_vertices, show_scheme)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: show_md5sum

```



```

logical, intent(in), optional :: show_variables
logical, intent(in), optional :: show_parameters
logical, intent(in), optional :: show_particles
logical, intent(in), optional :: show_vertices
logical, intent(in), optional :: show_scheme
logical :: show_sch, show_par, show_prt, show_vtx
integer :: u, i
u = given_output_unit (unit)
show_sch = .false.; if (present (show_scheme)) &
    show_sch = show_scheme
show_par = .true.; if (present (show_parameters)) &
    show_par = show_parameters
show_prt = .true.; if (present (show_particles)) &
    show_prt = show_particles
show_vtx = .true.; if (present (show_vertices)) &
    show_vtx = show_vertices
if (show_sch) then
    write (u, "(3x,A,1X,I0)") "scheme =", model%scheme
end if
if (show_par) then
    do i = 1, size (model%par_real)
        call model%par_real(i)%write (u)
        write (u, "(A)")
    end do
    do i = 1, size (model%par_complex)
        call model%par_complex(i)%write (u)
        write (u, "(A)")
    end do
end if
if (show_prt) then
    write (u, "(A)")
    call model%write_fields (u)
end if
if (show_vtx) then
    write (u, "(A)")
    call model%write_vertices (u, verbose)
end if
end subroutine model_data_write

```

Initialize, allocating pointer arrays. The second version makes a deep copy.

```

<Model data: model data: TBP>+≡
generic :: init => model_data_init
procedure, private :: model_data_init

<Model data: sub interfaces>+≡
module subroutine model_data_init (model, name, &
    n_par_real, n_par_complex, n_field, n_vtx)
class(model_data_t), intent(out) :: model
type(string_t), intent(in) :: name
integer, intent(in) :: n_par_real, n_par_complex
integer, intent(in) :: n_field
integer, intent(in) :: n_vtx
end subroutine model_data_init

<Model data: procedures>+≡

```

```

module subroutine model_data_init (model, name, &
    n_par_real, n_par_complex, n_field, n_vtx)
    class(model_data_t), intent(out) :: model
    type(string_t), intent(in) :: name
    integer, intent(in) :: n_par_real, n_par_complex
    integer, intent(in) :: n_field
    integer, intent(in) :: n_vtx
    model%name = name
    allocate (model%par_real (n_par_real))
    allocate (model%par_complex (n_par_complex))
    allocate (model%field (n_field))
    allocate (model%vtx (n_vtx))
end subroutine model_data_init

```

Set the scheme ID.

```

<Model data: model data: TBP>+≡
    procedure :: set_scheme_num => model_data_set_scheme_num

<Model data: sub interfaces>+≡
    module subroutine model_data_set_scheme_num (model, scheme)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: scheme
    end subroutine model_data_set_scheme_num

<Model data: procedures>+≡
    module subroutine model_data_set_scheme_num (model, scheme)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: scheme
        model%scheme = scheme
    end subroutine model_data_set_scheme_num

```

Complete model data initialization.

```

<Model data: model data: TBP>+≡
    procedure :: freeze_fields => model_data_freeze_fields

<Model data: sub interfaces>+≡
    module subroutine model_data_freeze_fields (model)
        class(model_data_t), intent(inout) :: model
    end subroutine model_data_freeze_fields

<Model data: procedures>+≡
    module subroutine model_data_freeze_fields (model)
        class(model_data_t), intent(inout) :: model
        call model%field%freeze ()
    end subroutine model_data_freeze_fields

```

Deep copy. The new model should already be initialized, so we do not allocate memory.

```

<Model data: model data: TBP>+≡
    procedure :: copy_from => model_data_copy

<Model data: sub interfaces>+≡
    module subroutine model_data_copy (model, src)
        class(model_data_t), intent(inout), target :: model
        class(model_data_t), intent(in), target :: src
    end subroutine model_data_copy

```

```

<Model data: procedures>+≡
module subroutine model_data_copy (model, src)
  class(model_data_t), intent(inout), target :: model
  class(model_data_t), intent(in), target :: src
  class(modelpar_data_t), pointer :: data, src_data
  integer :: i
  model%scheme = src%scheme
  model%par_real = src%par_real
  model%par_complex = src%par_complex
  do i = 1, size (src%field)
    associate (field => model%field(i), src_field => src%field(i))
      call field%init (src_field%get_longname (), src_field%get_pdg ())
      call field%copy_from (src_field)
      src_data => src_field%mass_data
      if (associated (src_data)) then
        data => model%get_par_data_ptr (src_data%get_name ())
        call field%set (mass_data = data)
      end if
      src_data => src_field%width_data
      if (associated (src_data)) then
        data => model%get_par_data_ptr (src_data%get_name ())
        call field%set (width_data = data)
      end if
      call field%set_multiplicity ()
    end associate
  end do
  do i = 1, size (src%vtx)
    call model%vtx(i)%copy_from (src%vtx(i), model)
  end do
  call model%freeze_vertices ()
end subroutine model_data_copy

```

Return the model name and numeric scheme.

```

<Model data: model data: TBP>+≡
  procedure :: get_name => model_data_get_name
  procedure :: get_scheme_num => model_data_get_scheme_num

<Model data: sub interfaces>+≡
  module function model_data_get_name (model) result (name)
    class(model_data_t), intent(in) :: model
    type(string_t) :: name
  end function model_data_get_name
  module function model_data_get_scheme_num (model) result (scheme)
    class(model_data_t), intent(in) :: model
    integer :: scheme
  end function model_data_get_scheme_num

<Model data: procedures>+≡
  module function model_data_get_name (model) result (name)
    class(model_data_t), intent(in) :: model
    type(string_t) :: name
    name = model%name
  end function model_data_get_name

  module function model_data_get_scheme_num (model) result (scheme)

```

```

class(model_data_t), intent(in) :: model
integer :: scheme
scheme = model%scheme
end function model_data_get_scheme_num

```

Retrieve a MD5 sum for the current model parameter values and decay/polarization settings. This is done by writing them to a temporary file, using a standard format. If the model scheme is nonzero, it is also written.

```

<Model data: model data: TBP>+≡
  procedure :: get_parameters_md5sum => model_data_get_parameters_md5sum

<Model data: sub interfaces>+≡
  module function model_data_get_parameters_md5sum (model) result (par_md5sum)
    character(32) :: par_md5sum
    class(model_data_t), intent(in) :: model
  end function model_data_get_parameters_md5sum

<Model data: procedures>+≡
  module function model_data_get_parameters_md5sum (model) result (par_md5sum)
    character(32) :: par_md5sum
    class(model_data_t), intent(in) :: model
    real(default), dimension(:), allocatable :: par
    type(field_data_t), pointer :: field
    integer :: unit, i
    allocate (par (model%get_n_real ()))
    call model%real_parameters_to_array (par)
    unit = free_unit ()
    open (unit, status="scratch", action="readwrite")
    if (model%scheme /= 0) write (unit, "(I0)") model%scheme
    write (unit, "(" // FMT_19 // ")") par
    do i = 1, model%get_n_field ()
      field => model%get_field_ptr_by_index (i)
      if (.not. field%is_stable (.false.) .or. .not. field%is_stable (.true.) &
        .or. field%is_polarized (.false.) .or. field%is_polarized (.true.))&
        then
        write (unit, "(3x,A)") char (field%get_longname ())
        call field%write_decays (unit)
      end if
    end do
    rewind (unit)
    par_md5sum = md5sum (unit)
    close (unit)
  end function model_data_get_parameters_md5sum

```

Return the MD5 sum. This is a placeholder, to be overwritten for the complete model definition.

```

<Model data: model data: TBP>+≡
  procedure :: get_md5sum => model_data_get_md5sum

<Model data: sub interfaces>+≡
  module function model_data_get_md5sum (model) result (md5sum)
    class(model_data_t), intent(in) :: model
    character(32) :: md5sum
  end function model_data_get_md5sum

```

```

<Model data: procedures>+≡
  module function model_data_get_md5sum (model) result (md5sum)
    class(model_data_t), intent(in) :: model
    character(32) :: md5sum
    md5sum = model%get_parameters_md5sum ()
  end function model_data_get_md5sum

```

Initialize a real or complex parameter.

```

<Model data: model data: TBP>+≡
  generic :: init_par => model_data_init_par_real, model_data_init_par_complex
  procedure, private :: model_data_init_par_real
  procedure, private :: model_data_init_par_complex

```

```

<Model data: sub interfaces>+≡
  module subroutine model_data_init_par_real (model, i, name, value)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
  end subroutine model_data_init_par_real
  module subroutine model_data_init_par_complex (model, i, name, value)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: value
  end subroutine model_data_init_par_complex

```

```

<Model data: procedures>+≡
  module subroutine model_data_init_par_real (model, i, name, value)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    call model%par_real(i)%init (name, value)
  end subroutine model_data_init_par_real

  module subroutine model_data_init_par_complex (model, i, name, value)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: value
    call model%par_complex(i)%init (name, value)
  end subroutine model_data_init_par_complex

```

After initialization, return size of parameter array.

```

<Model data: model data: TBP>+≡
  procedure :: get_n_real => model_data_get_n_real
  procedure :: get_n_complex => model_data_get_n_complex

```

```

<Model data: sub interfaces>+≡
  module function model_data_get_n_real (model) result (n)
    class(model_data_t), intent(in) :: model
    integer :: n
  end function model_data_get_n_real

```

```

        module function model_data_get_n_complex (model) result (n)
            class(model_data_t), intent(in) :: model
            integer :: n
        end function model_data_get_n_complex
    <Model data: procedures>+≡
    module function model_data_get_n_real (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%par_real)
    end function model_data_get_n_real

    module function model_data_get_n_complex (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%par_complex)
    end function model_data_get_n_complex

```

After initialization, extract the whole parameter array.

```

    <Model data: model data: TBP>+≡
    procedure :: real_parameters_to_array &
        => model_data_real_par_to_array
    procedure :: complex_parameters_to_array &
        => model_data_complex_par_to_array

    <Model data: sub interfaces>+≡
    module subroutine model_data_real_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        real(default), dimension(:), intent(inout) :: array
    end subroutine model_data_real_par_to_array
    module subroutine model_data_complex_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        complex(default), dimension(:), intent(inout) :: array
    end subroutine model_data_complex_par_to_array

    <Model data: procedures>+≡
    module subroutine model_data_real_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        real(default), dimension(:), intent(inout) :: array
        array = model%par_real%get_real ()
    end subroutine model_data_real_par_to_array

    module subroutine model_data_complex_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        complex(default), dimension(:), intent(inout) :: array
        array = model%par_complex%get_complex ()
    end subroutine model_data_complex_par_to_array

```

After initialization, set the whole parameter array.

```

    <Model data: model data: TBP>+≡
    procedure :: real_parameters_from_array &
        => model_data_real_par_from_array
    procedure :: complex_parameters_from_array &
        => model_data_complex_par_from_array

```

```

<Model data: sub interfaces>+≡
    module subroutine model_data_real_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        real(default), dimension(:), intent(in) :: array
    end subroutine model_data_real_par_from_array
    module subroutine model_data_complex_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        complex(default), dimension(:), intent(in) :: array
    end subroutine model_data_complex_par_from_array

<Model data: procedures>+≡
    module subroutine model_data_real_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        real(default), dimension(:), intent(in) :: array
        model%par_real = array
    end subroutine model_data_real_par_from_array

    module subroutine model_data_complex_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        complex(default), dimension(:), intent(in) :: array
        model%par_complex = array
    end subroutine model_data_complex_par_from_array

```

Analogous, for a C parameter array.

```

<Model data: model data: TBP>+≡
    procedure :: real_parameters_to_c_array &
        => model_data_real_par_to_c_array

<Model data: sub interfaces>+≡
    module subroutine model_data_real_par_to_c_array (model, array)
        class(model_data_t), intent(in) :: model
        real(c_default_float), dimension(:), intent(inout) :: array
    end subroutine model_data_real_par_to_c_array

<Model data: procedures>+≡
    module subroutine model_data_real_par_to_c_array (model, array)
        class(model_data_t), intent(in) :: model
        real(c_default_float), dimension(:), intent(inout) :: array
        array = model%par_real%get_real ()
    end subroutine model_data_real_par_to_c_array

```

After initialization, set the whole parameter array.

```

<Model data: model data: TBP>+≡
    procedure :: real_parameters_from_c_array &
        => model_data_real_par_from_c_array

<Model data: sub interfaces>+≡
    module subroutine model_data_real_par_from_c_array (model, array)
        class(model_data_t), intent(inout) :: model
        real(c_default_float), dimension(:), intent(in) :: array
    end subroutine model_data_real_par_from_c_array

<Model data: procedures>+≡
    module subroutine model_data_real_par_from_c_array (model, array)
        class(model_data_t), intent(inout) :: model

```

```

    real(c_default_float), dimension(:), intent(in) :: array
    model%par_real = real (array, default)
end subroutine model_data_real_par_from_c_array

```

After initialization, get pointer to a real or complex parameter, directly by index.

```

<Model data: model data: TBP>+≡
    procedure :: get_par_real_ptr => model_data_get_par_real_ptr_index
    procedure :: get_par_complex_ptr => model_data_get_par_complex_ptr_index

<Model data: sub interfaces>+≡
    module function model_data_get_par_real_ptr_index (model, i) result (ptr)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        class(modelpar_data_t), pointer :: ptr
    end function model_data_get_par_real_ptr_index
    module function model_data_get_par_complex_ptr_index (model, i) result (ptr)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        class(modelpar_data_t), pointer :: ptr
    end function model_data_get_par_complex_ptr_index

<Model data: procedures>+≡
    module function model_data_get_par_real_ptr_index (model, i) result (ptr)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        class(modelpar_data_t), pointer :: ptr
        ptr => model%par_real(i)
    end function model_data_get_par_real_ptr_index

    module function model_data_get_par_complex_ptr_index (model, i) result (ptr)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        class(modelpar_data_t), pointer :: ptr
        ptr => model%par_complex(i)
    end function model_data_get_par_complex_ptr_index

```

After initialization, get pointer to a parameter by name.

```

<Model data: model data: TBP>+≡
    procedure :: get_par_data_ptr => model_data_get_par_data_ptr_name

<Model data: sub interfaces>+≡
    module function model_data_get_par_data_ptr_name (model, name) result (ptr)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        class(modelpar_data_t), pointer :: ptr
    end function model_data_get_par_data_ptr_name

<Model data: procedures>+≡
    module function model_data_get_par_data_ptr_name (model, name) result (ptr)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        class(modelpar_data_t), pointer :: ptr
        integer :: i
        do i = 1, size (model%par_real)

```



```

        if (model%par_real(i)%name == name) then
            ptr => model%par_real(i)
            return
        end if
    end do
do i = 1, size (model%par_complex)
    if (model%par_complex(i)%name == name) then
        ptr => model%par_complex(i)
        return
    end if
end do
ptr => null ()
end function model_data_get_par_data_ptr_name

```

Return the value by name. Again, type conversion is allowed.

<Model data: model data: TBP>+≡

```

    procedure :: get_real => model_data_get_par_real_value
    procedure :: get_complex => model_data_get_par_complex_value

```

<Model data: sub interfaces>+≡

```

    module function model_data_get_par_real_value (model, name) result (value)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        real(default) :: value
    end function model_data_get_par_real_value
    module function model_data_get_par_complex_value &
        (model, name) result (value)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        complex(default) :: value
    end function model_data_get_par_complex_value

```

<Model data: procedures>+≡

```

    module function model_data_get_par_real_value (model, name) result (value)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        class(modelpar_data_t), pointer :: par
        real(default) :: value
        par => model%get_par_data_ptr (name)
        value = par%get_real ()
    end function model_data_get_par_real_value

    module function model_data_get_par_complex_value (model, name) result (value)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        class(modelpar_data_t), pointer :: par
        complex(default) :: value
        par => model%get_par_data_ptr (name)
        value = par%get_complex ()
    end function model_data_get_par_complex_value

```

Modify a real or complex parameter.

<Model data: model data: TBP>+≡

```

    generic :: set_par => model_data_set_par_real, model_data_set_par_complex

```

```

    procedure, private :: model_data_set_par_real
    procedure, private :: model_data_set_par_complex
<Model data: sub interfaces>+≡
    module subroutine model_data_set_par_real (model, name, value)
        class(model_data_t), intent(inout) :: model
        type(string_t), intent(in) :: name
        real(default), intent(in) :: value
    end subroutine model_data_set_par_real
    module subroutine model_data_set_par_complex (model, name, value)
        class(model_data_t), intent(inout) :: model
        type(string_t), intent(in) :: name
        complex(default), intent(in) :: value
    end subroutine model_data_set_par_complex
<Model data: procedures>+≡
    module subroutine model_data_set_par_real (model, name, value)
        class(model_data_t), intent(inout) :: model
        type(string_t), intent(in) :: name
        real(default), intent(in) :: value
        class(modelpar_data_t), pointer :: par
        par => model%get_par_data_ptr (name)
        par = value
    end subroutine model_data_set_par_real

    module subroutine model_data_set_par_complex (model, name, value)
        class(model_data_t), intent(inout) :: model
        type(string_t), intent(in) :: name
        complex(default), intent(in) :: value
        class(modelpar_data_t), pointer :: par
        par => model%get_par_data_ptr (name)
        par = value
    end subroutine model_data_set_par_complex

```

List all fields in the model.

```

<Model data: model data: TBP>+≡
    procedure :: write_fields => model_data_write_fields
<Model data: sub interfaces>+≡
    module subroutine model_data_write_fields (model, unit)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
    end subroutine model_data_write_fields
<Model data: procedures>+≡
    module subroutine model_data_write_fields (model, unit)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        integer :: i
        do i = 1, size (model%field)
            call model%field(i)%write (unit)
        end do
    end subroutine model_data_write_fields

```

After initialization, return number of fields (particles):

```

<Model data: model data: TBP>+≡
    procedure :: get_n_field => model_data_get_n_field

<Model data: sub interfaces>+≡
    module function model_data_get_n_field (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
    end function model_data_get_n_field

<Model data: procedures>+≡
    module function model_data_get_n_field (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%field)
    end function model_data_get_n_field

```

Return the PDG code of a field. The field is identified by name or by index. If the field is not found, return zero.

```

<Model data: model data: TBP>+≡
    generic :: get_pdg => &
        model_data_get_field_pdg_index, &
        model_data_get_field_pdg_name
    procedure, private :: model_data_get_field_pdg_index
    procedure, private :: model_data_get_field_pdg_name

<Model data: sub interfaces>+≡
    module function model_data_get_field_pdg_index (model, i) result (pdg)
        class(model_data_t), intent(in) :: model
        integer, intent(in) :: i
        integer :: pdg
    end function model_data_get_field_pdg_index
    module function model_data_get_field_pdg_name &
        (model, name, check) result (pdg)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        logical, intent(in), optional :: check
        integer :: pdg
    end function model_data_get_field_pdg_name

<Model data: procedures>+≡
    module function model_data_get_field_pdg_index (model, i) result (pdg)
        class(model_data_t), intent(in) :: model
        integer, intent(in) :: i
        integer :: pdg
        pdg = model%field(i)%get_pdg ()
    end function model_data_get_field_pdg_index

    module function model_data_get_field_pdg_name &
        (model, name, check) result (pdg)
        class(model_data_t), intent(in) :: model
        type(string_t), intent(in) :: name
        logical, intent(in), optional :: check
        integer :: pdg
        integer :: i

```

```

do i = 1, size (model%field)
  associate (field => model%field(i))
    if (field%matches_name (name, .false.)) then
      pdg = field%get_pdg ()
      return
    else if (field%matches_name (name, .true.)) then
      pdg = - field%get_pdg ()
      return
    end if
  end associate
end do
pdg = 0
call model%field_error (check, name)
end function model_data_get_field_pdg_name

```

Return an array of all PDG codes, including antiparticles. The antiparticle are sorted after all particles.

```

<Model data: model data: TBP>+≡
  procedure :: get_all_pdg => model_data_get_all_pdg

<Model data: sub interfaces>+≡
  module subroutine model_data_get_all_pdg (model, pdg)
    class(model_data_t), intent(in) :: model
    integer, dimension(:), allocatable, intent(inout) :: pdg
  end subroutine model_data_get_all_pdg

<Model data: procedures>+≡
  module subroutine model_data_get_all_pdg (model, pdg)
    class(model_data_t), intent(in) :: model
    integer, dimension(:), allocatable, intent(inout) :: pdg
    integer :: n0, n1, i, k
    n0 = size (model%field)
    n1 = n0 + count (model%field%has_antiparticle ())
    allocate (pdg (n1))
    pdg(1:n0) = model%field%get_pdg ()
    k = n0
    do i = 1, size (model%field)
      associate (field => model%field(i))
        if (field%has_antiparticle ()) then
          k = k + 1
          pdg(k) = - field%get_pdg ()
        end if
      end associate
    end do
  end subroutine model_data_get_all_pdg

```

Return pointer to the field array.

```

<Model data: model data: TBP>+≡
  procedure :: get_field_array_ptr => model_data_get_field_array_ptr

<Model data: sub interfaces>+≡
  module function model_data_get_field_array_ptr (model) result (ptr)
    class(model_data_t), intent(in), target :: model
    type(field_data_t), dimension(:), pointer :: ptr
  end function model_data_get_field_array_ptr

```

```

<Model data: procedures>+≡
module function model_data_get_field_array_ptr (model) result (ptr)
  class(model_data_t), intent(in), target :: model
  type(field_data_t), dimension(:), pointer :: ptr
  ptr => model%field
end function model_data_get_field_array_ptr

```

Return pointer to a field. The identifier should be the unique long name, the PDG code, or the index.

We can issue an error message, if the `check` flag is set. We never return an error if the PDG code is zero, this yields just a null pointer.

```

<Model data: model data: TBP>+≡
generic :: get_field_ptr => &
  model_data_get_field_ptr_name, &
  model_data_get_field_ptr_pdg
procedure, private :: model_data_get_field_ptr_name
procedure, private :: model_data_get_field_ptr_pdg
procedure :: get_field_ptr_by_index => model_data_get_field_ptr_index

```

```

<Model data: sub interfaces>+≡
module function model_data_get_field_ptr_name &
  (model, name, check) result (ptr)
  class(model_data_t), intent(in), target :: model
  type(string_t), intent(in) :: name
  logical, intent(in), optional :: check
  type(field_data_t), pointer :: ptr
end function model_data_get_field_ptr_name
module function model_data_get_field_ptr_pdg &
  (model, pdg, check) result (ptr)
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: pdg
  logical, intent(in), optional :: check
  type(field_data_t), pointer :: ptr
end function model_data_get_field_ptr_pdg
module function model_data_get_field_ptr_index (model, i) result (ptr)
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: i
  type(field_data_t), pointer :: ptr
end function model_data_get_field_ptr_index

```

```

<Model data: procedures>+≡
module function model_data_get_field_ptr_name &
  (model, name, check) result (ptr)
  class(model_data_t), intent(in), target :: model
  type(string_t), intent(in) :: name
  logical, intent(in), optional :: check
  type(field_data_t), pointer :: ptr
  integer :: i
  do i = 1, size (model%field)
    if (model%field(i)%matches_name (name, .false.)) then
      ptr => model%field(i)
      return
    else if (model%field(i)%matches_name (name, .true.)) then
      ptr => model%field(i)
    end if
  end do
end function model_data_get_field_ptr_name

```

```

        return
    end if
end do
ptr => null ()
call model%field_error (check, name)
end function model_data_get_field_ptr_name

module function model_data_get_field_ptr_pdg (model, pdg, check) result (ptr)
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: pdg
    logical, intent(in), optional :: check
    type(field_data_t), pointer :: ptr
    integer :: i, pdg_abs
    if (pdg == 0) then
        ptr => null ()
        return
    end if
    pdg_abs = abs (pdg)
    do i = 1, size (model%field)
        if (abs(model%field(i)%get_pdg ()) == pdg_abs) then
            ptr => model%field(i)
            return
        end if
    end do
    ptr => null ()
    call model%field_error (check, pdg=pdg)
end function model_data_get_field_ptr_pdg

module function model_data_get_field_ptr_index (model, i) result (ptr)
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: i
    type(field_data_t), pointer :: ptr
    ptr => model%field(i)
end function model_data_get_field_ptr_index

```

Do not assign a pointer, just check.

<Model data: model data: TBP>+≡

```

    procedure :: test_field => model_data_test_field_pdg

```

<Model data: sub interfaces>+≡

```

    module function model_data_test_field_pdg (model, pdg, check) result (exist)
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: pdg
        logical, intent(in), optional :: check
        logical :: exist
    end function model_data_test_field_pdg

```

<Model data: procedures>+≡

```

    module function model_data_test_field_pdg (model, pdg, check) result (exist)
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: pdg
        logical, intent(in), optional :: check
        logical :: exist
        exist = associated (model%get_field_ptr (pdg, check))
    end function model_data_test_field_pdg

```

Error message, if `check` is set.

<Model data: model data: TBP>+≡

```
procedure :: field_error => model_data_field_error
```

<Model data: sub interfaces>+≡

```
module subroutine model_data_field_error (model, check, name, pdg)
  class(model_data_t), intent(in) :: model
  logical, intent(in), optional :: check
  type(string_t), intent(in), optional :: name
  integer, intent(in), optional :: pdg
end subroutine model_data_field_error
```

<Model data: procedures>+≡

```
module subroutine model_data_field_error (model, check, name, pdg)
  class(model_data_t), intent(in) :: model
  logical, intent(in), optional :: check
  type(string_t), intent(in), optional :: name
  integer, intent(in), optional :: pdg
  if (present (check)) then
    if (check) then
      if (present (name)) then
        write (msg_buffer, "(A,1x,A,1x,A,1x,A)") &
          "No particle with name", char (name), &
          "is contained in model", char (model%name)
      else if (present (pdg)) then
        write (msg_buffer, "(A,1x,I0,1x,A,1x,A)") &
          "No particle with PDG code", pdg, &
          "is contained in model", char (model%name)
      else
        write (msg_buffer, "(A,1x,A,1x,A)") &
          "Particle missing", &
          "in model", char (model%name)
      end if
      call msg_fatal ()
    end if
  end if
end subroutine model_data_field_error
```

Assign mass and width value, which are associated via pointer. Identify the particle via `pdg`.

<Model data: model data: TBP>+≡

```
procedure :: set_field_mass => model_data_set_field_mass_pdg
procedure :: set_field_width => model_data_set_field_width_pdg
```

<Model data: sub interfaces>+≡

```
module subroutine model_data_set_field_mass_pdg (model, pdg, value)
  class(model_data_t), intent(inout) :: model
  integer, intent(in) :: pdg
  real(default), intent(in) :: value
end subroutine model_data_set_field_mass_pdg
module subroutine model_data_set_field_width_pdg (model, pdg, value)
  class(model_data_t), intent(inout) :: model
  integer, intent(in) :: pdg
```

```

        real(default), intent(in) :: value
    end subroutine model_data_set_field_width_pdg
<Model data: procedures>+≡
    module subroutine model_data_set_field_mass_pdg (model, pdg, value)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: pdg
        real(default), intent(in) :: value
        type(field_data_t), pointer :: field
        field => model%get_field_ptr (pdg, check = .true.)
        call field%set_mass (value)
    end subroutine model_data_set_field_mass_pdg

    module subroutine model_data_set_field_width_pdg (model, pdg, value)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: pdg
        real(default), intent(in) :: value
        type(field_data_t), pointer :: field
        field => model%get_field_ptr (pdg, check = .true.)
        call field%set_width (value)
    end subroutine model_data_set_field_width_pdg

```

Mark a particle as unstable and provide a list of names for its decay processes. In contrast with the previous subroutine which is for internal use, we address the particle by its PDG code. If the index is negative, we address the antiparticle.

```

<Model data: model data: TBP>+≡
    procedure :: set_unstable => model_data_set_unstable
    procedure :: set_stable => model_data_set_stable
<Model data: sub interfaces>+≡
    module subroutine model_data_set_unstable &
        (model, pdg, decay, isotropic, diagonal, decay_helicity)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
        type(string_t), dimension(:), intent(in) :: decay
        logical, intent(in), optional :: isotropic, diagonal
        integer, intent(in), optional :: decay_helicity
    end subroutine model_data_set_unstable
    module subroutine model_data_set_stable (model, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
    end subroutine model_data_set_stable
<Model data: procedures>+≡
    module subroutine model_data_set_unstable &
        (model, pdg, decay, isotropic, diagonal, decay_helicity)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
        type(string_t), dimension(:), intent(in) :: decay
        logical, intent(in), optional :: isotropic, diagonal
        integer, intent(in), optional :: decay_helicity
        type(field_data_t), pointer :: field
        field => model%get_field_ptr (pdg)
        if (pdg > 0) then
            call field%set ( &

```



```

        p_is_stable = .false., p_decay = decay, &
        p_decays_isotropically = isotropic, &
        p_decays_diagonal = diagonal, &
        p_decay_helicity = decay_helicity)
    else
        call field%set ( &
            a_is_stable = .false., a_decay = decay, &
            a_decays_isotropically = isotropic, &
            a_decays_diagonal = diagonal, &
            a_decay_helicity = decay_helicity)
    end if
end subroutine model_data_set_unstable

module subroutine model_data_set_stable (model, pdg)
    class(model_data_t), intent(inout), target :: model
    integer, intent(in) :: pdg
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg)
    if (pdg > 0) then
        call field%set (p_is_stable = .true.)
    else
        call field%set (a_is_stable = .true.)
    end if
end subroutine model_data_set_stable

```

Mark a particle as polarized.

```

<Model data: model data: TBP>+≡
    procedure :: set_polarized => model_data_set_polarized
    procedure :: set_unpolarized => model_data_set_unpolarized

<Model data: sub interfaces>+≡
    module subroutine model_data_set_polarized (model, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
    end subroutine model_data_set_polarized
    module subroutine model_data_set_unpolarized (model, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
    end subroutine model_data_set_unpolarized

<Model data: procedures>+≡
    module subroutine model_data_set_polarized (model, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: pdg
        type(field_data_t), pointer :: field
        field => model%get_field_ptr (pdg)
        if (pdg > 0) then
            call field%set (p_polarized = .true.)
        else
            call field%set (a_polarized = .true.)
        end if
    end subroutine model_data_set_polarized

    module subroutine model_data_set_unpolarized (model, pdg)
        class(model_data_t), intent(inout), target :: model

```

```

integer, intent(in) :: pdg
type(field_data_t), pointer :: field
field => model%get_field_ptr (pdg)
if (pdg > 0) then
    call field%set (p_polarized = .false.)
else
    call field%set (a_polarized = .false.)
end if
end subroutine model_data_set_unpolarized

```

Revert all polarized (unstable) particles to unpolarized (stable) status, respectively.

```

<Model data: model data: TBP>+=
    procedure :: clear_unstable => model_clear_unstable
    procedure :: clear_polarized => model_clear_polarized

<Model data: sub interfaces>+=
    module subroutine model_clear_unstable (model)
        class(model_data_t), intent(inout), target :: model
    end subroutine model_clear_unstable
    module subroutine model_clear_polarized (model)
        class(model_data_t), intent(inout), target :: model
    end subroutine model_clear_polarized

<Model data: procedures>+=
    module subroutine model_clear_unstable (model)
        class(model_data_t), intent(inout), target :: model
        integer :: i
        type(field_data_t), pointer :: field
        do i = 1, model%get_n_field ()
            field => model%get_field_ptr_by_index (i)
            call field%set (p_is_stable = .true.)
            if (field%has_antiparticle ()) then
                call field%set (a_is_stable = .true.)
            end if
        end do
    end subroutine model_clear_unstable

    module subroutine model_clear_polarized (model)
        class(model_data_t), intent(inout), target :: model
        integer :: i
        type(field_data_t), pointer :: field
        do i = 1, model%get_n_field ()
            field => model%get_field_ptr_by_index (i)
            call field%set (p_polarized = .false.)
            if (field%has_antiparticle ()) then
                call field%set (a_polarized = .false.)
            end if
        end do
    end subroutine model_clear_polarized

```

List all vertices, optionally also the hash table.

```

<Model data: model data: TBP>+=
    procedure :: write_vertices => model_data_write_vertices

```

```

<Model data: sub interfaces>+≡
    module subroutine model_data_write_vertices (model, unit, verbose)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine model_data_write_vertices

<Model data: procedures>+≡
    module subroutine model_data_write_vertices (model, unit, verbose)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: i, u
        u = given_output_unit (unit)
        do i = 1, size (model%vtx)
            call vertex_write (model%vtx(i), unit)
        end do
        if (present (verbose)) then
            if (verbose) then
                write (u, *)
                call vertex_table_write (model%vt, unit)
            end if
        end if
    end subroutine model_data_write_vertices

```

Vertex definition.

```

<Model data: model data: TBP>+≡
    generic :: set_vertex => &
        model_data_set_vertex_pdg, model_data_set_vertex_names
    procedure, private :: model_data_set_vertex_pdg
    procedure, private :: model_data_set_vertex_names

<Model data: sub interfaces>+≡
    module subroutine model_data_set_vertex_pdg (model, i, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: pdg
    end subroutine model_data_set_vertex_pdg
    module subroutine model_data_set_vertex_names (model, i, name)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), dimension(:), intent(in) :: name
    end subroutine model_data_set_vertex_names

<Model data: procedures>+≡
    module subroutine model_data_set_vertex_pdg (model, i, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: pdg
        call vertex_init (model%vtx(i), pdg, model)
    end subroutine model_data_set_vertex_pdg

    module subroutine model_data_set_vertex_names (model, i, name)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i

```

```

type(string_t), dimension(:), intent(in) :: name
integer, dimension(size(name)) :: pdg
integer :: j
do j = 1, size (name)
    pdg(j) = model%get_pdg (name(j))
end do
call model%set_vertex (i, pdg)
end subroutine model_data_set_vertex_names

```

Finalize vertex definition: set up the hash table.

```

<Model data: model data: TBP>+≡
    procedure :: freeze_vertices => model_data_freeze_vertices

<Model data: sub interfaces>+≡
    module subroutine model_data_freeze_vertices (model)
        class(model_data_t), intent(inout) :: model
    end subroutine model_data_freeze_vertices

<Model data: procedures>+≡
    module subroutine model_data_freeze_vertices (model)
        class(model_data_t), intent(inout) :: model
        call model%vt%init (model%field, model%vtx)
    end subroutine model_data_freeze_vertices

```

Number of vertices in model

```

<Model data: model data: TBP>+≡
    procedure :: get_n_vtx => model_data_get_n_vtx

<Model data: sub interfaces>+≡
    module function model_data_get_n_vtx (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
    end function model_data_get_n_vtx

<Model data: procedures>+≡
    module function model_data_get_n_vtx (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%vtx)
    end function model_data_get_n_vtx

```

Lookup functions

```

<Model data: model data: TBP>+≡
    procedure :: match_vertex => model_data_match_vertex

<Model data: sub interfaces>+≡
    module subroutine model_data_match_vertex (model, pdg1, pdg2, pdg3)
        class(model_data_t), intent(in) :: model
        integer, intent(in) :: pdg1, pdg2
        integer, dimension(:), allocatable, intent(out) :: pdg3
    end subroutine model_data_match_vertex

```

```

<Model data: procedures>+≡
module subroutine model_data_match_vertex (model, pdg1, pdg2, pdg3)
  class(model_data_t), intent(in) :: model
  integer, intent(in) :: pdg1, pdg2
  integer, dimension(:), allocatable, intent(out) :: pdg3
  call model%vt%match (pdg1, pdg2, pdg3)
end subroutine model_data_match_vertex

<Model data: model data: TBP>+≡
procedure :: check_vertex => model_data_check_vertex

<Model data: sub interfaces>+≡
module function model_data_check_vertex &
  (model, pdg1, pdg2, pdg3) result (flag)
  logical :: flag
  class(model_data_t), intent(in) :: model
  integer, intent(in) :: pdg1, pdg2, pdg3
end function model_data_check_vertex

<Model data: procedures>+≡
module function model_data_check_vertex &
  (model, pdg1, pdg2, pdg3) result (flag)
  logical :: flag
  class(model_data_t), intent(in) :: model
  integer, intent(in) :: pdg1, pdg2, pdg3
  flag = model%vt%check (pdg1, pdg2, pdg3)
end function model_data_check_vertex

```

11.1.6 Toy Models

This is a stripped-down version of the (already trivial) model 'Test'.

```

<Model data: model data: TBP>+≡
procedure :: init_test => model_data_init_test

<Model data: sub interfaces>+≡
module subroutine model_data_init_test (model)
  class(model_data_t), intent(out) :: model
end subroutine model_data_init_test

<Model data: procedures>+≡
module subroutine model_data_init_test (model)
  class(model_data_t), intent(out) :: model
  type(field_data_t), pointer :: field
  integer, parameter :: n_real = 4
  integer, parameter :: n_field = 2
  integer, parameter :: n_vertex = 2
  integer :: i
  call model%init (var_str ("Test"), &
    n_real, 0, n_field, n_vertex)
  i = 0
  i = i + 1
  call model%init_par (i, var_str ("gy"), 1._default)
  i = i + 1
  call model%init_par (i, var_str ("ms"), 125._default)

```

```

i = i + 1
call model%init_par (i, var_str ("ff"), 1.5_default)
i = i + 1
call model%init_par (i, var_str ("mf"), 1.5_default * 125._default)
i = 0
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("SCALAR"), 25)
call field%set (spin_type=1)
call field%set (mass_data=model%get_par_real_ptr (2))
call field%set (name = [var_str ("s")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("FERMION"), 6)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (4))
call field%set (name = [var_str ("f")], anti = [var_str ("fbar")])
call model%freeze_fields ()
i = 0
i = i + 1
call model%set_vertex (i, [var_str ("fbar"), var_str ("f"), var_str ("s")])
i = i + 1
call model%set_vertex (i, [var_str ("s"), var_str ("s"), var_str ("s")])
call model%freeze_vertices ()
end subroutine model_data_init_test

```

This procedure prepares a subset of QED for testing purposes.

(Model data: model data: TBP)+≡

```

procedure :: init_qed_test => model_data_init_qed_test

```

(Model data: sub interfaces)+≡

```

module subroutine model_data_init_qed_test (model)
  class(model_data_t), intent(out) :: model
end subroutine model_data_init_qed_test

```

(Model data: procedures)+≡

```

module subroutine model_data_init_qed_test (model)
  class(model_data_t), intent(out) :: model
  type(field_data_t), pointer :: field
  integer, parameter :: n_real = 1
  integer, parameter :: n_field = 2
  integer :: i
  call model%init (var_str ("QED_test"), &
    n_real, 0, n_field, 0)
  i = 0
  i = i + 1
  call model%init_par (i, var_str ("me"), 0.000510997_default)
  i = 0
  i = i + 1
  field => model%get_field_ptr_by_index (i)
  call field%init (var_str ("E_LEPTON"), 11)
  call field%set (spin_type=2, charge_type=-4)
  call field%set (mass_data=model%get_par_real_ptr (1))
  call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
  i = i + 1

```

```

    field => model%get_field_ptr_by_index (i)
    call field%init (var_str ("PHOTON"), 22)
    call field%set (spin_type=3)
    call field%set (name = [var_str ("A")])
    call model%freeze_fields ()
    call model%freeze_vertices ()
end subroutine model_data_init_qed_test

```

This procedure prepares a subset of the Standard Model for testing purposes. We can thus avoid dependencies on model I/O, which is not defined here.

(Model data: model data: TBP)+≡

```

    procedure :: init_sm_test => model_data_init_sm_test

```

(Model data: sub interfaces)+≡

```

    module subroutine model_data_init_sm_test (model)
        class(model_data_t), intent(out) :: model
    end subroutine model_data_init_sm_test

```

(Model data: procedures)+≡

```

    module subroutine model_data_init_sm_test (model)
        class(model_data_t), intent(out) :: model
        type(field_data_t), pointer :: field
        integer, parameter :: n_real = 11
        integer, parameter :: n_field = 19
        integer, parameter :: n_vtx = 9
        integer :: i
        call model%init (var_str ("SM_test"), &
            n_real, 0, n_field, n_vtx)
        i = 0
        i = i + 1
        call model%init_par (i, var_str ("mZ"), 91.1882_default)
        i = i + 1
        call model%init_par (i, var_str ("mW"), 80.419_default)
        i = i + 1
        call model%init_par (i, var_str ("me"), 0.000510997_default)
        i = i + 1
        call model%init_par (i, var_str ("mmu"), 0.105658389_default)
        i = i + 1
        call model%init_par (i, var_str ("mb"), 4.2_default)
        i = i + 1
        call model%init_par (i, var_str ("mtop"), 173.1_default)
        i = i + 1
        call model%init_par (i, var_str ("wZ"), 2.443_default)
        i = i + 1
        call model%init_par (i, var_str ("wW"), 2.049_default)
        i = i + 1
        call model%init_par (i, var_str ("ee"), 0.3079561542961_default)
        i = i + 1
        call model%init_par (i, var_str ("cw"), 8.819013863636E-01_default)
        i = i + 1
        call model%init_par (i, var_str ("sw"), 4.714339240339E-01_default)
        i = 0
        i = i + 1
        field => model%get_field_ptr_by_index (i)
        call field%init (var_str ("D_QUARK"), 1)
    end subroutine model_data_init_sm_test

```

```

call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (name = [var_str ("d")], anti = [var_str ("dbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("U_QUARK"), 2)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (name = [var_str ("u")], anti = [var_str ("ubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("S_QUARK"), 3)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (name = [var_str ("s")], anti = [var_str ("sbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("C_QUARK"), 4)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (name = [var_str ("c")], anti = [var_str ("cbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("B_QUARK"), 5)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (mass_data=model%get_par_real_ptr (5))
call field%set (name = [var_str ("b")], anti = [var_str ("bbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("T_QUARK"), 6)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (6))
call field%set (name = [var_str ("t")], anti = [var_str ("tbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_LEPTON"), 11)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (3))
call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_NEUTRINO"), 12)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nue")], anti = [var_str ("nuebar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_LEPTON"), 13)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (4))
call field%set (name = [var_str ("mu-")], anti = [var_str ("mu+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_NEUTRINO"), 14)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("numu")], anti = [var_str ("numubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("GLUON"), 21)

```



```

call field%set (spin_type=3, color_type=8)
call field%set (name = [var_str ("gl")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PHOTON"), 22)
call field%set (spin_type=3)
call field%set (name = [var_str ("A")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("Z_BOSON"), 23)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (1))
call field%set (width_data=model%get_par_real_ptr (7))
call field%set (name = [var_str ("Z")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("W_BOSON"), 24)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (2))
call field%set (width_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("W+")], anti = [var_str ("W-")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HIGGS"), 25)
call field%set (spin_type=1)
!   call field%set (mass_data=model%get_par_real_ptr (2))
!   call field%set (width_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("H")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PROTON"), 2212)
call field%set (spin_type=2)
call field%set (name = [var_str ("p")], anti = [var_str ("pbar")])
!   call field%set (mass_data=model%get_par_real_ptr (12))
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_SINGLET"), 91)
call field%set (color_type=1)
call field%set (name = [var_str ("hr1")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_TRIPLET"), 92)
call field%set (color_type=3)
call field%set (name = [var_str ("hr3")], anti = [var_str ("hr3bar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_OCTET"), 93)
call field%set (color_type=8)
call field%set (name = [var_str ("hr8")])
call model%freeze_fields ()
i = 0
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("A")])
i = i + 1

```

```

call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("d"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("u"), var_str ("W-")])
call model%freeze_vertices ()
end subroutine model_data_init_sm_test

```

11.2 Model Testbed

The standard way of defining a model uses concrete variables and expressions to interpret the model file. Some of this is not available at the point of use. This is no problem for the WHIZARD program as a whole, but unit tests are kept local to their respective module and don't access all definitions.

Instead, we introduce a separate module that provides hooks, one for initializing a model and one for finalizing a model. The main program can assign real routines to the hooks (procedure pointers of abstract type) before unit tests are called. The unit tests can call the abstract routines without knowing about their implementation.

```
<model_testbed.f90>≡  
  <File header>  
  
  module model_testbed  
  
    <Use strings>  
    use model_data  
    use var_base  
  
    <Standard module head>  
  
    <Model testbed: public>  
  
    <Model testbed: variables>  
  
    <Model testbed: interfaces>  
  
  end module model_testbed
```

11.2.1 Abstract Model Handlers

Both routines take a polymorphic model (data) target, which is not allocated/deallocated inside the subroutine. The model constructor `prepare_model` requires the model name as input. It can, optionally, return a link to the variable list of the model.

```
<Model testbed: public>≡  
  public :: prepare_model  
  public :: cleanup_model  
  
<Model testbed: variables>≡  
  procedure (prepare_model_proc), pointer :: prepare_model => null ()  
  procedure (cleanup_model_proc), pointer :: cleanup_model => null ()  
  
<Model testbed: interfaces>≡  
  abstract interface  
    subroutine prepare_model_proc (model, name, vars)  
      import  
      class(model_data_t), intent(inout), pointer :: model  
      type(string_t), intent(in) :: name  
      class(vars_t), pointer, intent(out), optional :: vars  
    end subroutine prepare_model_proc  
  end interface
```

```
abstract interface
  subroutine cleanup_model_proc (model)
    import
    class(model_data_t), intent(inout), target :: model
  end subroutine cleanup_model_proc
end interface
```

11.3 Helicities

This module defines types and tools for dealing with helicity information.

```
<helicities.f90>≡  
  <File header>  
  
  module helicities  
  
    <Standard module head>  
  
    <Helicities: public>  
  
    <Helicities: types>  
  
    <Helicities: interfaces>  
  
    interface  
    <Helicities: sub interfaces>  
    end interface  
  
  end module helicities  
<helicities_sub.f90>≡  
  <File header>  
  
  submodule (helicities) helicities_s  
  
    use io_units  
  
    implicit none  
  
    contains  
  
    <Helicities: procedures>  
  
  end submodule helicities_s
```

11.3.1 Helicity types

Helicities may be defined or undefined, corresponding to a polarized or unpolarized state. Each helicity is actually a pair of helicities, corresponding to an entry in the spin density matrix. Obviously, diagonal entries are distinguished.

```
<Helicities: public>≡  
  public :: helicity_t  
<Helicities: types>≡  
  type :: helicity_t  
    private  
    logical :: defined = .false.  
    integer :: h1, h2  
    contains  
    <Helicities: helicity: TBP>  
  end type helicity_t
```

Constructor functions, for convenience:

```

<Helicities: public>+≡
    public :: helicity

<Helicities: interfaces>≡
    interface helicity
        module procedure helicity0, helicity1, helicity2
    end interface helicity

<Helicities: sub interfaces>≡
    pure module function helicity0 () result (hel)
        type(helicity_t) :: hel
    end function helicity0
    elemental module function helicity1 (h) result (hel)
        type(helicity_t) :: hel
        integer, intent(in) :: h
    end function helicity1
    elemental module function helicity2 (h2, h1) result (hel)
        type(helicity_t) :: hel
        integer, intent(in) :: h1, h2
    end function helicity2

<Helicities: procedures>≡
    pure module function helicity0 () result (hel)
        type(helicity_t) :: hel
    end function helicity0

    elemental module function helicity1 (h) result (hel)
        type(helicity_t) :: hel
        integer, intent(in) :: h
        call hel%init (h)
    end function helicity1

    elemental module function helicity2 (h2, h1) result (hel)
        type(helicity_t) :: hel
        integer, intent(in) :: h1, h2
        call hel%init (h2, h1)
    end function helicity2

```

Initializers.

Note: conceptually, the argument to initializers should be INTENT(OUT). However, Interp. F08/0033 prohibited this. The reason is that, in principle, the call could result in the execution of an impure finalizer for a type extension of `hel` (ugh).

```

<Helicities: helicity: TBP>≡
    generic :: init => helicity_init_empty, helicity_init_same, helicity_init_different
    procedure, private :: helicity_init_empty
    procedure, private :: helicity_init_same
    procedure, private :: helicity_init_different

<Helicities: sub interfaces>+≡
    elemental module subroutine helicity_init_empty (hel)
        class(helicity_t), intent(inout) :: hel

```

```

end subroutine helicity_init_empty
elemental module subroutine helicity_init_same (hel, h)
  class(helicity_t), intent(inout) :: hel
  integer, intent(in) :: h
end subroutine helicity_init_same
elemental module subroutine helicity_init_different (hel, h2, h1)
  class(helicity_t), intent(inout) :: hel
  integer, intent(in) :: h1, h2
end subroutine helicity_init_different

<Helicities: procedures>+≡
elemental module subroutine helicity_init_empty (hel)
  class(helicity_t), intent(inout) :: hel
  hel%defined = .false.
end subroutine helicity_init_empty

elemental module subroutine helicity_init_same (hel, h)
  class(helicity_t), intent(inout) :: hel
  integer, intent(in) :: h
  hel%defined = .true.
  hel%h1 = h
  hel%h2 = h
end subroutine helicity_init_same

elemental module subroutine helicity_init_different (hel, h2, h1)
  class(helicity_t), intent(inout) :: hel
  integer, intent(in) :: h1, h2
  hel%defined = .true.
  hel%h2 = h2
  hel%h1 = h1
end subroutine helicity_init_different

```

Undefine:

```

<Helicities: helicity: TBP>+≡
  procedure :: undefine => helicity_undefine

<Helicities: sub interfaces>+≡
  elemental module subroutine helicity_undefine (hel)
    class(helicity_t), intent(inout) :: hel
  end subroutine helicity_undefine

<Helicities: procedures>+≡
  elemental module subroutine helicity_undefine (hel)
    class(helicity_t), intent(inout) :: hel
    hel%defined = .false.
  end subroutine helicity_undefine

```

Diagonalize by removing the second entry (use with care!)

```

<Helicities: helicity: TBP>+≡
  procedure :: diagonalize => helicity_diagonalize

<Helicities: sub interfaces>+≡
  elemental module subroutine helicity_diagonalize (hel)
    class(helicity_t), intent(inout) :: hel
  end subroutine helicity_diagonalize

```

```

<Helicities: procedures>+≡
  elemental module subroutine helicity_diagonalize (hel)
    class(helicity_t), intent(inout) :: hel
    hel%h2 = hel%h1
  end subroutine helicity_diagonalize

```

Flip helicity indices by sign.

```

<Helicities: helicity: TBP>+≡
  procedure :: flip => helicity_flip

<Helicities: sub interfaces>+≡
  elemental module subroutine helicity_flip (hel)
    class(helicity_t), intent(inout) :: hel
  end subroutine helicity_flip

<Helicities: procedures>+≡
  elemental module subroutine helicity_flip (hel)
    class(helicity_t), intent(inout) :: hel
    hel%h1 = - hel%h1
    hel%h2 = - hel%h2
  end subroutine helicity_flip

```

```

<Helicities: helicity: TBP>+≡
  procedure :: get_indices => helicity_get_indices

<Helicities: sub interfaces>+≡
  module subroutine helicity_get_indices (hel, h1, h2)
    class(helicity_t), intent(in) :: hel
    integer, intent(out) :: h1, h2
  end subroutine helicity_get_indices

<Helicities: procedures>+≡
  module subroutine helicity_get_indices (hel, h1, h2)
    class(helicity_t), intent(in) :: hel
    integer, intent(out) :: h1, h2
    h1 = hel%h1; h2 = hel%h2
  end subroutine helicity_get_indices

```

Output (no linebreak). No output if undefined.

```

<Helicities: helicity: TBP>+≡
  procedure :: write => helicity_write

<Helicities: sub interfaces>+≡
  module subroutine helicity_write (hel, unit)
    class(helicity_t), intent(in) :: hel
    integer, intent(in), optional :: unit
  end subroutine helicity_write

<Helicities: procedures>+≡
  module subroutine helicity_write (hel, unit)
    class(helicity_t), intent(in) :: hel
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    if (hel%defined) then

```



```

        write (u, "(A)", advance="no") "h("
        write (u, "(I0)", advance="no") hel%h1
        if (hel%h1 /= hel%h2) then
            write (u, "(A)", advance="no") "|"
            write (u, "(I0)", advance="no") hel%h2
        end if
        write (u, "(A)", advance="no") ")"
    end if
end subroutine helicity_write

```

Binary I/O. Write contents only if defined.

<Helicities: helicity: TBP>+≡

```

    procedure :: write_raw => helicity_write_raw
    procedure :: read_raw => helicity_read_raw

```

<Helicities: sub interfaces>+≡

```

    module subroutine helicity_write_raw (hel, u)
        class(helicity_t), intent(in) :: hel
        integer, intent(in) :: u
    end subroutine helicity_write_raw
    module subroutine helicity_read_raw (hel, u, iostat)
        class(helicity_t), intent(out) :: hel
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
    end subroutine helicity_read_raw

```

<Helicities: procedures>+≡

```

    module subroutine helicity_write_raw (hel, u)
        class(helicity_t), intent(in) :: hel
        integer, intent(in) :: u
        write (u) hel%defined
        if (hel%defined) then
            write (u) hel%h1, hel%h2
        end if
    end subroutine helicity_write_raw

    module subroutine helicity_read_raw (hel, u, iostat)
        class(helicity_t), intent(out) :: hel
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
        read (u, iostat=iostat) hel%defined
        if (hel%defined) then
            read (u, iostat=iostat) hel%h1, hel%h2
        end if
    end subroutine helicity_read_raw

```

11.3.2 Predicates

Check if the helicity is defined:

<Helicities: helicity: TBP>+≡

```

    procedure :: is_defined => helicity_is_defined

```

```

<Helicities: sub interfaces>+≡
  elemental module function helicity_is_defined (hel) result (defined)
    logical :: defined
    class(helicity_t), intent(in) :: hel
  end function helicity_is_defined

```

```

<Helicities: procedures>+≡
  elemental module function helicity_is_defined (hel) result (defined)
    logical :: defined
    class(helicity_t), intent(in) :: hel
    defined = hel%defined
  end function helicity_is_defined

```

Return true if the two helicities are equal or the particle is unpolarized:

```

<Helicities: helicity: TBP>+≡
  procedure :: is_diagonal => helicity_is_diagonal

```

```

<Helicities: sub interfaces>+≡
  elemental module function helicity_is_diagonal (hel) result (diagonal)
    logical :: diagonal
    class(helicity_t), intent(in) :: hel
  end function helicity_is_diagonal

```

```

<Helicities: procedures>+≡
  elemental module function helicity_is_diagonal (hel) result (diagonal)
    logical :: diagonal
    class(helicity_t), intent(in) :: hel
    if (hel%defined) then
      diagonal = hel%h1 == hel%h2
    else
      diagonal = .true.
    end if
  end function helicity_is_diagonal

```

11.3.3 Accessing contents

This returns a two-element array and thus cannot be elemental. The result is unpredictable if the helicity is undefined.

```

<Helicities: helicity: TBP>+≡
  procedure :: to_pair => helicity_to_pair

```

```

<Helicities: sub interfaces>+≡
  pure module function helicity_to_pair (hel) result (h)
    integer, dimension(2) :: h
    class(helicity_t), intent(in) :: hel
  end function helicity_to_pair

```

```

<Helicities: procedures>+≡
  pure module function helicity_to_pair (hel) result (h)
    integer, dimension(2) :: h
    class(helicity_t), intent(in) :: hel
    h(1) = hel%h2
    h(2) = hel%h1
  end function helicity_to_pair

```

11.3.4 Comparisons

When comparing helicities, if either one is undefined, they are considered to match. In other words, an unpolarized particle matches any polarization. In the `dmatch` variant, it matches only diagonal helicity.

```
(Helicities: helicity: TBP)+≡
  generic :: operator(.match.) => helicity_match
  generic :: operator(.dmatch.) => helicity_match_diagonal
  generic :: operator(==) => helicity_eq
  generic :: operator(/=) => helicity_neq
  procedure, private :: helicity_match
  procedure, private :: helicity_match_diagonal
  procedure, private :: helicity_eq
  procedure, private :: helicity_neq

(Helicities: sub interfaces)+≡
  elemental module function helicity_match (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
  end function helicity_match
  elemental module function helicity_match_diagonal (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
  end function helicity_match_diagonal

(Helicities: procedures)+≡
  elemental module function helicity_match (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
      eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
    else
      eq = .true.
    end if
  end function helicity_match

  elemental module function helicity_match_diagonal (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
      eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
    else if (hel1%defined) then
      eq = hel1%h1 == hel1%h2
    else if (hel2%defined) then
      eq = hel2%h1 == hel2%h2
    else
      eq = .true.
    end if
  end function helicity_match_diagonal

(Helicities: sub interfaces)+≡
  elemental module function helicity_eq (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
  end function helicity_eq
```

```

<Helicities: procedures>+=
  elemental module function helicity_eq (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
      eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
    else if (.not. hel1%defined .and. .not. hel2%defined) then
      eq = .true.
    else
      eq = .false.
    end if
  end function helicity_eq

<Helicities: sub interfaces>+=
  elemental module function helicity_neq (hel1, hel2) result (neq)
    logical :: neq
    class(helicity_t), intent(in) :: hel1, hel2
  end function helicity_neq

<Helicities: procedures>+=
  elemental module function helicity_neq (hel1, hel2) result (neq)
    logical :: neq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
      neq = (hel1%h1 /= hel2%h1) .or. (hel1%h2 /= hel2%h2)
    else if (.not. hel1%defined .and. .not. hel2%defined) then
      neq = .false.
    else
      neq = .true.
    end if
  end function helicity_neq

```

11.3.5 Tools

Merge two helicity objects by taking the first entry from the first and the second entry from the second argument. Makes sense only if the input helicities were defined and diagonal. The handling of ghost flags is not well-defined; one should verify beforehand that they match.

```

<Helicities: helicity: TBP>+=
  generic :: operator(.merge.) => merge_helicities
  procedure, private :: merge_helicities

<Helicities: sub interfaces>+=
  elemental module function merge_helicities (hel1, hel2) result (hel)
    type(helicity_t) :: hel
    class(helicity_t), intent(in) :: hel1, hel2
  end function merge_helicities

<Helicities: procedures>+=
  elemental module function merge_helicities (hel1, hel2) result (hel)
    type(helicity_t) :: hel
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then

```

```

        call hel%init (hel2%h1, hel1%h1)
    else if (hel1%defined) then
        call hel%init (hel1%h2, hel1%h1)
    else if (hel2%defined) then
        call hel%init (hel2%h2, hel2%h1)
    end if
end function merge_helicities

```

11.4 Colors

This module defines a type and tools for dealing with color information.

Each particle can have zero or more (in practice, usually not more than two) color indices. Color indices are positive; flow direction can be determined from the particle nature.

While parton shower matrix elements are diagonal in color, some special applications (e.g., subtractions for NLO matrix elements) require non-diagonal color matrices.

```
<colors.f90>≡  
  <File header>  
  
  module colors  
  
    <Use kinds>  
    <Use strings>  
  
    <Standard module head>  
  
    <Colors: public>  
  
    <Colors: types>  
  
    <Colors: interfaces>  
  
    interface  
    <Colors: sub interfaces>  
    end interface  
  
  end module colors  
<colors_sub.f90>≡  
  <File header>  
  
  submodule (colors) colors_s  
  
    use io_units  
    use diagnostics  
  
    implicit none  
  
  contains  
  
    <Colors: procedures>  
  
  end submodule colors_s
```

11.4.1 The color type

A particle may have an arbitrary number of color indices (in practice, from zero to two, but more are possible). This object acts as a container. (The current implementation has a fixed array of length two.)

The fact that color comes as an array prohibits elemental procedures in some places. (May add interfaces and multi versions where necessary.)

The color may be undefined.

NOTE: Due to a compiler bug in nagfor 5.2, we do not use allocatable but fixed-size arrays with dimension 2. Only nonzero entries count. This may be more efficient anyway, but gives up some flexibility. However, the squaring algorithm currently works only for singlets, (anti)triplets and octets anyway, so two components are enough.

This type has to be generalized (abstract type and specific implementations) when trying to pursue generalized color flows or Monte Carlo over continuous color.

```

<Colors: public>≡
  public :: color_t

<Colors: types>≡
  type :: color_t
    private
    logical :: defined = .false.
    integer, dimension(2) :: c1 = 0, c2 = 0
    logical :: ghost = .false.
  contains
    <Colors: color: TBP>
  end type color_t

<Colors: types>+≡
  type :: entry_t
    integer, dimension(:), allocatable :: map
    type(color_t), dimension(:), allocatable :: col
    type(entry_t), pointer :: next => null ()
    logical :: nlo_event = .false.
  end type entry_t
  type :: list_t
    integer :: n = 0
    type(entry_t), pointer :: first => null ()
    type(entry_t), pointer :: last => null ()
  end type list_t

```

Initializers:

```

<Colors: color: TBP>≡
  generic :: init => &
    color_init_trivial, color_init_trivial_ghost, &
    color_init_array, color_init_array_ghost, &
    color_init_arrays, color_init_arrays_ghost
  procedure, private :: color_init_trivial
  procedure, private :: color_init_trivial_ghost
  procedure, private :: color_init_array
  procedure, private :: color_init_array_ghost
  procedure, private :: color_init_arrays
  procedure, private :: color_init_arrays_ghost

```

Undefined color: array remains unallocated

```

<Colors: sub interfaces>≡
  pure module subroutine color_init_trivial (col)

```

```

        class(color_t), intent(inout) :: col
    end subroutine color_init_trivial
    pure module subroutine color_init_trivial_ghost (col, ghost)
        class(color_t), intent(inout) :: col
        logical, intent(in) :: ghost
    end subroutine color_init_trivial_ghost
<Colors: procedures>≡
    pure module subroutine color_init_trivial (col)
        class(color_t), intent(inout) :: col
        col%defined = .true.
        col%c1 = 0
        col%c2 = 0
        col%ghost = .false.
    end subroutine color_init_trivial

    pure module subroutine color_init_trivial_ghost (col, ghost)
        class(color_t), intent(inout) :: col
        logical, intent(in) :: ghost
        col%defined = .true.
        col%c1 = 0
        col%c2 = 0
        col%ghost = ghost
    end subroutine color_init_trivial_ghost

```

This defines color from an arbitrary length color array, suitable for any representation. We may have two color arrays (non-diagonal matrix elements). This cannot be elemental. The third version assigns an array of colors, using a two-dimensional array as input.

```

<Colors: sub interfaces>+≡
    pure module subroutine color_init_array (col, c1)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1
    end subroutine color_init_array
    pure module subroutine color_init_array_ghost (col, c1, ghost)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1
        logical, intent(in) :: ghost
    end subroutine color_init_array_ghost
    pure module subroutine color_init_arrays (col, c1, c2)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1, c2
    end subroutine color_init_arrays
    pure module subroutine color_init_arrays_ghost (col, c1, c2, ghost)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1, c2
        logical, intent(in) :: ghost
    end subroutine color_init_arrays_ghost
<Colors: procedures>+≡
    pure module subroutine color_init_array (col, c1)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1
        col%defined = .true.

```



```

col%c1 = pack (c1, c1 /= 0, [0,0])
col%c2 = col%c1
col%ghost = .false.
end subroutine color_init_array

pure module subroutine color_init_array_ghost (col, c1, ghost)
  class(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1
  logical, intent(in) :: ghost
  call color_init_array (col, c1)
  col%ghost = ghost
end subroutine color_init_array_ghost

pure module subroutine color_init_arrays (col, c1, c2)
  class(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1, c2
  col%defined = .true.
  if (size (c1) == size (c2)) then
    col%c1 = pack (c1, c1 /= 0, [0,0])
    col%c2 = pack (c2, c2 /= 0, [0,0])
  else if (size (c1) /= 0) then
    col%c1 = pack (c1, c1 /= 0, [0,0])
    col%c2 = col%c1
  else if (size (c2) /= 0) then
    col%c1 = pack (c2, c2 /= 0, [0,0])
    col%c2 = col%c1
  end if
  col%ghost = .false.
end subroutine color_init_arrays

pure module subroutine color_init_arrays_ghost (col, c1, c2, ghost)
  class(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1, c2
  logical, intent(in) :: ghost
  call color_init_arrays (col, c1, c2)
  col%ghost = ghost
end subroutine color_init_arrays_ghost

```

This version is restricted to singlets, triplets, antitriplets, and octets: The input contains the color and anticolor index, each of the may be zero.

```

<Colors: color: TBP>+≡
  procedure :: init_col_acl => color_init_col_acl

<Colors: sub interfaces>+≡
  elemental module subroutine color_init_col_acl (col, col_in, acl_in)
    class(color_t), intent(inout) :: col
    integer, intent(in) :: col_in, acl_in
  end subroutine color_init_col_acl

<Colors: procedures>+≡
  elemental module subroutine color_init_col_acl (col, col_in, acl_in)
    class(color_t), intent(inout) :: col
    integer, intent(in) :: col_in, acl_in
    integer, dimension(0) :: null_array
    select case (col_in)

```

```

case (0)
  select case (acl_in)
    case (0)
      call color_init_array (col, null_array)
    case default
      call color_init_array (col, [-acl_in])
    end select
case default
  select case (acl_in)
    case (0)
      call color_init_array (col, [col_in])
    case default
      call color_init_array (col, [col_in, -acl_in])
    end select
  end select
end select
end subroutine color_init_col_acl

```

This version is used for the external interface. We convert a fixed-size array of colors (for each particle) to the internal form by packing only the nonzero entries.

Some of these procedures produce an array, so they can't be all type-bound. We implement them as ordinary procedures.

<Colors: public>+≡

```
public :: color_init_from_array
```

<Colors: interfaces>≡

```

interface color_init_from_array
  module procedure color_init_from_array1
  module procedure color_init_from_array1g
  module procedure color_init_from_array2
  module procedure color_init_from_array2g
end interface color_init_from_array

```

<Colors: sub interfaces>+≡

```

pure module subroutine color_init_from_array1 (col, c1)
  type(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1
end subroutine color_init_from_array1
pure module subroutine color_init_from_array1g (col, c1, ghost)
  type(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1
  logical, intent(in) :: ghost
end subroutine color_init_from_array1g
pure module subroutine color_init_from_array2 (col, c1)
  integer, dimension(:,:), intent(in) :: c1
  type(color_t), dimension(:), intent(inout) :: col
end subroutine color_init_from_array2
pure module subroutine color_init_from_array2g (col, c1, ghost)
  integer, dimension(:,:), intent(in) :: c1
  type(color_t), dimension(:), intent(out) :: col
  logical, intent(in), dimension(:) :: ghost
end subroutine color_init_from_array2g

```

```

<Colors: procedures>+≡
  pure module subroutine color_init_from_array1 (col, c1)
    type(color_t), intent(inout) :: col
    integer, dimension(:), intent(in) :: c1
    logical, dimension(size(c1)) :: mask
    mask = c1 /= 0
    col%defined = .true.
    col%c1 = pack (c1, mask, col%c1)
    col%c2 = col%c1
    col%ghost = .false.
  end subroutine color_init_from_array1

  pure module subroutine color_init_from_array1g (col, c1, ghost)
    type(color_t), intent(inout) :: col
    integer, dimension(:), intent(in) :: c1
    logical, intent(in) :: ghost
    call color_init_from_array1 (col, c1)
    col%ghost = ghost
  end subroutine color_init_from_array1g

  pure module subroutine color_init_from_array2 (col, c1)
    integer, dimension(:, :), intent(in) :: c1
    type(color_t), dimension(:), intent(inout) :: col
    integer :: i
    do i = 1, size (c1,2)
      call color_init_from_array1 (col(i), c1(:,i))
    end do
  end subroutine color_init_from_array2

  pure module subroutine color_init_from_array2g (col, c1, ghost)
    integer, dimension(:, :), intent(in) :: c1
    type(color_t), dimension(:), intent(out) :: col
    logical, intent(in), dimension(:) :: ghost
    call color_init_from_array2 (col, c1)
    col%ghost = ghost
  end subroutine color_init_from_array2g

```

Set the ghost property

```

<Colors: color: TBP>+≡
  procedure :: set_ghost => color_set_ghost

<Colors: sub interfaces>+≡
  elemental module subroutine color_set_ghost (col, ghost)
    class(color_t), intent(inout) :: col
    logical, intent(in) :: ghost
  end subroutine color_set_ghost

<Colors: procedures>+≡
  elemental module subroutine color_set_ghost (col, ghost)
    class(color_t), intent(inout) :: col
    logical, intent(in) :: ghost
    col%ghost = ghost
  end subroutine color_set_ghost

```

Undefine the color state:

```

<Colors: color: TBP>+≡
    procedure :: undefine => color_undefine

<Colors: sub interfaces>+≡
    elemental module subroutine color_undefine (col, undefine_ghost)
        class(color_t), intent(inout) :: col
        logical, intent(in), optional :: undefine_ghost
    end subroutine color_undefine

<Colors: procedures>+≡
    elemental module subroutine color_undefine (col, undefine_ghost)
        class(color_t), intent(inout) :: col
        logical, intent(in), optional :: undefine_ghost
        col%defined = .false.
        if (present (undefine_ghost)) then
            if (undefine_ghost) col%ghost = .false.
        else
            col%ghost = .false.
        end if
    end subroutine color_undefine

```

Output. As dense as possible, no linebreak. If color is undefined, no output.

The separate version for a color array suggest two distinct interfaces.

```

<Colors: public>+≡
    public :: color_write

<Colors: interfaces>+≡
    interface color_write
        module procedure color_write_single
        module procedure color_write_array
    end interface color_write

<Colors: color: TBP>+≡
    procedure :: write => color_write_single

<Colors: sub interfaces>+≡
    module subroutine color_write_single (col, unit)
        class(color_t), intent(in) :: col
        integer, intent(in), optional :: unit
    end subroutine color_write_single
    module subroutine color_write_array (col, unit)
        type(color_t), dimension(:), intent(in) :: col
        integer, intent(in), optional :: unit
    end subroutine color_write_array

<Colors: procedures>+≡
    module subroutine color_write_single (col, unit)
        class(color_t), intent(in) :: col
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (col%ghost) then
            write (u, "(A)", advance="no") "c*"
        else if (col%defined) then

```

```

        write (u, "(A)", advance="no") "c("
        if (col%c1(1) /= 0) write (u, "(I0)", advance="no") col%c1(1)
        if (any (col%c1 /= 0)) write (u, "(1x)", advance="no")
        if (col%c1(2) /= 0) write (u, "(I0)", advance="no") col%c1(2)
        if (.not. col%is_diagonal ()) then
            write (u, "(A)", advance="no") "|"
            if (col%c2(1) /= 0) write (u, "(I0)", advance="no") col%c2(1)
            if (any (col%c2 /= 0)) write (u, "(1x)", advance="no")
            if (col%c2(2) /= 0) write (u, "(I0)", advance="no") col%c2(2)
        end if
        write (u, "(A)", advance="no") ")"
    end if
end subroutine color_write_single

module subroutine color_write_array (col, unit)
    type(color_t), dimension(:), intent(in) :: col
    integer, intent(in), optional :: unit
    integer :: u
    integer :: i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A)", advance="no") "["
    do i = 1, size (col)
        if (i > 1) write (u, "(1x)", advance="no")
        call color_write_single (col(i), u)
    end do
    write (u, "(A)", advance="no") "]"
end subroutine color_write_array

```

Binary I/O. For allocatable colors, this would have to be modified.

```

<Colors: color: TBP>+≡
    procedure :: write_raw => color_write_raw
    procedure :: read_raw => color_read_raw

<Colors: sub interfaces>+≡
    module subroutine color_write_raw (col, u)
        class(color_t), intent(in) :: col
        integer, intent(in) :: u
    end subroutine color_write_raw
    module subroutine color_read_raw (col, u, iostat)
        class(color_t), intent(inout) :: col
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
    end subroutine color_read_raw

<Colors: procedures>+≡
    module subroutine color_write_raw (col, u)
        class(color_t), intent(in) :: col
        integer, intent(in) :: u
        logical :: defined
        defined = col%is_defined () .or. col%is_ghost ()
        write (u) defined
        if (defined) then
            write (u) col%c1, col%c2
            write (u) col%ghost
        end if
    end subroutine color_write_raw

```

```

end subroutine color_write_raw

module subroutine color_read_raw (col, u, iostat)
  class(color_t), intent(inout) :: col
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
  logical :: defined
  read (u, iostat=iostat) col%defined
  if (col%defined) then
    read (u, iostat=iostat) col%c1, col%c2
    read (u, iostat=iostat) col%ghost
  end if
end subroutine color_read_raw

```

11.4.2 Predicates

Return the definition status. A color state may be defined but trivial.

```

<Colors: color: TBP>+≡
  procedure :: is_defined => color_is_defined
  procedure :: is_nonzero => color_is_nonzero

<Colors: sub interfaces>+≡
  elemental module function color_is_defined (col) result (defined)
    logical :: defined
    class(color_t), intent(in) :: col
  end function color_is_defined
  elemental module function color_is_nonzero (col) result (flag)
    logical :: flag
    class(color_t), intent(in) :: col
  end function color_is_nonzero

<Colors: procedures>+≡
  elemental module function color_is_defined (col) result (defined)
    logical :: defined
    class(color_t), intent(in) :: col
    defined = col%defined
  end function color_is_defined

  elemental module function color_is_nonzero (col) result (flag)
    logical :: flag
    class(color_t), intent(in) :: col
    flag = col%defined &
      .and. .not. col%ghost &
      .and. any (col%c1 /= 0 .or. col%c2 /= 0)
  end function color_is_nonzero

```

Diagonal color objects have only one array allocated:

```

<Colors: color: TBP>+≡
  procedure :: is_diagonal => color_is_diagonal

<Colors: sub interfaces>+≡
  elemental module function color_is_diagonal (col) result (diagonal)
    logical :: diagonal

```

```

        class(color_t), intent(in) :: col
    end function color_is_diagonal
<Colors: procedures>+≡
    elemental module function color_is_diagonal (col) result (diagonal)
        logical :: diagonal
        class(color_t), intent(in) :: col
        if (col%defined) then
            diagonal = all (col%c1 == col%c2)
        else
            diagonal = .true.
        end if
    end function color_is_diagonal

```

Return the ghost flag

```

<Colors: color: TBP>+≡
    procedure :: is_ghost => color_is_ghost
<Colors: sub interfaces>+≡
    elemental module function color_is_ghost (col) result (ghost)
        logical :: ghost
        class(color_t), intent(in) :: col
    end function color_is_ghost
<Colors: procedures>+≡
    elemental module function color_is_ghost (col) result (ghost)
        logical :: ghost
        class(color_t), intent(in) :: col
        ghost = col%ghost
    end function color_is_ghost

```

The ghost parity: true if the color-ghost flag is set. Again, no TBP since this is an array.

```

<Colors: procedures>+≡
    pure function color_ghost_parity (col) result (parity)
        type(color_t), dimension(:), intent(in) :: col
        logical :: parity
        parity = mod (count (col%ghost), 2) == 1
    end function color_ghost_parity

```

Determine the color representation, given a color object. We allow only singlet (1), (anti)triplet (± 3), and octet states (8). A color ghost must not have color assigned, but the color type is 8. For non-diagonal color, representations must match. If the color type is undefined, return 0. If it is invalid or unsupported, return -1 .

Assumption: nonzero entries precede nonzero ones.

```

<Colors: color: TBP>+≡
    procedure :: get_type => color_get_type
<Colors: sub interfaces>+≡
    elemental module function color_get_type (col) result (ctype)
        class(color_t), intent(in) :: col
        integer :: ctype
    end function color_get_type

```

```

<Colors: procedures>+≡
  elemental module function color_get_type (col) result (ctype)
    class(color_t), intent(in) :: col
    integer :: ctype
    if (col%defined) then
      ctype = -1
      if (col%ghost) then
        if (all (col%c1 == 0 .and. col%c2 == 0)) then
          ctype = 8
        end if
      else
        if (all ((col%c1 == 0 .and. col%c2 == 0) &
          & .or. (col%c1 > 0 .and. col%c2 > 0) &
          & .or. (col%c1 < 0 .and. col%c2 < 0))) then
          if (all (col%c1 == 0)) then
            ctype = 1
          else if ((col%c1(1) > 0 .and. col%c1(2) == 0)) then
            ctype = 3
          else if ((col%c1(1) < 0 .and. col%c1(2) == 0)) then
            ctype = -3
          else if ((col%c1(1) > 0 .and. col%c1(2) < 0) &
            .or. (col%c1(1) < 0 .and. col%c1(2) > 0)) then
            ctype = 8
          end if
        end if
      end if
    else
      ctype = 0
    end if
  end function color_get_type

```

11.4.3 Accessing contents

Return the number of color indices. We assume that it is identical for both arrays.

```

<Colors: color: TBP>+≡
  procedure, private :: get_number_of_indices => color_get_number_of_indices

<Colors: sub interfaces>+≡
  elemental module function color_get_number_of_indices (col) result (n)
    integer :: n
    class(color_t), intent(in) :: col
  end function color_get_number_of_indices

<Colors: procedures>+≡
  elemental module function color_get_number_of_indices (col) result (n)
    integer :: n
    class(color_t), intent(in) :: col
    if (col%defined .and. .not. col%ghost) then
      n = count (col%c1 /= 0)
    else
      n = 0
    end if
  end function

```



```
end function color_get_number_of_indices
```

Return the (first) color/anticolor entry (assuming that color is diagonal). The result is a positive color index.

<Colors: color: TBP>+≡

```
procedure :: get_col => color_get_col
procedure :: get_acl => color_get_acl
```

<Colors: sub interfaces>+≡

```
elemental module function color_get_col (col) result (c)
  integer :: c
  class(color_t), intent(in) :: col
end function color_get_col
elemental module function color_get_acl (col) result (c)
  integer :: c
  class(color_t), intent(in) :: col
end function color_get_acl
```

<Colors: procedures>+≡

```
elemental module function color_get_col (col) result (c)
  integer :: c
  class(color_t), intent(in) :: col
  integer :: i
  if (col%defined .and. .not. col%ghost) then
    do i = 1, size (col%c1)
      if (col%c1(i) > 0) then
        c = col%c1(i)
        return
      end if
    end do
  end if
  c = 0
end function color_get_col
```

```
elemental module function color_get_acl (col) result (c)
  integer :: c
  class(color_t), intent(in) :: col
  integer :: i
  if (col%defined .and. .not. col%ghost) then
    do i = 1, size (col%c1)
      if (col%c1(i) < 0) then
        c = - col%c1(i)
        return
      end if
    end do
  end if
  c = 0
end function color_get_acl
```

Return the color index with highest absolute value

<Colors: public>+≡

```
public :: color_get_max_value
```

```

<Colors: interfaces>+≡
    interface color_get_max_value
        module procedure color_get_max_value0
        module procedure color_get_max_value1
        module procedure color_get_max_value2
    end interface color_get_max_value

<Colors: sub interfaces>+≡
    elemental module function color_get_max_value0 (col) result (cmax)
        integer :: cmax
        type(color_t), intent(in) :: col
    end function color_get_max_value0
    pure module function color_get_max_value1 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:), intent(in) :: col
    end function color_get_max_value1
    pure module function color_get_max_value2 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:, :), intent(in) :: col
    end function color_get_max_value2

<Colors: procedures>+≡
    elemental module function color_get_max_value0 (col) result (cmax)
        integer :: cmax
        type(color_t), intent(in) :: col
        if (col%defined .and. .not. col%ghost) then
            cmax = maxval (abs (col%c1))
        else
            cmax = 0
        end if
    end function color_get_max_value0

    pure module function color_get_max_value1 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:), intent(in) :: col
        cmax = maxval (color_get_max_value0 (col))
    end function color_get_max_value1

    pure module function color_get_max_value2 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:, :), intent(in) :: col
        integer, dimension(size(col, 2)) :: cm
        integer :: i
        forall (i = 1:size(col, 2))
            cm(i) = color_get_max_value1 (col(:,i))
        end forall
        cmax = maxval (cm)
    end function color_get_max_value2

```

11.4.4 Comparisons

Similar to helicities, colors match if they are equal, or if either one is undefined.

```

<Colors: color: TBP>+≡

```

```

generic :: operator(.match.) => color_match
generic :: operator(==) => color_eq
generic :: operator(/=) => color_neq
procedure, private :: color_match
procedure, private :: color_eq
procedure, private :: color_neq

<Colors: sub interfaces>+≡
    elemental module function color_match (col1, col2) result (eq)
        logical :: eq
        class(color_t), intent(in) :: col1, col2
    end function color_match
    elemental module function color_eq (col1, col2) result (eq)
        logical :: eq
        class(color_t), intent(in) :: col1, col2
    end function color_eq

<Colors: procedures>+≡
    elemental module function color_match (col1, col2) result (eq)
        logical :: eq
        class(color_t), intent(in) :: col1, col2
        if (col1%defined .and. col2%defined) then
            if (col1%ghost .and. col2%ghost) then
                eq = .true.
            else if (.not. col1%ghost .and. .not. col2%ghost) then
                eq = all (col1%c1 == col2%c1) .and. all (col1%c2 == col2%c2)
            else
                eq = .false.
            end if
        else
            eq = .true.
        end if
    end function color_match

    elemental module function color_eq (col1, col2) result (eq)
        logical :: eq
        class(color_t), intent(in) :: col1, col2
        if (col1%defined .and. col2%defined) then
            if (col1%ghost .and. col2%ghost) then
                eq = .true.
            else if (.not. col1%ghost .and. .not. col2%ghost) then
                eq = all (col1%c1 == col2%c1) .and. all (col1%c2 == col2%c2)
            else
                eq = .false.
            end if
        else if (.not. col1%defined &
            .and. .not. col2%defined) then
            eq = col1%ghost .eqv. col2%ghost
        else
            eq = .false.
        end if
    end function color_eq

<Colors: sub interfaces>+≡
    elemental module function color_neq (col1, col2) result (neq)

```

```

        logical :: neq
        class(color_t), intent(in) :: col1, col2
    end function color_neq
<Colors: procedures>+≡
    elemental module function color_neq (col1, col2) result (neq)
        logical :: neq
        class(color_t), intent(in) :: col1, col2
        if (col1%defined .and. col2%defined) then
            if (col1%ghost .and. col2%ghost) then
                neq = .false.
            else if (.not. col1%ghost .and. .not. col2%ghost) then
                neq = any (col1%c1 /= col2%c1) .or. any (col1%c2 /= col2%c2)
            else
                neq = .true.
            end if
        else if (.not. col1%defined &
            .and. .not. col2%defined) then
            neq = col1%ghost .neqv. col2%ghost
        else
            neq = .true.
        end if
    end function color_neq

```

11.4.5 Tools

Shift color indices by a common offset.

```

<Colors: color: TBP>+≡
    procedure :: add_offset => color_add_offset
<Colors: sub interfaces>+≡
    elemental module subroutine color_add_offset (col, offset)
        class(color_t), intent(inout) :: col
        integer, intent(in) :: offset
    end subroutine color_add_offset
<Colors: procedures>+≡
    elemental module subroutine color_add_offset (col, offset)
        class(color_t), intent(inout) :: col
        integer, intent(in) :: offset
        if (col%defined .and. .not. col%ghost) then
            where (col%c1 /= 0) col%c1 = col%c1 + sign (offset, col%c1)
            where (col%c2 /= 0) col%c2 = col%c2 + sign (offset, col%c2)
        end if
    end subroutine color_add_offset

```

Reassign color indices for an array of colored particle in canonical order. The allocated size of the color map is such that two colors per particle can be accommodated.

The algorithm works directly on the contents of the color objects, it

```

<Colors: public>+≡
    public :: color_canonicalize

```

```

<Colors: sub interfaces>+≡
  module subroutine color_canonicalize (col)
    type(color_t), dimension(:), intent(inout) :: col
  end subroutine color_canonicalize

<Colors: procedures>+≡
  module subroutine color_canonicalize (col)
    type(color_t), dimension(:), intent(inout) :: col
    integer, dimension(2*size(col)) :: map
    integer :: n_col, i, j, k
    n_col = 0
    do i = 1, size (col)
      if (col(i)%defined .and. .not. col(i)%ghost) then
        do j = 1, size (col(i)%c1)
          if (col(i)%c1(j) /= 0) then
            k = find (abs (col(i)%c1(j)), map(:n_col))
            if (k == 0) then
              n_col = n_col + 1
              map(n_col) = abs (col(i)%c1(j))
              k = n_col
            end if
            col(i)%c1(j) = sign (k, col(i)%c1(j))
          end if
          if (col(i)%c2(j) /= 0) then
            k = find (abs (col(i)%c2(j)), map(:n_col))
            if (k == 0) then
              n_col = n_col + 1
              map(n_col) = abs (col(i)%c2(j))
              k = n_col
            end if
            col(i)%c2(j) = sign (k, col(i)%c2(j))
          end if
        end do
      end if
    end do
  contains
    function find (c, array) result (k)
      integer :: k
      integer, intent(in) :: c
      integer, dimension(:), intent(in) :: array
      integer :: i
      k = 0
      do i = 1, size (array)
        if (c == array (i)) then
          k = i
          return
        end if
      end do
    end function find
  end subroutine color_canonicalize

```

Return an array of different color indices from an array of colors. The last argument is a pseudo-color array, where the color entries correspond to the position of the corresponding index entry in the index array. The colors are

assumed to be diagonal.

The algorithm works directly on the contents of the color objects.

```

<Colors: procedures>+≡
  subroutine extract_color_line_indices (col, c_index, col_pos)
    type(color_t), dimension(:), intent(in) :: col
    integer, dimension(:), intent(out), allocatable :: c_index
    type(color_t), dimension(size(col)), intent(out) :: col_pos
    integer, dimension(:), allocatable :: c_tmp
    integer :: i, j, k, n, c
    allocate (c_tmp (sum (col%get_number_of_indices ())), source=0)
    n = 0
    SCAN1: do i = 1, size (col)
      if (col(i)%defined .and. .not. col(i)%ghost) then
        SCAN2: do j = 1, 2
          c = abs (col(i)%c1(j))
          if (c /= 0) then
            do k = 1, n
              if (c_tmp(k) == c) then
                col_pos(i)%c1(j) = k
                cycle SCAN2
              end if
            end do
            n = n + 1
            c_tmp(n) = c
            col_pos(i)%c1(j) = n
          end if
        end do SCAN2
      end if
    end do SCAN1
    allocate (c_index (n))
    c_index = c_tmp(1:n)
  end subroutine extract_color_line_indices

```

Given a color array, pairwise contract the color lines in all possible ways and return the resulting array of arrays. The input color array must be diagonal, and each color should occur exactly twice, once as color and once as anticolor.

Gluon entries with equal color and anticolor are explicitly excluded.

This algorithm is generic, but for long arrays it is neither efficient, nor does it avoid duplicates. It is intended for small arrays, in particular for the state matrix of a structure-function pair.

The algorithm works directly on the contents of the color objects, it thus depends on the implementation.

```

<Colors: public>+≡
  public :: color_array_make_contractions

<Colors: sub interfaces>+≡
  module subroutine color_array_make_contractions (col_in, col_out)
    type(color_t), dimension(:), intent(in) :: col_in
    type(color_t), dimension(:, :), intent(out), allocatable :: col_out
  end subroutine color_array_make_contractions

<Colors: procedures>+≡
  module subroutine color_array_make_contractions (col_in, col_out)
    type(color_t), dimension(:), intent(in) :: col_in

```

```

type(color_t), dimension(:,:), intent(out), allocatable :: col_out
type(list_t) :: list
type(entry_t), pointer :: entry
integer, dimension(:), allocatable :: c_index
type(color_t), dimension(size(col_in)) :: col_pos
integer :: n_prt, n_c_index
integer, dimension(:), allocatable :: map
integer :: i, j, c
n_prt = size (col_in)
call extract_color_line_indices (col_in, c_index, col_pos)
n_c_index = size (c_index)
allocate (map (n_c_index))
map = 0
call list_append_if_valid (list, map)
entry => list%first
do while (associated (entry))
    do i = 1, n_c_index
        if (entry%map(i) == 0) then
            c = c_index(i)
            do j = i + 1, n_c_index
                if (entry%map(j) == 0) then
                    map = entry%map
                    map(i) = c
                    map(j) = c
                    call list_append_if_valid (list, map)
                end if
            end do
        end if
    end do
    entry => entry%next
end do
call list_to_array (list, col_out)
contains
subroutine list_append_if_valid (list, map)
    type(list_t), intent(inout) :: list
    integer, dimension(:), intent(in) :: map
    type(entry_t), pointer :: entry
    integer :: i, j, c, p
    entry => list%first
    do while (associated (entry))
        if (all (map == entry%map)) return
        entry => entry%next
    end do
    allocate (entry)
    allocate (entry%map (n_c_index))
    entry%map = map
    allocate (entry%col (n_prt))
    do i = 1, n_prt
        do j = 1, 2
            c = col_in(i)%c1(j)
            if (c /= 0) then
                p = col_pos(i)%c1(j)
                entry%col(i)%defined = .true.
                if (map(p) /= 0) then

```

```

        entry%col(i)%c1(j) = sign (map(p), c)
    else
        entry%col(i)%c1(j) = c
    endif
    entry%col(i)%c2(j) = entry%col(i)%c1(j)
end if
end do
if (any (entry%col(i)%c1 /= 0) .and. &
    entry%col(i)%c1(1) == - entry%col(i)%c1(2)) return
end do
if (associated (list%last)) then
    list%last%next => entry
else
    list%first => entry
end if
list%last => entry
list%n = list%n + 1
end subroutine list_append_if_valid
subroutine list_to_array (list, col)
    type(list_t), intent(inout) :: list
    type(color_t), dimension(:,,:), intent(out), allocatable :: col
    type(entry_t), pointer :: entry
    integer :: i
    allocate (col (n_prt, list%n - 1))
    do i = 0, list%n - 1
        entry => list%first
        list%first => list%first%next
        if (i /= 0) col(:,i) = entry%col
        deallocate (entry)
    end do
    list%last => null ()
end subroutine list_to_array
end subroutine color_array_make_contractions

```

Invert the color index, switching from particle to antiparticle. For gluons, we have to swap the order of color entries.

```

<Colors: color: TBP>+≡
    procedure :: invert => color_invert

<Colors: sub interfaces>+≡
    elemental module subroutine color_invert (col)
        class(color_t), intent(inout) :: col
    end subroutine color_invert

<Colors: procedures>+≡
    elemental module subroutine color_invert (col)
        class(color_t), intent(inout) :: col
        if (col%defined .and. .not. col%ghost) then
            col%c1 = - col%c1
            col%c2 = - col%c2
            if (col%c1(1) < 0 .and. col%c1(2) > 0) then
                col%c1 = col%c1(2:1:-1)
                col%c2 = col%c2(2:1:-1)
            end if
        end if
    end if
end if

```



```
end subroutine color_invert
```

Make a color map for two matching color arrays. The result is an array of integer pairs.

```
<Colors: public>+≡
```

```
public :: make_color_map
```

```
<Colors: interfaces>+≡
```

```
interface make_color_map
```

```
module procedure color_make_color_map
```

```
end interface make_color_map
```

```
<Colors: sub interfaces>+≡
```

```
module subroutine color_make_color_map (map, col1, col2)
  integer, dimension(:,:), intent(out), allocatable :: map
  type(color_t), dimension(:), intent(in) :: col1, col2
end subroutine color_make_color_map
```

```
<Colors: procedures>+≡
```

```
module subroutine color_make_color_map (map, col1, col2)
  integer, dimension(:,:), intent(out), allocatable :: map
  type(color_t), dimension(:), intent(in) :: col1, col2
  integer, dimension(:,:), allocatable :: map1
  integer :: i, j, k
  allocate (map1 (2, 2 * sum (col1%get_number_of_indices ())))
  k = 0
  do i = 1, size (col1)
    if (col1(i)%defined .and. .not. col1(i)%ghost) then
      do j = 1, size (col1(i)%c1)
        if (col1(i)%c1(j) /= 0 &
          .and. all (map1(1,:k) /= abs (col1(i)%c1(j)))) then
          k = k + 1
          map1(1,k) = abs (col1(i)%c1(j))
          map1(2,k) = abs (col2(i)%c1(j))
        end if
        if (col1(i)%c2(j) /= 0 &
          .and. all (map1(1,:k) /= abs (col1(i)%c2(j)))) then
          k = k + 1
          map1(1,k) = abs (col1(i)%c2(j))
          map1(2,k) = abs (col2(i)%c2(j))
        end if
      end do
    end do
  end do
  allocate (map (2, k))
  map(:, :) = map1(:, :k)
end subroutine color_make_color_map
```

Translate colors which have a match in the translation table (an array of integer pairs). Color that do not match an entry are simply transferred; this is done by first transferring all components, then modifying entries where appropriate.

```
<Colors: public>+≡
```

```
public :: color_translate
```

```

<Colors: interfaces>+≡
interface color_translate
  module procedure color_translate0
  module procedure color_translate0_offset
  module procedure color_translate1
end interface color_translate

<Colors: sub interfaces>+≡
module subroutine color_translate0 (col, map)
  type(color_t), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
end subroutine color_translate0
module subroutine color_translate0_offset (col, map, offset)
  type(color_t), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
  integer, intent(in) :: offset
end subroutine color_translate0_offset
module subroutine color_translate1 (col, map, offset)
  type(color_t), dimension(:), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
  integer, intent(in), optional :: offset
end subroutine color_translate1

<Colors: procedures>+≡
module subroutine color_translate0 (col, map)
  type(color_t), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
  type(color_t) :: col_tmp
  integer :: i
  if (col%defined .and. .not. col%ghost) then
    col_tmp = col
    do i = 1, size (map,2)
      where (abs (col%c1) == map(1,i))
        col_tmp%c1 = sign (map(2,i), col%c1)
      end where
      where (abs (col%c2) == map(1,i))
        col_tmp%c2 = sign (map(2,i), col%c2)
      end where
    end do
    col = col_tmp
  end if
end subroutine color_translate0

module subroutine color_translate0_offset (col, map, offset)
  type(color_t), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
  integer, intent(in) :: offset
  logical, dimension(size(col%c1)) :: mask1, mask2
  type(color_t) :: col_tmp
  integer :: i
  if (col%defined .and. .not. col%ghost) then
    col_tmp = col
    mask1 = col%c1 /= 0
    mask2 = col%c2 /= 0

```

```

do i = 1, size (map,2)
  where (abs (col%c1) == map(1,i))
    col_tmp%c1 = sign (map(2,i), col%c1)
    mask1 = .false.
  end where
  where (abs (col%c2) == map(1,i))
    col_tmp%c2 = sign (map(2,i), col%c2)
    mask2 = .false.
  end where
end do
col = col_tmp
where (mask1) col%c1 = sign (abs (col%c1) + offset, col%c1)
where (mask2) col%c2 = sign (abs (col%c2) + offset, col%c2)
end if
end subroutine color_translate0_offset

module subroutine color_translate1 (col, map, offset)
  type(color_t), dimension(:), intent(inout) :: col
  integer, dimension(:,:), intent(in) :: map
  integer, intent(in), optional :: offset
  integer :: i
  if (present (offset)) then
    do i = 1, size (col)
      call color_translate0_offset (col(i), map, offset)
    end do
  else
    do i = 1, size (col)
      call color_translate0 (col(i), map)
    end do
  end if
end if
end subroutine color_translate1

```

Merge two color objects by taking the first entry from the first and the first entry from the second argument. Makes sense only if the input colors are defined (and diagonal). If either one is undefined, transfer the defined one.

```

<Colors: color: TBP>+≡
  generic :: operator(.merge.) => merge_colors
  procedure, private :: merge_colors

<Colors: sub interfaces>+≡
  elemental module function merge_colors (col1, col2) result (col)
    type(color_t) :: col
    class(color_t), intent(in) :: col1, col2
  end function merge_colors

<Colors: procedures>+≡
  elemental module function merge_colors (col1, col2) result (col)
    type(color_t) :: col
    class(color_t), intent(in) :: col1, col2
    if (color_is_defined (col1) .and. color_is_defined (col2)) then
      if (color_is_ghost (col1) .and. color_is_ghost (col2)) then
        call color_init_trivial_ghost (col, .true.)
      else
        call color_init_arrays (col, col1%c1, col2%c1)
      end if
    end if
  end function merge_colors

```

```

        end if
    else if (color_is_defined (col1)) then
        call color_init_array (col, col1%c1)
    else if (color_is_defined (col2)) then
        call color_init_array (col, col2%c1)
    end if
end function merge_colors

```

Merge up to two (diagonal!) color objects. The result inherits the unmatched color lines of the input colors. If one of the input colors is undefined, the output is undefined as well. It must be in a supported color representation.

A color-ghost object should not actually occur in real-particle events, but for completeness we define its behavior. For simplicity, it is identified as a color-octet with zero color/anticolor. It can only couple to a triplet or antitriplet. A fusion of triplet with matching antitriplet will yield a singlet, not a ghost, however.

If the fusion fails, the result is undefined.

```

<Colors: color: TBP>+≡
    generic :: operator (.fuse.) => color_fusion
    procedure, private :: color_fusion

<Colors: sub interfaces>+≡
    module function color_fusion (col1, col2) result (col)
        class(color_t), intent(in) :: col1, col2
        type(color_t) :: col
    end function color_fusion

<Colors: procedures>+≡
    module function color_fusion (col1, col2) result (col)
        class(color_t), intent(in) :: col1, col2
        type(color_t) :: col
        integer, dimension(2) :: ctype
        if (col1%is_defined () .and. col2%is_defined ()) then
            if (col1%is_diagonal () .and. col2%is_diagonal ()) then
                ctype = [col1%get_type (), col2%get_type ()]
                select case (ctype(1))
                    case (1)
                        select case (ctype(2))
                            case (1,3,-3,8)
                                col = col2
                        end select
                    case (3)
                        select case (ctype(2))
                            case (1)
                                col = col1
                            case (-3)
                                call t_a (col1%get_col (), col2%get_acl ())
                            case (8)
                                call t_o (col1%get_col (), col2%get_acl (), &
                                    & col2%get_col ())
                        end select
                    case (-3)
                        select case (ctype(2))
                            case (1)

```

```

        col = col1
    case (3)
        call t_a (col2%get_col (), col1%get_acl ())
    case (8)
        call a_o (col1%get_acl (), col2%get_col (), &
            & col2%get_acl ())
    end select
case (8)
    select case (ctype(2))
    case (1)
        col = col1
    case (3)
        call t_o (col2%get_col (), col1%get_acl (), &
            & col1%get_col ())
    case (-3)
        call a_o (col2%get_acl (), col1%get_col (), &
            & col1%get_acl ())
    case (8)
        call o_o (col1%get_col (), col1%get_acl (), &
            & col2%get_col (), col2%get_acl ())
    end select
    end select
end if
end if
contains
subroutine t_a (c1, c2)
    integer, intent(in) :: c1, c2
    if (c1 == c2) then
        call col%init_col_acl (0, 0)
    else
        call col%init_col_acl (c1, c2)
    end if
end subroutine t_a
subroutine t_o (c1, c2, c3)
    integer, intent(in) :: c1, c2, c3
    if (c1 == c2) then
        call col%init_col_acl (c3, 0)
    else if (c2 == 0 .and. c3 == 0) then
        call col%init_col_acl (c1, 0)
    end if
end subroutine t_o
subroutine a_o (c1, c2, c3)
    integer, intent(in) :: c1, c2, c3
    if (c1 == c2) then
        call col%init_col_acl (0, c3)
    else if (c2 == 0 .and. c3 == 0) then
        call col%init_col_acl (0, c1)
    end if
end subroutine a_o
subroutine o_o (c1, c2, c3, c4)
    integer, intent(in) :: c1, c2, c3, c4
    if (all ([c1,c2,c3,c4] /= 0)) then
        if (c2 == c3 .and. c4 == c1) then
            call col%init_col_acl (0, 0)

```

```

        else if (c2 == c3) then
            call col%init_col_acl (c1, c4)
        else if (c4 == c1) then
            call col%init_col_acl (c3, c2)
        end if
    end if
end subroutine o_o
end function color_fusion

```

Compute the color factor, given two interfering color arrays.

<Colors: public>+≡

```
public :: compute_color_factor
```

<Colors: sub interfaces>+≡

```

module function compute_color_factor (col1, col2, nc) result (factor)
    real(default) :: factor
    type(color_t), dimension(:), intent(in) :: col1, col2
    integer, intent(in), optional :: nc
end function compute_color_factor

```

<Colors: procedures>+≡

```

module function compute_color_factor (col1, col2, nc) result (factor)
    real(default) :: factor
    type(color_t), dimension(:), intent(in) :: col1, col2
    integer, intent(in), optional :: nc
    type(color_t), dimension(size(col1)) :: col
    integer :: ncol, nloops, nghost
    ncol = 3; if (present(nc)) ncol = nc
    col = col1 .merge. col2
    nloops = count_color_loops (col)
    nghost = count (col%is_ghost ())
    factor = real (ncol, default) ** (nloops - nghost)
    if (color_ghost_parity (col)) factor = - factor
end function compute_color_factor

```

We have a pair of color index arrays which corresponds to a squared matrix element. We want to determine the number of color loops in this square matrix element. So we first copy the colors (stored in a single color array with a pair of color lists in each entry) to a temporary where the color indices are shifted by some offset. We then recursively follow each loop, starting at the first color that has the offset, resetting the first color index to the loop index and each further index to zero as we go. We check that (a) each color index occurs twice within the left (right) color array, (b) the loops are closed, so we always come back to a line which has the loop index.

In order for the algorithm to work we have to conjugate the colors of initial state particles (one for decays, two for scatterings) into their corresponding anticolors of outgoing particles.

<Colors: public>+≡

```
public :: count_color_loops
```

<Colors: sub interfaces>+≡

```

module function count_color_loops (col) result (count)
    integer :: count

```

```

        type(color_t), dimension(:), intent(in) :: col
    end function count_color_loops

(Colors: procedures)+≡
module function count_color_loops (col) result (count)
    integer :: count
    type(color_t), dimension(:), intent(in) :: col
    type(color_t), dimension(size(col)) :: cc
    integer :: i, n, offset
    cc = col
    n = size (cc)
    offset = n
    call color_add_offset (cc, offset)
    count = 0
    SCAN_LOOPS: do
        do i = 1, n
            if (color_is_nonzero (cc(i))) then
                if (any (cc(i)%c1 > offset)) then
                    count = count + 1
                    call follow_line1 (pick_new_line (cc(i)%c1, count, 1))
                    cycle SCAN_LOOPS
                end if
            end if
        end do
        exit SCAN_LOOPS
    end do SCAN_LOOPS
contains
    function pick_new_line (c, reset_val, sgn) result (line)
        integer :: line
        integer, dimension(:), intent(inout) :: c
        integer, intent(in) :: reset_val
        integer, intent(in) :: sgn
        integer :: i
        if (any (c == count)) then
            line = count
        else
            do i = 1, size (c)
                if (sign (1, c(i)) == sgn .and. abs (c(i)) > offset) then
                    line = c(i)
                    c(i) = reset_val
                    return
                end if
            end do
            call color_mismatch
        end if
    end function pick_new_line

    subroutine reset_line (c, line)
        integer, dimension(:), intent(inout) :: c
        integer, intent(in) :: line
        integer :: i
        do i = 1, size (c)
            if (c(i) == line) then
                c(i) = 0
            end if
        end do
    end subroutine reset_line

```

```

        end if
    end do
end subroutine reset_line

recursive subroutine follow_line1 (line)
    integer, intent(in) :: line
    integer :: i
    if (line == count) return
    do i = 1, n
        if (any (cc(i)%c1 == -line)) then
            call reset_line (cc(i)%c1, -line)
            call follow_line2 (pick_new_line (cc(i)%c2, 0, sign (1, -line)))
            return
        end if
    end do
    call color_mismatch ()
end subroutine follow_line1

recursive subroutine follow_line2 (line)
    integer, intent(in) :: line
    integer :: i
    do i = 1, n
        if (any (cc(i)%c2 == -line)) then
            call reset_line (cc(i)%c2, -line)
            call follow_line1 (pick_new_line (cc(i)%c1, 0, sign (1, -line)))
            return
        end if
    end do
    call color_mismatch ()
end subroutine follow_line2

subroutine color_mismatch ()
    call color_write (col)
    print *
    call msg_fatal ("Color flow mismatch: Non-closed color lines appear during ", &
        [var_str ("the evaluation of color correlations. This can happen if there "), &
        var_str ("are different color structures in the initial or final state of "), &
        var_str ("the process definition. If so, please use separate processes for "), &
        var_str ("the different initial / final states. In a future WHIZARD version "), &
        var_str ("this will be fixed.")])
end subroutine color_mismatch
end function count_color_loops

```

11.4.6 Unit tests

Test module, followed by the corresponding implementation module.

```

(colors_ut.f90)≡
    <File header>

```

```

module colors_ut
    use unit_tests
    use colors_uti

```



```

    <Standard module head>

    <Colors: public test>

    contains

    <Colors: test driver>

    end module colors_ut
<colors_uti.f90>≡
    <File header>

    module colors_uti

        use colors

    <Standard module head>

    <Colors: test declarations>

    contains

    <Colors: tests>

    end module colors_uti
API: driver for the unit tests below.
<Colors: public test>≡
    public :: color_test
<Colors: test driver>≡
    subroutine color_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Colors: execute tests>
    end subroutine color_test

This is a color counting test.
<Colors: execute tests>≡
    call test (color_1, "color_1", &
        "check color counting", &
        u, results)
<Colors: test declarations>≡
    public :: color_1
<Colors: tests>≡
    subroutine color_1 (u)
        integer, intent(in) :: u
        type(color_t), dimension(4) :: col1, col2, col
        type(color_t), dimension(:), allocatable :: col3
        type(color_t), dimension(:,:), allocatable :: col_array
        integer :: count, i
        call col1%init_col_acl ([1, 0, 2, 3], [0, 1, 3, 2])

```

```

col2 = col1
call color_write (col1, u)
write (u, "(A)")
call color_write (col2, u)
write (u, "(A)")
col = col1 .merge. col2
call color_write (col, u)
write (u, "(A)")
count = count_color_loops (col)
write (u, "(A,I1)") "Number of color loops (3): ", count
call col2%init_col_acl ([1, 0, 2, 3], [0, 2, 3, 1])
call color_write (col1, u)
write (u, "(A)")
call color_write (col2, u)
write (u, "(A)")
col = col1 .merge. col2
call color_write (col, u)
write (u, "(A)")
count = count_color_loops (col)
write (u, "(A,I1)") "Number of color loops (2): ", count
write (u, "(A)")
allocate (col3 (4))
call color_init_from_array (col3, &
    reshape ([1, 0, 0, -1, 2, -3, 3, -2], &
        [2, 4]))
call color_write (col3, u)
write (u, "(A)")
call color_array_make_contractions (col3, col_array)
write (u, "(A)") "Contractions:"
do i = 1, size (col_array, 2)
    call color_write (col_array(:,i), u)
    write (u, "(A)")
end do
deallocate (col3)
write (u, "(A)")
allocate (col3 (6))
call color_init_from_array (col3, &
    reshape ([1, -2, 3, 0, 0, -1, 2, -4, -3, 0, 4, 0], &
        [2, 6]))
call color_write (col3, u)
write (u, "(A)")
call color_array_make_contractions (col3, col_array)
write (u, "(A)") "Contractions:"
do i = 1, size (col_array, 2)
    call color_write (col_array(:,i), u)
    write (u, "(A)")
end do
end subroutine color_1

```

A color fusion test.

```

<Colors: execute tests>+=
    call test (color_2, "color_2", &
        "color fusion", &

```

```

        u, results)
<Colors: test declarations>+≡
    public :: color_2
<Colors: tests>+≡
    subroutine color_2 (u)
        integer, intent(in) :: u
        type(color_t) :: s1, t1, t2, a1, a2, o1, o2, o3, o4, g1

        write (u, "(A)")  "*" Test output: color_2"
        write (u, "(A)")  "*"  Purpose: test all combinations for color-object fusion"
        write (u, "(A)")

        call s1%init_col_acl (0,0)
        call t1%init_col_acl (1,0)
        call t2%init_col_acl (2,0)
        call a1%init_col_acl (0,1)
        call a2%init_col_acl (0,2)
        call o1%init_col_acl (1,2)
        call o2%init_col_acl (1,3)
        call o3%init_col_acl (2,3)
        call o4%init_col_acl (2,1)
        call g1%init (ghost=.true.)

        call wrt ("s1", s1)
        call wrt ("t1", t1)
        call wrt ("t2", t2)
        call wrt ("a1", a1)
        call wrt ("a2", a2)
        call wrt ("o1", o1)
        call wrt ("o2", o2)
        call wrt ("o3", o3)
        call wrt ("o4", o4)
        call wrt ("g1", g1)

        write (u, *)

        call wrt ("s1 * s1", s1 .fuse. s1)

        write (u, *)

        call wrt ("s1 * t1", s1 .fuse. t1)
        call wrt ("s1 * a1", s1 .fuse. a1)
        call wrt ("s1 * o1", s1 .fuse. o1)

        write (u, *)

        call wrt ("t1 * s1", t1 .fuse. s1)
        call wrt ("a1 * s1", a1 .fuse. s1)
        call wrt ("o1 * s1", o1 .fuse. s1)

        write (u, *)

        call wrt ("t1 * t1", t1 .fuse. t1)

```

```

write (u, *)

call wrt ("t1 * t2", t1 .fuse. t2)
call wrt ("t1 * a1", t1 .fuse. a1)
call wrt ("t1 * a2", t1 .fuse. a2)
call wrt ("t1 * o1", t1 .fuse. o1)
call wrt ("t2 * o1", t2 .fuse. o1)

write (u, *)

call wrt ("t2 * t1", t2 .fuse. t1)
call wrt ("a1 * t1", a1 .fuse. t1)
call wrt ("a2 * t1", a2 .fuse. t1)
call wrt ("o1 * t1", o1 .fuse. t1)
call wrt ("o1 * t2", o1 .fuse. t2)

write (u, *)

call wrt ("a1 * a1", a1 .fuse. a1)

write (u, *)

call wrt ("a1 * a2", a1 .fuse. a2)
call wrt ("a1 * o1", a1 .fuse. o1)
call wrt ("a2 * o2", a2 .fuse. o2)

write (u, *)

call wrt ("a2 * a1", a2 .fuse. a1)
call wrt ("o1 * a1", o1 .fuse. a1)
call wrt ("o2 * a2", o2 .fuse. a2)

write (u, *)

call wrt ("o1 * o1", o1 .fuse. o1)

write (u, *)

call wrt ("o1 * o2", o1 .fuse. o2)
call wrt ("o1 * o3", o1 .fuse. o3)
call wrt ("o1 * o4", o1 .fuse. o4)

write (u, *)

call wrt ("o2 * o1", o2 .fuse. o1)
call wrt ("o3 * o1", o3 .fuse. o1)
call wrt ("o4 * o1", o4 .fuse. o1)

write (u, *)

call wrt ("g1 * g1", g1 .fuse. g1)

write (u, *)

```

```

call wrt ("g1 * s1", g1 .fuse. s1)
call wrt ("g1 * t1", g1 .fuse. t1)
call wrt ("g1 * a1", g1 .fuse. a1)
call wrt ("g1 * o1", g1 .fuse. o1)

write (u, *)

call wrt ("s1 * g1", s1 .fuse. g1)
call wrt ("t1 * g1", t1 .fuse. g1)
call wrt ("a1 * g1", a1 .fuse. g1)
call wrt ("o1 * g1", o1 .fuse. g1)

write (u, "(A)")
write (u, "(A)")  "** Test output end: color_2"

contains

subroutine wrt (s, col)
  character(*), intent(in) :: s
  class(color_t), intent(in) :: col
  write (u, "(A,1x,'=',1x)", advance="no")  s
  call col%write (u)
  write (u, *)
end subroutine wrt

end subroutine color_2

```

11.4.7 The Madgraph color model

This section describes the method for matrix element and color flow calculation within Madgraph.

For each Feynman diagram, the colorless amplitude for a specified helicity and momentum configuration (in- and out- combined) is computed:

$$A_d(p, h) \quad (11.1)$$

Inserting color, the squared matrix element for definite helicity and momentum is

$$M^2(p, h) = \sum_{dd'} A_d(p, h) C_{dd'} A_{d'}^*(p, h) \quad (11.2)$$

where $C_{dd'}$ describes the color interference of the two diagrams A_d and $A_{d'}$, which is independent of momentum and helicity and can be calculated for each Feynman diagram pair by reducing it to the corresponding color graph. Obviously, one could combine all diagrams with identical color structure, such that the index d runs only over different color graphs. For colorless diagrams all elements of $C_{dd'}$ are equal to unity.

The hermitian matrix $C_{dd'}$ is diagonalized once and for all, such that it can be written in the form

$$C_{dd'} = \sum_{\lambda} c_d^{\lambda} \lambda c_{d'}^{\lambda*}, \quad (11.3)$$

where the eigenvectors c_d are normalized,

$$\sum_d |c_d^\lambda|^2 = 1, \quad (11.4)$$

and the λ values are the corresponding eigenvalues. In the colorless case, this means $c_d = 1/\sqrt{N_d}$ for all diagrams (N_d = number of diagrams), and $\lambda = N_d$ is the only nonzero eigenvalue.

Consequently, the squared matrix element for definite helicity and momentum can also be written as

$$M^2(p, h) = \sum_\lambda A_\lambda(p, h) \lambda A_\lambda(p, h)^* \quad (11.5)$$

with

$$A_\lambda(p, h) = \sum_d c_d^\lambda A_d(p, h). \quad (11.6)$$

For generic spin density matrices, this is easily generalized to

$$M^2(p, h, h') = \sum_\lambda A_\lambda(p, h) \lambda A_\lambda(p, h')^* \quad (11.7)$$

To determine the color flow probabilities of a given momentum-helicity configuration, the color flow amplitudes are calculated as

$$a_f(p, h) = \sum_d \beta_d^f A_d(p, h), \quad (11.8)$$

where the coefficients β_d^f describe the amplitude for a given Feynman diagram (or color graph) d to correspond to a definite color flow f . They are computed from $C_{dd'}$ by transforming this matrix into the color flow basis and neglecting all off-diagonal elements. Again, these coefficients do not depend on momentum or helicity and can therefore be calculated in advance. This gives the color flow transition matrix

$$F^f(p, h, h') = a_f(p, h) a_f^*(p, h') \quad (11.9)$$

which is assumed diagonal in color flow space and is separate from the color-summed transition matrix M^2 . They are, however, equivalent (up to a factor) to leading order in $1/N_c$, and using the color flow transition matrix is appropriate for matching to hadronization.

Note that the color flow transition matrix is not normalized at this stage. To make use of it, we have to fold it with the in-state density matrix to get a pseudo density matrix

$$\hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}}) = \sum_{h_{\text{in}} h'_{\text{in}}} F^f(p, h, h') \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}) \quad (11.10)$$

which gets a meaning only after contracted with projections on the outgoing helicity states k_{out} , given as linear combinations of helicity states with the unitary coefficient matrix $c(k_{\text{out}}, h_{\text{out}})$. Then the probability of finding color flow f when the helicity state k_{out} is measured is given by

$$P^f(p, k_{\text{out}}) = Q^f(p, k_{\text{out}}) / \sum_f Q^f(p, k_{\text{out}}) \quad (11.11)$$

where

$$Q^f(p, k_{\text{out}}) = \sum_{h_{\text{out}} h'_{\text{out}}} c(k_{\text{out}}, h_{\text{out}}) \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}}) c^*(k_{\text{out}}, h'_{\text{out}}) \quad (11.12)$$

However, if we can assume that the out-state helicity basis is the canonical one, we can throw away the off diagonal elements in the color flow density matrix and normalize the ones on the diagonal to obtain

$$P^f(p, h_{\text{out}}) = \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h_{\text{out}}) / \sum_f \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h_{\text{out}}) \quad (11.13)$$

Finally, the color-summed out-state density matrix is computed by the scattering formula

$$\rho_{\text{out}}(p, h_{\text{out}}, h'_{\text{out}}) = \sum_{h_{\text{in}} h'_{\text{in}}} M^2(p, h, h') \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}) \quad (11.14)$$

$$= \sum_{h_{\text{in}} h'_{\text{in}} \lambda} A_\lambda(p, h) \lambda A_\lambda(p, h')^* \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}), \quad (11.15)$$

The trace of ρ_{out} is the squared matrix element, summed over all internal degrees of freedom. To get the squared matrix element for a definite helicity k_{out} and color flow f , one has to project the density matrix onto the given helicity state and multiply with $P^f(p, k_{\text{out}})$.

For diagonal helicities the out-state density reduces to

$$\rho_{\text{out}}(p, h_{\text{out}}) = \sum_{h_{\text{in}} \lambda} \lambda |A_\lambda(p, h)|^2 \rho_{\text{in}}(p, h_{\text{in}}). \quad (11.16)$$

Since no basis transformation is involved, we can use the normalized color flow probability $P^f(p, h_{\text{out}})$ and express the result as

$$\rho_{\text{out}}^f(p, h_{\text{out}}) = \rho_{\text{out}}(p, h_{\text{out}}) P^f(p, h_{\text{out}}) \quad (11.17)$$

$$= \sum_{h_{\text{in}} \lambda} \frac{|a^f(p, h)|^2}{\sum_f |a^f(p, h)|^2} \lambda |A_\lambda(p, h)|^2 \rho_{\text{in}}(p, h_{\text{in}}). \quad (11.18)$$

From these considerations, the following calculation strategy can be derived:

- Before the first event is generated, the color interference matrix $C_{dd'}$ is computed and diagonalized, so the eigenvectors c_d^λ , eigenvalues λ and color flow coefficients β_d^f are obtained. In practice, these calculations are done when the matrix element code is generated, and the results are hardcoded in the matrix element subroutine as **DATA** statements.
- For each event, one loops over helicities once and stores the matrices $A_\lambda(p, h)$ and $a^f(p, h)$. The allowed color flows, helicity combinations and eigenvalues are each labeled by integer indices, so one has to store complex matrices of dimension $N_\lambda \times N_h$ and $N_f \times N_h$, respectively.
- The further strategy depends on the requested information.

1. If colorless diagonal helicity amplitudes are required, the eigenvalues $A_\lambda(p, h)$ are squared, summed with weight λ , and the result contracted with the in-state probability vector $\rho_{\text{in}}(p, h_{\text{in}})$. The result is a probability vector $\rho_{\text{out}}(p, h_{\text{out}})$.
2. For colored diagonal helicity amplitudes, the color coefficients $a^f(p, h)$ are also squared and used as weights to obtain the color-flow probability vector $\rho_{\text{out}}^f(p, h_{\text{out}})$.
3. For colorless non-diagonal helicity amplitudes, we contract the tensor product of $A_\lambda(p, h)$ with $A_\lambda(p, h')$, weighted with λ , with the correlated in-state density matrix, to obtain a correlated out-state density matrix.
4. In the general (colored, non-diagonal) case, we do the same as in the colorless case, but return the un-normalized color flow density matrix $\hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}})$ in addition. When the relevant helicity basis is known, the latter can be used by the caller program to determine flow probabilities. (In reality, we assume the canonical basis and reduce the correlated out-state density to its diagonal immediately.)

11.5 Flavors: Particle properties

This module contains a type for holding the flavor code, and all functions that depend on the model, i.e., that determine particle properties.

The PDG code is packed in a special `flavor` type. (This prohibits meaningless operations, and it allows for a different implementation, e.g., some non-PDG scheme internally, if appropriate at some point.)

There are lots of further particle properties that depend on the model. Implementing a flyweight pattern, the associated field data object is to be stored in a central area, the `flavor` object just receives a pointer to this, so all queries can be delegated.

```
<flavors.f90>≡
  <File header>

  module flavors

    <Use kinds>
    <Use strings>
    use physics_defs, only: UNDEFINED
    use model_data
    use colors, only: color_t

    <Standard module head>

    <Flavors: public>

    <Flavors: types>

    <Flavors: interfaces>

    interface
    <Flavors: sub interfaces>
    end interface

  end module flavors

<flavors_sub.f90>≡
  <File header>

  submodule (flavors) flavors_s

    use io_units
    use diagnostics
    use physics_defs, only: INVALID
    use physics_defs, only: HADRON_REMNANT
    use physics_defs, only: HADRON_REMNANT_SINGLET
    use physics_defs, only: HADRON_REMNANT_TRIPLET
    use physics_defs, only: HADRON_REMNANT_OCTET

    implicit none

  contains

    <Flavors: procedures>
```

```
end submodule flavors_s
```

11.5.1 The flavor type

The flavor type is an integer representing the PDG code, or undefined (zero). Negative codes represent antiparticles. They should be used only for particles which do have a distinct antiparticle.

The `hard_process` flag can be set for particles that are participating in the hard interaction.

The `radiated` flag can be set for particles that are the result of a beam-structure interaction (hadron beam remnant, ISR photon, etc.), not of the hard interaction itself.

Further properties of the given flavor can be retrieved via the particle-data pointer, if it is associated.

```
<Flavors: public>≡
  public :: flavor_t

<Flavors: types>≡
  type :: flavor_t
    private
    integer :: f = UNDEFINED
    logical :: hard_process = .false.
    logical :: radiated = .false.
    type(field_data_t), pointer :: field_data => null ()
  contains
    <Flavors: flavor: TBP>
  end type flavor_t
```

Initializer form. If the model is assigned, the procedure is impure, therefore we have to define a separate array version.

Note: The pure elemental subroutines can't have an `intent(out)` CLASS argument (because of the potential for an impure finalizer in a type extension), so we stick to `intent(inout)` and (re)set all components explicitly.

```
<Flavors: flavor: TBP>≡
  generic :: init => &
    flavor_init_empty, &
    flavor_init, &
    flavor_init_field_data, &
    flavor_init_model, &
    flavor_init_model_alt, &
    flavor_init_name_model
  procedure, private :: flavor_init_empty
  procedure, private :: flavor_init
  procedure, private :: flavor_init_field_data
  procedure, private :: flavor_init_model
  procedure, private :: flavor_init_model_alt
  procedure, private :: flavor_init_name_model

<Flavors: sub interfaces>≡
  elemental module subroutine flavor_init_empty (flv)
    class(flavor_t), intent(inout) :: flv
```

```

end subroutine flavor_init_empty
elemental module subroutine flavor_init (flv, f)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
end subroutine flavor_init
impure elemental module subroutine flavor_init_field_data (flv, field_data)
  class(flavor_t), intent(inout) :: flv
  type(field_data_t), intent(in), target :: field_data
end subroutine flavor_init_field_data
impure elemental module subroutine flavor_init_model (flv, f, model)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
  class(model_data_t), intent(in), target :: model
end subroutine flavor_init_model
impure elemental module subroutine flavor_init_model_alt (flv, f, model, alt_model)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
  class(model_data_t), intent(in), target :: model, alt_model
end subroutine flavor_init_model_alt
impure elemental module subroutine flavor_init_name_model (flv, name, model)
  class(flavor_t), intent(inout) :: flv
  type(string_t), intent(in) :: name
  class(model_data_t), intent(in), target :: model
end subroutine flavor_init_name_model

```

(Flavors: procedures)≡

```

elemental module subroutine flavor_init_empty (flv)
  class(flavor_t), intent(inout) :: flv
  flv%f = UNDEFINED
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => null ()
end subroutine flavor_init_empty

elemental module subroutine flavor_init (flv, f)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
  flv%f = f
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => null ()
end subroutine flavor_init

impure elemental module subroutine flavor_init_field_data (flv, field_data)
  class(flavor_t), intent(inout) :: flv
  type(field_data_t), intent(in), target :: field_data
  flv%f = field_data%get_pdg ()
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => field_data
end subroutine flavor_init_field_data

impure elemental module subroutine flavor_init_model (flv, f, model)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f

```

```

class(model_data_t), intent(in), target :: model
flv%f = f
flv%hard_process = .false.
flv%radiated = .false.
flv%field_data => model%get_field_ptr (f, check=.true.)
end subroutine flavor_init_model

impure elemental module subroutine flavor_init_model_alt (flv, f, model, alt_model)
class(flavor_t), intent(inout) :: flv
integer, intent(in) :: f
class(model_data_t), intent(in), target :: model, alt_model
flv%f = f
flv%hard_process = .false.
flv%radiated = .false.
flv%field_data => model%get_field_ptr (f, check=.false.)
if (.not. associated (flv%field_data)) then
  flv%field_data => alt_model%get_field_ptr (f, check=.false.)
  if (.not. associated (flv%field_data)) then
    write (msg_buffer, "(A,1x,I0,1x,A,1x,A,1x,A,1x,A)") &
      "Particle with code", f, &
      "found neither in model", char (model%get_name ()), &
      "nor in model", char (alt_model%get_name ())
    call msg_fatal ()
  end if
end if
end subroutine flavor_init_model_alt

impure elemental module subroutine flavor_init_name_model (flv, name, model)
class(flavor_t), intent(inout) :: flv
type(string_t), intent(in) :: name
class(model_data_t), intent(in), target :: model
flv%f = model%get_pdg (name)
flv%hard_process = .false.
flv%radiated = .false.
flv%field_data => model%get_field_ptr (name, check=.true.)
end subroutine flavor_init_name_model

```

Set the radiated flag.

```

<Flavors: flavor: TBP>+≡
  procedure :: tag_radiated => flavor_tag_radiated

<Flavors: sub interfaces>+≡
  elemental module subroutine flavor_tag_radiated (flv)
    class(flavor_t), intent(inout) :: flv
  end subroutine flavor_tag_radiated

<Flavors: procedures>+≡
  elemental module subroutine flavor_tag_radiated (flv)
    class(flavor_t), intent(inout) :: flv
    flv%radiated = .true.
  end subroutine flavor_tag_radiated

```

Set the hard_process flag.

```

<Flavors: flavor: TBP>+≡

```

```

    procedure :: tag_hard_process => flavor_tag_hard_process
<Flavors: sub interfaces>+≡
    elemental module subroutine flavor_tag_hard_process (flv, hard)
        class(flavor_t), intent(inout) :: flv
        logical, intent(in), optional :: hard
    end subroutine flavor_tag_hard_process
<Flavors: procedures>+≡
    elemental module subroutine flavor_tag_hard_process (flv, hard)
        class(flavor_t), intent(inout) :: flv
        logical, intent(in), optional :: hard
        if (present (hard)) then
            flv%hard_process = hard
        else
            flv%hard_process = .true.
        end if
    end subroutine flavor_tag_hard_process

```

Undefine the flavor state:

```

<Flavors: flavor: TBP>+≡
    procedure :: undefine => flavor_undefine
<Flavors: sub interfaces>+≡
    elemental module subroutine flavor_undefine (flv)
        class(flavor_t), intent(inout) :: flv
    end subroutine flavor_undefine
<Flavors: procedures>+≡
    elemental module subroutine flavor_undefine (flv)
        class(flavor_t), intent(inout) :: flv
        flv%f = UNDEFINED
        flv%field_data => null ()
    end subroutine flavor_undefine

```

Output: dense, no linebreak

A hard-process tag is only shown if debugging is on.

```

<Flavors: flavor: TBP>+≡
    procedure :: write => flavor_write
<Flavors: sub interfaces>+≡
    module subroutine flavor_write (flv, unit)
        class(flavor_t), intent(in) :: flv
        integer, intent(in), optional :: unit
    end subroutine flavor_write
<Flavors: procedures>+≡
    module subroutine flavor_write (flv, unit)
        class(flavor_t), intent(in) :: flv
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (associated (flv%field_data)) then
            write (u, "(A)", advance="no") "f("
        else
            write (u, "(A)", advance="no") "p("

```

```

end if
write (u, "(I0)", advance="no") flv%f
if (flv%radiated) then
    write (u, "('*')", advance="no")
end if
if (msg_level (D_FLAVOR) >= DEBUG) then
    if (flv%hard_process) then
        write (u, "('#')", advance="no")
    end if
end if
write (u, "(A)", advance="no") " "
end subroutine flavor_write

```

<Flavors: public>+≡

```
public :: flavor_write_array
```

<Flavors: sub interfaces>+≡

```

module subroutine flavor_write_array (flv, unit)
    type(flavor_t), intent(in), dimension(:) :: flv
    integer, intent(in), optional :: unit
end subroutine flavor_write_array

```

<Flavors: procedures>+≡

```

module subroutine flavor_write_array (flv, unit)
    type(flavor_t), intent(in), dimension(:) :: flv
    integer, intent(in), optional :: unit
    integer :: u, i_flv
    u = given_output_unit (unit); if (u < 0) return
    do i_flv = 1, size (flv)
        call flv(i_flv)%write (u)
        if (i_flv /= size (flv)) write (u,"(A)", advance = "no") " / "
    end do
    write (u,"(A)")
end subroutine flavor_write_array

```

Binary I/O. Currently, the model information is not written/read, so after reading the particle-data pointer is empty.

<Flavors: flavor: TBP>+≡

```

procedure :: write_raw => flavor_write_raw
procedure :: read_raw => flavor_read_raw

```

<Flavors: sub interfaces>+≡

```

module subroutine flavor_write_raw (flv, u)
    class(flavor_t), intent(in) :: flv
    integer, intent(in) :: u
end subroutine flavor_write_raw
module subroutine flavor_read_raw (flv, u, iostat)
    class(flavor_t), intent(out) :: flv
    integer, intent(in) :: u
    integer, intent(out), optional :: iostat
end subroutine flavor_read_raw

```

<Flavors: procedures>+≡

```

module subroutine flavor_write_raw (flv, u)
    class(flavor_t), intent(in) :: flv

```

```

integer, intent(in) :: u
write (u) flv%f
write (u) flv%radiated
write (u) flv%hard_process
end subroutine flavor_write_raw

module subroutine flavor_read_raw (flv, u, iostat)
class(flavor_t), intent(out) :: flv
integer, intent(in) :: u
integer, intent(out), optional :: iostat
read (u, iostat=iostat) flv%f
if (present (iostat)) then
  if (iostat /= 0) return
end if
read (u, iostat=iostat) flv%radiated
read (u, iostat=iostat) flv%hard_process
end subroutine flavor_read_raw

```

Assignment

Default assignment of flavor objects is possible, but cannot be used in pure procedures, because a pointer assignment is involved.

Assign the particle pointer separately. This cannot be elemental, so we define a scalar and an array version explicitly. We refer to an array of flavors, not an array of models.

```

<Flavors: flavor: TBP> +=
  procedure :: set_model => flavor_set_model_single

<Flavors: sub interfaces> +=
  impure elemental module subroutine flavor_set_model_single (flv, model)
    class(flavor_t), intent(inout) :: flv
    class(model_data_t), intent(in), target :: model
  end subroutine flavor_set_model_single

<Flavors: procedures> +=
  impure elemental module subroutine flavor_set_model_single (flv, model)
    class(flavor_t), intent(inout) :: flv
    class(model_data_t), intent(in), target :: model
    if (flv%f /= UNDEFINED) &
      flv%field_data => model%get_field_ptr (flv%f)
  end subroutine flavor_set_model_single

```

Predicates

Return the definition status. By definition, the flavor object is defined if the flavor PDG code is nonzero.

```

<Flavors: flavor: TBP> +=
  procedure :: is_defined => flavor_is_defined

```

```

<Flavors: sub interfaces>+≡
    elemental module function flavor_is_defined (flv) result (defined)
        class(flavor_t), intent(in) :: flv
        logical :: defined
    end function flavor_is_defined

```

```

<Flavors: procedures>+≡
    elemental module function flavor_is_defined (flv) result (defined)
        class(flavor_t), intent(in) :: flv
        logical :: defined
        defined = flv%f /= UNDEFINED
    end function flavor_is_defined

```

Check for valid flavor (including undefined). This is distinct from the `is_defined` status. Invalid flavor is actually a specific PDG code.

```

<Flavors: flavor: TBP>+≡
    procedure :: is_valid => flavor_is_valid

<Flavors: sub interfaces>+≡
    elemental module function flavor_is_valid (flv) result (valid)
        class(flavor_t), intent(in) :: flv
        logical :: valid
    end function flavor_is_valid

<Flavors: procedures>+≡
    elemental module function flavor_is_valid (flv) result (valid)
        class(flavor_t), intent(in) :: flv
        logical :: valid
        valid = flv%f /= INVALID
    end function flavor_is_valid

```

Return true if the particle-data pointer is associated. (Debugging aid)

```

<Flavors: flavor: TBP>+≡
    procedure :: is_associated => flavor_is_associated

<Flavors: sub interfaces>+≡
    elemental module function flavor_is_associated (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
    end function flavor_is_associated

<Flavors: procedures>+≡
    elemental module function flavor_is_associated (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
        flag = associated (flv%field_data)
    end function flavor_is_associated

```

Check the `radiated` flag. A radiated particle has a definite PDG flavor status, but it is actually a pseudoparticle (a beam remnant) which may be subject to fragmentation.

```

<Flavors: flavor: TBP>+≡
    procedure :: is_radiated => flavor_is_radiated

```



```

<Flavors: sub interfaces>+≡
    elemental module function flavor_is_radiated (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
    end function flavor_is_radiated

```

```

<Flavors: procedures>+≡
    elemental module function flavor_is_radiated (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
        flag = flv%radiated
    end function flavor_is_radiated

```

Check the `hard_process` flag. A particle is tagged with this flag if it participates in the hard interaction and is not a beam remnant.

```

<Flavors: flavor: TBP>+≡
    procedure :: is_hard_process => flavor_is_hard_process

<Flavors: sub interfaces>+≡
    elemental module function flavor_is_hard_process (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
    end function flavor_is_hard_process

<Flavors: procedures>+≡
    elemental module function flavor_is_hard_process (flv) result (flag)
        class(flavor_t), intent(in) :: flv
        logical :: flag
        flag = flv%hard_process
    end function flavor_is_hard_process

```

Accessing contents

With the exception of the PDG code, all particle property enquiries are delegated to the `field_data` pointer. If this is unassigned, some access function will crash.

Return the flavor as an integer

```

<Flavors: flavor: TBP>+≡
    procedure :: get_pdg => flavor_get_pdg

<Flavors: sub interfaces>+≡
    elemental module function flavor_get_pdg (flv) result (f)
        integer :: f
        class(flavor_t), intent(in) :: flv
    end function flavor_get_pdg

<Flavors: procedures>+≡
    elemental module function flavor_get_pdg (flv) result (f)
        integer :: f
        class(flavor_t), intent(in) :: flv
        f = flv%f
    end function flavor_get_pdg

```

Return the flavor of the antiparticle

```
(Flavors: flavor: TBP)+≡
  procedure :: get_pdg_anti => flavor_get_pdg_anti

(Flavors: sub interfaces)+≡
  elemental module function flavor_get_pdg_anti (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
  end function flavor_get_pdg_anti

(Flavors: procedures)+≡
  elemental module function flavor_get_pdg_anti (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
      if (flv%field_data%has_antiparticle ()) then
        f = -flv%f
      else
        f = flv%f
      end if
    else
      f = 0
    end if
  end function flavor_get_pdg_anti
```

Absolute value:

```
(Flavors: flavor: TBP)+≡
  procedure :: get_pdg_abs => flavor_get_pdg_abs

(Flavors: sub interfaces)+≡
  elemental module function flavor_get_pdg_abs (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
  end function flavor_get_pdg_abs

(Flavors: procedures)+≡
  elemental module function flavor_get_pdg_abs (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
    f = abs (flv%f)
  end function flavor_get_pdg_abs
```

Generic properties

```
(Flavors: flavor: TBP)+≡
  procedure :: is_visible => flavor_is_visible
  procedure :: is_parton => flavor_is_parton
  procedure :: is_beam_remnant => flavor_is_beam_remnant
  procedure :: is_gauge => flavor_is_gauge
  procedure :: is_left_handed => flavor_is_left_handed
  procedure :: is_right_handed => flavor_is_right_handed
  procedure :: is_antiparticle => flavor_is_antiparticle
  procedure :: has_antiparticle => flavor_has_antiparticle
  procedure :: is_stable => flavor_is_stable
  procedure :: get_decays => flavor_get_decays
  procedure :: decays_isotropically => flavor_decays_isotropically
```

```

procedure :: decays_diagonal => flavor_decays_diagonal
procedure :: has_decay_helicity => flavor_has_decay_helicity
procedure :: get_decay_helicity => flavor_get_decay_helicity
procedure :: is_polarized => flavor_is_polarized

```

(Flavors: sub interfaces)+≡

```

elemental module function flavor_is_visible (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_visible
elemental module function flavor_is_parton (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_parton
elemental module function flavor_is_beam_remnant (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_beam_remnant
elemental module function flavor_is_gauge (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_gauge
elemental module function flavor_is_left_handed (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_left_handed
elemental module function flavor_is_right_handed (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_right_handed
elemental module function flavor_is_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_antiparticle
elemental module function flavor_has_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_has_antiparticle
elemental module function flavor_is_stable (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_is_stable
module subroutine flavor_get_decays (flv, decay)
  class(flavor_t), intent(in) :: flv
  type(string_t), dimension(:), intent(out), allocatable :: decay
  logical :: anti
end subroutine flavor_get_decays
elemental module function flavor_decays_isotropically (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_decays_isotropically
elemental module function flavor_decays_diagonal (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
end function flavor_decays_diagonal

```

```

elemental module function flavor_has_decay_helicity (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
end function flavor_has_decay_helicity
elemental module function flavor_get_decay_helicity (flv) result (hel)
    integer :: hel
    class(flavor_t), intent(in) :: flv
end function flavor_get_decay_helicity
elemental module function flavor_is_polarized (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
end function flavor_is_polarized

<Flavors: procedures>+≡
elemental module function flavor_is_visible (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%is_visible ()
    else
        flag = .false.
    end if
end function flavor_is_visible

elemental module function flavor_is_parton (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%is_parton ()
    else
        flag = .false.
    end if
end function flavor_is_parton

elemental module function flavor_is_beam_remnant (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    select case (abs (flv%f))
    case (HADRON_REMNANT, &
           HADRON_REMNANT_SINGLET, HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET)
        flag = .true.
    case default
        flag = .false.
    end select
end function flavor_is_beam_remnant

elemental module function flavor_is_gauge (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%is_gauge ()
    else
        flag = .false.
    end if
end function flavor_is_gauge

```

```

elemental module function flavor_is_left_handed (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    if (flv%f > 0) then
      flag = flv%field_data%is_left_handed ()
    else
      flag = flv%field_data%is_right_handed ()
    end if
  else
    flag = .false.
  end if
end function flavor_is_left_handed

elemental module function flavor_is_right_handed (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    if (flv%f > 0) then
      flag = flv%field_data%is_right_handed ()
    else
      flag = flv%field_data%is_left_handed ()
    end if
  else
    flag = .false.
  end if
end function flavor_is_right_handed

elemental module function flavor_is_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  flag = flv%f < 0
end function flavor_is_antiparticle

elemental module function flavor_has_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%has_antiparticle ()
  else
    flag = .false.
  end if
end function flavor_has_antiparticle

elemental module function flavor_is_stable (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%is_stable (anti = flv%f < 0)
  else
    flag = .true.
  end if
end function flavor_is_stable

```

```

module subroutine flavor_get_decays (flv, decay)
  class(flavor_t), intent(in) :: flv
  type(string_t), dimension(:), intent(out), allocatable :: decay
  logical :: anti
  anti = flv%f < 0
  if (.not. flv%field_data%is_stable (anti)) then
    call flv%field_data%get_decays (decay, anti)
  end if
end subroutine flavor_get_decays

elemental module function flavor_decays_isotropically (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%decays_isotropically (anti = flv%f < 0)
  else
    flag = .true.
  end if
end function flavor_decays_isotropically

elemental module function flavor_decays_diagonal (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%decays_diagonal (anti = flv%f < 0)
  else
    flag = .true.
  end if
end function flavor_decays_diagonal

elemental module function flavor_has_decay_helicity (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%has_decay_helicity (anti = flv%f < 0)
  else
    flag = .false.
  end if
end function flavor_has_decay_helicity

elemental module function flavor_get_decay_helicity (flv) result (hel)
  integer :: hel
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    hel = flv%field_data%decay_helicity (anti = flv%f < 0)
  else
    hel = 0
  end if
end function flavor_get_decay_helicity

elemental module function flavor_is_polarized (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv

```

```

    if (associated (flv%field_data)) then
        flag = flv%field_data%is_polarized (anti = flv%f < 0)
    else
        flag = .false.
    end if
end function flavor_is_polarized

```

Names:

```

<Flavors: flavor: TBP>+≡
    procedure :: get_name => flavor_get_name
    procedure :: get_tex_name => flavor_get_tex_name

<Flavors: sub interfaces>+≡
    elemental module function flavor_get_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
    end function flavor_get_name
    elemental module function flavor_get_tex_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
    end function flavor_get_tex_name

<Flavors: procedures>+≡
    elemental module function flavor_get_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then
            name = flv%field_data%get_name (flv%f < 0)
        else
            name = "?"
        end if
    end function flavor_get_name

    elemental module function flavor_get_tex_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then
            name = flv%field_data%get_tex_name (flv%f < 0)
        else
            name = "?"
        end if
    end function flavor_get_tex_name

<Flavors: flavor: TBP>+≡
    procedure :: get_spin_type => flavor_get_spin_type
    procedure :: get_multiplicity => flavor_get_multiplicity
    procedure :: get_isospin_type => flavor_get_isospin_type
    procedure :: get_charge_type => flavor_get_charge_type
    procedure :: get_color_type => flavor_get_color_type

<Flavors: sub interfaces>+≡
    elemental module function flavor_get_spin_type (flv) result (type)
        integer :: type
        class(flavor_t), intent(in) :: flv
    end function flavor_get_spin_type

```

```

elemental module function flavor_get_multiplicity (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
end function flavor_get_multiplicity
elemental module function flavor_get_isospin_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
end function flavor_get_isospin_type
elemental module function flavor_get_charge_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
end function flavor_get_charge_type
elemental module function flavor_get_color_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
end function flavor_get_color_type

<Flavors: procedures>+≡
elemental module function flavor_get_spin_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    type = flv%field_data%get_spin_type ()
  else
    type = 1
  end if
end function flavor_get_spin_type

elemental module function flavor_get_multiplicity (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    type = flv%field_data%get_multiplicity ()
  else
    type = 1
  end if
end function flavor_get_multiplicity

elemental module function flavor_get_isospin_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    type = flv%field_data%get_isospin_type ()
  else
    type = 1
  end if
end function flavor_get_isospin_type

elemental module function flavor_get_charge_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    type = flv%field_data%get_charge_type ()
  else
    type = 1
  end if
end function flavor_get_charge_type

```



```

        end if
    end function flavor_get_charge_type

    elemental module function flavor_get_color_type (flv) result (type)
        integer :: type
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then
            if (flavor_is_antiparticle (flv)) then
                type = - flv%field_data%get_color_type ()
            else
                type = flv%field_data%get_color_type ()
            end if
            select case (type)
            case (-1,-8); type = abs (type)
            end select
        else
            type = 1
        end if
    end function flavor_get_color_type

```

These functions return real values:

(Flavors: flavor: TBP)+≡

```

    procedure :: get_charge => flavor_get_charge
    procedure :: get_mass => flavor_get_mass
    procedure :: get_width => flavor_get_width
    procedure :: get_isospin => flavor_get_isospin

```

(Flavors: sub interfaces)+≡

```

    elemental module function flavor_get_charge (flv) result (charge)
        real(default) :: charge
        class(flavor_t), intent(in) :: flv
    end function flavor_get_charge
    elemental module function flavor_get_mass (flv) result (mass)
        real(default) :: mass
        class(flavor_t), intent(in) :: flv
    end function flavor_get_mass
    elemental module function flavor_get_width (flv) result (width)
        real(default) :: width
        class(flavor_t), intent(in) :: flv
    end function flavor_get_width
    elemental module function flavor_get_isospin (flv) result (isospin)
        real(default) :: isospin
        class(flavor_t), intent(in) :: flv
    end function flavor_get_isospin

```

(Flavors: procedures)+≡

```

    elemental module function flavor_get_charge (flv) result (charge)
        real(default) :: charge
        class(flavor_t), intent(in) :: flv
        integer :: charge_type
        if (associated (flv%field_data)) then
            charge_type = flv%get_charge_type ()
            if (charge_type == 0 .or. charge_type == 1) then
                charge = 0
            else

```

```

        if (flavor_is_antiparticle (flv)) then
            charge = - flv%field_data%get_charge ()
        else
            charge = flv%field_data%get_charge ()
        end if
    end if
else
    charge = 0
end if
end function flavor_get_charge

elemental module function flavor_get_mass (flv) result (mass)
    real(default) :: mass
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        mass = flv%field_data%get_mass ()
    else
        mass = 0
    end if
end function flavor_get_mass

elemental module function flavor_get_width (flv) result (width)
    real(default) :: width
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        width = flv%field_data%get_width ()
    else
        width = 0
    end if
end function flavor_get_width

elemental module function flavor_get_isospin (flv) result (isospin)
    real(default) :: isospin
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        if (flavor_is_antiparticle (flv)) then
            isospin = - flv%field_data%get_isospin ()
        else
            isospin = flv%field_data%get_isospin ()
        end if
    else
        isospin = 0
    end if
end function flavor_get_isospin

```

Comparisons

If one of the flavors is undefined, the other defined, they match.

$\langle \text{Flavors: flavor: TBP} \rangle + \equiv$

```

generic :: operator(.match.) => flavor_match
generic :: operator(==) => flavor_eq
generic :: operator(/=) => flavor_neq

```

```

procedure, private :: flavor_match
procedure, private :: flavor_eq
procedure, private :: flavor_neq

<Flavors: sub interfaces>+≡
    elemental module function flavor_match (flv1, flv2) result (eq)
        logical :: eq
        class(flavor_t), intent(in) :: flv1, flv2
    end function flavor_match
    elemental module function flavor_eq (flv1, flv2) result (eq)
        logical :: eq
        class(flavor_t), intent(in) :: flv1, flv2
    end function flavor_eq

<Flavors: procedures>+≡
    elemental module function flavor_match (flv1, flv2) result (eq)
        logical :: eq
        class(flavor_t), intent(in) :: flv1, flv2
        if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
            eq = flv1%f == flv2%f
        else
            eq = .true.
        end if
    end function flavor_match

    elemental module function flavor_eq (flv1, flv2) result (eq)
        logical :: eq
        class(flavor_t), intent(in) :: flv1, flv2
        if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
            eq = flv1%f == flv2%f
        else if (flv1%f == UNDEFINED .and. flv2%f == UNDEFINED) then
            eq = .true.
        else
            eq = .false.
        end if
    end function flavor_eq

<Flavors: sub interfaces>+≡
    elemental module function flavor_neq (flv1, flv2) result (neq)
        logical :: neq
        class(flavor_t), intent(in) :: flv1, flv2
    end function flavor_neq

<Flavors: procedures>+≡
    elemental module function flavor_neq (flv1, flv2) result (neq)
        logical :: neq
        class(flavor_t), intent(in) :: flv1, flv2
        if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
            neq = flv1%f /= flv2%f
        else if (flv1%f == UNDEFINED .and. flv2%f == UNDEFINED) then
            neq = .false.
        else
            neq = .true.
        end if
    end function flavor_neq

```

Tools

Merge two flavor indices. This works only if both are equal or either one is undefined, because we have no off-diagonal flavor entries. Otherwise, generate an invalid flavor.

We cannot use elemental procedures because of the pointer component.

```
<Flavors: public>+≡
    public :: operator(.merge.)

<Flavors: interfaces>≡
    interface operator(.merge.)
        module procedure merge_flavors0
        module procedure merge_flavors1
    end interface

<Flavors: sub interfaces>+≡
    module function merge_flavors0 (flv1, flv2) result (flv)
        type(flavor_t) :: flv
        type(flavor_t), intent(in) :: flv1, flv2
    end function merge_flavors0
    module function merge_flavors1 (flv1, flv2) result (flv)
        type(flavor_t), dimension(:), intent(in) :: flv1, flv2
        type(flavor_t), dimension(size(flv1)) :: flv
    end function merge_flavors1

<Flavors: procedures>+≡
    module function merge_flavors0 (flv1, flv2) result (flv)
        type(flavor_t) :: flv
        type(flavor_t), intent(in) :: flv1, flv2
        if (flavor_is_defined (flv1) .and. flavor_is_defined (flv2)) then
            if (flv1 == flv2) then
                flv = flv1
            else
                flv%f = INVALID
            end if
        else if (flavor_is_defined (flv1)) then
            flv = flv1
        else if (flavor_is_defined (flv2)) then
            flv = flv2
        end if
    end function merge_flavors0

    module function merge_flavors1 (flv1, flv2) result (flv)
        type(flavor_t), dimension(:), intent(in) :: flv1, flv2
        type(flavor_t), dimension(size(flv1)) :: flv
        integer :: i
        do i = 1, size (flv1)
            flv(i) = flv1(i) .merge. flv2(i)
        end do
    end function merge_flavors1
```

Generate consecutive color indices for a given flavor. The indices are counted starting with the stored value of c, so new indices are created each time this (impure) function is called. The counter can be reset by the optional argument

`c_seed` if desired. The optional flag `reverse` is used only for octets. If set, the color and anticolor entries of the octet particle are exchanged.

```

<Flavors: public>+≡
    public :: color_from_flavor

<Flavors: interfaces>+≡
    interface color_from_flavor
        module procedure color_from_flavor0
        module procedure color_from_flavor1
    end interface

<Flavors: sub interfaces>+≡
    module function color_from_flavor0 (flv, c_seed, reverse) result (col)
        type(color_t) :: col
        type(flavor_t), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
    end function color_from_flavor0
    module function color_from_flavor1 (flv, c_seed, reverse) result (col)
        type(flavor_t), dimension(:), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
        type(color_t), dimension(size(flv)) :: col
    end function color_from_flavor1

<Flavors: procedures>+≡
    module function color_from_flavor0 (flv, c_seed, reverse) result (col)
        type(color_t) :: col
        type(flavor_t), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
        integer, save :: c = 1
        logical :: rev
        if (present (c_seed)) c = c_seed
        rev = .false.; if (present (reverse)) rev = reverse
        select case (flavor_get_color_type (flv))
        case (1)
            call col%init ()
        case (3)
            call col%init ([c]); c = c + 1
        case (-3)
            call col%init ([-c]); c = c + 1
        case (8)
            if (rev) then
                call col%init ([c+1, -c]); c = c + 2
            else
                call col%init ([c, -(c+1)]); c = c + 2
            end if
        end select
    end function color_from_flavor0

    module function color_from_flavor1 (flv, c_seed, reverse) result (col)
        type(flavor_t), dimension(:), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
        type(color_t), dimension(size(flv)) :: col

```

```

integer :: i
col(1) = color_from_flavor0 (flv(1), c_seed, reverse)
do i = 2, size (flv)
    col(i) = color_from_flavor0 (flv(i), reverse=reverse)
end do
end function color_from_flavor1

```

This procedure returns the flavor object for the antiparticle. The antiparticle code may either be the same code or its negative.

```

<Flavors: flavor: TBP>+=
    procedure :: anti => flavor_anti

<Flavors: sub interfaces>+=
    module function flavor_anti (flv) result (aflv)
        type(flavor_t) :: aflv
        class(flavor_t), intent(in) :: flv
    end function flavor_anti

<Flavors: procedures>+=
    module function flavor_anti (flv) result (aflv)
        type(flavor_t) :: aflv
        class(flavor_t), intent(in) :: flv
        if (flavor_has_antiparticle (flv)) then
            aflv%f = - flv%f
        else
            aflv%f = flv%f
        end if
        aflv%field_data => flv%field_data
    end function flavor_anti

```

11.6 Quantum numbers

This module collects helicity, color, and flavor in a single type and defines procedures

```
<quantum_numbers.f90>≡  
  <File header>  
  
  module quantum_numbers  
  
    use model_data  
    use helicities  
    use colors  
    use flavors  
  
    <Standard module head>  
  
    <Quantum numbers: public>  
  
    <Quantum numbers: types>  
  
    <Quantum numbers: interfaces>  
  
    interface  
    <Quantum numbers: sub interfaces>  
    end interface  
  
  end module quantum_numbers  
  
<quantum_numbers_sub.f90>≡  
  <File header>  
  
  submodule (quantum_numbers) quantum_numbers_s  
  
    use io_units  
  
    implicit none  
  
    contains  
  
    <Quantum numbers: procedures>  
  
  end submodule quantum_numbers_s
```

11.6.1 The quantum number type

```
<Quantum numbers: public>≡  
  public :: quantum_numbers_t  
  
<Quantum numbers: types>≡  
  type :: quantum_numbers_t  
    private  
    type(flavor_t) :: f  
    type(color_t) :: c
```

```

    type(helicity_t) :: h
    integer :: sub = 0
contains
  <Quantum numbers: quantum numbers: TBP>
end type quantum_numbers_t

```

Define quantum numbers: Initializer form. All arguments may be present or absent.

Some elemental initializers are impure because they set the `flv` component. This implies transfer of a pointer behind the scenes.

```

<Quantum numbers: quantum numbers: TBP>≡
  generic :: init => &
    quantum_numbers_init_f, &
    quantum_numbers_init_c, &
    quantum_numbers_init_h, &
    quantum_numbers_init_fc, &
    quantum_numbers_init_fh, &
    quantum_numbers_init_ch, &
    quantum_numbers_init_fch, &
    quantum_numbers_init_fs, &
    quantum_numbers_init_fhs, &
    quantum_numbers_init_fcs, &
    quantum_numbers_init_fhcs
  procedure, private :: quantum_numbers_init_f
  procedure, private :: quantum_numbers_init_c
  procedure, private :: quantum_numbers_init_h
  procedure, private :: quantum_numbers_init_fc
  procedure, private :: quantum_numbers_init_fh
  procedure, private :: quantum_numbers_init_ch
  procedure, private :: quantum_numbers_init_fch
  procedure, private :: quantum_numbers_init_fs
  procedure, private :: quantum_numbers_init_fhs
  procedure, private :: quantum_numbers_init_fcs
  procedure, private :: quantum_numbers_init_fhcs

<Quantum numbers: sub interfaces>≡
  impure elemental module subroutine quantum_numbers_init_f (qn, flv)
    class(quantum_numbers_t), intent(out) :: qn
    type(flavor_t), intent(in) :: flv
  end subroutine quantum_numbers_init_f
  impure elemental module subroutine quantum_numbers_init_c (qn, col)
    class(quantum_numbers_t), intent(out) :: qn
    type(color_t), intent(in) :: col
  end subroutine quantum_numbers_init_c
  impure elemental module subroutine quantum_numbers_init_h (qn, hel)
    class(quantum_numbers_t), intent(out) :: qn
    type(helicity_t), intent(in) :: hel
  end subroutine quantum_numbers_init_h
  impure elemental module subroutine quantum_numbers_init_fc (qn, flv, col)
    class(quantum_numbers_t), intent(out) :: qn
    type(flavor_t), intent(in) :: flv
    type(color_t), intent(in) :: col
  end subroutine quantum_numbers_init_fc
  impure elemental module subroutine quantum_numbers_init_fh (qn, flv, hel)

```



```

        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
    end subroutine quantum_numbers_init_fh
    impure elemental module subroutine quantum_numbers_init_ch (qn, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
    end subroutine quantum_numbers_init_ch
    impure elemental module subroutine quantum_numbers_init_fch (qn, flv, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
    end subroutine quantum_numbers_init_fch
    impure elemental module subroutine quantum_numbers_init_fs (qn, flv, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        integer, intent(in) :: sub
    end subroutine quantum_numbers_init_fs
    impure elemental module subroutine quantum_numbers_init_fhs (qn, flv, hel, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
        integer, intent(in) :: sub
    end subroutine quantum_numbers_init_fhs
    impure elemental module subroutine quantum_numbers_init_fcs (qn, flv, col, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        integer, intent(in) :: sub
    end subroutine quantum_numbers_init_fcs
    impure elemental module subroutine quantum_numbers_init_fhcs (qn, flv, hel, col, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
        type(color_t), intent(in) :: col
        integer, intent(in) :: sub
    end subroutine quantum_numbers_init_fhcs

```

(Quantum numbers: procedures)≡

```

    impure elemental module subroutine quantum_numbers_init_f (qn, flv)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        qn%f = flv
        call qn%c%undefine ()
        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_f

    impure elemental module subroutine quantum_numbers_init_c (qn, col)
        class(quantum_numbers_t), intent(out) :: qn
        type(color_t), intent(in) :: col
        call qn%f%undefine ()
        qn%c = col
    end subroutine quantum_numbers_init_c

```

```

        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_c

    impure elemental module subroutine quantum_numbers_init_h (qn, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(helicity_t), intent(in) :: hel
        call qn%f%undefine ()
        call qn%c%undefine ()
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_h

    impure elemental module subroutine quantum_numbers_init_fc (qn, flv, col)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        qn%f = flv
        qn%c = col
        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_fc

    impure elemental module subroutine quantum_numbers_init_fh (qn, flv, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
        qn%f = flv
        call qn%c%undefine ()
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_fh

    impure elemental module subroutine quantum_numbers_init_ch (qn, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
        call qn%f%undefine ()
        qn%c = col
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_ch

    impure elemental module subroutine quantum_numbers_init_fch (qn, flv, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
        qn%f = flv
        qn%c = col
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_fch

```

```

impure elemental module subroutine quantum_numbers_init_fs (qn, flv, sub)
  class(quantum_numbers_t), intent(out) :: qn
  type(flavor_t), intent(in) :: flv
  integer, intent(in) :: sub
  qn%f = flv; qn%sub = sub
end subroutine quantum_numbers_init_fs

impure elemental module subroutine quantum_numbers_init_fhs (qn, flv, hel, sub)
  class(quantum_numbers_t), intent(out) :: qn
  type(flavor_t), intent(in) :: flv
  type(helicity_t), intent(in) :: hel
  integer, intent(in) :: sub
  qn%f = flv; qn%h = hel; qn%sub = sub
end subroutine quantum_numbers_init_fhs

impure elemental module subroutine quantum_numbers_init_fcs (qn, flv, col, sub)
  class(quantum_numbers_t), intent(out) :: qn
  type(flavor_t), intent(in) :: flv
  type(color_t), intent(in) :: col
  integer, intent(in) :: sub
  qn%f = flv; qn%c = col; qn%sub = sub
end subroutine quantum_numbers_init_fcs

impure elemental module subroutine quantum_numbers_init_fhcs (qn, flv, hel, col, sub)
  class(quantum_numbers_t), intent(out) :: qn
  type(flavor_t), intent(in) :: flv
  type(helicity_t), intent(in) :: hel
  type(color_t), intent(in) :: col
  integer, intent(in) :: sub
  qn%f = flv; qn%h = hel; qn%c = col; qn%sub = sub
end subroutine quantum_numbers_init_fhcs

```

11.6.2 I/O

Write the quantum numbers in condensed form, enclosed by square brackets. Color is written only if nontrivial. For convenience, introduce also an array version.

If the `col_verbose` option is set, show the quantum number color also if it is zero, but defined. Otherwise, suppress zero color.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_write

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: write => quantum_numbers_write_single

<Quantum numbers: interfaces>≡
  interface quantum_numbers_write
    module procedure quantum_numbers_write_single
    module procedure quantum_numbers_write_array
  end interface

<Quantum numbers: sub interfaces>+≡
  module subroutine quantum_numbers_write_single (qn, unit, col_verbose)
    class(quantum_numbers_t), intent(in) :: qn

```

```

        integer, intent(in), optional :: unit
        logical, intent(in), optional :: col_verbose
end subroutine quantum_numbers_write_single
module subroutine quantum_numbers_write_array (qn, unit, col_verbose)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: col_verbose
end subroutine quantum_numbers_write_array

(Quantum numbers: procedures)+≡
module subroutine quantum_numbers_write_single (qn, unit, col_verbose)
    class(quantum_numbers_t), intent(in) :: qn
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: col_verbose
    integer :: u
    logical :: col_verb
    u = given_output_unit (unit); if (u < 0) return
    col_verb = .false.; if (present (col_verbose)) col_verb = col_verbose
    write (u, "(A)", advance = "no") "["
    if (qn%f%is_defined ()) then
        call qn%f%write (u)
        if (qn%c%is_nonzero () .or. qn%h%is_defined ()) &
            write (u, "(1x)", advance = "no")
    end if
    if (col_verb) then
        if (qn%c%is_defined () .or. qn%c%is_ghost ()) then
            call color_write (qn%c, u)
            if (qn%h%is_defined ()) write (u, "(1x)", advance = "no")
        end if
    else
        if (qn%c%is_nonzero () .or. qn%c%is_ghost ()) then
            call color_write (qn%c, u)
            if (qn%h%is_defined ()) write (u, "(1x)", advance = "no")
        end if
    end if
    if (qn%h%is_defined ()) then
        call qn%h%write (u)
    end if
    if (qn%sub > 0) &
        write (u, "(A,I0)", advance = "no") " SUB = ", qn%sub
    write (u, "(A)", advance="no") "]"
end subroutine quantum_numbers_write_single

module subroutine quantum_numbers_write_array (qn, unit, col_verbose)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: col_verbose
    integer :: i
    integer :: u
    logical :: col_verb
    u = given_output_unit (unit); if (u < 0) return
    col_verb = .false.; if (present (col_verbose)) col_verb = col_verbose
    write (u, "(A)", advance="no") "["
    do i = 1, size (qn)
        if (i > 1) write (u, "(A)", advance="no") " / "

```

```

        if (qn(i)%f%is_defined ()) then
            call qn(i)%f%write (u)
            if (qn(i)%c%is_nonzero () .or. qn(i)%h%is_defined ()) &
                write (u, "(1x)", advance="no")
        end if
        if (col_verb) then
            if (qn(i)%c%is_defined () .or. qn(i)%c%is_ghost ()) then
                call color_write (qn(i)%c, u)
                if (qn(i)%h%is_defined ()) write (u, "(1x)", advance="no")
            end if
        else
            if (qn(i)%c%is_nonzero () .or. qn(i)%c%is_ghost ()) then
                call color_write (qn(i)%c, u)
                if (qn(i)%h%is_defined ()) write (u, "(1x)", advance="no")
            end if
        end if
        if (qn(i)%h%is_defined ()) then
            call qn(i)%h%write (u)
        end if
        if (qn(i)%sub > 0) &
            write (u, "(A,I2)", advance = "no") " SUB = ", qn(i)%sub
    end do
    write (u, "(A)", advance = "no") "]"
end subroutine quantum_numbers_write_array

```

Binary I/O.

(Quantum numbers: quantum numbers: TBP)+≡

```

    procedure :: write_raw => quantum_numbers_write_raw
    procedure :: read_raw => quantum_numbers_read_raw

```

(Quantum numbers: sub interfaces)+≡

```

    module subroutine quantum_numbers_write_raw (qn, u)
        class(quantum_numbers_t), intent(in) :: qn
        integer, intent(in) :: u
    end subroutine quantum_numbers_write_raw
    module subroutine quantum_numbers_read_raw (qn, u, iostat)
        class(quantum_numbers_t), intent(out) :: qn
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
    end subroutine quantum_numbers_read_raw

```

(Quantum numbers: procedures)+≡

```

    module subroutine quantum_numbers_write_raw (qn, u)
        class(quantum_numbers_t), intent(in) :: qn
        integer, intent(in) :: u
        call qn%f%write_raw (u)
        call qn%c%write_raw (u)
        call qn%h%write_raw (u)
    end subroutine quantum_numbers_write_raw

    module subroutine quantum_numbers_read_raw (qn, u, iostat)
        class(quantum_numbers_t), intent(out) :: qn
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
        call qn%f%read_raw (u, iostat=iostat)
    end subroutine quantum_numbers_read_raw

```

```

        call qn%c%read_raw (u, iostat=iostat)
        call qn%h%read_raw (u, iostat=iostat)
    end subroutine quantum_numbers_read_raw

```

11.6.3 Accessing contents

Color and helicity can be done by elemental functions. Flavor needs impure elemental. We export also the functions directly, this allows us to avoid temporaries in some places.

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_get_flavor
    public :: quantum_numbers_get_color
    public :: quantum_numbers_get_helicity

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: get_flavor => quantum_numbers_get_flavor
    procedure :: get_color => quantum_numbers_get_color
    procedure :: get_helicity => quantum_numbers_get_helicity
    procedure :: get_sub => quantum_numbers_get_sub

<Quantum numbers: sub interfaces>+≡
    impure elemental module function quantum_numbers_get_flavor (qn) result (flv)
        type(flavor_t) :: flv
        class(quantum_numbers_t), intent(in) :: qn
    end function quantum_numbers_get_flavor
    elemental module function quantum_numbers_get_color (qn) result (col)
        type(color_t) :: col
        class(quantum_numbers_t), intent(in) :: qn
    end function quantum_numbers_get_color
    elemental module function quantum_numbers_get_helicity (qn) result (hel)
        type(helicity_t) :: hel
        class(quantum_numbers_t), intent(in) :: qn
    end function quantum_numbers_get_helicity
    elemental module function quantum_numbers_get_sub (qn) result (sub)
        integer :: sub
        class(quantum_numbers_t), intent(in) :: qn
    end function quantum_numbers_get_sub

<Quantum numbers: procedures>+≡
    impure elemental module function quantum_numbers_get_flavor (qn) result (flv)
        type(flavor_t) :: flv
        class(quantum_numbers_t), intent(in) :: qn
        flv = qn%f
    end function quantum_numbers_get_flavor

    elemental module function quantum_numbers_get_color (qn) result (col)
        type(color_t) :: col
        class(quantum_numbers_t), intent(in) :: qn
        col = qn%c
    end function quantum_numbers_get_color

    elemental module function quantum_numbers_get_helicity (qn) result (hel)
        type(helicity_t) :: hel
        class(quantum_numbers_t), intent(in) :: qn

```

```

        hel = qn%h
    end function quantum_numbers_get_helicity

    elemental module function quantum_numbers_get_sub (qn) result (sub)
        integer :: sub
        class(quantum_numbers_t), intent(in) :: qn
        sub = qn%sub
    end function quantum_numbers_get_sub

```

This just resets the ghost property of the color part:

```

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: set_color_ghost => quantum_numbers_set_color_ghost

<Quantum numbers: sub interfaces>+≡
    elemental module subroutine quantum_numbers_set_color_ghost (qn, ghost)
        class(quantum_numbers_t), intent(inout) :: qn
        logical, intent(in) :: ghost
    end subroutine quantum_numbers_set_color_ghost

<Quantum numbers: procedures>+≡
    elemental module subroutine quantum_numbers_set_color_ghost (qn, ghost)
        class(quantum_numbers_t), intent(inout) :: qn
        logical, intent(in) :: ghost
        call qn%c%set_ghost (ghost)
    end subroutine quantum_numbers_set_color_ghost

```

Assign a model to the flavor part of quantum numbers.

```

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: set_model => quantum_numbers_set_model

<Quantum numbers: sub interfaces>+≡
    impure elemental module subroutine quantum_numbers_set_model (qn, model)
        class(quantum_numbers_t), intent(inout) :: qn
        class(model_data_t), intent(in), target :: model
    end subroutine quantum_numbers_set_model

<Quantum numbers: procedures>+≡
    impure elemental module subroutine quantum_numbers_set_model (qn, model)
        class(quantum_numbers_t), intent(inout) :: qn
        class(model_data_t), intent(in), target :: model
        call qn%f%set_model (model)
    end subroutine quantum_numbers_set_model

```

Set the radiated flag for the flavor component.

```

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: tag_radiated => quantum_numbers_tag_radiated

<Quantum numbers: sub interfaces>+≡
    elemental module subroutine quantum_numbers_tag_radiated (qn)
        class(quantum_numbers_t), intent(inout) :: qn
    end subroutine quantum_numbers_tag_radiated

```

```

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_tag_radiated (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%f%tag_radiated ()
  end subroutine quantum_numbers_tag_radiated

```

Set the `hard_process` flag for the flavor component.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: tag_hard_process => quantum_numbers_tag_hard_process

```

```

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_tag_hard_process (qn, hard)
    class(quantum_numbers_t), intent(inout) :: qn
    logical, intent(in), optional :: hard
  end subroutine quantum_numbers_tag_hard_process

```

```

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_tag_hard_process (qn, hard)
    class(quantum_numbers_t), intent(inout) :: qn
    logical, intent(in), optional :: hard
    call qn%f%tag_hard_process (hard)
  end subroutine quantum_numbers_tag_hard_process

```

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: set_subtraction_index => &
    quantum_numbers_set_subtraction_index

```

```

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_set_subtraction_index (qn, i)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: i
  end subroutine quantum_numbers_set_subtraction_index

```

```

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_set_subtraction_index (qn, i)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: i
    qn%sub = i
  end subroutine quantum_numbers_set_subtraction_index

```

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: get_subtraction_index => &
    quantum_numbers_get_subtraction_index

```

```

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_get_subtraction_index &
    (qn) result (sub)
    integer :: sub
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_get_subtraction_index

```

```

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_get_subtraction_index &
    (qn) result (sub)
    integer :: sub

```



```

class(quantum_numbers_t), intent(in) :: qn
sub = qn%sub
end function quantum_numbers_get_subtraction_index

```

This is a convenience function: return the color type for the flavor (array).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: get_color_type => quantum_numbers_get_color_type

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_get_color_type (qn) result (color_type)
    integer :: color_type
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_get_color_type

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_get_color_type (qn) result (color_type)
    integer :: color_type
    class(quantum_numbers_t), intent(in) :: qn
    color_type = qn%f%get_color_type ()
  end function quantum_numbers_get_color_type

```

11.6.4 Predicates

Check if the flavor index is valid (including UNDEFINED).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_valid => quantum_numbers_are_valid

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_are_valid (qn) result (valid)
    logical :: valid
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_are_valid

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_are_valid (qn) result (valid)
    logical :: valid
    class(quantum_numbers_t), intent(in) :: qn
    valid = qn%f%is_valid ()
  end function quantum_numbers_are_valid

```

Check if the flavor part has its particle-data pointer associated (debugging aid).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_associated => quantum_numbers_are_associated

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_are_associated (qn) result (flag)
    logical :: flag
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_are_associated

```

```

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_are_associated (qn) result (flag)
    logical :: flag
    class(quantum_numbers_t), intent(in) :: qn
    flag = qn%f%is_associated ()
  end function quantum_numbers_are_associated

```

Check if the helicity and color quantum numbers are diagonal. (Unpolarized/colorless also counts as diagonal.) Flavor is diagonal by definition.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_diagonal => quantum_numbers_are_diagonal

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_are_diagonal (qn) result (diagonal)
    logical :: diagonal
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_are_diagonal

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_are_diagonal (qn) result (diagonal)
    logical :: diagonal
    class(quantum_numbers_t), intent(in) :: qn
    diagonal = qn%h%is_diagonal () .and. qn%c%is_diagonal ()
  end function quantum_numbers_are_diagonal

```

Check if the color part has the ghost property.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: is_color_ghost => quantum_numbers_is_color_ghost

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_is_color_ghost (qn) result (ghost)
    logical :: ghost
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_is_color_ghost

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_is_color_ghost (qn) result (ghost)
    logical :: ghost
    class(quantum_numbers_t), intent(in) :: qn
    ghost = qn%c%is_ghost ()
  end function quantum_numbers_is_color_ghost

```

Check if the flavor participates in the hard interaction.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_hard_process => quantum_numbers_are_hard_process

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_are_hard_process &
    (qn) result (hard_process)
    logical :: hard_process
    class(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_are_hard_process

```

```

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_are_hard_process &
    (qn) result (hard_process)
    logical :: hard_process
    class(quantum_numbers_t), intent(in) :: qn
    hard_process = qn%f%is_hard_process ()
  end function quantum_numbers_are_hard_process

```

11.6.5 Comparisons

Matching and equality is derived from the individual quantum numbers. The variant `fhmatch` matches only flavor and helicity. The variant `dhmatch` matches only diagonal helicity, if the matching helicity is undefined.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_eq_wo_sub

<Quantum numbers: quantum numbers: TBP>+≡
  generic :: operator(.match.) => quantum_numbers_match
  generic :: operator(.fmatch.) => quantum_numbers_match_f
  generic :: operator(.hmatch.) => quantum_numbers_match_h
  generic :: operator(.fhmatch.) => quantum_numbers_match_fh
  generic :: operator(.dhmatch.) => quantum_numbers_match_hel_diag
  generic :: operator(==) => quantum_numbers_eq
  generic :: operator(/=) => quantum_numbers_neq
  procedure, private :: quantum_numbers_match
  procedure, private :: quantum_numbers_match_f
  procedure, private :: quantum_numbers_match_h
  procedure, private :: quantum_numbers_match_fh
  procedure, private :: quantum_numbers_match_hel_diag
  procedure, private :: quantum_numbers_eq
  procedure, private :: quantum_numbers_neq

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_match (qn1, qn2) result (match)
    logical :: match
    class(quantum_numbers_t), intent(in) :: qn1, qn2
  end function quantum_numbers_match
  elemental module function quantum_numbers_match_f (qn1, qn2) result (match)
    logical :: match
    class(quantum_numbers_t), intent(in) :: qn1, qn2
  end function quantum_numbers_match_f
  elemental module function quantum_numbers_match_h (qn1, qn2) result (match)
    logical :: match
    class(quantum_numbers_t), intent(in) :: qn1, qn2
  end function quantum_numbers_match_h
  elemental module function quantum_numbers_match_fh (qn1, qn2) result (match)
    logical :: match
    class(quantum_numbers_t), intent(in) :: qn1, qn2
  end function quantum_numbers_match_fh
  elemental module function quantum_numbers_match_hel_diag (qn1, qn2) result (match)
    logical :: match
    class(quantum_numbers_t), intent(in) :: qn1, qn2
  end function quantum_numbers_match_hel_diag

```

```

elemental module function quantum_numbers_eq_wo_sub (qn1, qn2) result (eq)
  logical :: eq
  type(quantum_numbers_t), intent(in) :: qn1, qn2
end function quantum_numbers_eq_wo_sub
elemental module function quantum_numbers_eq (qn1, qn2) result (eq)
  logical :: eq
  class(quantum_numbers_t), intent(in) :: qn1, qn2
end function quantum_numbers_eq
elemental module function quantum_numbers_neq (qn1, qn2) result (neq)
  logical :: neq
  class(quantum_numbers_t), intent(in) :: qn1, qn2
end function quantum_numbers_neq

<Quantum numbers: procedures>+≡
elemental module function quantum_numbers_match (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
    (qn1%c .match. qn2%c) .and. &
    (qn1%h .match. qn2%h)
end function quantum_numbers_match

elemental module function quantum_numbers_match_f (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f)
end function quantum_numbers_match_f

elemental module function quantum_numbers_match_h (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%h .match. qn2%h)
end function quantum_numbers_match_h

elemental module function quantum_numbers_match_fh (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
    (qn1%h .match. qn2%h)
end function quantum_numbers_match_fh

elemental module function quantum_numbers_match_hel_diag (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
    (qn1%c .match. qn2%c) .and. &
    (qn1%h .dmatch. qn2%h)
end function quantum_numbers_match_hel_diag

elemental module function quantum_numbers_eq_wo_sub (qn1, qn2) result (eq)
  logical :: eq
  type(quantum_numbers_t), intent(in) :: qn1, qn2
  eq = (qn1%f == qn2%f) .and. &
    (qn1%c == qn2%c) .and. &
    (qn1%h == qn2%h)

```

```

end function quantum_numbers_eq_wo_sub

elemental module function quantum_numbers_eq (qn1, qn2) result (eq)
  logical :: eq
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  eq = (qn1%f == qn2%f) .and. &
        (qn1%c == qn2%c) .and. &
        (qn1%h == qn2%h) .and. &
        (qn1%sub == qn2%sub)
end function quantum_numbers_eq

elemental module function quantum_numbers_neq (qn1, qn2) result (neq)
  logical :: neq
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  neq = (qn1%f /= qn2%f) .or. &
        (qn1%c /= qn2%c) .or. &
        (qn1%h /= qn2%h) .or. &
        (qn1%sub /= qn2%sub)
end function quantum_numbers_neq

<Quantum numbers: public>+≡
  public :: assignment(=)

<Quantum numbers: interfaces>+≡
  interface assignment(=)
    module procedure quantum_numbers_assign
  end interface

<Quantum numbers: sub interfaces>+≡
  module subroutine quantum_numbers_assign (qn_out, qn_in)
    type(quantum_numbers_t), intent(out) :: qn_out
    type(quantum_numbers_t), intent(in) :: qn_in
  end subroutine quantum_numbers_assign

<Quantum numbers: procedures>+≡
  module subroutine quantum_numbers_assign (qn_out, qn_in)
    type(quantum_numbers_t), intent(out) :: qn_out
    type(quantum_numbers_t), intent(in) :: qn_in
    qn_out%f = qn_in%f
    qn_out%c = qn_in%c
    qn_out%h = qn_in%h
    qn_out%sub = qn_in%sub
  end subroutine quantum_numbers_assign

```

Two sets of quantum numbers are compatible if the individual quantum numbers are compatible, depending on the mask. Flavor has to match, regardless of the flavor mask.

If the color flag is set, color is compatible if the ghost property is identical. If the color flag is unset, color has to be identical. I.e., if the flag is set, the color amplitudes can interfere. If it is not set, they must be identical, and there must be no ghost. The latter property is used for expanding physical color flows.

Helicity is compatible if the mask is unset, otherwise it has to match. This determines if two amplitudes can be multiplied (no mask) or traced (mask).

```

<Quantum numbers: public>+≡

```

```

public :: quantum_numbers_are_compatible
<Quantum numbers: sub interfaces>+≡
    elemental module function quantum_numbers_are_compatible &
        (qn1, qn2, mask) result (flag)
        logical :: flag
        type(quantum_numbers_t), intent(in) :: qn1, qn2
        type(quantum_numbers_mask_t), intent(in) :: mask
        end function quantum_numbers_are_compatible

<Quantum numbers: procedures>+≡
    elemental module function quantum_numbers_are_compatible &
        (qn1, qn2, mask) result (flag)
        logical :: flag
        type(quantum_numbers_t), intent(in) :: qn1, qn2
        type(quantum_numbers_mask_t), intent(in) :: mask
        if (mask%h .or. mask%hd) then
            flag = (qn1%f .match. qn2%f) .and. (qn1%h .match. qn2%h)
        else
            flag = (qn1%f .match. qn2%f)
        end if
        if (mask%c) then
            flag = flag .and. (qn1%c%is_ghost () .eqv. qn2%c%is_ghost ())
        else
            flag = flag .and. &
                .not. (qn1%c%is_ghost () .or. qn2%c%is_ghost ()) .and. &
                (qn1%c == qn2%c)
        end if
    end function quantum_numbers_are_compatible

```

This is the analog for a single quantum-number set. We just check for color ghosts; they are excluded if the color mask is unset (color-flow expansion).

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_are_physical

<Quantum numbers: sub interfaces>+≡
    elemental module function quantum_numbers_are_physical (qn, mask) result (flag)
        logical :: flag
        type(quantum_numbers_t), intent(in) :: qn
        type(quantum_numbers_mask_t), intent(in) :: mask
        end function quantum_numbers_are_physical

<Quantum numbers: procedures>+≡
    elemental module function quantum_numbers_are_physical (qn, mask) result (flag)
        logical :: flag
        type(quantum_numbers_t), intent(in) :: qn
        type(quantum_numbers_mask_t), intent(in) :: mask
        if (mask%c) then
            flag = .true.
        else
            flag = .not. qn%c%is_ghost ()
        end if
    end function quantum_numbers_are_physical

```

11.6.6 Operations

Inherited from the color component: reassign color indices in canonical order.

```
<Quantum numbers: public>+≡
    public :: quantum_numbers_canonicalize_color

<Quantum numbers: sub interfaces>+≡
    module subroutine quantum_numbers_canonicalize_color (qn)
        type(quantum_numbers_t), dimension(:), intent(inout) :: qn
    end subroutine quantum_numbers_canonicalize_color

<Quantum numbers: procedures>+≡
    module subroutine quantum_numbers_canonicalize_color (qn)
        type(quantum_numbers_t), dimension(:), intent(inout) :: qn
        call color_canonicalize (qn%c)
    end subroutine quantum_numbers_canonicalize_color
```

Inherited from the color component: make a color map for two matching quantum-number arrays.

```
<Quantum numbers: public>+≡
    public :: make_color_map

<Quantum numbers: interfaces>+≡
    interface make_color_map
        module procedure quantum_numbers_make_color_map
    end interface make_color_map

<Quantum numbers: sub interfaces>+≡
    module subroutine quantum_numbers_make_color_map (map, qn1, qn2)
        integer, dimension(:,:), intent(out), allocatable :: map
        type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
    end subroutine quantum_numbers_make_color_map

<Quantum numbers: procedures>+≡
    module subroutine quantum_numbers_make_color_map (map, qn1, qn2)
        integer, dimension(:,:), intent(out), allocatable :: map
        type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
        call make_color_map (map, qn1%c, qn2%c)
    end subroutine quantum_numbers_make_color_map
```

Inherited from the color component: translate the color part using a color-map array

```
<Quantum numbers: public>+≡
    public :: quantum_numbers_translate_color

<Quantum numbers: interfaces>+≡
    interface quantum_numbers_translate_color
        module procedure quantum_numbers_translate_color0
        module procedure quantum_numbers_translate_color1
    end interface
```

```

<Quantum numbers: sub interfaces>+≡
  module subroutine quantum_numbers_translate_color0 (qn, map, offset)
    type(quantum_numbers_t), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
  end subroutine quantum_numbers_translate_color0
  module subroutine quantum_numbers_translate_color1 (qn, map, offset)
    type(quantum_numbers_t), dimension(:), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
  end subroutine quantum_numbers_translate_color1

<Quantum numbers: procedures>+≡
  module subroutine quantum_numbers_translate_color0 (qn, map, offset)
    type(quantum_numbers_t), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
    call color_translate (qn%c, map, offset)
  end subroutine quantum_numbers_translate_color0

  module subroutine quantum_numbers_translate_color1 (qn, map, offset)
    type(quantum_numbers_t), dimension(:), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
    call color_translate (qn%c, map, offset)
  end subroutine quantum_numbers_translate_color1

```

Inherited from the color component: return the color index with highest absolute value.

Since the algorithm is not elemental, we keep the separate procedures for different array rank.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_get_max_color_value

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_get_max_color_value
    module procedure quantum_numbers_get_max_color_value0
    module procedure quantum_numbers_get_max_color_value1
    module procedure quantum_numbers_get_max_color_value2
  end interface

<Quantum numbers: sub interfaces>+≡
  pure module function quantum_numbers_get_max_color_value0 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), intent(in) :: qn
  end function quantum_numbers_get_max_color_value0
  pure module function quantum_numbers_get_max_color_value1 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
  end function quantum_numbers_get_max_color_value1
  pure module function quantum_numbers_get_max_color_value2 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), dimension(:,:), intent(in) :: qn
  end function quantum_numbers_get_max_color_value2

```



```

<Quantum numbers: procedures>+≡
  pure module function quantum_numbers_get_max_color_value0 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), intent(in) :: qn
    cmax = color_get_max_value (qn%c)
  end function quantum_numbers_get_max_color_value0

  pure module function quantum_numbers_get_max_color_value1 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    cmax = color_get_max_value (qn%c)
  end function quantum_numbers_get_max_color_value1

  pure module function quantum_numbers_get_max_color_value2 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), dimension(:,:), intent(in) :: qn
    cmax = color_get_max_value (qn%c)
  end function quantum_numbers_get_max_color_value2

```

Inherited from the color component: add an offset to the indices of the color part

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: add_color_offset => quantum_numbers_add_color_offset

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_add_color_offset (qn, offset)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: offset
  end subroutine quantum_numbers_add_color_offset

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_add_color_offset (qn, offset)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: offset
    call qn%c%add_offset (offset)
  end subroutine quantum_numbers_add_color_offset

```

Given a quantum number array, return all possible color contractions, leaving the other quantum numbers intact.

```

<Quantum numbers: public>+≡
  public :: quantum_number_array_make_color_contractions

<Quantum numbers: sub interfaces>+≡
  module subroutine quantum_number_array_make_color_contractions (qn_in, qn_out)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    type(quantum_numbers_t), dimension(:,:), intent(out), allocatable :: qn_out
  end subroutine quantum_number_array_make_color_contractions

<Quantum numbers: procedures>+≡
  module subroutine quantum_number_array_make_color_contractions (qn_in, qn_out)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    type(quantum_numbers_t), dimension(:,:), intent(out), allocatable :: qn_out
    type(color_t), dimension(:,:), allocatable :: col
    integer :: i
    call color_array_make_contractions (qn_in%c, col)
  end subroutine quantum_number_array_make_color_contractions

```

```

allocate (qn_out (size (col, 1), size (col, 2)))
do i = 1, size (qn_out, 2)
  qn_out(:,i)%f = qn_in%f
  qn_out(:,i)%c = col(:,i)
  qn_out(:,i)%h = qn_in%h
end do
end subroutine quantum_number_array_make_color_contractions

```

Inherited from the color component: invert the color, switching particle/antiparticle.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: invert_color => quantum_numbers_invert_color

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_invert_color (qn)
    class(quantum_numbers_t), intent(inout) :: qn
  end subroutine quantum_numbers_invert_color

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_invert_color (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%c%invert ()
  end subroutine quantum_numbers_invert_color

```

Flip helicity.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: flip_helicity => quantum_numbers_flip_helicity

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_flip_helicity (qn)
    class(quantum_numbers_t), intent(inout) :: qn
  end subroutine quantum_numbers_flip_helicity

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_flip_helicity (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%h%flip ()
  end subroutine quantum_numbers_flip_helicity

```

Merge two quantum number sets: for each entry, if both are defined, combine them to an off-diagonal entry (meaningful only if the input was diagonal). If either entry is undefined, take the defined one.

For flavor, off-diagonal entries are invalid, so both flavors must be equal, otherwise an invalid flavor is inserted.

```

<Quantum numbers: public>+≡
  public :: operator(.merge.)

<Quantum numbers: interfaces>+≡
  interface operator(.merge.)
    module procedure merge_quantum_numbers0
    module procedure merge_quantum_numbers1
  end interface

```

```

<Quantum numbers: sub interfaces>+≡
    module function merge_quantum_numbers0 (qn1, qn2) result (qn3)
        type(quantum_numbers_t) :: qn3
        type(quantum_numbers_t), intent(in) :: qn1, qn2
    end function merge_quantum_numbers0
    module function merge_quantum_numbers1 (qn1, qn2) result (qn3)
        type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
        type(quantum_numbers_t), dimension(size(qn1)) :: qn3
    end function merge_quantum_numbers1

<Quantum numbers: procedures>+≡
    module function merge_quantum_numbers0 (qn1, qn2) result (qn3)
        type(quantum_numbers_t) :: qn3
        type(quantum_numbers_t), intent(in) :: qn1, qn2
        qn3%f = qn1%f .merge. qn2%f
        qn3%c = qn1%c .merge. qn2%c
        qn3%h = qn1%h .merge. qn2%h
        qn3%sub = merge_subtraction_index (qn1%sub, qn2%sub)
    end function merge_quantum_numbers0

    module function merge_quantum_numbers1 (qn1, qn2) result (qn3)
        type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
        type(quantum_numbers_t), dimension(size(qn1)) :: qn3
        qn3%f = qn1%f .merge. qn2%f
        qn3%c = qn1%c .merge. qn2%c
        qn3%h = qn1%h .merge. qn2%h
        qn3%sub = merge_subtraction_index (qn1%sub, qn2%sub)
    end function merge_quantum_numbers1

<Quantum numbers: procedures>+≡
    elemental function merge_subtraction_index (sub1, sub2) result (sub3)
        integer :: sub3
        integer, intent(in) :: sub1, sub2
        if (sub1 > 0 .and. sub2 > 0) then
            if (sub1 == sub2) then
                sub3 = sub1
            else
                sub3 = 0
            end if
        else if (sub1 > 0) then
            sub3 = sub1
        else if (sub2 > 0) then
            sub3 = sub2
        else
            sub3 = 0
        end if
    end function merge_subtraction_index

```

11.6.7 The quantum number mask

The quantum numbers mask is true for quantum numbers that should be ignored or summed over. The three mandatory entries correspond to flavor, color, and helicity, respectively.

There is an additional entry `cg`: If false, the color-ghosts property should be kept even if color is ignored. This is relevant only if `c` is set, otherwise it is always false.

The flag `hd` tells that only diagonal entries in helicity should be kept. If `h` is set, `hd` is irrelevant and will be kept `.false`.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_mask_t

<Quantum numbers: types>+≡
  type :: quantum_numbers_mask_t
    private
    logical :: f = .false.
    logical :: c = .false.
    logical :: cg = .false.
    logical :: h = .false.
    logical :: hd = .false.
    integer :: sub = 0
  contains
    <Quantum numbers: quantum numbers mask: TBP>
  end type quantum_numbers_mask_t

```

Define a quantum number mask: Constructor form

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_mask

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_mask &
    (mask_f, mask_c, mask_h, mask_cg, mask_hd) result (mask)
    type(quantum_numbers_mask_t) :: mask
    logical, intent(in) :: mask_f, mask_c, mask_h
    logical, intent(in), optional :: mask_cg
    logical, intent(in), optional :: mask_hd
  end function quantum_numbers_mask

<Quantum numbers: procedures>+≡
  elemental module function quantum_numbers_mask &
    (mask_f, mask_c, mask_h, mask_cg, mask_hd) result (mask)
    type(quantum_numbers_mask_t) :: mask
    logical, intent(in) :: mask_f, mask_c, mask_h
    logical, intent(in), optional :: mask_cg
    logical, intent(in), optional :: mask_hd
    call quantum_numbers_mask_init &
      (mask, mask_f, mask_c, mask_h, mask_cg, mask_hd)
  end function quantum_numbers_mask

```

Define quantum numbers: Initializer form

```

<Quantum numbers: quantum numbers mask: TBP>≡
  procedure :: init => quantum_numbers_mask_init

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_mask_init &
    (mask, mask_f, mask_c, mask_h, mask_cg, mask_hd)
    class(quantum_numbers_mask_t), intent(inout) :: mask
    logical, intent(in) :: mask_f, mask_c, mask_h

```

```

        logical, intent(in), optional :: mask_cg, mask_hd
    end subroutine quantum_numbers_mask_init

<Quantum numbers: procedures>+≡
    elemental module subroutine quantum_numbers_mask_init &
        (mask, mask_f, mask_c, mask_h, mask_cg, mask_hd)
        class(quantum_numbers_mask_t), intent(inout) :: mask
        logical, intent(in) :: mask_f, mask_c, mask_h
        logical, intent(in), optional :: mask_cg, mask_hd
        mask%f = mask_f
        mask%c = mask_c
        mask%h = mask_h
        mask%cg = .false.
        if (present (mask_cg)) then
            if (mask%c) mask%cg = mask_cg
        else
            mask%cg = mask_c
        end if
        mask%hd = .false.
        if (present (mask_hd)) then
            if (.not. mask%h) mask%hd = mask_hd
        end if
    end subroutine quantum_numbers_mask_init

```

Write a quantum numbers mask. We need the stand-alone subroutine for the array case.

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_mask_write

<Quantum numbers: interfaces>+≡
    interface quantum_numbers_mask_write
        module procedure quantum_numbers_mask_write_single
        module procedure quantum_numbers_mask_write_array
    end interface

<Quantum numbers: quantum numbers mask: TBP>+≡
    procedure :: write => quantum_numbers_mask_write_single

<Quantum numbers: sub interfaces>+≡
    module subroutine quantum_numbers_mask_write_single (mask, unit)
        class(quantum_numbers_mask_t), intent(in) :: mask
        integer, intent(in), optional :: unit
    end subroutine quantum_numbers_mask_write_single
    module subroutine quantum_numbers_mask_write_array (mask, unit)
        type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
        integer, intent(in), optional :: unit
    end subroutine quantum_numbers_mask_write_array

<Quantum numbers: procedures>+≡
    module subroutine quantum_numbers_mask_write_single (mask, unit)
        class(quantum_numbers_mask_t), intent(in) :: mask
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(A)", advance="no") "["
        write (u, "(L1)", advance="no") mask%f
    end subroutine quantum_numbers_mask_write_single

```

```

write (u, "(L1)", advance="no") mask%c
if (.not.mask%cg) write (u, "('g')", advance="no")
write (u, "(L1)", advance="no") mask%h
if (mask%hd) write (u, "('d')", advance="no")
write (u, "(A)", advance="no") "]"
end subroutine quantum_numbers_mask_write_single

module subroutine quantum_numbers_mask_write_array (mask, unit)
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)", advance="no") "["
  do i = 1, size (mask)
    if (i > 1) write (u, "(A)", advance="no") "/"
    write (u, "(L1)", advance="no") mask(i)%f
    write (u, "(L1)", advance="no") mask(i)%c
    if (.not.mask(i)%cg) write (u, "('g')", advance="no")
    write (u, "(L1)", advance="no") mask(i)%h
    if (mask(i)%hd) write (u, "('d')", advance="no")
  end do
  write (u, "(A)", advance="no") "]"
end subroutine quantum_numbers_mask_write_array

```

11.6.8 Setting mask components

(Quantum numbers: quantum numbers mask: TBP)+≡

```

procedure :: set_flavor => quantum_numbers_mask_set_flavor
procedure :: set_color  => quantum_numbers_mask_set_color
procedure :: set_helicity => quantum_numbers_mask_set_helicity
procedure :: set_sub    => quantum_numbers_mask_set_sub

```

(Quantum numbers: sub interfaces)+≡

```

elemental module subroutine quantum_numbers_mask_set_flavor (mask, mask_f)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_f
end subroutine quantum_numbers_mask_set_flavor
elemental module subroutine quantum_numbers_mask_set_color (mask, mask_c, mask_cg)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_c
  logical, intent(in), optional :: mask_cg
end subroutine quantum_numbers_mask_set_color
elemental module subroutine quantum_numbers_mask_set_helicity (mask, mask_h, mask_hd)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_h
  logical, intent(in), optional :: mask_hd
end subroutine quantum_numbers_mask_set_helicity
elemental module subroutine quantum_numbers_mask_set_sub (mask, sub)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  integer, intent(in) :: sub
end subroutine quantum_numbers_mask_set_sub

```

(Quantum numbers: procedures)+≡

```

elemental module subroutine quantum_numbers_mask_set_flavor (mask, mask_f)

```

```

class(quantum_numbers_mask_t), intent(inout) :: mask
logical, intent(in) :: mask_f
mask%f = mask_f
end subroutine quantum_numbers_mask_set_flavor

elemental module subroutine quantum_numbers_mask_set_color (mask, mask_c, mask_cg)
class(quantum_numbers_mask_t), intent(inout) :: mask
logical, intent(in) :: mask_c
logical, intent(in), optional :: mask_cg
mask%c = mask_c
if (present (mask_cg)) then
    if (mask%c) mask%cg = mask_cg
else
    mask%cg = mask_c
end if
end subroutine quantum_numbers_mask_set_color

elemental module subroutine quantum_numbers_mask_set_helicity (mask, mask_h, mask_hd)
class(quantum_numbers_mask_t), intent(inout) :: mask
logical, intent(in) :: mask_h
logical, intent(in), optional :: mask_hd
mask%h = mask_h
if (present (mask_hd)) then
    if (.not. mask%h) mask%hd = mask_hd
end if
end subroutine quantum_numbers_mask_set_helicity

elemental module subroutine quantum_numbers_mask_set_sub (mask, sub)
class(quantum_numbers_mask_t), intent(inout) :: mask
integer, intent(in) :: sub
mask%sub = sub
end subroutine quantum_numbers_mask_set_sub

```

The following routines assign part of a mask, depending on the flags given.

```

<Quantum numbers: quantum numbers mask: TBP>+≡
    procedure :: assign => quantum_numbers_mask_assign

<Quantum numbers: sub interfaces>+≡
    elemental module subroutine quantum_numbers_mask_assign &
        (mask, mask_in, flavor, color, helicity)
        class(quantum_numbers_mask_t), intent(inout) :: mask
        class(quantum_numbers_mask_t), intent(in) :: mask_in
        logical, intent(in), optional :: flavor, color, helicity
    end subroutine quantum_numbers_mask_assign

<Quantum numbers: procedures>+≡
    elemental module subroutine quantum_numbers_mask_assign &
        (mask, mask_in, flavor, color, helicity)
        class(quantum_numbers_mask_t), intent(inout) :: mask
        class(quantum_numbers_mask_t), intent(in) :: mask_in
        logical, intent(in), optional :: flavor, color, helicity
    if (present (flavor)) then
        if (flavor) then
            mask%f = mask_in%f
        end if
    end if

```

```

end if
if (present (color)) then
  if (color) then
    mask%c = mask_in%c
    mask%cg = mask_in%cg
  end if
end if
if (present (helicity)) then
  if (helicity) then
    mask%h = mask_in%h
    mask%hd = mask_in%hd
  end if
end if
end subroutine quantum_numbers_mask_assign

```

11.6.9 Mask predicates

Return true if either one of the entries is set:

```

<Quantum numbers: public>+≡
  public :: any

<Quantum numbers: interfaces>+≡
  interface any
    module procedure quantum_numbers_mask_any
  end interface

<Quantum numbers: sub interfaces>+≡
  module function quantum_numbers_mask_any (mask) result (match)
    logical :: match
    type(quantum_numbers_mask_t), intent(in) :: mask
  end function quantum_numbers_mask_any

<Quantum numbers: procedures>+≡
  module function quantum_numbers_mask_any (mask) result (match)
    logical :: match
    type(quantum_numbers_mask_t), intent(in) :: mask
    match = mask%f .or. mask%c .or. mask%h .or. mask%hd
  end function quantum_numbers_mask_any

```

11.6.10 Operators

The OR operation is applied to all components.

```

<Quantum numbers: quantum numbers mask: TBP>+≡
  generic :: operator(.or.) => quantum_numbers_mask_or
  procedure, private :: quantum_numbers_mask_or

<Quantum numbers: sub interfaces>+≡
  elemental module function quantum_numbers_mask_or (mask1, mask2) result (mask)
    type(quantum_numbers_mask_t) :: mask
    class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
  end function quantum_numbers_mask_or

```



```

<Quantum numbers: procedures>+≡
elemental module function quantum_numbers_mask_or (mask1, mask2) result (mask)
  type(quantum_numbers_mask_t) :: mask
  class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
  mask%f = mask1%f .or. mask2%f
  mask%c = mask1%c .or. mask2%c
  if (mask%c) mask%cg = mask1%cg .or. mask2%cg
  mask%h = mask1%h .or. mask2%h
  if (.not. mask%h) mask%hd = mask1%hd .or. mask2%hd
end function quantum_numbers_mask_or

```

11.6.11 Mask comparisons

Return true if the two masks are equivalent / differ:

```

<Quantum numbers: quantum numbers mask: TBP>+≡
generic :: operator(.eqv.) => quantum_numbers_mask_eqv
generic :: operator(.neqv.) => quantum_numbers_mask_neqv
procedure, private :: quantum_numbers_mask_eqv
procedure, private :: quantum_numbers_mask_neqv

<Quantum numbers: sub interfaces>+≡
elemental module function quantum_numbers_mask_eqv (mask1, mask2) result (eqv)
  logical :: eqv
  class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
end function quantum_numbers_mask_eqv
elemental module function quantum_numbers_mask_neqv (mask1, mask2) result (neqv)
  logical :: neqv
  class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
end function quantum_numbers_mask_neqv

<Quantum numbers: procedures>+≡
elemental module function quantum_numbers_mask_eqv (mask1, mask2) result (eqv)
  logical :: eqv
  class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
  eqv = (mask1%f .eqv. mask2%f) .and. &
        (mask1%c .eqv. mask2%c) .and. &
        (mask1%cg .eqv. mask2%cg) .and. &
        (mask1%h .eqv. mask2%h) .and. &
        (mask1%hd .eqv. mask2%hd)
end function quantum_numbers_mask_eqv

elemental module function quantum_numbers_mask_neqv (mask1, mask2) result (neqv)
  logical :: neqv
  class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
  neqv = (mask1%f .neqv. mask2%f) .or. &
        (mask1%c .neqv. mask2%c) .or. &
        (mask1%cg .neqv. mask2%cg) .or. &
        (mask1%h .neqv. mask2%h) .or. &
        (mask1%hd .neqv. mask2%hd)
end function quantum_numbers_mask_neqv

```

11.6.12 Apply a mask

Applying a mask to the quantum number object means undefining those entries where the mask is set. The others remain unaffected.

The `hd` mask has the special property that it “diagonalizes” helicity, i.e., the second helicity entry is dropped and the result is a diagonal helicity quantum number.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: undefine => quantum_numbers_undefine
  procedure :: undefined => quantum_numbers_undefined0

<Quantum numbers: public>+≡
  public :: quantum_numbers_undefined

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_undefined
    module procedure quantum_numbers_undefined0
    module procedure quantum_numbers_undefined1
    module procedure quantum_numbers_undefined11
  end interface

<Quantum numbers: sub interfaces>+≡
  elemental module subroutine quantum_numbers_undefine (qn, mask)
    class(quantum_numbers_t), intent(inout) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
  end subroutine quantum_numbers_undefine
  module function quantum_numbers_undefined0 (qn, mask) result (qn_new)
    class(quantum_numbers_t), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t) :: qn_new
  end function quantum_numbers_undefined0
  module function quantum_numbers_undefined1 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new
  end function quantum_numbers_undefined1
  module function quantum_numbers_undefined11 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new
  end function quantum_numbers_undefined11

<Quantum numbers: procedures>+≡
  elemental module subroutine quantum_numbers_undefine (qn, mask)
    class(quantum_numbers_t), intent(inout) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    if (mask%f) call qn%f%undefine ()
    if (mask%c) call qn%c%undefine (undefine_ghost = mask%cg)
    if (mask%h) then
      call qn%h%undefine ()
    else if (mask%hd) then
      if (.not. qn%h%is_diagonal ()) then
        call qn%h%diagonalize ()
      end if
    end if
  end if

```

```

        if (mask%sub > 0) qn%sub = 0
    end subroutine quantum_numbers_undefine

module function quantum_numbers_undefined0 (qn, mask) result (qn_new)
    class(quantum_numbers_t), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t) :: qn_new
    select type (qn)
    type is (quantum_numbers_t); qn_new = qn
    end select
    call quantum_numbers_undefine (qn_new, mask)
end function quantum_numbers_undefined0

module function quantum_numbers_undefined1 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new
    qn_new = qn
    call quantum_numbers_undefine (qn_new, mask)
end function quantum_numbers_undefined1

module function quantum_numbers_undefined11 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new
    qn_new = qn
    call quantum_numbers_undefine (qn_new, mask)
end function quantum_numbers_undefined11

```

Return true if the input quantum number set has entries that would be removed by the applied mask, e.g., if polarization is defined but mask%h is set:

```

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: are_redundant => quantum_numbers_are_redundant

<Quantum numbers: sub interfaces>+≡
    elemental module function quantum_numbers_are_redundant (qn, mask) &
        result (redundant)
        logical :: redundant
        class(quantum_numbers_t), intent(in) :: qn
        type(quantum_numbers_mask_t), intent(in) :: mask
    end function quantum_numbers_are_redundant

<Quantum numbers: procedures>+≡
    elemental module function quantum_numbers_are_redundant (qn, mask) &
        result (redundant)
        logical :: redundant
        class(quantum_numbers_t), intent(in) :: qn
        type(quantum_numbers_mask_t), intent(in) :: mask
        redundant = .false.
        if (mask%f) then
            redundant = qn%f%is_defined ()
        end if
        if (mask%c) then
            redundant = qn%c%is_defined ()
        end if
    end function

```

```

    if (mask%h) then
        redundant = qn%h%is_defined ()
    else if (mask%hd) then
        redundant = .not. qn%h%is_diagonal ()
    end if
    if (mask%sub > 0) redundant = qn%sub >= mask%sub
end function quantum_numbers_are_redundant

```

Return true if the helicity flag is set or the diagonal-helicity flag is set.

```

<Quantum numbers: quantum numbers mask: TBP>+≡
    procedure :: diagonal_helicity => quantum_numbers_mask_diagonal_helicity

<Quantum numbers: sub interfaces>+≡
    elemental module function quantum_numbers_mask_diagonal_helicity (mask) &
        result (flag)
        logical :: flag
        class(quantum_numbers_mask_t), intent(in) :: mask
    end function quantum_numbers_mask_diagonal_helicity

<Quantum numbers: procedures>+≡
    elemental module function quantum_numbers_mask_diagonal_helicity (mask) &
        result (flag)
        logical :: flag
        class(quantum_numbers_mask_t), intent(in) :: mask
        flag = mask%h .or. mask%hd
    end function quantum_numbers_mask_diagonal_helicity

```

Chapter 12

Transition Matrices and Evaluation

The modules in this chapter implement transition matrices and calculations. The functionality is broken down in three modules

state_matrices represent state and transition density matrices built from particle quantum numbers (helicity, color, flavor)

interactions extend state matrices with the record of particle momenta. They also distinguish in- and out-particles and store parent-child relations.

evaluators These objects extend interaction objects by the information how to calculate matrix elements from products and squares of other interactions. They implement the methods to actually compute those matrix elements.

12.1 State matrices

This module deals with the internal state of a particle system, i.e., with its density matrix in flavor, color, and helicity space.

```
<state_matrices.f90>≡  
  <File header>  
  
  module state_matrices  
  
    <Use kinds>  
    use model_data  
    use flavors  
    use colors  
    use helicities  
    use quantum_numbers  
  
    <Standard module head>  
  
    <State matrices: public>  
  
    <State matrices: parameters>  
  
    <State matrices: types>  
  
    <State matrices: interfaces>  
  
    interface  
    <State matrices: sub interfaces>  
    end interface  
  
  end module state_matrices  
<state_matrices_sub.f90>≡  
  <File header>  
  
  submodule (state_matrices) state_matrices_s  
  
    use constants, only: zero  
    use format_utils, only: pac_fmt  
    use format_defs, only: FMT_17, FMT_19  
    use io_units  
    use diagnostics  
    use sorting  
  
    implicit none  
  
  contains  
  
    <State matrices: procedures>  
  
  end submodule state_matrices_s
```

12.1.1 Nodes of the quantum state trie

A quantum state object represents an unnormalized density matrix, i.e., an array of possibilities for flavor, color, and helicity indices with associated complex values. Physically, the trace of this matrix is the summed squared matrix element for an interaction, and the matrix elements divided by this value correspond to the flavor-color-helicity density matrix. (Flavor and color are diagonal.)

We store density matrices as tries, that is, as trees where each branching represents the possible quantum numbers of a particle. The first branching is the first particle in the system. A leaf (the node corresponding to the last particle) contains the value of the matrix element.

Each node contains a flavor, color, and helicity entry. Note that each of those entries may be actually undefined, so we can also represent, e.g., unpolarized particles.

The value is meaningful only for leaves, which have no child nodes. There is a pointer to the parent node which allows for following the trie downwards from a leaf, it is null for a root node. The child nodes are implemented as a list, so there is a pointer to the first and last child, and each node also has a `next` pointer to the next sibling.

The root node does not correspond to a particle, only its children do. The quantum numbers of the root node are irrelevant and will not be set. However, we use a common type for the three classes (root, branch, leaf); they may easily be distinguished by the association status of parent and child.

Node type

The node is linked in all directions: the parent, the first and last in the list of children, and the previous and next sibling. This allows us for adding and removing nodes and whole branches anywhere in the trie. (Circular links are not allowed, however.). The node holds its associated set of quantum numbers. The integer index, which is set only for leaf nodes, is the index of the corresponding matrix element value within the state matrix.

Temporarily, matrix-element values may be stored within a leaf node. This is used during state-matrix factorization. When the state matrix is `frozen`, these values are transferred to the matrix-element array within the host state matrix.

(State matrices: types)≡

```
type :: node_t
  private
  type(quantum_numbers_t) :: qn
  type(node_t), pointer :: parent => null ()
  type(node_t), pointer :: child_first => null ()
  type(node_t), pointer :: child_last => null ()
  type(node_t), pointer :: next => null ()
  type(node_t), pointer :: previous => null ()
  integer :: me_index = 0
  integer, dimension(:), allocatable :: me_count
  complex(default) :: me = 0
end type node_t
```

Operations on nodes

Recursively deallocate all children of the current node. This includes any values associated with the children.

(State matrices: procedures)≡

```
pure recursive subroutine node_delete_offspring (node)
  type(node_t), pointer :: node
  type(node_t), pointer :: child
  child => node%child_first
  do while (associated (child))
    node%child_first => node%child_first%next
    call node_delete_offspring (child)
    deallocate (child)
    child => node%child_first
  end do
  node%child_last => null ()
end subroutine node_delete_offspring
```

Remove a node including its offspring. Adjust the pointers of parent and siblings, if necessary.

(State matrices: procedures)+≡

```
pure subroutine node_delete (node)
  type(node_t), pointer :: node
  call node_delete_offspring (node)
  if (associated (node%previous)) then
    node%previous%next => node%next
  else if (associated (node%parent)) then
    node%parent%child_first => node%next
  end if
  if (associated (node%next)) then
    node%next%previous => node%previous
  else if (associated (node%parent)) then
    node%parent%child_last => node%previous
  end if
  deallocate (node)
end subroutine node_delete
```

Append a child node

(State matrices: procedures)+≡

```
subroutine node_append_child (node, child)
  type(node_t), target, intent(inout) :: node
  type(node_t), pointer :: child
  allocate (child)
  if (associated (node%child_last)) then
    node%child_last%next => child
    child%previous => node%child_last
  else
    node%child_first => child
  end if
  node%child_last => child
  child%parent => node
end subroutine node_append_child
```


I/O

Output of a single node, no recursion. We print the quantum numbers in square brackets, then the value (if any).

(State matrices: procedures)+≡

```

subroutine node_write (node, me_array, verbose, unit, col_verbose, testflag)
  type(node_t), intent(in) :: node
  complex(default), dimension(:), intent(in), optional :: me_array
  logical, intent(in), optional :: verbose, col_verbose, testflag
  integer, intent(in), optional :: unit
  logical :: verb
  integer :: u
  character(len=7) :: fmt
  call pac_fmt (fmt, FMT_19, FMT_17, testflag)
  verb = .false.; if (present (verbose)) verb = verbose
  u = given_output_unit (unit); if (u < 0) return
  call node%qn%write (u, col_verbose)
  if (node%me_index /= 0) then
    write (u, "(A,I0,A)", advance="no") " => ME(", node%me_index, ")"
    if (present (me_array)) then
      write (u, "(A)", advance="no") " = "
      write (u, "('(', " // fmt // ",',', " // fmt // ",')')", &
        advance="no") pacify_complex (me_array(node%me_index))
    end if
  end if
  write (u, *)
  if (verb) then
    call ptr_write ("parent      ", node%parent)
    call ptr_write ("child_first", node%child_first)
    call ptr_write ("child_last ", node%child_last)
    call ptr_write ("next       ", node%next)
    call ptr_write ("previous   ", node%previous)
  end if
contains
  subroutine ptr_write (label, node)
    character(*), intent(in) :: label
    type(node_t), pointer :: node
    if (associated (node)) then
      write (u, "(10x,A,1x,'->',1x)", advance="no") label
      call node%qn%write (u, col_verbose)
      write (u, *)
    end if
  end subroutine ptr_write
end subroutine node_write

```

Recursive output of a node:

(State matrices: procedures)+≡

```

recursive subroutine node_write_rec (node, me_array, verbose, &
  indent, unit, col_verbose, testflag)
  type(node_t), intent(in), target :: node
  complex(default), dimension(:), intent(in), optional :: me_array
  logical, intent(in), optional :: verbose, col_verbose, testflag
  integer, intent(in), optional :: indent
  integer, intent(in), optional :: unit

```

```

type(node_t), pointer :: current
logical :: verb
integer :: i, u
verb = .false.; if (present (verbose)) verb = verbose
i = 0; if (present (indent)) i = indent
u = given_output_unit (unit); if (u < 0) return
current => node%child_first
do while (associated (current))
  write (u, "(A)", advance="no") repeat (" ", i)
  call node_write (current, me_array, verbose = verb, &
    unit = u, col_verbose = col_verbose, testflag = testflag)
  call node_write_rec (current, me_array, verbose = verb, &
    indent = i + 2, unit = u, col_verbose = col_verbose, testflag = testflag)
  current => current%next
end do
end subroutine node_write_rec

```

Binary I/O. Matrix elements are written only for leaf nodes.

(State matrices: procedures)+≡

```

recursive subroutine node_write_raw_rec (node, u)
  type(node_t), intent(in), target :: node
  integer, intent(in) :: u
  logical :: associated_child_first, associated_next
  call node%qn%write_raw (u)
  associated_child_first = associated (node%child_first)
  write (u) associated_child_first
  associated_next = associated (node%next)
  write (u) associated_next
  if (associated_child_first) then
    call node_write_raw_rec (node%child_first, u)
  else
    write (u) node%me_index
    write (u) node%me
  end if
  if (associated_next) then
    call node_write_raw_rec (node%next, u)
  end if
end subroutine node_write_raw_rec

recursive subroutine node_read_raw_rec (node, u, parent, iostat)
  type(node_t), intent(out), target :: node
  integer, intent(in) :: u
  type(node_t), intent(in), optional, target :: parent
  integer, intent(out), optional :: iostat
  logical :: associated_child_first, associated_next
  type(node_t), pointer :: child
  call node%qn%read_raw (u, iostat=iostat)
  read (u, iostat=iostat) associated_child_first
  read (u, iostat=iostat) associated_next
  if (present (parent)) node%parent => parent
  if (associated_child_first) then
    allocate (child)
    node%child_first => child
    node%child_last => null ()
  end if
end subroutine node_read_raw_rec

```

```

        call node_read_raw_rec (child, u, node, iostat=iostat)
        do while (associated (child))
            child%previous => node%child_last
            node%child_last => child
            child => child%next
        end do
    else
        read (u, iostat=iostat) node%me_index
        read (u, iostat=iostat) node%me
    end if
    if (associated_next) then
        allocate (node%next)
        call node_read_raw_rec (node%next, u, parent, iostat=iostat)
    end if
end subroutine node_read_raw_rec

```

12.1.2 State matrix

Definition

The quantum state object is a container that keeps and hides the root node. For direct accessibility of values, they are stored in a separate array. The leaf nodes of the quantum-number tree point to those values, once the state matrix is finalized.

The norm component is redefined if a common factor is extracted from all nodes.

```

<State matrices: public>≡
    public :: state_matrix_t

<State matrices: types>+≡
    type :: state_matrix_t
        private
        type(node_t), pointer :: root => null ()
        integer :: depth = 0
        integer :: n_matrix_elements = 0
        logical :: leaf_nodes_store_values = .false.
        integer :: n_counters = 0
        complex(default), dimension(:), allocatable :: me
        real(default) :: norm = 1
        integer :: n_sub = -1
    contains
        <State matrices: state matrix: TBP>
    end type state_matrix_t

```

This initializer allocates the root node but does not fill anything. We declare whether values are stored within the nodes during state-matrix construction, and how many counters should be maintained (default: none).

```

<State matrices: state matrix: TBP>≡
    procedure :: init => state_matrix_init

<State matrices: sub interfaces>≡
    module subroutine state_matrix_init (state, store_values, n_counters)

```

```

        class(state_matrix_t), intent(out) :: state
        logical, intent(in), optional :: store_values
        integer, intent(in), optional :: n_counters
    end subroutine state_matrix_init

```

<State matrices: procedures>+≡

```

    module subroutine state_matrix_init (state, store_values, n_counters)
        class(state_matrix_t), intent(out) :: state
        logical, intent(in), optional :: store_values
        integer, intent(in), optional :: n_counters
        allocate (state%root)
        if (present (store_values)) &
            state%leaf_nodes_store_values = store_values
        if (present (n_counters)) state%n_counters = n_counters
    end subroutine state_matrix_init

```

This recursively deletes all children of the root node, restoring the initial state. The matrix element array is not finalized, since it does not contain physical entries, just pointers.

<State matrices: state matrix: TBP>+≡

```

    procedure :: final => state_matrix_final

```

<State matrices: sub interfaces>+≡

```

    module subroutine state_matrix_final (state)
        class(state_matrix_t), intent(inout) :: state
    end subroutine state_matrix_final

```

<State matrices: procedures>+≡

```

    module subroutine state_matrix_final (state)
        class(state_matrix_t), intent(inout) :: state
        if (allocated (state%me)) deallocate (state%me)
        if (associated (state%root)) call node_delete (state%root)
        state%depth = 0
        state%n_matrix_elements = 0
    end subroutine state_matrix_final

```

Output: Present the tree as a nested list with appropriate indentation.

<State matrices: state matrix: TBP>+≡

```

    procedure :: write => state_matrix_write

```

<State matrices: sub interfaces>+≡

```

    module subroutine state_matrix_write (state, unit, write_value_list, &
        verbose, col_verbose, testflag)
        class(state_matrix_t), intent(in) :: state
        logical, intent(in), optional :: write_value_list, verbose, col_verbose
        logical, intent(in), optional :: testflag
        integer, intent(in), optional :: unit
    end subroutine state_matrix_write

```

<State matrices: procedures>+≡

```

    module subroutine state_matrix_write (state, unit, write_value_list, &
        verbose, col_verbose, testflag)
        class(state_matrix_t), intent(in) :: state
        logical, intent(in), optional :: write_value_list, verbose, col_verbose
        logical, intent(in), optional :: testflag

```

```

integer, intent(in), optional :: unit
complex(default) :: me_dum
character(len=7) :: fmt
integer :: u
integer :: i
call pac_fmt (fmt, FMT_19, FMT_17, testflag)
u = given_output_unit (unit); if (u < 0) return
write (u, "(1x,A," // fmt // ")") "State matrix: norm = ", state%norm
if (associated (state%root)) then
  if (allocated (state%me)) then
    call node_write_rec (state%root, state%me, verbose = verbose, &
      indent = 1, unit = u, col_verbose = col_verbose, &
      testflag = testflag)
  else
    call node_write_rec (state%root, verbose = verbose, indent = 1, &
      unit = u, col_verbose = col_verbose, testflag = testflag)
  end if
end if
if (present (write_value_list)) then
  if (write_value_list .and. allocated (state%me)) then
    do i = 1, size (state%me)
      write (u, "(1x,I0,A)", advance="no") i, ":"
      me_dum = state%me(i)
      if (real(state%me(i)) == -real(state%me(i))) then
        me_dum = &
          cmplx (0._default, aimag(me_dum), kind=default)
      end if
      if (aimag(me_dum) == -aimag(me_dum)) then
        me_dum = &
          cmplx (real(me_dum), 0._default, kind=default)
      end if
      write (u, "(','," // fmt // ",','," // fmt // &
        ",')')") me_dum
    end do
  end if
end if
end subroutine state_matrix_write

```

Binary I/O. The auxiliary matrix-element array is not written, but reconstructed after reading the tree.

Note: To be checked. Might be broken, don't use (unless trivial).

(State matrices: state matrix: TBP)+≡

```

procedure :: write_raw => state_matrix_write_raw
procedure :: read_raw => state_matrix_read_raw

```

(State matrices: sub interfaces)+≡

```

module subroutine state_matrix_write_raw (state, u)
  class(state_matrix_t), intent(in), target :: state
  integer, intent(in) :: u
end subroutine state_matrix_write_raw
module subroutine state_matrix_read_raw (state, u, iostat)
  class(state_matrix_t), intent(out) :: state
  integer, intent(in) :: u
  integer, intent(out) :: iostat

```

```

end subroutine state_matrix_read_raw

<State matrices: procedures>+≡
module subroutine state_matrix_write_raw (state, u)
  class(state_matrix_t), intent(in), target :: state
  integer, intent(in) :: u
  logical :: is_defined
  integer :: depth, j
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  is_defined = state%is_defined ()
  write (u) is_defined
  if (is_defined) then
    write (u) state%get_norm ()
    write (u) state%get_n_leaves ()
    depth = state%get_depth ()
    write (u) depth
    allocate (qn (depth))
    call it%init (state)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      do j = 1, depth
        call qn(j)%write_raw (u)
      end do
      write (u) it%get_me_index ()
      write (u) it%get_matrix_element ()
      call it%advance ()
    end do
  end if
end subroutine state_matrix_write_raw

module subroutine state_matrix_read_raw (state, u, iostat)
  class(state_matrix_t), intent(out) :: state
  integer, intent(in) :: u
  integer, intent(out) :: iostat
  logical :: is_defined
  real(default) :: norm
  integer :: n_leaves, depth, i, j
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  integer :: me_index
  complex(default) :: me
  read (u, iostat=iostat) is_defined
  if (iostat /= 0) goto 1
  if (is_defined) then
    call state%init (store_values = .true.)
    read (u, iostat=iostat) norm
    if (iostat /= 0) goto 1
    call state_matrix_set_norm (state, norm)
    read (u) n_leaves
    if (iostat /= 0) goto 1
    read (u) depth
    if (iostat /= 0) goto 1
    allocate (qn (depth))
    do i = 1, n_leaves
      do j = 1, depth

```

```

        call qn(j)%read_raw (u, iostat=iostat)
        if (iostat /= 0) goto 1
    end do
    read (u, iostat=iostat) me_index
    if (iostat /= 0) goto 1
    read (u, iostat=iostat) me
    if (iostat /= 0) goto 1
    call state%add_state (qn, index = me_index, value = me)
end do
call state_matrix_freeze (state)
end if
return

! Clean up on error
1 continue
call state%final ()
end subroutine state_matrix_read_raw

```

Assign a model pointer to all flavor entries. This will become necessary when we have read a state matrix from file.

```

<State matrices: state matrix: TBP>+≡
    procedure :: set_model => state_matrix_set_model

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_set_model (state, model)
        class(state_matrix_t), intent(inout), target :: state
        class(model_data_t), intent(in), target :: model
    end subroutine state_matrix_set_model

<State matrices: procedures>+≡
    module subroutine state_matrix_set_model (state, model)
        class(state_matrix_t), intent(inout), target :: state
        class(model_data_t), intent(in), target :: model
        type(state_iterator_t) :: it
        call it%init (state)
        do while (it%is_valid ())
            call it%set_model (model)
            call it%advance ()
        end do
    end subroutine state_matrix_set_model

```

Iterate over **state**, get the quantum numbers array **qn** for each iteration, and tag all array elements of **qn** with the indices given by **tag** as part of the hard interaction. Then add them to **tagged_state** and return it. If no **tag** is given, tag all **qn** as part of the hard process.

```

<State matrices: state matrix: TBP>+≡
    procedure :: tag_hard_process => state_matrix_tag_hard_process

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_tag_hard_process (state, tagged_state, tag)
        class(state_matrix_t), intent(in), target :: state
        type(state_matrix_t), intent(out) :: tagged_state
        integer, dimension(:), intent(in), optional :: tag
    end subroutine state_matrix_tag_hard_process

```

```

<State matrices: procedures>+≡
module subroutine state_matrix_tag_hard_process (state, tagged_state, tag)
  class(state_matrix_t), intent(in), target :: state
  type(state_matrix_t), intent(out) :: tagged_state
  integer, dimension(:), intent(in), optional :: tag
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  complex(default) :: value
  integer :: i
  call tagged_state%init (store_values = .true.)
  call it%init (state)
  do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    value = it%get_matrix_element ()
    if (present (tag)) then
      do i = 1, size (tag)
        call qn(tag(i))%tag_hard_process ()
      end do
    else
      call qn%tag_hard_process ()
    end if
    call tagged_state%add_state (qn, index = it%get_me_index (), value = value)
    call it%advance ()
  end do
  call tagged_state%freeze ()
end subroutine state_matrix_tag_hard_process

```

Properties of the quantum state

A state is defined if its root is allocated:

```

<State matrices: state matrix: TBP>+≡
  procedure :: is_defined => state_matrix_is_defined

<State matrices: sub interfaces>+≡
  elemental module function state_matrix_is_defined (state) result (defined)
    logical :: defined
    class(state_matrix_t), intent(in) :: state
  end function state_matrix_is_defined

<State matrices: procedures>+≡
  elemental module function state_matrix_is_defined (state) result (defined)
    logical :: defined
    class(state_matrix_t), intent(in) :: state
    defined = associated (state%root)
  end function state_matrix_is_defined

```

A state is empty if its depth is zero:

```

<State matrices: state matrix: TBP>+≡
  procedure :: is_empty => state_matrix_is_empty

<State matrices: sub interfaces>+≡
  elemental module function state_matrix_is_empty (state) result (flag)
    logical :: flag

```



```

        class(state_matrix_t), intent(in) :: state
    end function state_matrix_is_empty

<State matrices: procedures>+≡
    elemental module function state_matrix_is_empty (state) result (flag)
        logical :: flag
        class(state_matrix_t), intent(in) :: state
        flag = state%depth == 0
    end function state_matrix_is_empty

```

Return the number of matrix-element values.

```

<State matrices: state matrix: TBP>+≡
    generic :: get_n_matrix_elements => get_n_matrix_elements_all, get_n_matrix_elements_mask
    procedure :: get_n_matrix_elements_all => state_matrix_get_n_matrix_elements_all
    procedure :: get_n_matrix_elements_mask => state_matrix_get_n_matrix_elements_mask

<State matrices: sub interfaces>+≡
    pure module function state_matrix_get_n_matrix_elements_all (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_n_matrix_elements_all

<State matrices: procedures>+≡
    pure module function state_matrix_get_n_matrix_elements_all (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        n = state%n_matrix_elements
    end function state_matrix_get_n_matrix_elements_all

<State matrices: sub interfaces>+≡
    module function state_matrix_get_n_matrix_elements_mask (state, qn_mask) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
    end function state_matrix_get_n_matrix_elements_mask

<State matrices: procedures>+≡
    module function state_matrix_get_n_matrix_elements_mask (state, qn_mask) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
        type(state_iterator_t) :: it
        type(quantum_numbers_t), dimension(size(qn_mask)) :: qn
        type(state_matrix_t) :: state_tmp
        call state_tmp%init ()
        call it%init (state)
        do while (it%is_valid ())
            qn = it%get_quantum_numbers ()
            call qn%undefine (qn_mask)
            call state_tmp%add_state (qn)
            call it%advance ()
        end do
        n = state_tmp%n_matrix_elements
        call state_tmp%final ()
    end function state_matrix_get_n_matrix_elements_mask

```

Return the size of the me-array for debugging purposes.

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_me_size => state_matrix_get_me_size

<State matrices: sub interfaces>+≡
    pure module function state_matrix_get_me_size (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_me_size

<State matrices: procedures>+≡
    pure module function state_matrix_get_me_size (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        if (allocated (state%me)) then
            n = size (state%me)
        else
            n = 0
        end if
    end function state_matrix_get_me_size

<State matrices: state matrix: TBP>+≡
    procedure :: compute_n_sub => state_matrix_compute_n_sub

<State matrices: sub interfaces>+≡
    module function state_matrix_compute_n_sub (state) result (n_sub)
        integer :: n_sub
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_compute_n_sub

<State matrices: procedures>+≡
    module function state_matrix_compute_n_sub (state) result (n_sub)
        integer :: n_sub
        class(state_matrix_t), intent(in) :: state
        type(state_iterator_t) :: it
        type(quantum_numbers_t), dimension(state%depth) :: qn
        integer :: sub, sub_pos
        n_sub = 0
        call it%init (state)
        do while (it%is_valid ())
            qn = it%get_quantum_numbers ()
            sub = 0
            sub_pos = qn_array_sub_pos ()
            if (sub_pos > 0) sub = qn(sub_pos)%get_sub ()
            if (sub > n_sub) n_sub = sub
            call it%advance ()
        end do
    contains
        function qn_array_sub_pos () result (pos)
            integer :: pos
            integer :: i
            pos = 0
            do i = 1, state%depth
                if (qn(i)%get_sub () > 0) then
                    pos = i
                    exit
                end if
            end do
        end function
    end module

```

```

        end if
    end do
end function qn_array_sub_pos
end function state_matrix_compute_n_sub

```

```

<State matrices: state matrix: TBP>+≡
    procedure :: set_n_sub => state_matrix_set_n_sub

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_set_n_sub (state)
        class(state_matrix_t), intent(inout) :: state
    end subroutine state_matrix_set_n_sub

<State matrices: procedures>+≡
    module subroutine state_matrix_set_n_sub (state)
        class(state_matrix_t), intent(inout) :: state
        state%n_sub = state%compute_n_sub ()
    end subroutine state_matrix_set_n_sub

```

Return number of subtractions.

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_n_sub => state_matrix_get_n_sub

<State matrices: sub interfaces>+≡
    module function state_matrix_get_n_sub (state) result (n_sub)
        integer :: n_sub
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_n_sub

<State matrices: procedures>+≡
    module function state_matrix_get_n_sub (state) result (n_sub)
        integer :: n_sub
        class(state_matrix_t), intent(in) :: state
        if (state%n_sub < 0) then
            call msg_bug ("[state_matrix_get_n_sub] number of subtractions not set.")
        end if
        n_sub = state%n_sub
    end function state_matrix_get_n_sub

```

Return the number of leaves. This can be larger than the number of independent matrix elements.

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_n_leaves => state_matrix_get_n_leaves

<State matrices: sub interfaces>+≡
    module function state_matrix_get_n_leaves (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        type(state_iterator_t) :: it
    end function state_matrix_get_n_leaves

<State matrices: procedures>+≡
    module function state_matrix_get_n_leaves (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state

```

```

type(state_iterator_t) :: it
n = 0
call it%init (state)
do while (it%is_valid ())
    n = n + 1
    call it%advance ()
end do
end function state_matrix_get_n_leaves

```

Return the depth:

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: get_depth => state_matrix_get_depth

⟨State matrices: sub interfaces⟩+≡
    pure module function state_matrix_get_depth (state) result (depth)
        integer :: depth
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_depth

⟨State matrices: procedures⟩+≡
    pure module function state_matrix_get_depth (state) result (depth)
        integer :: depth
        class(state_matrix_t), intent(in) :: state
        depth = state%depth
    end function state_matrix_get_depth

```

Return the norm:

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: get_norm => state_matrix_get_norm

⟨State matrices: sub interfaces⟩+≡
    pure module function state_matrix_get_norm (state) result (norm)
        real(default) :: norm
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_norm

⟨State matrices: procedures⟩+≡
    pure module function state_matrix_get_norm (state) result (norm)
        real(default) :: norm
        class(state_matrix_t), intent(in) :: state
        norm = state%norm
    end function state_matrix_get_norm

```

Retrieving contents

Return the quantum number array, using an index. We have to scan the state matrix since there is no shortcut.

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: get_quantum_number => &
        state_matrix_get_quantum_number

```

<State matrices: sub interfaces>+≡

```

module function state_matrix_get_quantum_number (state, i, by_me_index) result (qn)
  class(state_matrix_t), intent(in), target :: state
  integer, intent(in) :: i
  logical, intent(in), optional :: by_me_index
  type(quantum_numbers_t), dimension(state%depth) :: qn
end function state_matrix_get_quantum_number

```

<State matrices: procedures>+≡

```

module function state_matrix_get_quantum_number (state, i, by_me_index) result (qn)
  class(state_matrix_t), intent(in), target :: state
  integer, intent(in) :: i
  logical, intent(in), optional :: by_me_index
  logical :: opt_by_me_index
  type(quantum_numbers_t), dimension(state%depth) :: qn
  type(state_iterator_t) :: it
  integer :: k
  opt_by_me_index = .false.
  if (present (by_me_index)) opt_by_me_index = by_me_index
  k = 0
  call it%init (state)
  do while (it%is_valid ())
    if (opt_by_me_index) then
      k = it%get_me_index ()
    else
      k = k + 1
    end if
    if (k == i) then
      qn = it%get_quantum_numbers ()
      exit
    end if
    call it%advance ()
  end do
end function state_matrix_get_quantum_number

```

<State matrices: state matrix: TBP>+≡

```

generic :: get_quantum_numbers => get_quantum_numbers_all, get_quantum_numbers_mask
procedure :: get_quantum_numbers_all => state_matrix_get_quantum_numbers_all
procedure :: get_quantum_numbers_mask => state_matrix_get_quantum_numbers_mask

```

<State matrices: sub interfaces>+≡

```

module subroutine state_matrix_get_quantum_numbers_all (state, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
end subroutine state_matrix_get_quantum_numbers_all

```

<State matrices: procedures>+≡

```

module subroutine state_matrix_get_quantum_numbers_all (state, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
  integer :: i
  allocate (qn (state%get_n_matrix_elements (), &
    state%get_depth()))
  do i = 1, state%get_n_matrix_elements ()
    qn (i, :) = state%get_quantum_number (i)
  end do

```

```
end subroutine state_matrix_get_quantum_numbers_all
```

(State matrices: sub interfaces)+≡

```
module subroutine state_matrix_get_quantum_numbers_mask (state, qn_mask, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
end subroutine state_matrix_get_quantum_numbers_mask
```

(State matrices: procedures)+≡

```
module subroutine state_matrix_get_quantum_numbers_mask (state, qn_mask, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
  type(quantum_numbers_t), dimension(:), allocatable :: qn_tmp
  type(state_matrix_t) :: state_tmp
  type(state_iterator_t) :: it
  integer :: i, n
  n = state%get_n_matrix_elements (qn_mask)
  allocate (qn (n, state%get_depth ()))
  allocate (qn_tmp (state%get_depth ()))
  call it%init (state)
  call state_tmp%init ()
  do while (it%is_valid ())
    qn_tmp = it%get_quantum_numbers ()
    call qn_tmp%undefine (qn_mask)
    call state_tmp%add_state (qn_tmp)
    call it%advance ()
  end do
  do i = 1, n
    qn (i, :) = state_tmp%get_quantum_number (i)
  end do
  call state_tmp%final ()
end subroutine state_matrix_get_quantum_numbers_mask
```

(State matrices: state matrix: TBP)+≡

```
procedure :: get_flavors => state_matrix_get_flavors
```

(State matrices: sub interfaces)+≡

```
module subroutine state_matrix_get_flavors (state, only_elementary, qn_mask, flv)
  class(state_matrix_t), intent(in), target :: state
  logical, intent(in) :: only_elementary
  type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
  integer, intent(out), dimension(:,:), allocatable :: flv
end subroutine state_matrix_get_flavors
```

(State matrices: procedures)+≡

```
module subroutine state_matrix_get_flavors (state, only_elementary, qn_mask, flv)
  class(state_matrix_t), intent(in), target :: state
  logical, intent(in) :: only_elementary
  type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
  integer, intent(out), dimension(:,:), allocatable :: flv
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  integer :: i_flv, n_partons
  type(flavor_t), dimension(:), allocatable :: flv_flv
```

```

if (present (qn_mask)) then
  call state%get_quantum_numbers (qn_mask, qn)
else
  call state%get_quantum_numbers (qn)
end if
allocate (flv_flv (size (qn, dim=2)))
if (only_elementary) then
  flv_flv = qn(1, :)%get_flavor ()
  n_partons = count (is_elementary (flv_flv%get_pdg ()))
end if
allocate (flv (n_partons, size (qn, dim=1)))
associate (n_flv => size (qn, dim=1))
do i_flv = 1, size (qn, dim=1)
  flv_flv = qn(i_flv, :)%get_flavor ()
  flv(:, i_flv) = pack (flv_flv%get_pdg (), is_elementary(flv_flv%get_pdg()))
end do
end associate
contains
elemental function is_elementary (pdg)
  logical :: is_elementary
  integer, intent(in) :: pdg
  is_elementary = abs(pdg) /= 2212 .and. abs(pdg) /= 92 .and. abs(pdg) /= 93
end function is_elementary
end subroutine state_matrix_get_flavors

```

Return a single matrix element using its index. Works only if the shortcut array is allocated.

<State matrices: state matrix: TBP>+≡

```

generic :: get_matrix_element => get_matrix_element_single
generic :: get_matrix_element => get_matrix_element_array
procedure :: get_matrix_element_single => &
  state_matrix_get_matrix_element_single
procedure :: get_matrix_element_array => &
  state_matrix_get_matrix_element_array

```

<State matrices: sub interfaces>+≡

```

elemental module function state_matrix_get_matrix_element_single (state, i) result (me)
  complex(default) :: me
  class(state_matrix_t), intent(in) :: state
  integer, intent(in) :: i
end function state_matrix_get_matrix_element_single

```

<State matrices: procedures>+≡

```

elemental module function state_matrix_get_matrix_element_single (state, i) result (me)
  complex(default) :: me
  class(state_matrix_t), intent(in) :: state
  integer, intent(in) :: i
  if (allocated (state%me)) then
    me = state%me(i)
  else
    me = 0
  end if
end function state_matrix_get_matrix_element_single

```

```

<State matrices: sub interfaces>+≡
  module function state_matrix_get_matrix_element_array (state) result (me)
    complex(default), dimension(:), allocatable :: me
    class(state_matrix_t), intent(in) :: state
  end function state_matrix_get_matrix_element_array

```

```

<State matrices: procedures>+≡
  module function state_matrix_get_matrix_element_array (state) result (me)
    complex(default), dimension(:), allocatable :: me
    class(state_matrix_t), intent(in) :: state
    if (associated (state%me)) then
      allocate (me (size (state%me)))
      me = state%me
    else
      me = 0
    end if
  end function state_matrix_get_matrix_element_array

```

Return the color index with maximum absolute value that is present within the state matrix.

```

<State matrices: state matrix: TBP>+≡
  procedure :: get_max_color_value => state_matrix_get_max_color_value

```

```

<State matrices: sub interfaces>+≡
  module function state_matrix_get_max_color_value (state) result (cmax)
    integer :: cmax
    class(state_matrix_t), intent(in) :: state
  end function state_matrix_get_max_color_value

```

```

<State matrices: procedures>+≡
  module function state_matrix_get_max_color_value (state) result (cmax)
    integer :: cmax
    class(state_matrix_t), intent(in) :: state
    if (associated (state%root)) then
      cmax = node_get_max_color_value (state%root)
    else
      cmax = 0
    end if
  contains
    recursive function node_get_max_color_value (node) result (cmax)
      integer :: cmax
      type(node_t), intent(in), target :: node
      type(node_t), pointer :: current
      cmax = quantum_numbers_get_max_color_value (node%qn)
      current => node%child_first
      do while (associated (current))
        cmax = max (cmax, node_get_max_color_value (current))
        current => current%next
      end do
    end function node_get_max_color_value
  end function state_matrix_get_max_color_value

```


Building the quantum state

The procedure generates a branch associated to the input array of quantum numbers. If the branch exists already, it is used.

Optionally, we set the matrix-element index, a value (which may be added to the previous one), and increment one of the possible counters. We may also return the matrix element index of the current node.

```

<State matrices: state matrix: TBP>+≡
    procedure :: add_state => state_matrix_add_state

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_add_state (state, qn, index, value, &
        sum_values, counter_index, ignore_sub_for_qn, me_index)
        class(state_matrix_t), intent(inout) :: state
        type(quantum_numbers_t), dimension(:), intent(in) :: qn
        integer, intent(in), optional :: index
        complex(default), intent(in), optional :: value
        logical, intent(in), optional :: sum_values
        integer, intent(in), optional :: counter_index
        logical, intent(in), optional :: ignore_sub_for_qn
        integer, intent(out), optional :: me_index
    end subroutine state_matrix_add_state

<State matrices: procedures>+≡
    module subroutine state_matrix_add_state (state, qn, index, value, &
        sum_values, counter_index, ignore_sub_for_qn, me_index)
        class(state_matrix_t), intent(inout) :: state
        type(quantum_numbers_t), dimension(:), intent(in) :: qn
        integer, intent(in), optional :: index
        complex(default), intent(in), optional :: value
        logical, intent(in), optional :: sum_values
        integer, intent(in), optional :: counter_index
        logical, intent(in), optional :: ignore_sub_for_qn
        integer, intent(out), optional :: me_index
        logical :: set_index, get_index, add
        set_index = present (index)
        get_index = present (me_index)
        add = .false.; if (present (sum_values)) add = sum_values
        if (state%depth == 0) then
            state%depth = size (qn)
        else if (state%depth /= size (qn)) then
            call state%write ()
            call msg_bug ("State matrix: depth mismatch")
        end if
        if (size (qn) > 0) call node_make_branch (state%root, qn)
contains
        recursive subroutine node_make_branch (parent, qn)
            type(node_t), pointer :: parent
            type(quantum_numbers_t), dimension(:), intent(in) :: qn
            type(node_t), pointer :: child
            logical :: match
            match = .false.
            child => parent%child_first
            SCAN_CHILDREN: do while (associated (child))
                if (present (ignore_sub_for_qn)) then

```

```

        if (ignore_sub_for_qn) then
            match = quantum_numbers_eq_wo_sub (child%qn, qn(1))
        else
            match = child%qn == qn(1)
        end if
    else
        match = child%qn == qn(1)
    end if
    if (match) exit SCAN_CHILDREN
    child => child%next
end do SCAN_CHILDREN
if (.not. match) then
    call node_append_child (parent, child)
    child%qn = qn(1)
end if
select case (size (qn))
case (1)
    if (.not. match) then
        state%n_matrix_elements = state%n_matrix_elements + 1
        child%me_index = state%n_matrix_elements
    end if
    if (set_index) then
        child%me_index = index
    end if
    if (get_index) then
        me_index = child%me_index
    end if
    if (present (counter_index)) then
        if (.not. allocated (child%me_count)) then
            allocate (child%me_count (state%n_counters))
            child%me_count = 0
        end if
        child%me_count(counter_index) = child%me_count(counter_index) + 1
    end if
    if (present (value)) then
        if (add) then
            child%me = child%me + value
        else
            child%me = value
        end if
    end if
case (2:)
    call node_make_branch (child, qn(2:))
end select
end subroutine node_make_branch
end subroutine state_matrix_add_state

```

Remove irrelevant flavor/color/helicity labels and the corresponding branchings. The masks indicate which particles are affected; the masks length should coincide with the depth of the trie (without the root node). Recursively scan the whole tree, starting from the leaf nodes and working up to the root node. If a mask entry is set for the current tree level, scan the children there. For each child within that level make a new empty branch where the masked quan-

tum number is undefined. Then recursively combine all following children with matching quantum number into this new node and move on.

```

<State matrices: state matrix: TBP>+≡
  procedure :: collapse => state_matrix_collapse

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_collapse (state, mask)
    class(state_matrix_t), intent(inout) :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
  end subroutine state_matrix_collapse

<State matrices: procedures>+≡
  module subroutine state_matrix_collapse (state, mask)
    class(state_matrix_t), intent(inout) :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(state_matrix_t) :: red_state
    if (state%is_defined ()) then
      call state%reduce (mask, red_state)
      call state%final ()
      state = red_state
    end if
  end subroutine state_matrix_collapse

```

Transform the given state matrix into a reduced state matrix where some quantum numbers are removed, as indicated by the mask. The procedure creates a new state matrix, so the old one can be deleted after this if it is no longer used.

It is said that the matrix element ordering is lost afterwards. We allow to keep the original matrix element index in the new state matrix. If the matrix element indices are kept, we do not freeze the state matrix. After reordering the matrix element indices by `state_matrix_reorder_me`, the state matrix can be frozen.

```

<State matrices: state matrix: TBP>+≡
  procedure :: reduce => state_matrix_reduce

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_reduce (state, mask, red_state, keep_me_index)
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(state_matrix_t), intent(out) :: red_state
    logical, optional, intent(in) :: keep_me_index
  end subroutine state_matrix_reduce

<State matrices: procedures>+≡
  module subroutine state_matrix_reduce (state, mask, red_state, keep_me_index)
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(state_matrix_t), intent(out) :: red_state
    logical, optional, intent(in) :: keep_me_index
    logical :: opt_keep_me_index
    type(state_iterator_t) :: it
    type(quantum_numbers_t), dimension(size(mask)) :: qn
    opt_keep_me_index = .false.
    if (present (keep_me_index)) opt_keep_me_index = keep_me_index
    call red_state%init ()
    call it%init (state)

```

```

do while (it%is_valid ())
  qn = it%get_quantum_numbers ()
  call qn%undefine (mask)
  if (opt_keep_me_index) then
    call red_state%add_state (qn, index = it%get_me_index ())
  else
    call red_state%add_state (qn)
  end if
  call it%advance ()
end do
if (.not. opt_keep_me_index) then
  call red_state%freeze ()
end if
end subroutine state_matrix_reduce

```

Reorder the matrix elements – not the tree itself. The procedure is necessary in case the matrix element indices were kept when reducing over quantum numbers and one wants to reintroduce the previous order of the matrix elements.

<State matrices: state matrix: TBP>+≡

```

procedure :: reorder_me => state_matrix_reorder_me

```

<State matrices: sub interfaces>+≡

```

module subroutine state_matrix_reorder_me (state, ordered_state)
  class(state_matrix_t), intent(in), target :: state
  type(state_matrix_t), intent(out) :: ordered_state
end subroutine state_matrix_reorder_me

```

<State matrices: procedures>+≡

```

module subroutine state_matrix_reorder_me (state, ordered_state)
  class(state_matrix_t), intent(in), target :: state
  type(state_matrix_t), intent(out) :: ordered_state
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(state%depth) :: qn
  integer, dimension(:), allocatable :: me_index
  integer :: i
  call ordered_state%init ()
  call get_me_index_sorted (state, me_index)
  i = 1; call it%init (state)
  do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    call ordered_state%add_state (qn, index = me_index(i))
    i = i + 1; call it%advance ()
  end do
  call ordered_state%freeze ()
contains
  subroutine get_me_index_sorted (state, me_index)
    class(state_matrix_t), intent(in), target :: state
    integer, dimension(:), allocatable, intent(out) :: me_index
    type(state_iterator_t) :: it
    integer :: i, j
    integer, dimension(:), allocatable :: me_index_unsorted, me_index_sorted
    associate (n_matrix_elements => state%get_n_matrix_elements ())
      allocate (me_index(n_matrix_elements), source = 0)
      allocate (me_index_unsorted(n_matrix_elements), source = 0)
    end associate
  end subroutine

```

```

allocate (me_index_unsorted(n_matrix_elements), source = 0)
i = 1; call it%init (state)
do while (it%is_valid ())
    me_index_unsorted(i) = it%get_me_index ()
    i = i + 1
    call it%advance ()
end do
me_index_sorted = sort (me_index_unsorted)
! We do not care about efficiency at this point.
UNSORTED: do i = 1, n_matrix_elements
    SORTED: do j = 1, n_matrix_elements
        if (me_index_unsorted(i) == me_index_sorted(j)) then
            me_index(i) = j
            cycle UNSORTED
        end if
    end do SORTED
end do UNSORTED
end associate
end subroutine get_me_index_sorted
end subroutine state_matrix_reorder_me

```

Sets all matrix elements whose flavor structure is a duplicate of another flavor structure to zero. We need this for the real finite to ignore duplicate flavor structures while keeping the indices identical to the singular real component. When comparing the flavor structures, we take into account permutations of final- state particles. To do this properly, we keep only the non-hard flavors and the initial-state flavors, i.e. the first two hard flavors fixed.

<State matrices: state matrix: TBP>+≡

```
procedure :: set_duplicate_flv_zero => state_matrix_set_duplicate_flv_zero
```

<State matrices: sub interfaces>+≡

```

module subroutine state_matrix_set_duplicate_flv_zero (state)
    class(state_matrix_t), intent(inout), target :: state
end subroutine state_matrix_set_duplicate_flv_zero

```

<State matrices: procedures>+≡

```

module subroutine state_matrix_set_duplicate_flv_zero (state)
    class(state_matrix_t), intent(inout), target :: state
    type(quantum_numbers_t), dimension(state%depth) :: qn
    type(flavor_t) :: flv
    type(state_flv_content_t), allocatable :: state_flv
    logical, dimension(:), allocatable :: hard_mask, sort_mask, duplicate_mask
    integer :: i, j, n_in, n_flvs
    n_flvs = state%get_depth ()
    n_in = 2
    !!! TODO (PS-28-07-21) n_in should not be hard coded to work for decays
    !!! This assumes that the positions of the non-hard flavors are the same for all flavor struct
    qn = state%get_quantum_number(1)
    allocate (hard_mask(n_flvs))
    do i = 1, n_flvs
        flv = qn(i)%get_flavor()
        hard_mask(i) = flv%is_hard_process ()
    end do
    allocate (sort_mask(n_flvs))

```

```

sort_mask = hard_mask
j = 0
do i = 1, n_flvs
  if (j == n_in) exit
  if (sort_mask(i)) then
    sort_mask(i) = .false.
    j = j + 1
  end if
end do
allocate (state_flv)
call state_flv%fill (state, sort_mask)
call state_flv%find_duplicates (duplicate_mask)
do i = 1, state%get_n_matrix_elements ()
  if (duplicate_mask(i)) then
    call state%set_matrix_element_single(i, cmplx(zero, zero, default))
  end if
end do
end subroutine state_matrix_set_duplicate_flv_zero

```

This subroutine sets up the matrix-element array. The leaf nodes acquire the index values that point to the appropriate matrix-element entry.

We recursively scan the trie. Once we arrive at a leaf node, the index is increased and associated to that node. Finally, we allocate the matrix-element array with the appropriate size.

If matrix element values are temporarily stored within the leaf nodes, we scan the state again and transfer them to the matrix-element array.

```

<State matrices: state matrix: TBP>+=
  procedure :: freeze => state_matrix_freeze

<State matrices: sub interfaces>+=
  module subroutine state_matrix_freeze (state)
    class(state_matrix_t), intent(inout), target :: state
  end subroutine state_matrix_freeze

<State matrices: procedures>+=
  module subroutine state_matrix_freeze (state)
    class(state_matrix_t), intent(inout), target :: state
    type(state_iterator_t) :: it
    if (associated (state%root)) then
      if (allocated (state%me)) deallocate (state%me)
      allocate (state%me (state%n_matrix_elements))
      state%me = 0
      call state%set_n_sub ()
    end if
    if (state%leaf_nodes_store_values) then
      call it%init (state)
      do while (it%is_valid ())
        state%me(it%get_me_index ()) = it%get_matrix_element ()
        call it%advance ()
      end do
      state%leaf_nodes_store_values = .false.
    end if
  end subroutine state_matrix_freeze

```

Direct access to the value array

Several methods for setting a value directly are summarized in this generic:

```
<State matrices: state matrix: TBP>+≡
generic :: set_matrix_element => set_matrix_element_qn
generic :: set_matrix_element => set_matrix_element_all
generic :: set_matrix_element => set_matrix_element_array
generic :: set_matrix_element => set_matrix_element_single
generic :: set_matrix_element => set_matrix_element_clone
procedure :: set_matrix_element_qn => state_matrix_set_matrix_element_qn
procedure :: set_matrix_element_all => state_matrix_set_matrix_element_all
procedure :: set_matrix_element_array => &
    state_matrix_set_matrix_element_array
procedure :: set_matrix_element_single => &
    state_matrix_set_matrix_element_single
procedure :: set_matrix_element_clone => &
    state_matrix_set_matrix_element_clone
```

Set a value that corresponds to a quantum number array:

```
<State matrices: sub interfaces>+≡
module subroutine state_matrix_set_matrix_element_qn (state, qn, value)
    class(state_matrix_t), intent(inout), target :: state
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    complex(default), intent(in) :: value
end subroutine state_matrix_set_matrix_element_qn

<State matrices: procedures>+≡
module subroutine state_matrix_set_matrix_element_qn (state, qn, value)
    class(state_matrix_t), intent(inout), target :: state
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    complex(default), intent(in) :: value
    type(state_iterator_t) :: it
    if (.not. allocated (state%me)) then
        allocate (state%me (size(qn)))
    end if
    call it%init (state)
    call it%go_to_qn (qn)
    call it%set_matrix_element (value)
end subroutine state_matrix_set_matrix_element_qn
```

Set all matrix elements to a single value

```
<State matrices: sub interfaces>+≡
module subroutine state_matrix_set_matrix_element_all (state, value)
    class(state_matrix_t), intent(inout) :: state
    complex(default), intent(in) :: value
end subroutine state_matrix_set_matrix_element_all

<State matrices: procedures>+≡
module subroutine state_matrix_set_matrix_element_all (state, value)
    class(state_matrix_t), intent(inout) :: state
    complex(default), intent(in) :: value
    if (.not. allocated (state%me)) then
        allocate (state%me (state%n_matrix_elements))
    end if
    state%me = value
```

```
end subroutine state_matrix_set_matrix_element_all
```

Set the matrix-element array directly.

<State matrices: sub interfaces>+≡

```
module subroutine state_matrix_set_matrix_element_array (state, value, range)
  class(state_matrix_t), intent(inout) :: state
  complex(default), intent(in), dimension(:) :: value
  integer, intent(in), dimension(:), optional :: range
end subroutine state_matrix_set_matrix_element_array
```

<State matrices: procedures>+≡

```
module subroutine state_matrix_set_matrix_element_array (state, value, range)
  class(state_matrix_t), intent(inout) :: state
  complex(default), intent(in), dimension(:) :: value
  integer, intent(in), dimension(:), optional :: range
  if (present (range)) then
    state%me(range) = value
  else
    if (.not. allocated (state%me)) &
      allocate (state%me (size (value)))
    state%me(:) = value
  end if
end subroutine state_matrix_set_matrix_element_array
```

Set a matrix element at position i to value.

<State matrices: sub interfaces>+≡

```
pure module subroutine state_matrix_set_matrix_element_single (state, i, value)
  class(state_matrix_t), intent(inout) :: state
  integer, intent(in) :: i
  complex(default), intent(in) :: value
end subroutine state_matrix_set_matrix_element_single
```

<State matrices: procedures>+≡

```
pure module subroutine state_matrix_set_matrix_element_single (state, i, value)
  class(state_matrix_t), intent(inout) :: state
  integer, intent(in) :: i
  complex(default), intent(in) :: value
  if (.not. allocated (state%me)) then
    allocate (state%me (state%n_matrix_elements))
  end if
  state%me(i) = value
end subroutine state_matrix_set_matrix_element_single
```

Clone the matrix elements from another (matching) state matrix.

<State matrices: sub interfaces>+≡

```
module subroutine state_matrix_set_matrix_element_clone (state, state1)
  class(state_matrix_t), intent(inout) :: state
  type(state_matrix_t), intent(in) :: state1
end subroutine state_matrix_set_matrix_element_clone
```

<State matrices: procedures>+≡

```
module subroutine state_matrix_set_matrix_element_clone (state, state1)
  class(state_matrix_t), intent(inout) :: state
  type(state_matrix_t), intent(in) :: state1
```



```

        if (.not. allocated (state1%me)) return
        if (.not. allocated (state%me)) allocate (state%me (size (state1%me)))
        state%me = state1%me
    end subroutine state_matrix_set_matrix_element_clone

```

Add a value to a matrix element

```

<State matrices: state matrix: TBP>+≡
    procedure :: add_to_matrix_element => state_matrix_add_to_matrix_element

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_add_to_matrix_element (state, qn, value, match_only_flavor)
        class(state_matrix_t), intent(inout), target :: state
        type(quantum_numbers_t), dimension(:), intent(in) :: qn
        complex(default), intent(in) :: value
        logical, intent(in), optional :: match_only_flavor
    end subroutine state_matrix_add_to_matrix_element

<State matrices: procedures>+≡
    module subroutine state_matrix_add_to_matrix_element (state, qn, value, match_only_flavor)
        class(state_matrix_t), intent(inout), target :: state
        type(quantum_numbers_t), dimension(:), intent(in) :: qn
        complex(default), intent(in) :: value
        logical, intent(in), optional :: match_only_flavor
        type(state_iterator_t) :: it
        call it%init (state)
        call it%go_to_qn (qn, match_only_flavor)
        if (it%is_valid ()) then
            call it%add_to_matrix_element (value)
        else
            call msg_fatal ("Cannot add to matrix element - it%node not allocated")
        end if
    end subroutine state_matrix_add_to_matrix_element

```

12.1.3 State iterators

Accessing the quantum state from outside is best done using a specialized iterator, i.e., a pointer to a particular branch of the quantum state trie. Technically, the iterator contains a pointer to a leaf node, but via parent pointers it allows to access the whole branch where the leaf is attached. For quick access, we also keep the branch depth (which is assumed to be universal for a quantum state).

```

<State matrices: public>+≡
    public :: state_iterator_t

<State matrices: types>+≡
    type :: state_iterator_t
        private
        integer :: depth = 0
        type(state_matrix_t), pointer :: state => null ()
        type(node_t), pointer :: node => null ()
    contains
        <State matrices: state iterator: TBP>
    end type state_iterator_t

```

The initializer: Point at the first branch. Note that this cannot be pure, thus not be elemental, because the iterator can be used to manipulate data in the state matrix.

```

<State matrices: state iterator: TBP>≡
  procedure :: init => state_iterator_init

<State matrices: sub interfaces>+≡
  module subroutine state_iterator_init (it, state)
    class(state_iterator_t), intent(out) :: it
    type(state_matrix_t), intent(in), target :: state
  end subroutine state_iterator_init

<State matrices: procedures>+≡
  module subroutine state_iterator_init (it, state)
    class(state_iterator_t), intent(out) :: it
    type(state_matrix_t), intent(in), target :: state
    it%state => state
    it%depth = state%depth
    if (state%is_defined ()) then
      it%node => state%root
      do while (associated (it%node%child_first))
        it%node => it%node%child_first
      end do
    else
      it%node => null ()
    end if
  end subroutine state_iterator_init

```

Go forward. Recursively programmed: if the next node does not exist, go back to the parent node and look at its successor (if present), etc.

There is a possible pitfall in the implementation: If the dummy pointer argument to the `find_next` routine is used directly, we still get the correct result for the iterator, but calling the recursion on `node%parent` means that we manipulate a parent pointer in the original state in addition to the iterator. Making a local copy of the pointer avoids this. Using pointer intent would be helpful, but we do not yet rely on this F2003 feature.

```

<State matrices: state iterator: TBP>+≡
  procedure :: advance => state_iterator_advance

<State matrices: sub interfaces>+≡
  module subroutine state_iterator_advance (it)
    class(state_iterator_t), intent(inout) :: it
  end subroutine state_iterator_advance

<State matrices: procedures>+≡
  module subroutine state_iterator_advance (it)
    class(state_iterator_t), intent(inout) :: it
    call find_next (it%node)
  contains
    recursive subroutine find_next (node_in)
      type(node_t), intent(in), target :: node_in
      type(node_t), pointer :: node
      node => node_in
      if (associated (node%next)) then
        node => node%next
      end if
    end subroutine find_next
  end subroutine state_iterator_advance

```

```

        do while (associated (node%child_first))
            node => node%child_first
        end do
        it%node => node
    else if (associated (node%parent)) then
        call find_next (node%parent)
    else
        it%node => null ()
    end if
end subroutine find_next
end subroutine state_iterator_advance

```

If all has been scanned, the iterator is at an undefined state. Check for this:

```

<State matrices: state iterator: TBP>+≡
    procedure :: is_valid => state_iterator_is_valid

<State matrices: sub interfaces>+≡
    module function state_iterator_is_valid (it) result (defined)
        logical :: defined
        class(state_iterator_t), intent(in) :: it
    end function state_iterator_is_valid

<State matrices: procedures>+≡
    module function state_iterator_is_valid (it) result (defined)
        logical :: defined
        class(state_iterator_t), intent(in) :: it
        defined = associated (it%node)
    end function state_iterator_is_valid

```

Return the matrix-element index that corresponds to the current node

```

<State matrices: state iterator: TBP>+≡
    procedure :: get_me_index => state_iterator_get_me_index

<State matrices: sub interfaces>+≡
    module function state_iterator_get_me_index (it) result (n)
        integer :: n
        class(state_iterator_t), intent(in) :: it
    end function state_iterator_get_me_index

<State matrices: procedures>+≡
    module function state_iterator_get_me_index (it) result (n)
        integer :: n
        class(state_iterator_t), intent(in) :: it
        n = it%node%me_index
    end function state_iterator_get_me_index

```

Return the number of times this quantum-number state has been added (noting that it is physically inserted only the first time). Note that for each state, there is an array of counters.

```

<State matrices: state iterator: TBP>+≡
    procedure :: get_me_count => state_iterator_get_me_count

```

<State matrices: sub interfaces>+≡

```
module function state_iterator_get_me_count (it) result (n)
  integer, dimension(:), allocatable :: n
  class(state_iterator_t), intent(in) :: it
end function state_iterator_get_me_count
```

<State matrices: procedures>+≡

```
module function state_iterator_get_me_count (it) result (n)
  integer, dimension(:), allocatable :: n
  class(state_iterator_t), intent(in) :: it
  if (allocated (it%node%me_count)) then
    allocate (n (size (it%node%me_count)))
    n = it%node%me_count
  else
    allocate (n (0))
  end if
end function state_iterator_get_me_count
```

<State matrices: state iterator: TBP>+≡

```
procedure :: get_depth => state_iterator_get_depth
```

<State matrices: sub interfaces>+≡

```
pure module function state_iterator_get_depth (state_iterator) result (depth)
  integer :: depth
  class(state_iterator_t), intent(in) :: state_iterator
end function state_iterator_get_depth
```

<State matrices: procedures>+≡

```
pure module function state_iterator_get_depth (state_iterator) result (depth)
  integer :: depth
  class(state_iterator_t), intent(in) :: state_iterator
  depth = state_iterator%depth
end function state_iterator_get_depth
```

Proceed to the state associated with the quantum numbers qn.

<State matrices: state iterator: TBP>+≡

```
procedure :: go_to_qn => state_iterator_go_to_qn
```

<State matrices: sub interfaces>+≡

```
module subroutine state_iterator_go_to_qn (it, qn, match_only_flavor)
  class(state_iterator_t), intent(inout) :: it
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  logical, intent(in), optional :: match_only_flavor
end subroutine state_iterator_go_to_qn
```

<State matrices: procedures>+≡

```
module subroutine state_iterator_go_to_qn (it, qn, match_only_flavor)
  class(state_iterator_t), intent(inout) :: it
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  logical, intent(in), optional :: match_only_flavor
  type(quantum_numbers_t), dimension(:), allocatable :: qn_hard, qn_tmp
  logical :: match_flg
  match_flg = .false.; if (present (match_only_flavor)) match_flg = .true.
  do while (it%is_valid ())
    if (match_flg) then
      qn_tmp = it%get_quantum_numbers ()
```

```

        qn_hard = pack (qn_tmp, qn_tmp%are_hard_process ())
        if (all (qn .fmatch. qn_hard)) then
            return
        else
            call it%advance ()
        end if
    else
        if (all (qn == it%get_quantum_numbers ())) then
            return
        else
            call it%advance ()
        end if
    end if
end do
end subroutine state_iterator_go_to_qn

```

Use the iterator to retrieve quantum-number information:

```

<State matrices: state iterator: TBP>+≡
    generic :: get_quantum_numbers => get_qn_multi, get_qn_slice, &
        get_qn_range, get_qn_single
    generic :: get_flavor => get_flv_multi, get_flv_slice, &
        get_flv_range, get_flv_single
    generic :: get_color => get_col_multi, get_col_slice, &
        get_col_range, get_col_single
    generic :: get_helicity => get_hel_multi, get_hel_slice, &
        get_hel_range, get_hel_single

<State matrices: state iterator: TBP>+≡
    procedure :: get_qn_multi => state_iterator_get_qn_multi
    procedure :: get_qn_slice => state_iterator_get_qn_slice
    procedure :: get_qn_range => state_iterator_get_qn_range
    procedure :: get_qn_single => state_iterator_get_qn_single
    procedure :: get_flv_multi => state_iterator_get_flv_multi
    procedure :: get_flv_slice => state_iterator_get_flv_slice
    procedure :: get_flv_range => state_iterator_get_flv_range
    procedure :: get_flv_single => state_iterator_get_flv_single
    procedure :: get_col_multi => state_iterator_get_col_multi
    procedure :: get_col_slice => state_iterator_get_col_slice
    procedure :: get_col_range => state_iterator_get_col_range
    procedure :: get_col_single => state_iterator_get_col_single
    procedure :: get_hel_multi => state_iterator_get_hel_multi
    procedure :: get_hel_slice => state_iterator_get_hel_slice
    procedure :: get_hel_range => state_iterator_get_hel_range
    procedure :: get_hel_single => state_iterator_get_hel_single

```

These versions return the whole quantum number array

```

<State matrices: sub interfaces>+≡
    module function state_iterator_get_qn_multi (it) result (qn)
        class(state_iterator_t), intent(in) :: it
        type(quantum_numbers_t), dimension(it%depth) :: qn
    end function state_iterator_get_qn_multi
    module function state_iterator_get_flv_multi (it) result (flv)
        class(state_iterator_t), intent(in) :: it
        type(flavor_t), dimension(it%depth) :: flv
    end function state_iterator_get_flv_multi

```

```

end function state_iterator_get_flv_multi
module function state_iterator_get_col_multi (it) result (col)
  class(state_iterator_t), intent(in) :: it
  type(color_t), dimension(it%depth) :: col
end function state_iterator_get_col_multi
module function state_iterator_get_hel_multi (it) result (hel)
  class(state_iterator_t), intent(in) :: it
  type(helicity_t), dimension(it%depth) :: hel
end function state_iterator_get_hel_multi

<State matrices: procedures>+≡
module function state_iterator_get_qn_multi (it) result (qn)
  class(state_iterator_t), intent(in) :: it
  type(quantum_numbers_t), dimension(it%depth) :: qn
  type(node_t), pointer :: node
  integer :: i
  node => it%node
  do i = it%depth, 1, -1
    qn(i) = node%qn
    node => node%parent
  end do
end function state_iterator_get_qn_multi

module function state_iterator_get_flv_multi (it) result (flv)
  class(state_iterator_t), intent(in) :: it
  type(flavor_t), dimension(it%depth) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers ())
end function state_iterator_get_flv_multi

module function state_iterator_get_col_multi (it) result (col)
  class(state_iterator_t), intent(in) :: it
  type(color_t), dimension(it%depth) :: col
  col = quantum_numbers_get_color &
    (it%get_quantum_numbers ())
end function state_iterator_get_col_multi

module function state_iterator_get_hel_multi (it) result (hel)
  class(state_iterator_t), intent(in) :: it
  type(helicity_t), dimension(it%depth) :: hel
  hel = quantum_numbers_get_helicity &
    (it%get_quantum_numbers ())
end function state_iterator_get_hel_multi

```

An array slice (derived from the above).

```

<State matrices: sub interfaces>+≡
module function state_iterator_get_qn_slice (it, index) result (qn)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index
  type(quantum_numbers_t), dimension(size(index)) :: qn
end function state_iterator_get_qn_slice
module function state_iterator_get_flv_slice (it, index) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index

```

```

        type(flavor_t), dimension(size(index)) :: flv
    end function state_iterator_get_flv_slice
    module function state_iterator_get_col_slice (it, index) result (col)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(color_t), dimension(size(index)) :: col
    end function state_iterator_get_col_slice
    module function state_iterator_get_hel_slice (it, index) result (hel)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(helicity_t), dimension(size(index)) :: hel
    end function state_iterator_get_hel_slice

    <State matrices: procedures>+≡
    module function state_iterator_get_qn_slice (it, index) result (qn)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(quantum_numbers_t), dimension(size(index)) :: qn
        type(quantum_numbers_t), dimension(it%depth) :: qn_tmp
        qn_tmp = state_iterator_get_qn_multi (it)
        qn = qn_tmp(index)
    end function state_iterator_get_qn_slice

    module function state_iterator_get_flv_slice (it, index) result (flv)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(flavor_t), dimension(size(index)) :: flv
        flv = quantum_numbers_get_flavor &
            (it%get_quantum_numbers (index))
    end function state_iterator_get_flv_slice

    module function state_iterator_get_col_slice (it, index) result (col)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(color_t), dimension(size(index)) :: col
        col = quantum_numbers_get_color &
            (it%get_quantum_numbers (index))
    end function state_iterator_get_col_slice

    module function state_iterator_get_hel_slice (it, index) result (hel)
        class(state_iterator_t), intent(in) :: it
        integer, dimension(:), intent(in) :: index
        type(helicity_t), dimension(size(index)) :: hel
        hel = quantum_numbers_get_helicity &
            (it%get_quantum_numbers (index))
    end function state_iterator_get_hel_slice

```

An array range (implemented directly).

```

    <State matrices: sub interfaces>+≡
    module function state_iterator_get_qn_range (it, k1, k2) result (qn)
        class(state_iterator_t), intent(in) :: it
        integer, intent(in) :: k1, k2
        type(quantum_numbers_t), dimension(k2-k1+1) :: qn
    end function state_iterator_get_qn_range

```

```

module function state_iterator_get_flv_range (it, k1, k2) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(flavor_t), dimension(k2-k1+1) :: flv
end function state_iterator_get_flv_range
module function state_iterator_get_col_range (it, k1, k2) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(color_t), dimension(k2-k1+1) :: col
end function state_iterator_get_col_range
module function state_iterator_get_hel_range (it, k1, k2) result (hel)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(helicity_t), dimension(k2-k1+1) :: hel
end function state_iterator_get_hel_range

```

(State matrices: procedures)+≡

```

module function state_iterator_get_qn_range (it, k1, k2) result (qn)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(quantum_numbers_t), dimension(k2-k1+1) :: qn
  type(node_t), pointer :: node
  integer :: i
  node => it%node
  SCAN: do i = it%depth, 1, -1
    if (k1 <= i .and. i <= k2) then
      qn(i-k1+1) = node%qn
    else
      node => node%parent
    end if
  end do SCAN
end function state_iterator_get_qn_range

module function state_iterator_get_flv_range (it, k1, k2) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(flavor_t), dimension(k2-k1+1) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_flv_range

module function state_iterator_get_col_range (it, k1, k2) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(color_t), dimension(k2-k1+1) :: col
  col = quantum_numbers_get_color &
    (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_col_range

module function state_iterator_get_hel_range (it, k1, k2) result (hel)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k1, k2
  type(helicity_t), dimension(k2-k1+1) :: hel
  hel = quantum_numbers_get_helicity &
    (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_hel_range

```



```
end function state_iterator_get_hel_range
```

Just a specific single element

<State matrices: sub interfaces>+≡

```
module function state_iterator_get_qn_single (it, k) result (qn)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(quantum_numbers_t) :: qn
end function state_iterator_get_qn_single
module function state_iterator_get_flv_single (it, k) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(flavor_t) :: flv
end function state_iterator_get_flv_single
module function state_iterator_get_col_single (it, k) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(color_t) :: col
end function state_iterator_get_col_single
module function state_iterator_get_hel_single (it, k) result (hel)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(helicity_t) :: hel
end function state_iterator_get_hel_single
```

<State matrices: procedures>+≡

```
module function state_iterator_get_qn_single (it, k) result (qn)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(quantum_numbers_t) :: qn
  type(node_t), pointer :: node
  integer :: i
  node => it%node
  SCAN: do i = it%depth, 1, -1
    if (i == k) then
      qn = node%qn
      exit SCAN
    else
      node => node%parent
    end if
  end do SCAN
end function state_iterator_get_qn_single

module function state_iterator_get_flv_single (it, k) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(flavor_t) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers(k))
end function state_iterator_get_flv_single

module function state_iterator_get_col_single (it, k) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
```

```

    type(color_t) :: col
    col = quantum_numbers_get_color &
        (it%get_quantum_numbers (k))
end function state_iterator_get_col_single

module function state_iterator_get_hel_single (it, k) result (hel)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k
    type(helicity_t) :: hel
    hel = quantum_numbers_get_helicity &
        (it%get_quantum_numbers (k))
end function state_iterator_get_hel_single

```

Assign a model pointer to the current flavor entries.

```

<State matrices: state iterator: TBP>+≡
    procedure :: set_model => state_iterator_set_model

<State matrices: sub interfaces>+≡
    module subroutine state_iterator_set_model (it, model)
        class(state_iterator_t), intent(inout) :: it
        class(model_data_t), intent(in), target :: model
    end subroutine state_iterator_set_model

<State matrices: procedures>+≡
    module subroutine state_iterator_set_model (it, model)
        class(state_iterator_t), intent(inout) :: it
        class(model_data_t), intent(in), target :: model
        type(node_t), pointer :: node
        integer :: i
        node => it%node
        do i = it%depth, 1, -1
            call node%qn%set_model (model)
            node => node%parent
        end do
    end subroutine state_iterator_set_model

```

Modify the hard-interaction tag of the current flavor entries at a specific position, in-place.

```

<State matrices: state iterator: TBP>+≡
    procedure :: retag_hard_process => state_iterator_retag_hard_process

<State matrices: sub interfaces>+≡
    module subroutine state_iterator_retag_hard_process (it, i, hard)
        class(state_iterator_t), intent(inout) :: it
        integer, intent(in) :: i
        logical, intent(in) :: hard
    end subroutine state_iterator_retag_hard_process

<State matrices: procedures>+≡
    module subroutine state_iterator_retag_hard_process (it, i, hard)
        class(state_iterator_t), intent(inout) :: it
        integer, intent(in) :: i
        logical, intent(in) :: hard
        type(node_t), pointer :: node
        integer :: j

```

```

node => it%node
do j = 1, it%depth-i
    node => node%parent
end do
call node%qn%tag_hard_process (hard)
end subroutine state_iterator_retag_hard_process

```

Retrieve the matrix element value associated with the current node.

```

<State matrices: state iterator: TBP>+≡
    procedure :: get_matrix_element => state_iterator_get_matrix_element

<State matrices: sub interfaces>+≡
    module function state_iterator_get_matrix_element (it) result (me)
        complex(default) :: me
        class(state_iterator_t), intent(in) :: it
    end function state_iterator_get_matrix_element

<State matrices: procedures>+≡
    module function state_iterator_get_matrix_element (it) result (me)
        complex(default) :: me
        class(state_iterator_t), intent(in) :: it
        if (it%state%leaf_nodes_store_values) then
            me = it%node%me
        else if (it%node%me_index /= 0) then
            me = it%state%me(it%node%me_index)
        else
            me = 0
        end if
    end function state_iterator_get_matrix_element

```

Set the matrix element value using the state iterator.

```

<State matrices: state iterator: TBP>+≡
    procedure :: set_matrix_element => state_iterator_set_matrix_element

<State matrices: sub interfaces>+≡
    module subroutine state_iterator_set_matrix_element (it, value)
        class(state_iterator_t), intent(inout) :: it
        complex(default), intent(in) :: value
    end subroutine state_iterator_set_matrix_element

<State matrices: procedures>+≡
    module subroutine state_iterator_set_matrix_element (it, value)
        class(state_iterator_t), intent(inout) :: it
        complex(default), intent(in) :: value
        if (it%node%me_index /= 0) it%state%me(it%node%me_index) = value
    end subroutine state_iterator_set_matrix_element

<State matrices: state iterator: TBP>+≡
    procedure :: add_to_matrix_element => state_iterator_add_to_matrix_element

<State matrices: sub interfaces>+≡
    module subroutine state_iterator_add_to_matrix_element (it, value)
        class(state_iterator_t), intent(inout) :: it
        complex(default), intent(in) :: value
    end subroutine state_iterator_add_to_matrix_element

```

```

<State matrices: procedures>+≡
module subroutine state_iterator_add_to_matrix_element (it, value)
  class(state_iterator_t), intent(inout) :: it
  complex(default), intent(in) :: value
  if (it%node%me_index /= 0) &
    it%state%me(it%node%me_index) = it%state%me(it%node%me_index) + value
end subroutine state_iterator_add_to_matrix_element

```

12.1.4 Operations on quantum states

Return a deep copy of a state matrix.

```

<State matrices: public>+≡
  public :: assignment(=)
<State matrices: interfaces>≡
  interface assignment(=)
    module procedure state_matrix_assign
  end interface

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_assign (state_out, state_in)
    type(state_matrix_t), intent(out) :: state_out
    type(state_matrix_t), intent(in), target :: state_in
  end subroutine state_matrix_assign

<State matrices: procedures>+≡
module subroutine state_matrix_assign (state_out, state_in)
  type(state_matrix_t), intent(out) :: state_out
  type(state_matrix_t), intent(in), target :: state_in
  type(state_iterator_t) :: it
  if (.not. state_in%is_defined ()) return
  call state_out%init ()
  call it%init (state_in)
  do while (it%is_valid ())
    call state_out%add_state (it%get_quantum_numbers (), &
      it%get_me_index ())
    call it%advance ()
  end do
  if (allocated (state_in%me)) then
    allocate (state_out%me (size (state_in%me)))
    state_out%me = state_in%me
  end if
  state_out%n_sub = state_in%n_sub
end subroutine state_matrix_assign

```

Determine the indices of all diagonal matrix elements.

```

<State matrices: state matrix: TBP>+≡
  procedure :: get_diagonal_entries => state_matrix_get_diagonal_entries
<State matrices: sub interfaces>+≡
  module subroutine state_matrix_get_diagonal_entries (state, i)
    class(state_matrix_t), intent(in) :: state
    integer, dimension(:), allocatable, intent(out) :: i
  end subroutine state_matrix_get_diagonal_entries

```

```

<State matrices: procedures>+≡
module subroutine state_matrix_get_diagonal_entries (state, i)
  class(state_matrix_t), intent(in) :: state
  integer, dimension(:), allocatable, intent(out) :: i
  integer, dimension(state%n_matrix_elements) :: tmp
  integer :: n
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  n = 0
  call it%init (state)
  allocate (qn (it%depth))
  do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    if (all (qn%are_diagonal ())) then
      n = n + 1
      tmp(n) = it%get_me_index ()
    end if
    call it%advance ()
  end do
  allocate (i(n))
  if (n > 0) i = tmp(:n)
end subroutine state_matrix_get_diagonal_entries

```

Normalize all matrix elements, i.e., multiply by a common factor. Assuming that the factor is nonzero, of course.

```

<State matrices: state matrix: TBP>+≡
  procedure :: renormalize => state_matrix_renormalize

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_renormalize (state, factor)
    class(state_matrix_t), intent(inout) :: state
    complex(default), intent(in) :: factor
  end subroutine state_matrix_renormalize

<State matrices: procedures>+≡
  module subroutine state_matrix_renormalize (state, factor)
    class(state_matrix_t), intent(inout) :: state
    complex(default), intent(in) :: factor
    state%me = state%me * factor
  end subroutine state_matrix_renormalize

```

Renormalize the state matrix by its trace, if nonzero. The renormalization is reflected in the state-matrix norm.

```

<State matrices: state matrix: TBP>+≡
  procedure :: normalize_by_trace => state_matrix_normalize_by_trace

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_normalize_by_trace (state)
    class(state_matrix_t), intent(inout) :: state
  end subroutine state_matrix_normalize_by_trace

<State matrices: procedures>+≡
  module subroutine state_matrix_normalize_by_trace (state)
    class(state_matrix_t), intent(inout) :: state
    real(default) :: trace

```

```

    trace = state%trace ()
    if (trace /= 0) then
        state%me = state%me / trace
        state%norm = state%norm * trace
    end if
end subroutine state_matrix_normalize_by_trace

```

Analogous, but renormalize by maximal (absolute) value.

```

<State matrices: state matrix: TBP>+≡
    procedure :: normalize_by_max => state_matrix_normalize_by_max

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_normalize_by_max (state)
        class(state_matrix_t), intent(inout) :: state
    end subroutine state_matrix_normalize_by_max

<State matrices: procedures>+≡
    module subroutine state_matrix_normalize_by_max (state)
        class(state_matrix_t), intent(inout) :: state
        real(default) :: m
        m = maxval (abs (state%me))
        if (m /= 0) then
            state%me = state%me / m
            state%norm = state%norm * m
        end if
    end subroutine state_matrix_normalize_by_max

```

Explicitly set the norm of a state matrix.

```

<State matrices: state matrix: TBP>+≡
    procedure :: set_norm => state_matrix_set_norm

<State matrices: sub interfaces>+≡
    module subroutine state_matrix_set_norm (state, norm)
        class(state_matrix_t), intent(inout) :: state
        real(default), intent(in) :: norm
    end subroutine state_matrix_set_norm

<State matrices: procedures>+≡
    module subroutine state_matrix_set_norm (state, norm)
        class(state_matrix_t), intent(inout) :: state
        real(default), intent(in) :: norm
        state%norm = norm
    end subroutine state_matrix_set_norm

```

Return the sum of all matrix element values.

```

<State matrices: state matrix: TBP>+≡
    procedure :: sum => state_matrix_sum

<State matrices: sub interfaces>+≡
    pure module function state_matrix_sum (state) result (value)
        complex(default) :: value
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_sum

```

```

<State matrices: procedures>+≡
  pure module function state_matrix_sum (state) result (value)
    complex(default) :: value
    class(state_matrix_t), intent(in) :: state
    value = sum (state%me)
  end function state_matrix_sum

```

Return the trace of a state matrix, i.e., the sum over all diagonal values.

If `qn_in` is provided, only branches that match this quantum-numbers array in flavor and helicity are considered. (This mode is used for selecting a color state.)

```

<State matrices: state matrix: TBP>+≡
  procedure :: trace => state_matrix_trace

```

```

<State matrices: sub interfaces>+≡
  module function state_matrix_trace (state, qn_in) result (trace)
    complex(default) :: trace
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
  end function state_matrix_trace

```

```

<State matrices: procedures>+≡
  module function state_matrix_trace (state, qn_in) result (trace)
    complex(default) :: trace
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    type(state_iterator_t) :: it
    allocate (qn (state%get_depth ()))
    trace = 0
    call it%init (state)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      if (present (qn_in)) then
        if (.not. all (qn .fhmatch. qn_in)) then
          call it%advance (); cycle
        end if
      end if
      if (all (qn%are_diagonal ())) then
        trace = trace + it%get_matrix_element ()
      end if
      call it%advance ()
    end do
  end function state_matrix_trace

```

Append new states which are color-contracted versions of the existing states. The matrix element index of each color contraction coincides with the index of its origin, so no new matrix elements are generated. After this operation, no `freeze` must be performed anymore.

```

<State matrices: state matrix: TBP>+≡
  procedure :: add_color_contractions => state_matrix_add_color_contractions

```

```

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_add_color_contractions (state)

```

```

        class(state_matrix_t), intent(inout), target :: state
    end subroutine state_matrix_add_color_contractions
<State matrices: procedures>+≡
module subroutine state_matrix_add_color_contractions (state)
    class(state_matrix_t), intent(inout), target :: state
    type(state_iterator_t) :: it
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_con
    integer, dimension(:), allocatable :: me_index
    integer :: depth, n_me, i, j
    depth = state%get_depth ()
    n_me = state%get_n_matrix_elements ()
    allocate (qn (depth, n_me))
    allocate (me_index (n_me))
    i = 0
    call it%init (state)
    do while (it%is_valid ())
        i = i + 1
        qn(:,i) = it%get_quantum_numbers ()
        me_index(i) = it%get_me_index ()
        call it%advance ()
    end do
    do i = 1, n_me
        call quantum_number_array_make_color_contractions (qn(:,i), qn_con)
        do j = 1, size (qn_con, 2)
            call state%add_state (qn_con(:,j), index = me_index(i))
        end do
    end do
end subroutine state_matrix_add_color_contractions

```

This procedure merges two state matrices of equal depth. For each quantum number (flavor, color, helicity), we take the entry from the first argument where defined, otherwise the second one. (If both are defined, we get an off-diagonal matrix.) The resulting trie combines the information of the input tries in all possible ways. Note that values are ignored, all values in the result are zero.

```

<State matrices: public>+≡
    public :: merge_state_matrices
<State matrices: sub interfaces>+≡
module subroutine merge_state_matrices (state1, state2, state3)
    type(state_matrix_t), intent(in), target :: state1, state2
    type(state_matrix_t), intent(out) :: state3
end subroutine merge_state_matrices
<State matrices: procedures>+≡
module subroutine merge_state_matrices (state1, state2, state3)
    type(state_matrix_t), intent(in), target :: state1, state2
    type(state_matrix_t), intent(out) :: state3
    type(state_iterator_t) :: it1, it2
    type(quantum_numbers_t), dimension(state1%depth) :: qn1, qn2
    if (state1%depth /= state2%depth) then
        call state1%write ()
        call state2%write ()
        call msg_bug ("State matrices merge impossible: incompatible depths")
    end if
end subroutine merge_state_matrices

```



```

end if
call state3%init ()
call it1%init (state1)
do while (it1%is_valid ())
  qn1 = it1%get_quantum_numbers ()
  call it2%init (state2)
  do while (it2%is_valid ())
    qn2 = it2%get_quantum_numbers ()
    call state3%add_state (qn1 .merge. qn2)
    call it2%advance ()
  end do
  call it1%advance ()
end do
call state3%freeze ()
end subroutine merge_state_matrices

```

Multiply matrix elements from two state matrices. Choose the elements as given by the integer index arrays, multiply them and store the sum of products in the indicated matrix element. The suffixes mean: c=conjugate first factor; f=include weighting factor.

Note that the `dot_product` intrinsic function conjugates its first complex argument. This is intended for the c suffix case, but must be reverted for the plain-product case.

We provide analogous subroutines for just summing over state matrix entries. The `evaluate_sum` variant includes the state-matrix norm in the evaluation, the `evaluate_me_sum` takes into account just the matrix elements proper.

(State matrices: state matrix: TBP)+≡

```

procedure :: evaluate_product => state_matrix_evaluate_product
procedure :: evaluate_product_cf => state_matrix_evaluate_product_cf
procedure :: evaluate_square_c => state_matrix_evaluate_square_c
procedure :: evaluate_sum => state_matrix_evaluate_sum
procedure :: evaluate_me_sum => state_matrix_evaluate_me_sum

```

(State matrices: sub interfaces)+≡

```

pure module subroutine state_matrix_evaluate_product &
  (state, i, state1, state2, index1, index2)
  class(state_matrix_t), intent(inout) :: state
  integer, intent(in) :: i
  type(state_matrix_t), intent(in) :: state1, state2
  integer, dimension(:), intent(in) :: index1, index2
end subroutine state_matrix_evaluate_product
pure module subroutine state_matrix_evaluate_product_cf &
  (state, i, state1, state2, index1, index2, factor)
  class(state_matrix_t), intent(inout) :: state
  integer, intent(in) :: i
  type(state_matrix_t), intent(in) :: state1, state2
  integer, dimension(:), intent(in) :: index1, index2
  complex(default), dimension(:), intent(in) :: factor
end subroutine state_matrix_evaluate_product_cf
pure module subroutine state_matrix_evaluate_square_c (state, i, state1, index1)
  class(state_matrix_t), intent(inout) :: state
  integer, intent(in) :: i
  type(state_matrix_t), intent(in) :: state1

```

```

        integer, dimension(:), intent(in) :: index1
    end subroutine state_matrix_evaluate_square_c
    pure module subroutine state_matrix_evaluate_sum (state, i, state1, index1)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1
        integer, dimension(:), intent(in) :: index1
    end subroutine state_matrix_evaluate_sum
    pure module subroutine state_matrix_evaluate_me_sum (state, i, state1, index1)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1
        integer, dimension(:), intent(in) :: index1
    end subroutine state_matrix_evaluate_me_sum

<State matrices: procedures>+≡
    pure module subroutine state_matrix_evaluate_product &
        (state, i, state1, state2, index1, index2)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1, state2
        integer, dimension(:), intent(in) :: index1, index2
        state%me(i) = &
            dot_product (conjg (state1%me(index1)), state2%me(index2))
        state%norm = state1%norm * state2%norm
    end subroutine state_matrix_evaluate_product

    pure module subroutine state_matrix_evaluate_product_cf &
        (state, i, state1, state2, index1, index2, factor)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1, state2
        integer, dimension(:), intent(in) :: index1, index2
        complex(default), dimension(:), intent(in) :: factor
        state%me(i) = &
            dot_product (state1%me(index1), factor * state2%me(index2))
        state%norm = state1%norm * state2%norm
    end subroutine state_matrix_evaluate_product_cf

    pure module subroutine state_matrix_evaluate_square_c (state, i, state1, index1)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1
        integer, dimension(:), intent(in) :: index1
        state%me(i) = &
            dot_product (state1%me(index1), state1%me(index1))
        state%norm = abs (state1%norm) ** 2
    end subroutine state_matrix_evaluate_square_c

    pure module subroutine state_matrix_evaluate_sum (state, i, state1, index1)
        class(state_matrix_t), intent(inout) :: state
        integer, intent(in) :: i
        type(state_matrix_t), intent(in) :: state1
        integer, dimension(:), intent(in) :: index1
        state%me(i) = &

```

```

        sum (state1%me(index1)) * state1%norm
end subroutine state_matrix_evaluate_sum

pure module subroutine state_matrix_evaluate_me_sum (state, i, state1, index1)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1
integer, dimension(:), intent(in) :: index1
state%me(i) = sum (state1%me(index1))
end subroutine state_matrix_evaluate_me_sum

```

Outer product (of states and matrix elements):

```

<State matrices: public>+≡
public :: outer_multiply

<State matrices: interfaces>+≡
interface outer_multiply
module procedure outer_multiply_pair
module procedure outer_multiply_array
end interface

```

This procedure constructs the outer product of two state matrices.

```

<State matrices: sub interfaces>+≡
module subroutine outer_multiply_pair (state1, state2, state3)
type(state_matrix_t), intent(in), target :: state1, state2
type(state_matrix_t), intent(out) :: state3
end subroutine outer_multiply_pair

<State matrices: procedures>+≡
module subroutine outer_multiply_pair (state1, state2, state3)
type(state_matrix_t), intent(in), target :: state1, state2
type(state_matrix_t), intent(out) :: state3
type(state_iterator_t) :: it1, it2
type(quantum_numbers_t), dimension(state1%depth) :: qn1
type(quantum_numbers_t), dimension(state2%depth) :: qn2
type(quantum_numbers_t), dimension(state1%depth+state2%depth) :: qn3
complex(default) :: val1, val2
call state3%init (store_values = .true.)
call it1%init (state1)
do while (it1%is_valid ())
qn1 = it1%get_quantum_numbers ()
val1 = it1%get_matrix_element ()
call it2%init (state2)
do while (it2%is_valid ())
qn2 = it2%get_quantum_numbers ()
val2 = it2%get_matrix_element ()
qn3(:state1%depth) = qn1
qn3(state1%depth+1:) = qn2
call state3%add_state (qn3, value=val1 * val2)
call it2%advance ()
end do
call it1%advance ()
end do
call state3%freeze ()

```

```
end subroutine outer_multiply_pair
```

This executes the above routine iteratively for an arbitrary number of state matrices.

(State matrices: sub interfaces)+≡

```
module subroutine outer_multiply_array (state_in, state_out)
  type(state_matrix_t), dimension(:), intent(in), target :: state_in
  type(state_matrix_t), intent(out) :: state_out
end subroutine outer_multiply_array
```

(State matrices: procedures)+≡

```
module subroutine outer_multiply_array (state_in, state_out)
  type(state_matrix_t), dimension(:), intent(in), target :: state_in
  type(state_matrix_t), intent(out) :: state_out
  type(state_matrix_t), dimension(:), allocatable, target :: state_tmp
  integer :: i, n
  n = size (state_in)
  select case (n)
  case (0)
    call state_out%init ()
  case (1)
    state_out = state_in(1)
  case (2)
    call outer_multiply_pair (state_in(1), state_in(2), state_out)
  case default
    allocate (state_tmp (n-2))
    call outer_multiply_pair (state_in(1), state_in(2), state_tmp(1))
    do i = 2, n - 2
      call outer_multiply_pair (state_tmp(i-1), state_in(i+1), state_tmp(i))
    end do
    call outer_multiply_pair (state_tmp(n-2), state_in(n), state_out)
    do i = 1, size(state_tmp)
      call state_tmp(i)%final ()
    end do
  end select
end subroutine outer_multiply_array
```

12.1.5 Factorization

In physical events, the state matrix is factorized into single-particle state matrices. This is essentially a measurement.

In a simulation, we select one particular branch of the state matrix with a probability that is determined by the matrix elements at the leaves. (This makes sense only if the state matrix represents a squared amplitude.) The selection is based on a (random) value x between 0 and one that is provided as the third argument.

For flavor and color, we select a unique value for each particle. For polarization, we have three options (modes). Option 1 is to drop helicity information altogether and sum over all diagonal helicities. Option 2 is to select a unique diagonal helicity in the same way as flavor and color. Option 3 is, for each

particle, to trace over all remaining helicities in order to obtain an array of independent single-particle helicity matrices.

Only branches that match the given quantum-number array `qn_in`, if present, are considered. For this array, color is ignored.

If the optional `correlated_state` is provided, it is assigned the correlated density matrix for the selected flavor-color branch, so multi-particle spin correlations remain available even if they are dropped in the single-particle density matrices. This should be done by the caller for the choice `FM_CORRELATED_HELICITY`, which otherwise is handled as `FM_IGNORE_HELICITY`.

The algorithm is as follows: First, we determine the normalization by summing over all diagonal matrix elements. In a second scan, we select one of the diagonal matrix elements by a cumulative comparison with the normalized random number. In the corresponding quantum number array, we undefine the helicity entries. Then, we scan the third time. For each branch that matches the selected quantum number array (i.e., definite flavor and color, arbitrary helicity), we determine its contribution to any of the single-particle state matrices. The matrix-element value is added if all other quantum numbers are diagonal, while the helicity of the chosen particle may be arbitrary; this helicity determines the branch in the single-particle state.

As a result, flavor and color quantum numbers are selected with the correct probability. Within this subset of states, each single-particle state matrix results from tracing over all other particles. Note that the single-particle state matrices are not normalized.

The flag `ok` is set to false if the matrix element sum is zero, so factorization is not possible. This can happen if an event did not pass cuts.

```

<State matrices: parameters>≡
  integer, parameter, public :: FM_IGNORE_HELICITY = 1
  integer, parameter, public :: FM_SELECT_HELICITY = 2
  integer, parameter, public :: FM_FACTOR_HELICITY = 3
  integer, parameter, public :: FM_CORRELATED_HELICITY = 4

<State matrices: state matrix: TBP>+≡
  procedure :: factorize => state_matrix_factorize

<State matrices: sub interfaces>+≡
  module subroutine state_matrix_factorize &
    (state, mode, x, ok, single_state, correlated_state, qn_in)
    class(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: mode
    real(default), intent(in) :: x
    logical, intent(out) :: ok
    type(state_matrix_t), &
      dimension(:), allocatable, intent(out) :: single_state
    type(state_matrix_t), intent(out), optional :: correlated_state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
  end subroutine state_matrix_factorize

<State matrices: procedures>+≡
  module subroutine state_matrix_factorize &
    (state, mode, x, ok, single_state, correlated_state, qn_in)
    class(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: mode

```

```

real(default), intent(in) :: x
logical, intent(out) :: ok
type(state_matrix_t), &
    dimension(:), allocatable, intent(out) :: single_state
type(state_matrix_t), intent(out), optional :: correlated_state
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
type(state_iterator_t) :: it
real(default) :: s, xt
complex(default) :: value
integer :: i, depth
type(quantum_numbers_t), dimension(:), allocatable :: qn, qn1
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
logical, dimension(:), allocatable :: diagonal
logical, dimension(:,:), allocatable :: mask
ok = .true.
if (x /= 0) then
    xt = x * abs (state%trace (qn_in))
else
    xt = 0
end if
s = 0
depth = state%get_depth ()
allocate (qn (depth), qn1 (depth), diagonal (depth))
call it%init (state)
do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    if (present (qn_in)) then
        if (.not. all (qn .fhmatch. qn_in)) then
            call it%advance (); cycle
        end if
    end if
    if (all (qn%are_diagonal ())) then
        value = abs (it%get_matrix_element ())
        s = s + value
        if (s > xt) exit
    end if
    call it%advance ()
end do
if (.not. it%is_valid ()) then
    if (s == 0) ok = .false.
    call it%init (state)
end if
allocate (single_state (depth))
do i = 1, depth
    call single_state(i)%init (store_values = .true.)
end do
if (present (correlated_state)) &
    call correlated_state%init (store_values = .true.)
qn = it%get_quantum_numbers ()
select case (mode)
case (FM_SELECT_HELICITY) ! single branch selected; shortcut
    do i = 1, depth
        call single_state(i)%add_state ([qn(i)], value=value)
    end do

```

```

        if (.not. present (correlated_state)) then
            do i = 1, size(single_state)
                call single_state(i)%freeze ()
            end do
            return
        end if
    end select
    allocate (qn_mask (depth))
    call qn_mask%init (.false., .false., .false., .true.)
    call qn%undefine (qn_mask)
    select case (mode)
    case (FM_FACTOR_HELICITY)
        allocate (mask (depth, depth))
        mask = .false.
        forall (i = 1:depth) mask(i,i) = .true.
    end select
    call it%init (state)
    do while (it%is_valid ())
        qn1 = it%get_quantum_numbers ()
        if (all (qn .match. qn1)) then
            diagonal = qn1%are_diagonal ()
            value = it%get_matrix_element ()
            select case (mode)
            case (FM_IGNORE_HELICITY, FM_CORRELATED_HELICITY)
                !!! trace over diagonal states that match qn
                if (all (diagonal)) then
                    do i = 1, depth
                        call single_state(i)%add_state &
                            ([qn(i)], value=value, sum_values=.true.)
                    end do
                end if
            case (FM_FACTOR_HELICITY) !!! trace over all other particles
                do i = 1, depth
                    if (all (diagonal .or. mask(:,i))) then
                        call single_state(i)%add_state &
                            ([qn1(i)], value=value, sum_values=.true.)
                    end if
                end do
            end select
            if (present (correlated_state)) &
                call correlated_state%add_state (qn1, value=value)
        end if
        call it%advance ()
    end do
    do i = 1, depth
        call single_state(i)%freeze ()
    end do
    if (present (correlated_state)) &
        call correlated_state%freeze ()
end subroutine state_matrix_factorize

```

Auxiliary functions

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_polarization_density_matrix &
        => state_matrix_get_polarization_density_matrix

<State matrices: sub interfaces>+≡
    module function state_matrix_get_polarization_density_matrix &
        (state) result (pol_matrix)
        real(default), dimension(:,:), allocatable :: pol_matrix
        class(state_matrix_t), intent(in) :: state
    end function state_matrix_get_polarization_density_matrix

<State matrices: procedures>+≡
    module function state_matrix_get_polarization_density_matrix &
        (state) result (pol_matrix)
        real(default), dimension(:,:), allocatable :: pol_matrix
        class(state_matrix_t), intent(in) :: state
        type(node_t), pointer :: current => null ()
        !!! What's the generic way to allocate the matrix?
        allocate (pol_matrix (4,4)); pol_matrix = 0
        if (associated (state%root%child_first)) then
            current => state%root%child_first
            do while (associated (current))
                call current%qn%write ()
                current => current%next
            end do
        else
            call msg_fatal ("Polarization state not allocated!")
        end if
    end function state_matrix_get_polarization_density_matrix

```

Quantum-number matching

This feature allows us to check whether a given string of PDG values matches, in any ordering, any of the flavor combinations that the state matrix provides. We will also request the permutation of the successful match.

This type provides an account of the state's flavor content. We store all flavor combinations, as `pdg` values, in an array, assuming that the length is uniform.

We check only the entries selected by `mask_match`. Among those, only the entries selected by `mask_sort` are sorted and thus matched without respecting array element order. The entries that correspond to a true value in the associated `mask` are sorted. The mapping from the original state to the sorted state is given by the index array `map`.

```

<State matrices: public>+≡
    public :: state_flv_content_t

<State matrices: types>+≡
    type :: state_flv_content_t
        private
        integer, dimension(:,:), allocatable :: pdg
        integer, dimension(:,:), allocatable :: map
        logical, dimension(:), allocatable :: mask

```



```

contains
  <State matrices: state flv content: TBP>
end type state_flv_content_t

```

Output (debugging aid).

```

<State matrices: state flv content: TBP>≡
  procedure :: write => state_flv_content_write

<State matrices: sub interfaces>+≡
  module subroutine state_flv_content_write (state_flv, unit)
    class(state_flv_content_t), intent(in), target :: state_flv
    integer, intent(in), optional :: unit
  end subroutine state_flv_content_write

<State matrices: procedures>+≡
  module subroutine state_flv_content_write (state_flv, unit)
    class(state_flv_content_t), intent(in), target :: state_flv
    integer, intent(in), optional :: unit
    integer :: u, n, d, i, j
    u = given_output_unit (unit)
    d = size (state_flv%pdg, 1)
    n = size (state_flv%pdg, 2)
    do i = 1, n
      write (u, "(2x,'PDG =')", advance="no")
      do j = 1, d
        write (u, "(1x,I0)", advance="no") state_flv%pdg(j,i)
      end do
      write (u, "(' :: map = (')", advance="no")
      do j = 1, d
        write (u, "(1x,I0)", advance="no") state_flv%map(j,i)
      end do
      write (u, "(' )')")
    end do
  end subroutine state_flv_content_write

```

Initialize with table length and mask. Each row of the map array, of length d , is initialized with $(0, 1, \dots, d)$.

```

<State matrices: state flv content: TBP>+≡
  procedure :: init => state_flv_content_init

<State matrices: sub interfaces>+≡
  module subroutine state_flv_content_init (state_flv, n, mask)
    class(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n
    logical, dimension(:), intent(in) :: mask
  end subroutine state_flv_content_init

<State matrices: procedures>+≡
  module subroutine state_flv_content_init (state_flv, n, mask)
    class(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n
    logical, dimension(:), intent(in) :: mask
    integer :: d, i
    d = size (mask)
    allocate (state_flv%pdg (d, n), source = 0)

```

```

        allocate (state_flv%map (d, n), source = spread ([i, i = 1, d], 2, n))
        allocate (state_flv%mask (d), source = mask)
    end subroutine state_flv_content_init

```

Manually fill the entries, one flavor set and mapping at a time.

```

<State matrices: state flv content: TBP>+≡
    procedure :: set_entry => state_flv_content_set_entry

<State matrices: sub interfaces>+≡
    module subroutine state_flv_content_set_entry (state_flv, i, pdg, map)
        class(state_flv_content_t), intent(inout) :: state_flv
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: pdg, map
    end subroutine state_flv_content_set_entry

<State matrices: procedures>+≡
    module subroutine state_flv_content_set_entry (state_flv, i, pdg, map)
        class(state_flv_content_t), intent(inout) :: state_flv
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: pdg, map
        state_flv%pdg(:,i) = pdg
        where (map /= 0)
            state_flv%map(:,i) = map
        end where
    end subroutine state_flv_content_set_entry

```

Given a state matrix, determine the flavor content. That is, scan the state matrix and extract flavor only, build a new state matrix from that.

```

<State matrices: state flv content: TBP>+≡
    procedure :: fill => state_flv_content_fill

<State matrices: sub interfaces>+≡
    module subroutine state_flv_content_fill &
        (state_flv, state_full, mask)
        class(state_flv_content_t), intent(out) :: state_flv
        type(state_matrix_t), intent(in), target :: state_full
        logical, dimension(:), intent(in) :: mask
    end subroutine state_flv_content_fill

<State matrices: procedures>+≡
    module subroutine state_flv_content_fill &
        (state_flv, state_full, mask)
        class(state_flv_content_t), intent(out) :: state_flv
        type(state_matrix_t), intent(in), target :: state_full
        logical, dimension(:), intent(in) :: mask
        type(state_matrix_t), target :: state_tmp
        type(state_iterator_t) :: it
        type(flavor_t), dimension(:), allocatable :: flv
        integer, dimension(:), allocatable :: pdg, pdg_subset
        integer, dimension(:), allocatable :: idx, map_subset, idx_subset, map
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        integer :: n, d, c, i
        call state_tmp%init ()
        d = state_full%get_depth ()
        allocate (flv (d), qn (d), pdg (d), idx (d), map (d))

```

```

idx = [(i, i = 1, d)]
c = count (mask)
allocate (pdg_subset (c), map_subset (c), idx_subset (c))
call it%init (state_full)
do while (it%is_valid ())
  flv = it%get_flavor ()
  call qn%init (flv)
  call state_tmp%add_state (qn)
  call it%advance ()
end do
n = state_tmp%get_n_leaves ()
call state_flv%init (n, mask)
i = 0
call it%init (state_tmp)
do while (it%is_valid ())
  i = i + 1
  flv = it%get_flavor ()
  pdg = flv%get_pdg ()
  idx_subset = pack (idx, mask)
  pdg_subset = pack (pdg, mask)
  map_subset = order_abs (pdg_subset)
  map = unpack (idx_subset (map_subset), mask, idx)
  call state_flv%set_entry (i, &
    unpack (pdg_subset(map_subset), mask, pdg), &
    order (map))
  call it%advance ()
end do
call state_tmp%final ()
end subroutine state_flv_content_fill

```

Match a given flavor string against the flavor content. We sort the input string and check whether it matches any of the stored strings. If yes, return the mapping.

Only PDG entries under the preset mask are sorted before matching. The other entries must match exactly (i.e., without reordering). A zero entry matches anything. In any case, the length of the PDG string must be equal to the length d of the individual flavor-state entries.

```

<State matrices: state flv content: TBP>+≡
  procedure :: match => state_flv_content_match

<State matrices: sub interfaces>+≡
  module subroutine state_flv_content_match (state_flv, pdg, success, map)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, dimension(:), intent(in) :: pdg
    logical, intent(out) :: success
    integer, dimension(:), intent(out) :: map
  end subroutine state_flv_content_match

<State matrices: procedures>+≡
  module subroutine state_flv_content_match (state_flv, pdg, success, map)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, dimension(:), intent(in) :: pdg
    logical, intent(out) :: success
    integer, dimension(:), intent(out) :: map

```

```

integer, dimension(:), allocatable :: pdg_subset, pdg_sorted, map1, map2
integer, dimension(:), allocatable :: idx, map_subset, idx_subset
integer :: i, n, c, d
c = count (state_flv%mask)
d = size (state_flv%pdg, 1)
n = size (state_flv%pdg, 2)
allocate (idx (d), source = [(i, i = 1, d)])
allocate (idx_subset (c), pdg_subset (c), map_subset (c))
allocate (pdg_sorted (d), map1 (d), map2 (d))
idx_subset = pack (idx, state_flv%mask)
pdg_subset = pack (pdg, state_flv%mask)
map_subset = order_abs (pdg_subset)
pdg_sorted = unpack (pdg_subset(map_subset), state_flv%mask, pdg)
success = .false.
do i = 1, n
  if (all (pdg_sorted == state_flv%pdg(:,i) &
    .or. pdg_sorted == 0)) then
    success = .true.
    exit
  end if
end do
if (success) then
  map1 = state_flv%map(:,i)
  map2 = unpack (idx_subset(map_subset), state_flv%mask, idx)
  map = map2(map1)
  where (pdg == 0) map = 0
end if
end subroutine state_flv_content_match

```

Check if a given PDG code occurs anywhere in the table.

```

<State matrices: state flv content: TBP>+≡
  procedure :: contains => state_flv_content_contains

<State matrices: sub interfaces>+≡
  module function state_flv_content_contains (state_flv, pdg) result (success)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, intent(in) :: pdg
    logical :: success
  end function state_flv_content_contains

<State matrices: procedures>+≡
  module function state_flv_content_contains (state_flv, pdg) result (success)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, intent(in) :: pdg
    logical :: success
    success = any (state_flv%pdg == pdg)
  end function state_flv_content_contains

<State matrices: procedures>+≡
  elemental function pacify_complex (c_in) result (c_pac)
    complex(default), intent(in) :: c_in
    complex(default) :: c_pac
    c_pac = c_in
    if (real(c_pac) == -real(c_pac)) then

```

```

        c_pac = &
            cmplx (0._default, aimag(c_pac), kind=default)
    end if
    if (aimag(c_pac) == -aimag(c_pac)) then
        c_pac = &
            cmplx (real(c_pac), 0._default, kind=default)
    end if
end function pacify_complex

```

Looks for flavor structures that only differ by a permutation of the masked flavors. The result is returned in form of a mask which is `.true.` at the positions of a duplicate flavor structure from the second encounter on. This routine implements the naive approach: We go through all flavor structures and compare each one with each preceding one. This works but is $\mathcal{O}(n^2)$ in the number of flavor structures. Using a table to remember which flavor structure has already been encountered, it would be possible to find the duplicates in $\mathcal{O}(n)$.

(State matrices: state flv content: TBP)+≡

```

    procedure :: find_duplicates => state_flv_content_find_duplicates

```

(State matrices: sub interfaces)+≡

```

    module subroutine state_flv_content_find_duplicates (state_flv, duplicate_mask)
        class(state_flv_content_t), intent(in) :: state_flv
        logical, dimension(:), allocatable, intent(out) :: duplicate_mask
    end subroutine state_flv_content_find_duplicates

```

(State matrices: procedures)+≡

```

    module subroutine state_flv_content_find_duplicates (state_flv, duplicate_mask)
        class(state_flv_content_t), intent(in) :: state_flv
        logical, dimension(:), allocatable, intent(out) :: duplicate_mask
        integer, dimension(:), allocatable :: flvst
        integer :: i1, i2, n_flvsts
        logical :: found_once
        n_flvsts = size (state_flv%pdg, 2)
        allocate (duplicate_mask (n_flvsts))
        duplicate_mask = .false.
        do i1 = 1, n_flvsts
            found_once = .false.
            flvst = state_flv%pdg(:,i1)
            do i2 = 1, i1
                if (all(flvst == state_flv%pdg(:,i2))) then
                    if (found_once) then
                        duplicate_mask(i1) = .true.
                        exit
                    else
                        found_once = .true.
                    end if
                end if
            end do
        end do
    end subroutine state_flv_content_find_duplicates

```

12.1.6 Unit tests

Test module, followed by the corresponding implementation module.

```
<state_matrices_ut.f90>≡  
  <File header>  
  
  module state_matrices_ut  
    use unit_tests  
    use state_matrices_uti  
  
    <Standard module head>  
  
    <State matrices: public test>  
  
    contains  
  
    <State matrices: test driver>  
  
  end module state_matrices_ut  
<state_matrices_uti.f90>≡  
  <File header>  
  
  module state_matrices_uti  
  
    <Use kinds>  
    use io_units  
    use format_defs, only: FMT_19  
    use flavors  
    use colors  
    use helicities  
    use quantum_numbers  
  
    use state_matrices  
  
    <Standard module head>  
  
    <State matrices: test declarations>  
  
    contains  
  
    <State matrices: tests>  
  
  end module state_matrices_uti  
API: driver for the unit tests below.  
<State matrices: public test>≡  
  public :: state_matrix_test  
<State matrices: test driver>≡  
  subroutine state_matrix_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <State matrices: execute tests>  
  end subroutine state_matrix_test
```

Create two quantum states of equal depth and merge them.

```

<State matrices: execute tests>≡
    call test (state_matrix_1, "state_matrix_1", &
        "check merge of quantum states of equal depth", &
        u, results)

<State matrices: test declarations>≡
    public :: state_matrix_1

<State matrices: tests>≡
    subroutine state_matrix_1 (u)
        integer, intent(in) :: u
        type(state_matrix_t) :: state1, state2, state3
        type(flavor_t), dimension(3) :: flv
        type(color_t), dimension(3) :: col
        type(quantum_numbers_t), dimension(3) :: qn

        write (u, "(A)")  "* Test output: state_matrix_1"
        write (u, "(A)")  "* Purpose: create and merge two quantum states"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        write (u, "(A)")  "* State matrix 1"
        write (u, "(A)")

        call state1%init ()
        call flv%init ([1, 2, 1])
        call qn%init (flv, helicity ([ 1, 1, 1]))
        call state1%add_state (qn)
        call qn%init (flv, helicity ([ 1, 1, 1], [-1, 1, -1]))
        call state1%add_state (qn)
        call state1%freeze ()
        call state1%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* State matrix 2"
        write (u, "(A)")

        call state2%init ()
        call col(1)%init ([501])
        call col(2)%init ([-501])
        call col(3)%init ([0])
        call qn%init (col, helicity ([-1, -1, 0]))
        call state2%add_state (qn)
        call col(3)%init ([99])
        call qn%init (col, helicity ([-1, -1, 0]))
        call state2%add_state (qn)
        call state2%freeze ()
        call state2%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Merge the state matrices"
        write (u, "(A)")

```

```

call merge_state_matrices (state1, state2, state3)
call state3%write (u)

write (u, "(A)")
write (u, "(A)")  "* Collapse the state matrix"
write (u, "(A)")

call state3%collapse (quantum_numbers_mask (.false., .false., &
      [.true., .false., .false.]))
call state3%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call state1%final ()
call state2%final ()
call state3%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_1"
write (u, "(A)")

end subroutine state_matrix_1

```

Create a correlated three-particle state matrix and factorize it.

```

<State matrices: execute tests>+≡
  call test (state_matrix_2, "state_matrix_2", &
    "check factorizing 3-particle state matrix", &
    u, results)

<State matrices: test declarations>+≡
  public :: state_matrix_2

<State matrices: tests>+≡
  subroutine state_matrix_2 (u)
    integer, intent(in) :: u
    type(state_matrix_t) :: state
    type(state_matrix_t), dimension(:), allocatable :: single_state
    type(state_matrix_t) :: correlated_state
    integer :: f, h11, h12, h21, h22, i, mode
    type(flavor_t), dimension(2) :: flv
    type(color_t), dimension(2) :: col
    type(helicity_t), dimension(2) :: hel
    type(quantum_numbers_t), dimension(2) :: qn
    logical :: ok

    write (u, "(A)")
    write (u, "(A)")  "* Test output: state_matrix_2"
    write (u, "(A)")  "* Purpose: factorize correlated 3-particle state"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

```



```

call state%init ()
do f = 1, 2
  do h11 = -1, 1, 2
    do h12 = -1, 1, 2
      do h21 = -1, 1, 2
        do h22 = -1, 1, 2
          call flv%init ([f, -f])
          call col(1)%init ([1])
          call col(2)%init ([-1])
          call hel%init ([h11,h12], [h21, h22])
          call qn%init (flv, col, hel)
          call state%add_state (qn)
        end do
      end do
    end do
  end do
end do
call state%freeze ()
call state%write (u)

write (u, "(A)")
write (u, "(A,'('," // FMT_19 // "',''," // FMT_19 // "','')')") &
  "Trace = ", state%trace ()
write (u, "(A)")

do mode = 1, 3
  write (u, "(A)")
  write (u, "(A,I1)")  "Mode = ", mode
  call state%factorize &
    (mode, 0.15_default, ok, single_state, correlated_state)
  do i = 1, size (single_state)
    write (u, "(A)")
    call single_state(i)%write (u)
    write (u, "(A,'('," // FMT_19 // "',''," // FMT_19 // "','')')") &
      "Trace = ", single_state(i)%trace ()
  end do
  write (u, "(A)")
  call correlated_state%write (u)
  write (u, "(A,'('," // FMT_19 // "',''," // FMT_19 // "','')')") &
    "Trace = ", correlated_state%trace ()
  do i = 1, size(single_state)
    call single_state(i)%final ()
  end do
  call correlated_state%final ()
end do

write (u, "(A)")
write (u, "(A)")  "Cleanup"

call state%final ()

write (u, "(A)")
write (u, "(A)")  "Test output end: state_matrix_2"

```

```
end subroutine state_matrix_2
```

Create a colored state matrix and add color contractions.

```
<State matrices: execute tests>+≡
  call test (state_matrix_3, "state_matrix_3", &
    "check factorizing 3-particle state matrix", &
    u, results)

<State matrices: test declarations>+≡
  public :: state_matrix_3

<State matrices: tests>+≡
  subroutine state_matrix_3 (u)
    use physics_defs, only: HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET
    integer, intent(in) :: u
    type(state_matrix_t) :: state
    type(flavor_t), dimension(4) :: flv
    type(color_t), dimension(4) :: col
    type(quantum_numbers_t), dimension(4) :: qn

    write (u, "(A)")  "* Test output: state_matrix_3"
    write (u, "(A)")  "* Purpose: add color connections to colored state"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call state%init ()
    call flv%init ([ 1, -HADRON_REMNANT_TRIPLET, -1, HADRON_REMNANT_TRIPLET ])
    call col(1)%init ([17])
    call col(2)%init ([-17])
    call col(3)%init ([-19])
    call col(4)%init ([19])
    call qn%init (flv, col)
    call state%add_state (qn)
    call flv%init ([ 1, -HADRON_REMNANT_TRIPLET, 21, HADRON_REMNANT_OCTET ])
    call col(1)%init ([17])
    call col(2)%init ([-17])
    call col(3)%init ([3, -5])
    call col(4)%init ([5, -3])
    call qn%init (flv, col)
    call state%add_state (qn)
    call state%freeze ()

    write (u, "(A)")  "* State:"
    write (u, "(A)")

    call state%write (u)
    call state%add_color_contractions ()

    write (u, "(A)")  "* State with contractions:"
    write (u, "(A)")

    call state%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call state%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrx_3"

end subroutine state_matrix_3

```

Create a correlated three-particle state matrix, write it to file and read again.

```

<State matrices: execute tests>+≡
call test (state_matrix_4, "state_matrix_4", &
  "check raw I/O", &
  u, results)

<State matrices: test declarations>+≡
public :: state_matrix_4

<State matrices: tests>+≡
subroutine state_matrix_4 (u)
  integer, intent(in) :: u
  type(state_matrix_t), allocatable :: state
  integer :: f, h11, h12, h21, h22, i
  type(flavor_t), dimension(2) :: flv
  type(color_t), dimension(2) :: col
  type(helicity_t), dimension(2) :: hel
  type(quantum_numbers_t), dimension(2) :: qn
  integer :: unit, iostat

  write (u, "(A)")
  write (u, "(A)")  "* Test output: state_matrix_4"
  write (u, "(A)")  "* Purpose: raw I/O for correlated 3-particle state"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  allocate (state)

  call state%init ()
  do f = 1, 2
    do h11 = -1, 1, 2
      do h12 = -1, 1, 2
        do h21 = -1, 1, 2
          do h22 = -1, 1, 2
            call flv%init ([f, -f])
            call col(1)%init ([1])
            call col(2)%init ([-1])
            call hel%init ([h11, h12], [h21, h22])
            call qn%init (flv, col, hel)
            call state%add_state (qn)
          end do
        end do
      end do
    end do
  end do
end do

```

```

        end do
    end do
end do
call state%freeze ()

call state%set_norm (3._default)
do i = 1, state%get_n_leaves ()
    call state%set_matrix_element (i, cmplx (2 * i, 2 * i + 1, default))
end do

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write to file and read again "
write (u, "(A)")

unit = free_unit ()
open (unit, action="readwrite", form="unformatted", status="scratch")
call state%write_raw (unit)
call state%final ()
deallocate (state)

allocate(state)
rewind (unit)
call state%read_raw (unit, iostat=iostat)
close (unit)

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call state%final ()
deallocate (state)

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_4"

end subroutine state_matrix_4

```

Create a flavor-content object for a given state matrix and match it against trial flavor (i.e., PDG) strings.

```

<State matrices: execute tests>+≡
    call test (state_matrix_5, "state_matrix_5", &
        "check flavor content", &
        u, results)

<State matrices: test declarations>+≡
    public :: state_matrix_5

<State matrices: tests>+≡
    subroutine state_matrix_5 (u)
        integer, intent(in) :: u
        type(state_matrix_t), allocatable, target :: state
        type(state_iterator_t) :: it

```

```

type(state_flv_content_t), allocatable :: state_flv
type(flavor_t), dimension(4) :: flv1, flv2, flv3, flv4
type(color_t), dimension(4) :: col1, col2
type(helicity_t), dimension(4) :: hel1, hel2, hel3
type(quantum_numbers_t), dimension(4) :: qn
logical, dimension(4) :: mask

write (u, "(A)")  "* Test output: state_matrix_5"
write (u, "(A)")  "* Purpose: check flavor-content state"
write (u, "(A)")

write (u, "(A)")  "* Set up arbitrary state matrix"
write (u, "(A)")

call flv1%init ([1, 4, 2, 7])
call flv2%init ([1, 3,-3, 8])
call flv3%init ([5, 6, 3, 7])
call flv4%init ([6, 3, 5, 8])
call hel1%init ([0, 1, -1, 0])
call hel2%init ([0, 1, 1, 1])
call hel3%init ([1, 0, 0, 0])
call col1(1)%init ([0])
call col1(2)%init ([0])
call col1(3)%init ([0])
call col1(4)%init ([0])
call col2(1)%init ([5, -6])
call col2(2)%init ([0])
call col2(3)%init ([6, -5])
call col2(4)%init ([0])

allocate (state)
call state%init ()
call qn%init (flv1, col1, hel1)
call state%add_state (qn)
call qn%init (flv1, col1, hel2)
call state%add_state (qn)
call qn%init (flv3, col1, hel3)
call state%add_state (qn)
call qn%init (flv4, col1, hel3)
call state%add_state (qn)
call qn%init (flv1, col2, hel3)
call state%add_state (qn)
call qn%init (flv2, col2, hel2)
call state%add_state (qn)
call qn%init (flv2, col2, hel1)
call state%add_state (qn)
call qn%init (flv2, col1, hel1)
call state%add_state (qn)
call qn%init (flv3, col1, hel1)
call state%add_state (qn)
call qn%init (flv3, col2, hel3)
call state%add_state (qn)
call qn%init (flv1, col1, hel1)
call state%add_state (qn)

```

```

write (u, "(A)")  "* Quantum number content"
write (u, "(A)")

call it%init (state)
do while (it%is_valid ())
    call quantum_numbers_write (it%get_quantum_numbers (), u)
    write (u, *)
    call it%advance ()
end do

write (u, "(A)")
write (u, "(A)")  "* Extract the flavor content"
write (u, "(A)")

mask = [.true., .true., .true., .false.]

allocate (state_flv)
call state_flv%fill (state, mask)
call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Match trial sets"
write (u, "(A)")

call check ([1, 2, 3, 0])
call check ([1, 4, 2, 0])
call check ([4, 2, 1, 0])
call check ([1, 3, -3, 0])
call check ([1, -3, 3, 0])
call check ([6, 3, 5, 0])

write (u, "(A)")
write (u, "(A)")  "* Determine the flavor content with mask"
write (u, "(A)")

mask = [.false., .true., .true., .false.]

call state_flv%fill (state, mask)
call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Match trial sets"
write (u, "(A)")

call check ([1, 2, 3, 0])
call check ([1, 4, 2, 0])
call check ([4, 2, 1, 0])
call check ([1, 3, -3, 0])
call check ([1, -3, 3, 0])
call check ([6, 3, 5, 0])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

deallocate (state_flv)

call state%final ()
deallocate (state)

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_5"

contains

subroutine check (pdg)
  integer, dimension(4), intent(in) :: pdg
  integer, dimension(4) :: map
  logical :: success
  call state_flv%match (pdg, success, map)
  write (u, "(2x,4(1x,I0),':',1x,L1)", advance="no")  pdg, success
  if (success) then
    write (u, "(2x,'map = (' ,4(1x,I0),' )')")  map
  else
    write (u, *)
  end if
end subroutine check

end subroutine state_matrix_5

```

Create a state matrix with full flavor, color and helicity information. Afterwards, reduce such that it is only differential in flavor and initial-state helicities. This is used when preparing states for beam- polarized computations with external matrix element providers.

```

<State matrices: execute tests>+≡
  call test (state_matrix_6, "state_matrix_6", &
    "check state matrix reduction", &
    u, results)

<State matrices: test declarations>+≡
  public :: state_matrix_6

<State matrices: tests>+≡
  subroutine state_matrix_6 (u)
    integer, intent(in) :: u
    type(state_matrix_t), allocatable :: state_orig, state_reduced
    type(flavor_t), dimension(4) :: flv
    type(helicity_t), dimension(4) :: hel
    type(color_t), dimension(4) :: col
    type(quantum_numbers_t), dimension(4) :: qn
    type(quantum_numbers_mask_t), dimension(4) :: qn_mask
    integer :: h1, h2, h3 , h4
    integer :: n_states = 0

    write (u, "(A)")  "* Test output: state_matrix_6"
    write (u, "(A)")  "* Purpose: Check state matrix reduction"
    write (u, "(A)")

```

```

write (u, "(A)") "* Set up helicity-diagonal state matrix"
write (u, "(A)")

allocate (state_orig)
call state_orig%init ()

call flv%init ([11, -11, 1, -1])
call col(3)%init ([1])
call col(4)%init ([-1])
do h1 = -1, 1, 2
  do h2 = -1, 1, 2
    do h3 = -1, 1, 2
      do h4 = -1, 1, 2
        n_states = n_states + 1
        call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
        call qn%init (flv, col, hel)
        call state_orig%add_state (qn)
      end do
    end do
  end do
end do
call state_orig%freeze ()

write (u, "(A)") "* Original state: "
write (u, "(A)")
call state_orig%write (u)

write (u, "(A)")
write (u, "(A)") "* Setup quantum mask: "

call qn_mask%init ([.false., .false., .false., .false.], &
                  [.true., .true., .true., .true.], &
                  [.false., .false., .true., .true.])
call quantum_numbers_mask_write (qn_mask, u)
write (u, "(A)")
write (u, "(A)") "* Reducing the state matrix using above mask"
write (u, "(A)")
allocate (state_reduced)
call state_orig%reduce (qn_mask, state_reduced)

write (u, "(A)") "* Reduced state matrix: "
call state_reduced%write (u)

write (u, "(A)") "* Test output end: state_matrix_6"
end subroutine state_matrix_6

```

Create a state matrix with full flavor, color and helicity information. Afterwards, reduce such that it is only differential in flavor and initial-state helicities, and keeping old indices. Afterwards reorder the reduced state matrix in accordance to the original state matrix.

```

<State matrices: execute tests>+=
call test (state_matrix_7, "state_matrix_7", &
          "check ordered state matrix reduction", &

```



```

        u, results)

<State matrices: test declarations>+≡
    public :: state_matrix_7

<State matrices: tests>+≡
    subroutine state_matrix_7 (u)
        integer, intent(in) :: u
        type(state_matrix_t), allocatable :: state_orig, state_reduced, &
            state_ordered
        type(flavor_t), dimension(4) :: flv
        type(helicity_t), dimension(4) :: hel
        type(color_t), dimension(4) :: col
        type(quantum_numbers_t), dimension(4) :: qn
        type(quantum_numbers_mask_t), dimension(4) :: qn_mask
        integer :: h1, h2, h3 , h4
        integer :: n_states = 0

        write (u, "(A)") "* Test output: state_matrix_7"
        write (u, "(A)") "* Purpose: Check ordered state matrix reduction"
        write (u, "(A)")

        write (u, "(A)") "* Set up helicity-diagonal state matrix"
        write (u, "(A)")

        allocate (state_orig)
        call state_orig%init ()

        call flv%init ([11, -11, 1, -1])
        call col(3)%init ([1])
        call col(4)%init ([-1])
        do h1 = -1, 1, 2
            do h2 = -1, 1, 2
                do h3 = -1, 1, 2
                    do h4 = -1, 1, 2
                        n_states = n_states + 1
                        call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
                        call qn%init (flv, col, hel)
                        call state_orig%add_state (qn)
                    end do
                end do
            end do
        end do
        call state_orig%freeze ()

        write (u, "(A)") "* Original state: "
        write (u, "(A)")
        call state_orig%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Setup quantum mask: "

        call qn_mask%init ([.false., .false., .false., .false.], &
            [.true., .true., .true., .true.], &
            [.false., .false., .true., .true.])

```

```

call quantum_numbers_mask_write (qn_mask, u)
write (u, "(A)")
write (u, "(A)") "* Reducing the state matrix using above mask and keeping the old indices:"
write (u, "(A)")
allocate (state_reduced)
call state_orig%reduce (qn_mask, state_reduced, keep_me_index = .true.)

write (u, "(A)") "* Reduced state matrix with kept indices: "
call state_reduced%write (u)

write (u, "(A)")
write (u, "(A)") "* Reordering reduced state matrix:"
write (u, "(A)")
allocate (state_ordered)
call state_reduced%reorder_me (state_ordered)

write (u, "(A)") "* Reduced and ordered state matrix:"
call state_ordered%write (u)

write (u, "(A)") "* Test output end: state_matrix_6"
end subroutine state_matrix_7

```

12.2 Interactions

This module defines the `interaction_t` type. It is an extension of the `state_matrix_t` type.

The state matrix is a representation of a multi-particle density matrix. It implements all possible flavor, color, and quantum-number assignments of the entries in a generic density matrix, and it can hold a complex matrix element for each entry. (Note that this matrix can hold non-diagonal entries in color and helicity space.) The `interaction_t` object associates this with a list of momenta, such that the whole object represents a multi-particle state.

The `interaction_t` holds information about which particles are incoming, virtual (i.e., kept for the records), or outgoing. Each particle can be associated to a source within another interaction. This allows us to automatically fill those interaction momenta which have been computed or defined elsewhere. It also contains internal parent-child relations and flags for (virtual) particles which are to be treated as resonances.

A quantum-number mask array summarizes, for each particle within the interaction, the treatment of flavor, color, or helicity (expose or ignore). A list of locks states which particles are bound to have an identical quantum-number mask. This is useful when the mask is changed at one place.

```

<interactions.f90>≡
  <File header>

```

```

module interactions

```

```

  <Use kinds>
  use lorentz
  use flavors

```

```

    use colors
    use helicities
    use quantum_numbers
    use state_matrices

    <Standard module head>

    <Interactions: public>

    <Interactions: types>

    <Interactions: interfaces>

    interface
    <Interactions: sub interfaces>
    end interface

    end module interactions
<interactions_sub.f90>≡
    <File header>

    submodule (interactions) interactions_s

        use io_units
        use diagnostics
        use sorting

        implicit none

    contains

    <Interactions: procedures>

    end submodule interactions_s

```

Given an ordered list of quantum numbers (without any subtraction index) map this list to a state matrix, such that each list index corresponds to an index of a set of quantum numbers in the state matrix, hence, the matrix element.

The (unphysical) subtraction index is not a genuine quantum number and as such handled specially.

```

<Interactions: public>≡
    public :: qn_index_map_t

<Interactions: types>≡
    type :: qn_index_map_t
        private
        type(quantum_numbers_t), dimension(:, :), allocatable :: qn_flv
        type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel
        logical :: flip_hel = .false.
        integer :: n_flv = 0, n_hel = 0, n_sub = 0
        integer, dimension(:, :, :), allocatable :: index
        integer, dimension(:, :, :), allocatable :: sf_index_born, sf_index_real
    contains

```

```

    <Interactions: qn index map: TBP>
end type qn_index_map_t

```

Construct a mapping from interaction to an array of (sorted) quantum numbers.

We strip all non-elementary particles (like beam) from the quantum numbers which we retrieve from the interaction.

We consider helicity matrix elements only, when `qn_hel` is allocated. Else the helicity index is handled trivially as 1.

For the rescaling of the structure functions in the real subtraction and DGLAP components we need a mapping (initialized by `qn_index_map_init_sf`) from the real and born flavor structure indices to the structure function chain interaction matrix element with the correct initial state quantum numbers. This is stored in `sf_index_born` and `sf_index_real`. The array `index` is only needed for the initialisation of the Born and real index arrays and is therefore deallocated again.

```

<Interactions: qn index map: TBP>≡

```

```

    generic :: init => init_trivial, &
                      init_involved, &
                      init_sf
    procedure, private :: init_trivial => qn_index_map_init_trivial
    procedure, private :: init_involved => qn_index_map_init_involved
    procedure, private :: init_sf => qn_index_map_init_sf

```

```

<Interactions: sub interfaces>≡

```

```

    module subroutine qn_index_map_init_trivial (self, int)
        class(qn_index_map_t), intent(out) :: self
        class(interaction_t), intent(in) :: int
    end subroutine qn_index_map_init_trivial
    module subroutine qn_index_map_init_involved (self, int, qn_flv, n_sub, qn_hel)
        class(qn_index_map_t), intent(out) :: self
        type(interaction_t), intent(in) :: int
        type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
        integer, intent(in) :: n_sub
        type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
    end subroutine qn_index_map_init_involved
    module subroutine qn_index_map_init_sf (self, int, qn_flv, n_flv_born, n_flv_real)
        class(qn_index_map_t), intent(out) :: self
        type(interaction_t), intent(in) :: int
        integer, intent(in) :: n_flv_born, n_flv_real
        type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
    end subroutine qn_index_map_init_sf

```

```

<Interactions: procedures>≡

```

```

    module subroutine qn_index_map_init_trivial (self, int)
        class(qn_index_map_t), intent(out) :: self
        class(interaction_t), intent(in) :: int
        integer :: qn
        self%n_flv = int%get_n_matrix_elements ()
        self%n_hel = 1
        self%n_sub = 0
        allocate (self%index(self%n_flv, self%n_hel, 0:self%n_sub), source = 0)
        do qn = 1, self%n_flv
            self%index(qn, 1, 0) = qn
        end do

```

```

end subroutine qn_index_map_init_trivial

module subroutine qn_index_map_init_involved (self, int, qn_flv, n_sub, qn_hel)
  class(qn_index_map_t), intent(out) :: self
  type(interaction_t), intent(in) :: int
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
  integer, intent(in) :: n_sub
  type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
  type(quantum_numbers_t), dimension(:), allocatable :: qn, qn_int
  integer :: i, i_flv, i_hel, i_sub
  self%qn_flv = qn_flv
  self%n_flv = size (qn_flv, dim=2)
  self%n_sub = n_sub
  if (present (qn_hel)) then
    if (size (qn_flv, dim=1) /= size (qn_hel, dim=1)) then
      call msg_bug ("[qn_index_map_init] number of particles does not match.")
    end if
    self%qn_hel = qn_hel
    self%n_hel = size (qn_hel, dim=2)
  else
    self%n_hel = 1
  end if
  allocate (self%index (self%n_flv, self%n_hel, 0:self%n_sub), source=0)
  associate (n_me => int%get_n_matrix_elements ())
    do i = 1, n_me
      qn_int = int%get_quantum_numbers (i, by_me_index = .true.)
      qn = pack (qn_int, qn_int%are_hard_process ())
      i_flv = find_flv_index (self, qn)
      i_hel = 1; if (allocated (self%qn_hel)) &
        i_hel = find_hel_index (self, qn)
      i_sub = find_sub_index (self, qn)
      self%index(i_flv, i_hel, i_sub) = i
    end do
  end associate
contains
  integer function find_flv_index (self, qn) result (i_flv)
    type(qn_index_map_t), intent(in) :: self
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer :: j
    i_flv = 0
    do j = 1, self%n_flv
      if (.not. all (qn .fmatch. self%qn_flv(:, j))) cycle
      i_flv = j
      exit
    end do
    if (i_flv < 1) then
      call msg_message ("QN:")
      call quantum_numbers_write (qn)
      call msg_message ("")
      call msg_message ("QN_FLV:")
      do j = 1, self%n_flv
        call quantum_numbers_write (self%qn_flv(:, j))
        call msg_message ("")
      end do
    end if
  end function find_flv_index
end module

```

```

        call msg_bug ("[find_flv_index] could not find flv in qn_flv.")
    end if
end function find_flv_index

integer function find_hel_index (self, qn) result (i_hel)
    type(qn_index_map_t), intent(in) :: self
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer :: j
    i_hel = 0
    do j = 1, self%n_hel
        if (.not. all (qn .hmatch. self%qn_hel(:, j))) cycle
        i_hel = j
        exit
    end do
    if (i_hel < 1) then
        call msg_message ("QN:")
        call quantum_numbers_write (qn)
        call msg_message ("")
        call msg_message ("QN_HEL:")
        do j = 1, self%n_hel
            call quantum_numbers_write (self%qn_hel(:, j))
            call msg_message ("")
        end do
        call msg_bug ("[find_hel_index] could not find hel in qn_hel.")
    end if
end function find_hel_index

integer function find_sub_index (self, qn) result (i_sub)
    type(qn_index_map_t), intent(in) :: self
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer :: s
    i_sub = -1
    do s = 0, self%n_sub
        if ((all (pack(qn%get_sub (), qn%get_sub () > 0) == s)) &
            .or. (all (qn%get_sub () == 0) .and. s == 0)) then
            i_sub = s
            exit
        end if
    end do
    if (i_sub < 0) then
        call msg_message ("QN:")
        call quantum_numbers_write (qn)
        call msg_bug ("[find_sub_index] could not find sub in qn.")
    end if
end function find_sub_index
end subroutine qn_index_map_init_involved

module subroutine qn_index_map_init_sf (self, int, qn_flv, n_flv_born, n_flv_real)
    class(qn_index_map_t), intent(out) :: self
    type(interaction_t), intent(in) :: int
    integer, intent(in) :: n_flv_born, n_flv_real
    type(quantum_numbers_t), dimension(:,:), intent(in) :: qn_flv
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_int
    type(quantum_numbers_t), dimension(:), allocatable :: qn_int_tmp

```

```

integer :: i, i_sub, n_flv, n_hard
n_flv = int%get_n_matrix_elements ()
qn_int_tmp = int%get_quantum_numbers (1, by_me_index = .true.)
n_hard = count (qn_int_tmp%are_hard_process ())
allocate (qn_int(n_hard, n_flv))
do i = 1, n_flv
    qn_int_tmp = int%get_quantum_numbers (i, by_me_index = .true.)
    qn_int(:, i) = pack (qn_int_tmp, qn_int_tmp%are_hard_process ())
end do
call self%init (int, qn_int, int%get_n_sub ())
allocate (self%sf_index_born(n_flv_born, 0:self%n_sub))
allocate (self%sf_index_real(n_flv_real, 0:self%n_sub))
do i_sub = 0, self%n_sub
    do i = 1, n_flv_born
        self%sf_index_born(i, i_sub) = self%get_index_by_qn (qn_flv(:,i), i_sub)
    end do
    do i = 1, n_flv_real
        self%sf_index_real(i, i_sub) = &
            self%get_index_by_qn (qn_flv(:,n_flv_born + i), i_sub)
    end do
end do
deallocate (self%index)
end subroutine qn_index_map_init_sf

```

Write the index map to unit.

<Interactions: qn index map: TBP>+≡

```

procedure :: write => qn_index_map_write

```

<Interactions: sub interfaces>+≡

```

module subroutine qn_index_map_write (self, unit)
    class(qn_index_map_t), intent(in) :: self
    integer, intent(in), optional :: unit
end subroutine qn_index_map_write

```

<Interactions: procedures>+≡

```

module subroutine qn_index_map_write (self, unit)
    class(qn_index_map_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer :: u, i_flv, i_hel, i_sub
    u = given_output_unit (unit); if (u < 0) return
    write (u, *) "flip_hel: ", self%flip_hel
    do i_flv = 1, self%n_flv
        if (allocated (self%qn_flv)) &
            call quantum_numbers_write (self%qn_flv(:, i_flv))
        write (u, *)
        do i_hel = 1, self%n_hel
            if (allocated (self%qn_hel)) then
                call quantum_numbers_write (self%qn_hel(:, i_hel))
                write (u, *)
            end if
            do i_sub = 0, self%n_sub
                write (u, *) &
                    "(" , i_flv , "," , i_hel , "," , i_sub , ")" => " , self%index(i_flv, i_hel, i_sub)
            end do
        end do
    end do
end subroutine qn_index_map_write

```

```

end do
end subroutine qn_index_map_write

```

Set helicity convention. If flip, then we flip the helicities of anti-particles and we remap the indices accordingly.

```

<Interactions: qn index map: TBP>+≡
  procedure :: set_helicity_flip => qn_index_map_set_helicity_flip

<Interactions: sub interfaces>+≡
  module subroutine qn_index_map_set_helicity_flip (self, yorn)
    class(qn_index_map_t), intent(inout) :: self
    logical, intent(in) :: yorn
  end subroutine qn_index_map_set_helicity_flip

<Interactions: procedures>+≡
  module subroutine qn_index_map_set_helicity_flip (self, yorn)
    class(qn_index_map_t), intent(inout) :: self
    logical, intent(in) :: yorn
    integer :: i, i_flv, i_hel, i_hel_new
    type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel_flip
    integer, dimension(:, :, :), allocatable :: index
    if (.not. allocated (self%qn_hel)) then
      call msg_bug ("[qn_index_map_set_helicity_flip] &
        &cannot flip not-given helicity.")
    end if
    allocate (index (self%n_flv, self%n_hel, 0:self%n_sub), &
      source=self%index)
    self%flip_hel = yorn
    if (self%flip_hel) then
      do i_flv = 1, self%n_flv
        qn_hel_flip = self%qn_hel
        do i_hel = 1, self%n_hel
          do i = 1, size (self%qn_flv, dim=1)
            if (is_anti_particle (self%qn_flv(i, i_flv))) then
              call qn_hel_flip(i, i_hel)%flip_helicity ()
            end if
          end do
        end do
        do i_hel = 1, self%n_hel
          i_hel_new = find_hel_index (qn_hel_flip, self%qn_hel(:, i_hel))
          self%index(i_flv, i_hel_new, :) = index(i_flv, i_hel, :)
        end do
      end do
    end if
  contains
    logical function is_anti_particle (qn) result (yorn)
      type(quantum_numbers_t), intent(in) :: qn
      type(flavor_t) :: flv
      flv = qn%get_flavor ()
      yorn = flv%get_pdg () < 0
    end function is_anti_particle

    integer function find_hel_index (qn_sort, qn) result (i_hel)
      type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_sort
      type(quantum_numbers_t), dimension(:, :), intent(in) :: qn

```



```

integer :: j
do j = 1, size(qn_sort, dim=2)
  if (.not. all (qn .hmatch. qn_sort(:, j))) cycle
  i_hel = j
  exit
end do
end function find_hel_index
end subroutine qn_index_map_set_helicity_flip

```

Map from the previously given quantum number and subtraction index (latter ranging from 0 to `n_sub`) to the (interaction) matrix element.

<Interactions: qn index map: TBP>+≡

```

procedure :: get_index => qn_index_map_get_index

```

<Interactions: sub interfaces>+≡

```

module function qn_index_map_get_index (self, i_flv, i_hel, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer :: index
  integer, intent(in) :: i_flv
  integer, intent(in), optional :: i_hel
  integer, intent(in), optional :: i_sub
end function qn_index_map_get_index

```

<Interactions: procedures>+≡

```

module function qn_index_map_get_index (self, i_flv, i_hel, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer :: index
  integer, intent(in) :: i_flv
  integer, intent(in), optional :: i_hel
  integer, intent(in), optional :: i_sub
  integer :: i_sub_opt, i_hel_opt
  i_sub_opt = 0; if (present (i_sub)) &
    i_sub_opt = i_sub
  i_hel_opt = 1; if (present (i_hel)) &
    i_hel_opt = i_hel
  index = 0
  if (.not. allocated (self%index)) then
    call msg_bug ("[qn_index_map_get_index] The index map is not allocated.")
  end if
  index = self%index(i_flv, i_hel_opt, i_sub_opt)
  if (index <= 0) then
    call self%write ()
    call msg_bug ("[qn_index_map_get_index] The index for the given quantum numbers could not b
  end if
end function qn_index_map_get_index

```

Get `n_flv`.

<Interactions: qn index map: TBP>+≡

```

procedure :: get_n_flv => qn_index_map_get_n_flv

```

<Interactions: sub interfaces>+≡

```

module function qn_index_map_get_n_flv (self) result (n_flv)
  class(qn_index_map_t), intent(in) :: self
  integer :: n_flv
end function qn_index_map_get_n_flv

```

```

<Interactions: procedures>+≡
  module function qn_index_map_get_n_flv (self) result (n_flv)
    class(qn_index_map_t), intent(in) :: self
    integer :: n_flv
    n_flv = self%n_flv
  end function qn_index_map_get_n_flv

```

Get n_hel.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_n_hel => qn_index_map_get_n_hel

<Interactions: sub interfaces>+≡
  module function qn_index_map_get_n_hel (self) result (n_hel)
    class(qn_index_map_t), intent(in) :: self
    integer :: n_hel
  end function qn_index_map_get_n_hel

<Interactions: procedures>+≡
  module function qn_index_map_get_n_hel (self) result (n_hel)
    class(qn_index_map_t), intent(in) :: self
    integer :: n_hel
    n_hel = self%n_hel
  end function qn_index_map_get_n_hel

```

Get n_sub.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_n_sub => qn_index_map_get_n_sub

<Interactions: sub interfaces>+≡
  module function qn_index_map_get_n_sub (self) result (n_sub)
    class(qn_index_map_t), intent(in) :: self
    integer :: n_sub
  end function qn_index_map_get_n_sub

<Interactions: procedures>+≡
  module function qn_index_map_get_n_sub (self) result (n_sub)
    class(qn_index_map_t), intent(in) :: self
    integer :: n_sub
    n_sub = self%n_sub
  end function qn_index_map_get_n_sub

```

Gets the index for the matrix element corresponding to a set of quantum numbers. So far, it ignores helicity (and color) indices.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_index_by_qn => qn_index_map_get_index_by_qn

<Interactions: sub interfaces>+≡
  module function qn_index_map_get_index_by_qn (self, qn, i_sub) result (index)
    class(qn_index_map_t), intent(in) :: self
    integer :: index
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: i_sub
  end function qn_index_map_get_index_by_qn

```

<Interactions: procedures>+≡

```

module function qn_index_map_get_index_by_qn (self, qn, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer :: index
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  integer, intent(in), optional :: i_sub
  integer :: i_qn
  if (size (qn) /= size (self%qn_flv, dim = 1)) &
    call msg_bug ("[qn_index_map_get_index_by_qn] number of particles does not match.")
  do i_qn = 1, self%n_flv
    if (all (qn .fmatch. self%qn_flv(:, i_qn))) then
      index = self%get_index (i_qn, i_sub = i_sub)
      return
    end if
  end do
  call self%write ()
  call msg_bug ("[qn_index_map_get_index_by_qn] The index for the given quantum &
    & numbers could not be retrieved.")
end function qn_index_map_get_index_by_qn

```

<Interactions: qn index map: TBP>+≡

```

procedure :: get_sf_index_born => qn_index_map_get_sf_index_born

```

<Interactions: sub interfaces>+≡

```

module function qn_index_map_get_sf_index_born (self, i_born, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer, intent(in) :: i_born, i_sub
  integer :: index
end function qn_index_map_get_sf_index_born

```

<Interactions: procedures>+≡

```

module function qn_index_map_get_sf_index_born (self, i_born, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer, intent(in) :: i_born, i_sub
  integer :: index
  index = self%sf_index_born(i_born, i_sub)
end function qn_index_map_get_sf_index_born

```

<Interactions: qn index map: TBP>+≡

```

procedure :: get_sf_index_real => qn_index_map_get_sf_index_real

```

<Interactions: sub interfaces>+≡

```

module function qn_index_map_get_sf_index_real (self, i_real, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer, intent(in) :: i_real, i_sub
  integer :: index
end function qn_index_map_get_sf_index_real

```

<Interactions: procedures>+≡

```

module function qn_index_map_get_sf_index_real (self, i_real, i_sub) result (index)
  class(qn_index_map_t), intent(in) :: self
  integer, intent(in) :: i_real, i_sub
  integer :: index
  index = self%sf_index_real(i_real, i_sub)
end function qn_index_map_get_sf_index_real

```

12.2.1 External interaction links

Each particle in an interaction can have a link to a corresponding particle in another interaction. This allows to fetch the momenta of incoming or virtual particles from the interaction where they are defined. The link object consists of a pointer to the interaction and an index.

```
<Interactions: types>+≡  
  type :: external_link_t  
  private  
    type(interaction_t), pointer :: int => null ()  
    integer :: i  
  end type external_link_t
```

Set an external link.

```
<Interactions: sub interfaces>+≡  
  module subroutine external_link_set (link, int, i)  
    type(external_link_t), intent(out) :: link  
    type(interaction_t), target, intent(in) :: int  
    integer, intent(in) :: i  
  end subroutine external_link_set
```

```
<Interactions: procedures>+≡  
  module subroutine external_link_set (link, int, i)  
    type(external_link_t), intent(out) :: link  
    type(interaction_t), target, intent(in) :: int  
    integer, intent(in) :: i  
    if (i /= 0) then  
      link%int => int  
      link%i = i  
    end if  
  end subroutine external_link_set
```

Reassign an external link to a new interaction (which should be an image of the original target).

```
<Interactions: sub interfaces>+≡  
  module subroutine external_link_reassign (link, int_src, int_target)  
    type(external_link_t), intent(inout) :: link  
    type(interaction_t), intent(in) :: int_src  
    type(interaction_t), intent(in), target :: int_target  
  end subroutine external_link_reassign
```

```
<Interactions: procedures>+≡  
  module subroutine external_link_reassign (link, int_src, int_target)  
    type(external_link_t), intent(inout) :: link  
    type(interaction_t), intent(in) :: int_src  
    type(interaction_t), intent(in), target :: int_target  
    if (associated (link%int)) then  
      if (link%int%tag == int_src%tag) link%int => int_target  
    end if  
  end subroutine external_link_reassign
```

Return true if the link is set

```
<Interactions: sub interfaces>+≡
```

```

module function external_link_is_set (link) result (flag)
  logical :: flag
  type(external_link_t), intent(in) :: link
end function external_link_is_set

```

<Interactions: procedures>+≡

```

module function external_link_is_set (link) result (flag)
  logical :: flag
  type(external_link_t), intent(in) :: link
  flag = associated (link%int)
end function external_link_is_set

```

Return the interaction pointer.

<Interactions: public>+≡

```

public :: external_link_get_ptr

```

<Interactions: sub interfaces>+≡

```

module function external_link_get_ptr (link) result (int)
  type(interaction_t), pointer :: int
  type(external_link_t), intent(in) :: link
end function external_link_get_ptr

```

<Interactions: procedures>+≡

```

module function external_link_get_ptr (link) result (int)
  type(interaction_t), pointer :: int
  type(external_link_t), intent(in) :: link
  int => link%int
end function external_link_get_ptr

```

Return the index within that interaction

<Interactions: public>+≡

```

public :: external_link_get_index

```

<Interactions: sub interfaces>+≡

```

module function external_link_get_index (link) result (i)
  integer :: i
  type(external_link_t), intent(in) :: link
end function external_link_get_index

```

<Interactions: procedures>+≡

```

module function external_link_get_index (link) result (i)
  integer :: i
  type(external_link_t), intent(in) :: link
  i = link%i
end function external_link_get_index

```

Return a pointer to the momentum of the corresponding particle. If there is no association, return a null pointer.

<Interactions: sub interfaces>+≡

```

module function external_link_get_momentum_ptr (link) result (p)
  type(vector4_t), pointer :: p
  type(external_link_t), intent(in) :: link
end function external_link_get_momentum_ptr

```

```

<Interactions: procedures>+≡
module function external_link_get_momentum_ptr (link) result (p)
  type(vector4_t), pointer :: p
  type(external_link_t), intent(in) :: link
  if (associated (link%int)) then
    p => link%int%p(link%i)
  else
    p => null ()
  end if
end function external_link_get_momentum_ptr

```

12.2.2 Internal relations

In addition to the external links, particles within the interaction have parent-child relations. Here, more than one link is possible, and we set up an array.

```

<Interactions: types>+≡
type :: internal_link_list_t
  private
  integer :: length = 0
  integer, dimension(:), allocatable :: link
contains
  <Interactions: internal link list: TBP>
end type internal_link_list_t

```

Output, non-advancing.

```

<Interactions: internal link list: TBP>≡
procedure :: write => internal_link_list_write

<Interactions: sub interfaces>+≡
module subroutine internal_link_list_write (object, unit)
  class(internal_link_list_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine internal_link_list_write

<Interactions: procedures>+≡
module subroutine internal_link_list_write (object, unit)
  class(internal_link_list_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  do i = 1, object%length
    write (u, "(1x,I0)", advance="no") object%link(i)
  end do
end subroutine internal_link_list_write

```

Append an item. Start with an array size of 2 and double the size if necessary.

Make sure that the indices are stored in ascending order. To this end, shift the existing entries right, starting from the end, as long as they are larger than the new entry.

```

<Interactions: internal link list: TBP>+≡
procedure :: append => internal_link_list_append

```

<Interactions: sub interfaces>+≡

```

module subroutine internal_link_list_append (link_list, link)
  class(internal_link_list_t), intent(inout) :: link_list
  integer, intent(in) :: link
end subroutine internal_link_list_append

```

<Interactions: procedures>+≡

```

module subroutine internal_link_list_append (link_list, link)
  class(internal_link_list_t), intent(inout) :: link_list
  integer, intent(in) :: link
  integer :: l, j
  integer, dimension(:), allocatable :: tmp
  l = link_list%length
  if (allocated (link_list%link)) then
    if (l == size (link_list%link)) then
      allocate (tmp (2 * l))
      tmp(:l) = link_list%link
      call move_alloc (from = tmp, to = link_list%link)
    end if
  else
    allocate (link_list%link (2))
  end if
  link_list%link(l+1) = link
  SHIFT_LINK_IN_PLACE: do j = l, 1, -1
    if (link >= link_list%link(j)) then
      exit SHIFT_LINK_IN_PLACE
    else
      link_list%link(j+1) = link_list%link(j)
      link_list%link(j) = link
    end if
  end do SHIFT_LINK_IN_PLACE
  link_list%length = l + 1
end subroutine internal_link_list_append

```

Return true if the link list is nonempty:

<Interactions: internal link list: TBP>+≡

```

procedure :: has_entries => internal_link_list_has_entries

```

<Interactions: sub interfaces>+≡

```

module function internal_link_list_has_entries (link_list) result (flag)
  class(internal_link_list_t), intent(in) :: link_list
  logical :: flag
end function internal_link_list_has_entries

```

<Interactions: procedures>+≡

```

module function internal_link_list_has_entries (link_list) result (flag)
  class(internal_link_list_t), intent(in) :: link_list
  logical :: flag
  flag = link_list%length > 0
end function internal_link_list_has_entries

```

Return the list length

<Interactions: internal link list: TBP>+≡

```

procedure :: get_length => internal_link_list_get_length

```

```

<Interactions: sub interfaces>+≡
    module function internal_link_list_get_length (link_list) result (length)
        class(internal_link_list_t), intent(in) :: link_list
        integer :: length
    end function internal_link_list_get_length

```

```

<Interactions: procedures>+≡
    module function internal_link_list_get_length (link_list) result (length)
        class(internal_link_list_t), intent(in) :: link_list
        integer :: length
        length = link_list%length
    end function internal_link_list_get_length

```

Return an entry.

```

<Interactions: internal link list: TBP>+≡
    procedure :: get_link => internal_link_list_get_link

```

```

<Interactions: sub interfaces>+≡
    module function internal_link_list_get_link (link_list, i) result (link)
        class(internal_link_list_t), intent(in) :: link_list
        integer, intent(in) :: i
        integer :: link
    end function internal_link_list_get_link

```

```

<Interactions: procedures>+≡
    module function internal_link_list_get_link (link_list, i) result (link)
        class(internal_link_list_t), intent(in) :: link_list
        integer, intent(in) :: i
        integer :: link
        if (i <= link_list%length) then
            link = link_list%link(i)
        else
            call msg_bug ("Internal link list: out of bounds")
        end if
    end function internal_link_list_get_link

```

12.2.3 The interaction type

An interaction is an entangled system of particles. Thus, the interaction object consists of two parts: the subevent, and the quantum state which technically is a trie. The subnode levels beyond the trie root node are in correspondence to the subevent, so both should be traversed in parallel.

The subevent is implemented as an allocatable array of four-momenta. The first **n_in** particles are incoming, **n_vir** particles in-between can be kept for bookkeeping, and the last **n_out** particles are outgoing.

Distinct interactions are linked by their particles: for each particle, we have the possibility of links to corresponding particles in other interactions. Furthermore, for bookkeeping purposes we have a self-link array **relations** where the parent-child relations are kept, and a flag array **resonant** which is set for an intermediate resonance.

Each momentum is associated with masks for flavor, color, and helicity. If a mask entry is set, the associated quantum number is to be ignored for that particle. If any mask has changed, the flag **update** is set.

We can have particle pairs locked together. If this is the case, the corresponding mask entries are bound to be equal. This is useful for particles that go through the interaction.

The interaction tag serves bookkeeping purposes. In particular, it identifies links in printout.

```

<Interactions: public>+≡
    public :: interaction_t

<Interactions: types>+≡
    type :: interaction_t
        private
        integer :: tag = 0
        type(state_matrix_t) :: state_matrix
        integer :: n_in = 0
        integer :: n_vir = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        logical, dimension(:), allocatable :: p_is_known
        type(vector4_t), dimension(:), allocatable :: p
        type(external_link_t), dimension(:), allocatable :: source
        type(internal_link_list_t), dimension(:), allocatable :: parents
        type(internal_link_list_t), dimension(:), allocatable :: children
        logical, dimension(:), allocatable :: resonant
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        integer, dimension(:), allocatable :: hel_lock
        logical :: update_state_matrix = .false.
        logical :: update_values = .false.
        type(qn_index_map_t) :: qn_index
    contains
    <Interactions: interaction: TBP>
end type interaction_t

```

Initialize the particle array with a fixed size. The first `n_in` particles are incoming, the rest outgoing. Masks are optional. There is also an optional tag. The interaction still needs fixing the values, but that is to be done after all branches have been added.

Interaction tags are assigned consecutively, using a `saved` variable local to this procedure. If desired, we can provide a seed for the interaction tags. Such a seed should be positive. The default seed is one. `tag=0` indicates an empty interaction.

If `set_relations` is set and true, we establish parent-child relations for all incoming and outgoing particles. Virtual particles are skipped; this option is normally used only for interactions without virtual particles.

```

<Interactions: interaction: TBP>≡
    procedure :: basic_init => interaction_init

<Interactions: sub interfaces>+≡
    module subroutine interaction_init &
        (int, n_in, n_vir, n_out, &
         tag, resonant, mask, hel_lock, set_relations, store_values)
    class(interaction_t), intent(out) :: int
    integer, intent(in) :: n_in, n_vir, n_out
    integer, intent(in), optional :: tag

```

```

    logical, dimension(:), intent(in), optional :: resonant
    type(quantum_numbers_mask_t), dimension(:), intent(in), optional :: mask
    integer, dimension(:), intent(in), optional :: hel_lock
    logical, intent(in), optional :: set_relations, store_values
end subroutine interaction_init

```

<Interactions: procedures>+≡

```

module subroutine interaction_init &
    (int, n_in, n_vir, n_out, &
     tag, resonant, mask, hel_lock, set_relations, store_values)
class(interaction_t), intent(out) :: int
integer, intent(in) :: n_in, n_vir, n_out
integer, intent(in), optional :: tag
logical, dimension(:), intent(in), optional :: resonant
type(quantum_numbers_mask_t), dimension(:), intent(in), optional :: mask
integer, dimension(:), intent(in), optional :: hel_lock
logical, intent(in), optional :: set_relations, store_values
logical :: set_rel
integer :: i, j
set_rel = .false.; if (present (set_relations)) set_rel = set_relations
call interaction_set_tag (int, tag)
call int%state_matrix%init (store_values)
int%n_in = n_in
int%n_vir = n_vir
int%n_out = n_out
int%n_tot = n_in + n_vir + n_out
allocate (int%p_is_known (int%n_tot))
int%p_is_known = .false.
allocate (int%p (int%n_tot))
allocate (int%source (int%n_tot))
allocate (int%parents (int%n_tot))
allocate (int%children (int%n_tot))
allocate (int%resonant (int%n_tot))
if (present (resonant)) then
    int%resonant = resonant
else
    int%resonant = .false.
end if
allocate (int%mask (int%n_tot))
allocate (int%hel_lock (int%n_tot))
if (present (mask)) then
    int%mask = mask
end if
if (present (hel_lock)) then
    int%hel_lock = hel_lock
else
    int%hel_lock = 0
end if
int%update_state_matrix = .false.
int%update_values = .true.
if (set_rel) then
    do i = 1, n_in
        do j = 1, n_out
            call int%relate (i, n_in + j)
        end do
    end do

```

```

        end do
    end if
end subroutine interaction_init

<Interactions: interaction: TBP>+≡
generic :: init_qn_index => init_qn_index_trivial, &
    init_qn_index_involved, &
    init_qn_index_sf
procedure :: init_qn_index_trivial => interaction_init_qn_index_trivial
procedure :: init_qn_index_involved => interaction_init_qn_index_involved
procedure :: init_qn_index_sf => interaction_init_qn_index_sf

<Interactions: sub interfaces>+≡
module subroutine interaction_init_qn_index_trivial (int)
    class(interaction_t), intent(inout) :: int
end subroutine interaction_init_qn_index_trivial
module subroutine interaction_init_qn_index_involved (int, qn_flv, n_sub, qn_hel)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
    integer, intent(in) :: n_sub
    type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
end subroutine interaction_init_qn_index_involved
module subroutine interaction_init_qn_index_sf (int, qn_flv, n_flv_born, n_flv_real)
    class(interaction_t), intent(inout) :: int
    integer, intent(in) :: n_flv_born, n_flv_real
    type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
end subroutine interaction_init_qn_index_sf

<Interactions: procedures>+≡
module subroutine interaction_init_qn_index_trivial (int)
    class(interaction_t), intent(inout) :: int
    call int%qn_index%init (int)
end subroutine interaction_init_qn_index_trivial

module subroutine interaction_init_qn_index_involved (int, qn_flv, n_sub, qn_hel)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
    integer, intent(in) :: n_sub
    type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
    call int%qn_index%init (int, qn_flv, n_sub, qn_hel)
end subroutine interaction_init_qn_index_involved

module subroutine interaction_init_qn_index_sf (int, qn_flv, n_flv_born, n_flv_real)
    class(interaction_t), intent(inout) :: int
    integer, intent(in) :: n_flv_born, n_flv_real
    type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
    call int%qn_index%init (int, qn_flv, n_flv_born, n_flv_real)
end subroutine interaction_init_qn_index_sf

<Interactions: interaction: TBP>+≡
procedure :: set_qn_index_helicity_flip => interaction_set_qn_index_helicity_flip

<Interactions: sub interfaces>+≡
module subroutine interaction_set_qn_index_helicity_flip (int, yorn)
    class(interaction_t), intent(inout) :: int

```

```

        logical, intent(in) :: yorn
    end subroutine interaction_set_qn_index_helicity_flip

<Interactions: procedures>+≡
    module subroutine interaction_set_qn_index_helicity_flip (int, yorn)
        class(interaction_t), intent(inout) :: int
        logical, intent(in) :: yorn
        call int%qn_index%set_helicity_flip (yorn)
    end subroutine interaction_set_qn_index_helicity_flip

<Interactions: interaction: TBP>+≡
    procedure :: get_qn_index => interaction_get_qn_index
    procedure :: get_sf_qn_index_born => interaction_get_sf_qn_index_born
    procedure :: get_sf_qn_index_real => interaction_get_sf_qn_index_real

<Interactions: sub interfaces>+≡
    module function interaction_get_qn_index (int, i_flv, i_hel, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_flv
        integer, intent(in), optional :: i_hel
        integer, intent(in), optional :: i_sub
    end function interaction_get_qn_index
    module function interaction_get_sf_qn_index_born (int, i_born, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_born, i_sub
    end function interaction_get_sf_qn_index_born
    module function interaction_get_sf_qn_index_real (int, i_real, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_real, i_sub
    end function interaction_get_sf_qn_index_real

<Interactions: procedures>+≡
    module function interaction_get_qn_index (int, i_flv, i_hel, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_flv
        integer, intent(in), optional :: i_hel
        integer, intent(in), optional :: i_sub
        index = int%qn_index%get_index (i_flv, i_hel, i_sub)
    end function interaction_get_qn_index

    module function interaction_get_sf_qn_index_born (int, i_born, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_born, i_sub
        index = int%qn_index%get_sf_index_born (i_born, i_sub)
    end function interaction_get_sf_qn_index_born

    module function interaction_get_sf_qn_index_real (int, i_real, i_sub) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        integer, intent(in) :: i_real, i_sub

```

```

        index = int%qn_index%get_sf_index_real (i_real, i_sub)
    end function interaction_get_sf_qn_index_real

```

<Interactions: interaction: TBP>+≡

```

    procedure :: get_qn_index_n_flv => interaction_get_qn_index_n_flv
    procedure :: get_qn_index_n_hel => interaction_get_qn_index_n_hel
    procedure :: get_qn_index_n_sub => interaction_get_qn_index_n_sub

```

<Interactions: sub interfaces>+≡

```

    module function interaction_get_qn_index_n_flv (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
    end function interaction_get_qn_index_n_flv
    module function interaction_get_qn_index_n_hel (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
    end function interaction_get_qn_index_n_hel
    module function interaction_get_qn_index_n_sub (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
    end function interaction_get_qn_index_n_sub

```

<Interactions: procedures>+≡

```

    module function interaction_get_qn_index_n_flv (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        index = int%qn_index%get_n_flv ()
    end function interaction_get_qn_index_n_flv

    module function interaction_get_qn_index_n_hel (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        index = int%qn_index%get_n_hel ()
    end function interaction_get_qn_index_n_hel

    module function interaction_get_qn_index_n_sub (int) result (index)
        class(interaction_t), intent(in) :: int
        integer :: index
        index = int%qn_index%get_n_sub ()
    end function interaction_get_qn_index_n_sub

```

Set or create a unique tag for the interaction. Without interaction, reset the tag counter.

<Interactions: sub interfaces>+≡

```

    module subroutine interaction_set_tag (int, tag)
        type(interaction_t), intent(inout), optional :: int
        integer, intent(in), optional :: tag
    end subroutine interaction_set_tag

```

<Interactions: procedures>+≡

```

    module subroutine interaction_set_tag (int, tag)
        type(interaction_t), intent(inout), optional :: int
        integer, intent(in), optional :: tag
        integer, save :: stored_tag = 1

```

```

if (present (int)) then
  if (present (tag)) then
    int%tag = tag
  else
    int%tag = stored_tag
    stored_tag = stored_tag + 1
  end if
else if (present (tag)) then
  stored_tag = tag
else
  stored_tag = 1
end if
end subroutine interaction_set_tag

```

The public interface for the previous procedure only covers the reset functionality.

```

<Interactions: public>+≡
public :: reset_interaction_counter

<Interactions: sub interfaces>+≡
module subroutine reset_interaction_counter (tag)
  integer, intent(in), optional :: tag
end subroutine reset_interaction_counter

<Interactions: procedures>+≡
module subroutine reset_interaction_counter (tag)
  integer, intent(in), optional :: tag
  call interaction_set_tag (tag=tag)
end subroutine reset_interaction_counter

```

Finalizer: The state-matrix object contains pointers.

```

<Interactions: interaction: TBP>+≡
procedure :: final => interaction_final

<Interactions: sub interfaces>+≡
module subroutine interaction_final (object)
  class(interaction_t), intent(inout) :: object
end subroutine interaction_final

<Interactions: procedures>+≡
module subroutine interaction_final (object)
  class(interaction_t), intent(inout) :: object
  call object%state_matrix%final ()
end subroutine interaction_final

```

Output. The `verbose` option refers to the state matrix output.

```

<Interactions: interaction: TBP>+≡
procedure :: basic_write => interaction_write

<Interactions: sub interfaces>+≡
module subroutine interaction_write &
  (int, unit, verbose, show_momentum_sum, show_mass, show_state, &
  col_verbose, testflag)
  class(interaction_t), intent(in) :: int
  integer, intent(in), optional :: unit

```

```

        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, col_verbose, testflag
    end subroutine interaction_write

    (Interactions: procedures)+≡
    module subroutine interaction_write &
        (int, unit, verbose, show_momentum_sum, show_mass, show_state, &
        col_verbose, testflag)
        class(interaction_t), intent(in) :: int
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, col_verbose, testflag
        integer :: u
        integer :: i, index_link
        type(interaction_t), pointer :: int_link
        logical :: show_st
        u = given_output_unit (unit); if (u < 0) return
        show_st = .true.; if (present (show_state)) show_st = show_state
        if (int%tag /= 0) then
            write (u, "(1x,A,I0)") "Interaction: ", int%tag
            do i = 1, int%n_tot
                if (i == 1 .and. int%n_in > 0) then
                    write (u, "(1x,A)") "Incoming:"
                else if (i == int%n_in + 1 .and. int%n_vir > 0) then
                    write (u, "(1x,A)") "Virtual:"
                else if (i == int%n_in + int%n_vir + 1 .and. int%n_out > 0) then
                    write (u, "(1x,A)") "Outgoing:"
                end if
                write (u, "(1x,A,1x,I0)", advance="no") "Particle", i
                if (allocated (int%resonant)) then
                    if (int%resonant(i)) then
                        write (u, "(A)") "[r]"
                    else
                        write (u, *)
                    end if
                else
                    write (u, *)
                end if
                if (allocated (int%p)) then
                    if (int%p_is_known(i)) then
                        call vector4_write (int%p(i), u, show_mass, testflag)
                    else
                        write (u, "(A)") " [momentum undefined]"
                    end if
                else
                    write (u, "(A)") " [momentum not allocated]"
                end if
                if (allocated (int%mask)) then
                    write (u, "(1x,A)", advance="no") "mask [fch] = "
                    call int%mask(i)%write (u)
                    write (u, *)
                end if
                if (int%parents(i)%has_entries () &
                    .or. int%children(i)%has_entries ()) then
                    write (u, "(1x,A)", advance="no") "internal links:"

```

```

        call int%parents(i)%write (u)
        if (int%parents(i)%has_entries ()) &
            write (u, "(1x,A)", advance="no") "=>"
        write (u, "(1x,A)", advance="no") "X"
        if (int%children(i)%has_entries ()) &
            write (u, "(1x,A)", advance="no") "=>"
        call int%children(i)%write (u)
        write (u, *)
    end if
    if (allocated (int%hel_lock)) then
        if (int%hel_lock(i) /= 0) then
            write (u, "(1x,A,1x,I0)") "helicity lock:", int%hel_lock(i)
        end if
    end if
    if (external_link_is_set (int%source(i))) then
        write (u, "(1x,A)", advance="no") "source:"
        int_link => external_link_get_ptr (int%source(i))
        index_link = external_link_get_index (int%source(i))
        write (u, "(1x,'(,IO,')',I0)", advance="no") &
            int_link%tag, index_link
        write (u, *)
    end if
end do
if (present (show_momentum_sum)) then
    if (allocated (int%p) .and. show_momentum_sum) then
        write (u, "(1x,A)") "Incoming particles (sum):"
        call vector4_write &
            (sum (int%p(1 : int%n_in)), u, show_mass = show_mass)
        write (u, "(1x,A)") "Outgoing particles (sum):"
        call vector4_write &
            (sum (int%p(int%n_in + int%n_vir + 1 : )), &
                u, show_mass = show_mass)
        write (u, *)
    end if
end if
if (show_st) then
    call int%write_state_matrix (write_value_list = verbose, &
        verbose = verbose, unit = unit, col_verbose = col_verbose, &
        testflag = testflag)
end if
else
    write (u, "(1x,A)") "Interaction: [empty]"
end if
end subroutine interaction_write

```

<Interactions: interaction: TBP>+≡

```
procedure :: write_state_matrix => interaction_write_state_matrix
```

<Interactions: sub interfaces>+≡

```

module subroutine interaction_write_state_matrix (int, unit, write_value_list, &
    verbose, col_verbose, testflag)
    class(interaction_t), intent(in) :: int
    logical, intent(in), optional :: write_value_list, verbose, col_verbose
    logical, intent(in), optional :: testflag

```



```

        integer, intent(in), optional :: unit
    end subroutine interaction_write_state_matrix

<Interactions: procedures>+=
    module subroutine interaction_write_state_matrix (int, unit, write_value_list, &
        verbose, col_verbose, testflag)
        class(interaction_t), intent(in) :: int
        logical, intent(in), optional :: write_value_list, verbose, col_verbose
        logical, intent(in), optional :: testflag
        integer, intent(in), optional :: unit
        call int%state_matrix%write (write_value_list = verbose, &
            verbose = verbose, unit = unit, col_verbose = col_verbose, &
            testflag = testflag)
    end subroutine interaction_write_state_matrix

```

Reduce the `state_matrix` over the quantum mask. During the reduce procedure the iterator does not conserve the order of the matrix element respective their quantum numbers. Setting the `keep_order` results in a reorder state matrix with reintroduced matrix element indices.

```

<Interactions: interaction: TBP>+=
    procedure :: reduce_state_matrix => interaction_reduce_state_matrix

<Interactions: sub interfaces>+=
    module subroutine interaction_reduce_state_matrix (int, qn_mask, keep_order)
        class(interaction_t), intent(inout) :: int
        type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
        logical, optional, intent(in) :: keep_order
    end subroutine interaction_reduce_state_matrix

<Interactions: procedures>+=
    module subroutine interaction_reduce_state_matrix (int, qn_mask, keep_order)
        class(interaction_t), intent(inout) :: int
        type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
        logical, optional, intent(in) :: keep_order
        type(state_matrix_t) :: state
        logical :: opt_keep_order
        opt_keep_order = .false.
        if (present (keep_order)) opt_keep_order = keep_order
        call int%state_matrix%reduce (qn_mask, state, keep_me_index = keep_order)
        int%state_matrix = state
        if (opt_keep_order) then
            call int%state_matrix%reorder_me (state)
            int%state_matrix = state
        end if
    end subroutine interaction_reduce_state_matrix

```

Assignment: We implement this as a deep copy. This applies, in particular, to the state-matrix and internal-link components. Furthermore, the new interaction acquires a new tag.

```

<Interactions: public>+=
    public :: assignment(=)

<Interactions: interfaces>=
    interface assignment(=)

```

```

    module procedure interaction_assign
end interface

```

(Interactions: sub interfaces)+≡

```

    module subroutine interaction_assign (int_out, int_in)
        type(interaction_t), intent(out) :: int_out
        type(interaction_t), intent(in), target :: int_in
    end subroutine interaction_assign

```

(Interactions: procedures)+≡

```

    module subroutine interaction_assign (int_out, int_in)
        type(interaction_t), intent(out) :: int_out
        type(interaction_t), intent(in), target :: int_in
        call interaction_set_tag (int_out)
        int_out%state_matrix = int_in%state_matrix
        int_out%n_in = int_in%n_in
        int_out%n_out = int_in%n_out
        int_out%n_vir = int_in%n_vir
        int_out%n_tot = int_in%n_tot
        if (allocated (int_in%p_is_known)) then
            allocate (int_out%p_is_known (size (int_in%p_is_known)))
            int_out%p_is_known = int_in%p_is_known
        end if
        if (allocated (int_in%p)) then
            allocate (int_out%p (size (int_in%p)))
            int_out%p = int_in%p
        end if
        if (allocated (int_in%source)) then
            allocate (int_out%source (size (int_in%source)))
            int_out%source = int_in%source
        end if
        if (allocated (int_in%parents)) then
            allocate (int_out%parents (size (int_in%parents)))
            int_out%parents = int_in%parents
        end if
        if (allocated (int_in%children)) then
            allocate (int_out%children (size (int_in%children)))
            int_out%children = int_in%children
        end if
        if (allocated (int_in%resonant)) then
            allocate (int_out%resonant (size (int_in%resonant)))
            int_out%resonant = int_in%resonant
        end if
        if (allocated (int_in%mask)) then
            allocate (int_out%mask (size (int_in%mask)))
            int_out%mask = int_in%mask
        end if
        if (allocated (int_in%hel_lock)) then
            allocate (int_out%hel_lock (size (int_in%hel_lock)))
            int_out%hel_lock = int_in%hel_lock
        end if
        int_out%update_state_matrix = int_in%update_state_matrix
        int_out%update_values = int_in%update_values
    end subroutine interaction_assign

```

12.2.4 Methods inherited from the state matrix member

Until F2003 is standard, we cannot implement inheritance directly. Therefore, we need wrappers for “inherited” methods.

Make a new branch in the state matrix if it does not yet exist. This is not just a wrapper but it introduces the interaction mask: where a quantum number is masked, it is not transferred but set undefined. After this, the value array has to be updated.

```

<Interactions: interaction: TBP>+≡
  procedure :: add_state => interaction_add_state

<Interactions: sub interfaces>+≡
  module subroutine interaction_add_state &
    (int, qn, index, value, sum_values, counter_index, ignore_sub_for_qn, me_index)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: index
    complex(default), intent(in), optional :: value
    logical, intent(in), optional :: sum_values
    integer, intent(in), optional :: counter_index
    logical, intent(in), optional :: ignore_sub_for_qn
    integer, intent(out), optional :: me_index
  end subroutine interaction_add_state

<Interactions: procedures>+≡
  module subroutine interaction_add_state &
    (int, qn, index, value, sum_values, counter_index, ignore_sub_for_qn, me_index)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: index
    complex(default), intent(in), optional :: value
    logical, intent(in), optional :: sum_values
    integer, intent(in), optional :: counter_index
    logical, intent(in), optional :: ignore_sub_for_qn
    integer, intent(out), optional :: me_index
    type(quantum_numbers_t), dimension(size(qn)) :: qn_tmp
    qn_tmp = qn
    call qn_tmp%undefine (int%mask)
    call int%state_matrix%add_state (qn_tmp, index, value, sum_values, &
      counter_index, ignore_sub_for_qn, me_index)
    int%update_values = .true.
  end subroutine interaction_add_state

<Interactions: interaction: TBP>+≡
  procedure :: set_duplicate_flv_zero => interaction_set_duplicate_flv_zero

<Interactions: sub interfaces>+≡
  module subroutine interaction_set_duplicate_flv_zero (int)
    class(interaction_t), intent(inout) :: int
  end subroutine interaction_set_duplicate_flv_zero

```

```

<Interactions: procedures>+≡
  module subroutine interaction_set_duplicate_flv_zero (int)
    class(interaction_t), intent(inout) :: int
    call int%state_matrix%set_duplicate_flv_zero ()
  end subroutine interaction_set_duplicate_flv_zero

```

Freeze the quantum state: First collapse the quantum state, i.e., remove quantum numbers if any mask has changed, then fix the array of value pointers.

```

<Interactions: interaction: TBP>+≡
  procedure :: freeze => interaction_freeze

<Interactions: sub interfaces>+≡
  module subroutine interaction_freeze (int)
    class(interaction_t), intent(inout) :: int
  end subroutine interaction_freeze

```

```

<Interactions: procedures>+≡
  module subroutine interaction_freeze (int)
    class(interaction_t), intent(inout) :: int
    if (int%update_state_matrix) then
      call int%state_matrix%collapse (int%mask)
      int%update_state_matrix = .false.
      int%update_values = .true.
    end if
    if (int%update_values) then
      call int%state_matrix%freeze ()
      int%update_values = .false.
    end if
  end subroutine interaction_freeze

```

Return true if the state matrix is empty.

```

<Interactions: interaction: TBP>+≡
  procedure :: is_empty => interaction_is_empty

<Interactions: sub interfaces>+≡
  pure module function interaction_is_empty (int) result (flag)
    logical :: flag
    class(interaction_t), intent(in) :: int
  end function interaction_is_empty

<Interactions: procedures>+≡
  pure module function interaction_is_empty (int) result (flag)
    logical :: flag
    class(interaction_t), intent(in) :: int
    flag = int%state_matrix%is_empty ()
  end function interaction_is_empty

```

Get the number of values stored in the state matrix:

```

<Interactions: interaction: TBP>+≡
  procedure :: get_n_matrix_elements => &
    interaction_get_n_matrix_elements

```

```

<Interactions: sub interfaces>+≡
    pure module function interaction_get_n_matrix_elements (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
    end function interaction_get_n_matrix_elements

<Interactions: procedures>+≡
    pure module function interaction_get_n_matrix_elements (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
        n = int%state_matrix%get_n_matrix_elements ()
    end function interaction_get_n_matrix_elements

<Interactions: interaction: TBP>+≡
    procedure :: get_state_depth => interaction_get_state_depth

<Interactions: sub interfaces>+≡
    module function interaction_get_state_depth (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
    end function interaction_get_state_depth

<Interactions: procedures>+≡
    module function interaction_get_state_depth (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
        n = int%state_matrix%get_depth ()
    end function interaction_get_state_depth

<Interactions: interaction: TBP>+≡
    procedure :: get_n_in_helicities => interaction_get_n_in_helicities

<Interactions: sub interfaces>+≡
    module function interaction_get_n_in_helicities (int) result (n_hel)
        integer :: n_hel
        class(interaction_t), intent(in) :: int
    end function interaction_get_n_in_helicities

<Interactions: procedures>+≡
    module function interaction_get_n_in_helicities (int) result (n_hel)
        integer :: n_hel
        class(interaction_t), intent(in) :: int
        type(interaction_t) :: int_copy
        type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
        type(quantum_numbers_t), dimension(:,:), allocatable :: qn
        integer :: i
        allocate (qn_mask (int%n_tot))
        do i = 1, int%n_tot
            if (i <= int%n_in) then
                call qn_mask(i)%init (.true., .true., .false.)
            else
                call qn_mask(i)%init (.true., .true., .true.)
            end if
        end do
        int_copy = int
        call int_copy%set_mask (qn_mask)
    end function interaction_get_n_in_helicities

```

```

call int_copy%freeze ()
allocate (qn (int_copy%state_matrix%get_n_matrix_elements (), &
            int_copy%state_matrix%get_depth ()))
qn = int_copy%get_quantum_numbers ()
n_hel = 0
do i = 1, size (qn, dim=1)
    if (all (qn(:, i)%get_subtraction_index () == 0)) n_hel = n_hel + 1
end do
call int_copy%final ()
deallocate (qn_mask)
deallocate (qn)
end function interaction_get_n_in_helicities

```

Get the size of the me-array of the associated state matrix for debugging purposes

```

<Interactions: interaction: TBP>+≡
    procedure :: get_me_size => interaction_get_me_size

<Interactions: sub interfaces>+≡
    pure module function interaction_get_me_size (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
    end function interaction_get_me_size

<Interactions: procedures>+≡
    pure module function interaction_get_me_size (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
        n = int%state_matrix%get_me_size ()
    end function interaction_get_me_size

```

Get the norm of the state matrix (if the norm has been taken out, otherwise this would be unity).

```

<Interactions: interaction: TBP>+≡
    procedure :: get_norm => interaction_get_norm

<Interactions: sub interfaces>+≡
    pure module function interaction_get_norm (int) result (norm)
        real(default) :: norm
        class(interaction_t), intent(in) :: int
    end function interaction_get_norm

<Interactions: procedures>+≡
    pure module function interaction_get_norm (int) result (norm)
        real(default) :: norm
        class(interaction_t), intent(in) :: int
        norm = int%state_matrix%get_norm ()
    end function interaction_get_norm

```

```

<Interactions: interaction: TBP>+≡
    procedure :: get_n_sub => interaction_get_n_sub

<Interactions: sub interfaces>+≡
    module function interaction_get_n_sub (int) result (n_sub)
        integer :: n_sub
        class(interaction_t), intent(in) :: int
    end function interaction_get_n_sub

```

<Interactions: procedures>+≡

```
module function interaction_get_n_sub (int) result (n_sub)
  integer :: n_sub
  class(interaction_t), intent(in) :: int
  n_sub = int%state_matrix%get_n_sub ()
end function interaction_get_n_sub
```

Get the quantum number array that corresponds to a given index.

<Interactions: interaction: TBP>+≡

```
generic :: get_quantum_numbers => get_quantum_numbers_single, &
                                     get_quantum_numbers_all, &
                                     get_quantum_numbers_all_qn_mask

procedure :: get_quantum_numbers_single => &
  interaction_get_quantum_numbers_single
procedure :: get_quantum_numbers_all => &
  interaction_get_quantum_numbers_all
procedure :: get_quantum_numbers_all_qn_mask => &
  interaction_get_quantum_numbers_all_qn_mask
```

<Interactions: sub interfaces>+≡

```
module function interaction_get_quantum_numbers_single (int, i, by_me_index) result (qn)
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  class(interaction_t), intent(in), target :: int
  integer, intent(in) :: i
  logical, intent(in), optional :: by_me_index
end function interaction_get_quantum_numbers_single
module function interaction_get_quantum_numbers_all (int) result (qn)
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  class(interaction_t), intent(in), target :: int
end function interaction_get_quantum_numbers_all
module function interaction_get_quantum_numbers_all_qn_mask (int, qn_mask) &
  result (qn)
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  class(interaction_t), intent(in) :: int
  type(quantum_numbers_mask_t), intent(in) :: qn_mask
end function interaction_get_quantum_numbers_all_qn_mask
```

<Interactions: procedures>+≡

```
module function interaction_get_quantum_numbers_single (int, i, by_me_index) result (qn)
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  class(interaction_t), intent(in), target :: int
  integer, intent(in) :: i
  logical, intent(in), optional :: by_me_index
  allocate (qn (int%state_matrix%get_depth ()))
  qn = int%state_matrix%get_quantum_number (i, by_me_index)
end function interaction_get_quantum_numbers_single
```

```
module function interaction_get_quantum_numbers_all (int) result (qn)
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  class(interaction_t), intent(in), target :: int
  integer :: i
```

<Interactions: get quantum numbers all>

<Interactions: get quantum numbers all>≡

```
allocate (qn (int%state_matrix%get_depth(), &
```

```

        int%state_matrix%get_n_matrix_elements ()))
    do i = 1, int%state_matrix%get_n_matrix_elements ()
        qn (:, i) = int%state_matrix%get_quantum_number (i)
    end do
<Interactions: procedures>+≡
    end function interaction_get_quantum_numbers_all

    module function interaction_get_quantum_numbers_all_qn_mask (int, qn_mask) &
        result (qn)
        type(quantum_numbers_t), dimension(:,:), allocatable :: qn
        class(interaction_t), intent(in) :: int
        type(quantum_numbers_mask_t), intent(in) :: qn_mask
        integer :: n_redundant, n_all, n_me
        integer :: i
        type(quantum_numbers_t), dimension(:,:), allocatable :: qn_all
    <Interactions: get quantum numbers all qn mask>
<Interactions: get quantum numbers all qn mask>≡
        call int%state_matrix%get_quantum_numbers (qn_all)
        n_redundant = count (qn_all%are_redundant (qn_mask))
        n_all = size (qn_all)
        !!! Number of matrix elements = survivors / n_particles
        n_me = (n_all - n_redundant) / int%state_matrix%get_depth ()
        allocate (qn (int%state_matrix%get_depth(), n_me))
        do i = 1, n_me
            if (.not. any (qn_all(i, :)%are_redundant (qn_mask))) &
                qn (:, i) = qn_all (i, :)
        end do
    <Interactions: procedures>+≡
        end function interaction_get_quantum_numbers_all_qn_mask

    <Interactions: interaction: TBP>+≡
        procedure :: get_quantum_numbers_all_sub => interaction_get_quantum_numbers_all_sub
    <Interactions: sub interfaces>+≡
        module subroutine interaction_get_quantum_numbers_all_sub (int, qn)
            class(interaction_t), intent(in) :: int
            type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
        end subroutine interaction_get_quantum_numbers_all_sub
    <Interactions: procedures>+≡
        module subroutine interaction_get_quantum_numbers_all_sub (int, qn)
            class(interaction_t), intent(in) :: int
            type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
            integer :: i
        <Interactions: get quantum numbers all>
        end subroutine interaction_get_quantum_numbers_all_sub

    <Interactions: interaction: TBP>+≡
        procedure :: get_flavors => interaction_get_flavors
    <Interactions: sub interfaces>+≡
        module subroutine interaction_get_flavors (int, only_elementary, qn_mask, flv)
            class(interaction_t), intent(in), target :: int

```



```

        logical, intent(in) :: only_elementary
        type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
        integer, intent(out), dimension(:,:), allocatable :: flv
    end subroutine interaction_get_flavors

<Interactions: procedures>+≡
    module subroutine interaction_get_flavors (int, only_elementary, qn_mask, flv)
        class(interaction_t), intent(in), target :: int
        logical, intent(in) :: only_elementary
        type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
        integer, intent(out), dimension(:,:), allocatable :: flv
        call int%state_matrix%get_flavors (only_elementary, qn_mask, flv)
    end subroutine interaction_get_flavors

<Interactions: interaction: TBP>+≡
    procedure :: get_quantum_numbers_mask => interaction_get_quantum_numbers_mask

<Interactions: sub interfaces>+≡
    module subroutine interaction_get_quantum_numbers_mask (int, qn_mask, qn)
        class(interaction_t), intent(in) :: int
        type(quantum_numbers_mask_t), intent(in) :: qn_mask
        type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
    end subroutine interaction_get_quantum_numbers_mask

<Interactions: procedures>+≡
    module subroutine interaction_get_quantum_numbers_mask (int, qn_mask, qn)
        class(interaction_t), intent(in) :: int
        type(quantum_numbers_mask_t), intent(in) :: qn_mask
        type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
        integer :: n_redundant, n_all, n_me
        integer :: i
        type(quantum_numbers_t), dimension(:,:), allocatable :: qn_all
    <Interactions: get quantum numbers all qn mask>
    end subroutine interaction_get_quantum_numbers_mask

```

Get the matrix element that corresponds to a set of quantum numbers, a given index, or return the whole array.

```

<Interactions: interaction: TBP>+≡
    generic :: get_matrix_element => get_matrix_element_single
    generic :: get_matrix_element => get_matrix_element_array
    procedure :: get_matrix_element_single => &
        interaction_get_matrix_element_single
    procedure :: get_matrix_element_array => &
        interaction_get_matrix_element_array

<Interactions: sub interfaces>+≡
    elemental module function interaction_get_matrix_element_single (int, i) result (me)
        complex(default) :: me
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
    end function interaction_get_matrix_element_single

<Interactions: procedures>+≡
    elemental module function interaction_get_matrix_element_single (int, i) result (me)
        complex(default) :: me

```

```

class(interaction_t), intent(in) :: int
integer, intent(in) :: i
me = int%state_matrix%get_matrix_element (i)
end function interaction_get_matrix_element_single

```

<Interactions: sub interfaces>+≡

```

module function interaction_get_matrix_element_array (int) result (me)
  complex(default), dimension(:), allocatable :: me
  class(interaction_t), intent(in) :: int
end function interaction_get_matrix_element_array

```

<Interactions: procedures>+≡

```

module function interaction_get_matrix_element_array (int) result (me)
  complex(default), dimension(:), allocatable :: me
  class(interaction_t), intent(in) :: int
  allocate (me (int%get_n_matrix_elements ()))
  me = int%state_matrix%get_matrix_element (i)
end function interaction_get_matrix_element_array

```

Set the complex value(s) stored in the quantum state.

<Interactions: interaction: TBP>+≡

```

generic :: set_matrix_element => interaction_set_matrix_element_qn, &
  interaction_set_matrix_element_all, &
  interaction_set_matrix_element_array, &
  interaction_set_matrix_element_single, &
  interaction_set_matrix_element_clone
procedure :: interaction_set_matrix_element_qn
procedure :: interaction_set_matrix_element_all
procedure :: interaction_set_matrix_element_array
procedure :: interaction_set_matrix_element_single
procedure :: interaction_set_matrix_element_clone

```

Indirect access via the quantum number array:

<Interactions: sub interfaces>+≡

```

module subroutine interaction_set_matrix_element_qn (int, qn, val)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  complex(default), intent(in) :: val
end subroutine interaction_set_matrix_element_qn

```

<Interactions: procedures>+≡

```

module subroutine interaction_set_matrix_element_qn (int, qn, val)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  complex(default), intent(in) :: val
  call int%state_matrix%set_matrix_element (qn, val)
end subroutine interaction_set_matrix_element_qn

```

Set all entries of the matrix-element array to a given value.

<Interactions: sub interfaces>+≡

```

module subroutine interaction_set_matrix_element_all (int, value)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in) :: value
end subroutine interaction_set_matrix_element_all

```

<Interactions: procedures>+≡

```
module subroutine interaction_set_matrix_element_all (int, value)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in) :: value
  call int%state_matrix%set_matrix_element (value)
end subroutine interaction_set_matrix_element_all
```

Set the matrix-element array directly.

<Interactions: sub interfaces>+≡

```
module subroutine interaction_set_matrix_element_array (int, value, range)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in), dimension(:) :: value
  integer, intent(in), dimension(:), optional :: range
end subroutine interaction_set_matrix_element_array
pure module subroutine interaction_set_matrix_element_single (int, i, value)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  complex(default), intent(in) :: value
end subroutine interaction_set_matrix_element_single
```

<Interactions: procedures>+≡

```
module subroutine interaction_set_matrix_element_array (int, value, range)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in), dimension(:) :: value
  integer, intent(in), dimension(:), optional :: range
  call int%state_matrix%set_matrix_element (value, range)
end subroutine interaction_set_matrix_element_array

pure module subroutine interaction_set_matrix_element_single (int, i, value)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  complex(default), intent(in) :: value
  call int%state_matrix%set_matrix_element (i, value)
end subroutine interaction_set_matrix_element_single
```

Clone from another (matching) interaction.

<Interactions: sub interfaces>+≡

```
module subroutine interaction_set_matrix_element_clone (int, int1)
  class(interaction_t), intent(inout) :: int
  class(interaction_t), intent(in) :: int1
end subroutine interaction_set_matrix_element_clone
```

<Interactions: procedures>+≡

```
module subroutine interaction_set_matrix_element_clone (int, int1)
  class(interaction_t), intent(inout) :: int
  class(interaction_t), intent(in) :: int1
  call int%state_matrix%set_matrix_element (int1%state_matrix)
end subroutine interaction_set_matrix_element_clone
```

<Interactions: interaction: TBP>+≡

```
procedure :: set_only_matrix_element => interaction_set_only_matrix_element
```

<Interactions: sub interfaces>+≡

```
module subroutine interaction_set_only_matrix_element (int, i, value)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  complex(default), intent(in) :: value
end subroutine interaction_set_only_matrix_element
```

<Interactions: procedures>+≡

```
module subroutine interaction_set_only_matrix_element (int, i, value)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  complex(default), intent(in) :: value
  call int%set_matrix_element (cmplx (0, 0, default))
  call int%set_matrix_element (i, value)
end subroutine interaction_set_only_matrix_element
```

<Interactions: interaction: TBP>+≡

```
procedure :: add_to_matrix_element => interaction_add_to_matrix_element
```

<Interactions: sub interfaces>+≡

```
module subroutine interaction_add_to_matrix_element (int, qn, value, match_only_flavor)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  complex(default), intent(in) :: value
  logical, intent(in), optional :: match_only_flavor
end subroutine interaction_add_to_matrix_element
```

<Interactions: procedures>+≡

```
module subroutine interaction_add_to_matrix_element (int, qn, value, match_only_flavor)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  complex(default), intent(in) :: value
  logical, intent(in), optional :: match_only_flavor
  call int%state_matrix%add_to_matrix_element (qn, value, match_only_flavor)
end subroutine interaction_add_to_matrix_element
```

Get the indices of any diagonal matrix elements.

<Interactions: interaction: TBP>+≡

```
procedure :: get_diagonal_entries => interaction_get_diagonal_entries
```

<Interactions: sub interfaces>+≡

```
module subroutine interaction_get_diagonal_entries (int, i)
  class(interaction_t), intent(in) :: int
  integer, dimension(:), allocatable, intent(out) :: i
end subroutine interaction_get_diagonal_entries
```

<Interactions: procedures>+≡

```
module subroutine interaction_get_diagonal_entries (int, i)
  class(interaction_t), intent(in) :: int
  integer, dimension(:), allocatable, intent(out) :: i
  call int%state_matrix%get_diagonal_entries (i)
end subroutine interaction_get_diagonal_entries
```

Renormalize the state matrix by its trace, if nonzero. The renormalization is reflected in the state-matrix norm.

```

<Interactions: interaction: TBP>+≡
    procedure :: normalize_by_trace => interaction_normalize_by_trace

<Interactions: sub interfaces>+≡
    module subroutine interaction_normalize_by_trace (int)
        class(interaction_t), intent(inout) :: int
    end subroutine interaction_normalize_by_trace

<Interactions: procedures>+≡
    module subroutine interaction_normalize_by_trace (int)
        class(interaction_t), intent(inout) :: int
        call int%state_matrix%normalize_by_trace ()
    end subroutine interaction_normalize_by_trace

```

Analogous, but renormalize by maximal (absolute) value.

```

<Interactions: interaction: TBP>+≡
    procedure :: normalize_by_max => interaction_normalize_by_max

<Interactions: sub interfaces>+≡
    module subroutine interaction_normalize_by_max (int)
        class(interaction_t), intent(inout) :: int
    end subroutine interaction_normalize_by_max

<Interactions: procedures>+≡
    module subroutine interaction_normalize_by_max (int)
        class(interaction_t), intent(inout) :: int
        call int%state_matrix%normalize_by_max ()
    end subroutine interaction_normalize_by_max

```

Explicitly set the norm value (of the state matrix).

```

<Interactions: interaction: TBP>+≡
    procedure :: set_norm => interaction_set_norm

<Interactions: sub interfaces>+≡
    module subroutine interaction_set_norm (int, norm)
        class(interaction_t), intent(inout) :: int
        real(default), intent(in) :: norm
    end subroutine interaction_set_norm

<Interactions: procedures>+≡
    module subroutine interaction_set_norm (int, norm)
        class(interaction_t), intent(inout) :: int
        real(default), intent(in) :: norm
        call int%state_matrix%set_norm (norm)
    end subroutine interaction_set_norm

<Interactions: interaction: TBP>+≡
    procedure :: set_state_matrix => interaction_set_state_matrix

<Interactions: sub interfaces>+≡
    module subroutine interaction_set_state_matrix (int, state)
        class(interaction_t), intent(inout) :: int
        type(state_matrix_t), intent(in) :: state
    end subroutine interaction_set_state_matrix

```

```

<Interactions: procedures>+≡
  module subroutine interaction_set_state_matrix (int, state)
    class(interaction_t), intent(inout) :: int
    type(state_matrix_t), intent(in) :: state
    int%state_matrix = state
  end subroutine interaction_set_state_matrix

```

Return the maximum absolute value of color indices.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_max_color_value => &
    interaction_get_max_color_value

<Interactions: sub interfaces>+≡
  module function interaction_get_max_color_value (int) result (cmax)
    class(interaction_t), intent(in) :: int
    integer :: cmax
  end function interaction_get_max_color_value

<Interactions: procedures>+≡
  module function interaction_get_max_color_value (int) result (cmax)
    class(interaction_t), intent(in) :: int
    integer :: cmax
    cmax = int%state_matrix%get_max_color_value ()
  end function interaction_get_max_color_value

```

Factorize the state matrix into single-particle state matrices, the branch selection depending on a (random) value between 0 and 1; optionally also return a correlated state matrix.

```

<Interactions: interaction: TBP>+≡
  procedure :: factorize => interaction_factorize

<Interactions: sub interfaces>+≡
  module subroutine interaction_factorize &
    (int, mode, x, ok, single_state, correlated_state, qn_in)
    class(interaction_t), intent(in), target :: int
    integer, intent(in) :: mode
    real(default), intent(in) :: x
    logical, intent(out) :: ok
    type(state_matrix_t), &
      dimension(:), allocatable, intent(out) :: single_state
    type(state_matrix_t), intent(out), optional :: correlated_state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
  end subroutine interaction_factorize

<Interactions: procedures>+≡
  module subroutine interaction_factorize &
    (int, mode, x, ok, single_state, correlated_state, qn_in)
    class(interaction_t), intent(in), target :: int
    integer, intent(in) :: mode
    real(default), intent(in) :: x
    logical, intent(out) :: ok
    type(state_matrix_t), &
      dimension(:), allocatable, intent(out) :: single_state
    type(state_matrix_t), intent(out), optional :: correlated_state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in

```

```

        call int%state_matrix%factorize &
            (mode, x, ok, single_state, correlated_state, qn_in)
    end subroutine interaction_factorize

```

Sum all matrix element values

```

<Interactions: interaction: TBP>+≡
    procedure :: sum => interaction_sum

<Interactions: sub interfaces>+≡
    module function interaction_sum (int) result (value)
        class(interaction_t), intent(in) :: int
        complex(default) :: value
    end function interaction_sum

<Interactions: procedures>+≡
    module function interaction_sum (int) result (value)
        class(interaction_t), intent(in) :: int
        complex(default) :: value
        value = int%state_matrix%sum ()
    end function interaction_sum

```

Append new states which are color-contracted versions of the existing states. The matrix element index of each color contraction coincides with the index of its origin, so no new matrix elements are generated. After this operation, no `freeze` must be performed anymore.

```

<Interactions: interaction: TBP>+≡
    procedure :: add_color_contractions => &
        interaction_add_color_contractions

<Interactions: sub interfaces>+≡
    module subroutine interaction_add_color_contractions (int)
        class(interaction_t), intent(inout) :: int
    end subroutine interaction_add_color_contractions

<Interactions: procedures>+≡
    module subroutine interaction_add_color_contractions (int)
        class(interaction_t), intent(inout) :: int
        call int%state_matrix%add_color_contractions ()
    end subroutine interaction_add_color_contractions

```

Multiply matrix elements from two interactions. Choose the elements as given by the integer index arrays, multiply them and store the sum of products in the indicated matrix element. The suffixes mean: c=conjugate first factor; f=include weighting factor.

```

<Interactions: interaction: TBP>+≡
    procedure :: evaluate_product => interaction_evaluate_product
    procedure :: evaluate_product_cf => interaction_evaluate_product_cf
    procedure :: evaluate_square_c => interaction_evaluate_square_c
    procedure :: evaluate_sum => interaction_evaluate_sum
    procedure :: evaluate_me_sum => interaction_evaluate_me_sum

<Interactions: sub interfaces>+≡
    pure module subroutine interaction_evaluate_product &
        (int, i, int1, int2, index1, index2)

```

```

class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1, int2
integer, dimension(:), intent(in) :: index1, index2
end subroutine interaction_evaluate_product
pure module subroutine interaction_evaluate_product_cf &
  (int, i, int1, int2, index1, index2, factor)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1, int2
integer, dimension(:), intent(in) :: index1, index2
complex(default), dimension(:), intent(in) :: factor
end subroutine interaction_evaluate_product_cf
pure module subroutine interaction_evaluate_square_c (int, i, int1, index1)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1
integer, dimension(:), intent(in) :: index1
end subroutine interaction_evaluate_square_c
pure module subroutine interaction_evaluate_sum (int, i, int1, index1)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1
integer, dimension(:), intent(in) :: index1
end subroutine interaction_evaluate_sum
pure module subroutine interaction_evaluate_me_sum (int, i, int1, index1)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1
integer, dimension(:), intent(in) :: index1
end subroutine interaction_evaluate_me_sum

```

(Interactions: procedures)+≡

```

pure module subroutine interaction_evaluate_product &
  (int, i, int1, int2, index1, index2)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1, int2
integer, dimension(:), intent(in) :: index1, index2
call int%state_matrix%evaluate_product &
  (i, int1%state_matrix, int2%state_matrix, &
   index1, index2)
end subroutine interaction_evaluate_product

pure module subroutine interaction_evaluate_product_cf &
  (int, i, int1, int2, index1, index2, factor)
class(interaction_t), intent(inout) :: int
integer, intent(in) :: i
type(interaction_t), intent(in) :: int1, int2
integer, dimension(:), intent(in) :: index1, index2
complex(default), dimension(:), intent(in) :: factor
call int%state_matrix%evaluate_product_cf &
  (i, int1%state_matrix, int2%state_matrix, &
   index1, index2, factor)
end subroutine interaction_evaluate_product_cf

```



```

pure module subroutine interaction_evaluate_square_c (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_square_c (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_square_c

pure module subroutine interaction_evaluate_sum (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_sum (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_sum

pure module subroutine interaction_evaluate_me_sum (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_me_sum (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_me_sum

```

Tag quantum numbers of the state matrix as part of the hard process, according to the indices specified in `tag`. If no `tag` is given, all quantum numbers are tagged as part of the hard process.

<Interactions: interaction: TBP>+≡

```

procedure :: tag_hard_process => interaction_tag_hard_process

```

<Interactions: sub interfaces>+≡

```

module subroutine interaction_tag_hard_process (int, tag)
  class(interaction_t), intent(inout) :: int
  integer, dimension(:), intent(in), optional :: tag
end subroutine interaction_tag_hard_process

```

<Interactions: procedures>+≡

```

module subroutine interaction_tag_hard_process (int, tag)
  class(interaction_t), intent(inout) :: int
  integer, dimension(:), intent(in), optional :: tag
  type(state_matrix_t) :: state
  call int%state_matrix%tag_hard_process (state, tag)
  call int%state_matrix%final ()
  int%state_matrix = state
end subroutine interaction_tag_hard_process

```

Modify hard-interaction flags at the specified particle-position, in-place.

<Interactions: interaction: TBP>+≡

```

procedure :: retag_hard_process => interaction_retag_hard_process

```

<Interactions: sub interfaces>+≡

```

module subroutine interaction_retag_hard_process (int, i, hard)
  class(interaction_t), intent(inout), target :: int

```

```

        integer, intent(in) :: i
        logical, intent(in) :: hard
    end subroutine interaction_retag_hard_process
<Interactions: procedures>+≡
    module subroutine interaction_retag_hard_process (int, i, hard)
        class(interaction_t), intent(inout), target :: int
        integer, intent(in) :: i
        logical, intent(in) :: hard
        type(state_iterator_t) :: it
        call it%init (int%get_state_matrix_ptr ())
        do while (it%is_valid ())
            call it%retag_hard_process (i, hard)
            call it%advance ()
        end do
    end subroutine interaction_retag_hard_process

```

12.2.5 Accessing contents

Return the integer tag.

```

<Interactions: interaction: TBP>+≡
    procedure :: get_tag => interaction_get_tag
<Interactions: sub interfaces>+≡
    module function interaction_get_tag (int) result (tag)
        class(interaction_t), intent(in) :: int
        integer :: tag
    end function interaction_get_tag
<Interactions: procedures>+≡
    module function interaction_get_tag (int) result (tag)
        class(interaction_t), intent(in) :: int
        integer :: tag
        tag = int%tag
    end function interaction_get_tag

```

Return the number of particles.

```

<Interactions: interaction: TBP>+≡
    procedure :: get_n_tot => interaction_get_n_tot
    procedure :: get_n_in => interaction_get_n_in
    procedure :: get_n_vir => interaction_get_n_vir
    procedure :: get_n_out => interaction_get_n_out
<Interactions: sub interfaces>+≡
    pure module function interaction_get_n_tot (object) result (n_tot)
        class(interaction_t), intent(in) :: object
        integer :: n_tot
    end function interaction_get_n_tot
    pure module function interaction_get_n_in (object) result (n_in)
        class(interaction_t), intent(in) :: object
        integer :: n_in
    end function interaction_get_n_in
    pure module function interaction_get_n_vir (object) result (n_vir)
        class(interaction_t), intent(in) :: object

```

```

        integer :: n_vir
    end function interaction_get_n_vir
    pure module function interaction_get_n_out (object) result (n_out)
        class(interaction_t), intent(in) :: object
        integer :: n_out
    end function interaction_get_n_out
<Interactions: procedures>+≡
    pure module function interaction_get_n_tot (object) result (n_tot)
        class(interaction_t), intent(in) :: object
        integer :: n_tot
        n_tot = object%n_tot
    end function interaction_get_n_tot

    pure module function interaction_get_n_in (object) result (n_in)
        class(interaction_t), intent(in) :: object
        integer :: n_in
        n_in = object%n_in
    end function interaction_get_n_in

    pure module function interaction_get_n_vir (object) result (n_vir)
        class(interaction_t), intent(in) :: object
        integer :: n_vir
        n_vir = object%n_vir
    end function interaction_get_n_vir

    pure module function interaction_get_n_out (object) result (n_out)
        class(interaction_t), intent(in) :: object
        integer :: n_out
        n_out = object%n_out
    end function interaction_get_n_out

```

Return a momentum index. The flags specify whether to keep/drop incoming, virtual, or outgoing momenta. Check for illegal values.

```

<Interactions: sub interfaces>+≡
    module function idx (int, i, outgoing)
        integer :: idx
        type(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        logical, intent(in), optional :: outgoing
    end function idx
<Interactions: procedures>+≡
    module function idx (int, i, outgoing)
        integer :: idx
        type(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        logical, intent(in), optional :: outgoing
        logical :: in, vir, out
        if (present (outgoing)) then
            in = .not. outgoing
            vir = .false.
            out = outgoing
        else
            in = .true.

```

```

        vir = .true.
        out = .true.
    end if
    idx = 0
    if (in) then
        if (vir) then
            if (out) then
                if (i <= int%n_tot) idx = i
            else
                if (i <= int%n_in + int%n_vir) idx = i
            end if
        else if (out) then
            if (i <= int%n_in) then
                idx = i
            else if (i <= int%n_in + int%n_out) then
                idx = int%n_vir + i
            end if
        else
            if (i <= int%n_in) idx = i
        end if
    else if (vir) then
        if (out) then
            if (i <= int%n_vir + int%n_out) idx = int%n_in + i
        else
            if (i <= int%n_vir) idx = int%n_in + i
        end if
    else if (out) then
        if (i <= int%n_out) idx = int%n_in + int%n_vir + i
    end if
    if (idx == 0) then
        call int%basic_write ()
        print *, i, in, vir, out
        call msg_bug (" Momentum index is out of range for this interaction")
    end if
end function idx

```

Return all or just a specific four-momentum.

(Interactions: interaction: TBP)+≡

```

generic :: get_momenta => get_momenta_all, get_momenta_idx
procedure :: get_momentum => interaction_get_momentum
procedure :: get_momenta_all => interaction_get_momenta_all
procedure :: get_momenta_idx => interaction_get_momenta_idx

```

(Interactions: sub interfaces)+≡

```

module function interaction_get_momenta_all (int, outgoing) result (p)
    class(interaction_t), intent(in) :: int
    type(vector4_t), dimension(:), allocatable :: p
    logical, intent(in), optional :: outgoing
end function interaction_get_momenta_all
module function interaction_get_momenta_idx (int, jj) result (p)
    class(interaction_t), intent(in) :: int
    type(vector4_t), dimension(:), allocatable :: p
    integer, dimension(:), intent(in) :: jj
end function interaction_get_momenta_idx

```

```

module function interaction_get_momentum (int, i, outgoing) result (p)
  class(interaction_t), intent(in) :: int
  type(vector4_t) :: p
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
end function interaction_get_momentum

```

<Interactions: procedures>+≡

```

module function interaction_get_momenta_all (int, outgoing) result (p)
  class(interaction_t), intent(in) :: int
  type(vector4_t), dimension(:), allocatable :: p
  logical, intent(in), optional :: outgoing
  integer :: i
  if (present (outgoing)) then
    if (outgoing) then
      allocate (p (int%n_out))
    else
      allocate (p (int%n_in))
    end if
  else
    allocate (p (int%n_tot))
  end if
  do i = 1, size (p)
    p(i) = int%p(idx (int, i, outgoing))
  end do
end function interaction_get_momenta_all

```

```

module function interaction_get_momenta_idx (int, jj) result (p)
  class(interaction_t), intent(in) :: int
  type(vector4_t), dimension(:), allocatable :: p
  integer, dimension(:), intent(in) :: jj
  allocate (p (size (jj)))
  p = int%p(jj)
end function interaction_get_momenta_idx

```

```

module function interaction_get_momentum (int, i, outgoing) result (p)
  class(interaction_t), intent(in) :: int
  type(vector4_t) :: p
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
  p = int%p(idx (int, i, outgoing))
end function interaction_get_momentum

```

Return a shallow copy of the state matrix:

<Interactions: interaction: TBP>+≡

```

procedure :: get_state_matrix_ptr => &
  interaction_get_state_matrix_ptr

```

<Interactions: sub interfaces>+≡

```

module function interaction_get_state_matrix_ptr (int) result (state)
  class(interaction_t), intent(in), target :: int
  type(state_matrix_t), pointer :: state
end function interaction_get_state_matrix_ptr

```

<Interactions: procedures>+≡

```

module function interaction_get_state_matrix_ptr (int) result (state)
  class(interaction_t), intent(in), target :: int
  type(state_matrix_t), pointer :: state
  state => int%state_matrix
end function interaction_get_state_matrix_ptr

```

Return the array of resonance flags

<Interactions: interaction: TBP>+≡

```

  procedure :: get_resonance_flags => interaction_get_resonance_flags

```

<Interactions: sub interfaces>+≡

```

  module function interaction_get_resonance_flags (int) result (resonant)
    class(interaction_t), intent(in) :: int
    logical, dimension(size(int%resonant)) :: resonant
  end function interaction_get_resonance_flags

```

<Interactions: procedures>+≡

```

  module function interaction_get_resonance_flags (int) result (resonant)
    class(interaction_t), intent(in) :: int
    logical, dimension(size(int%resonant)) :: resonant
    resonant = int%resonant
  end function interaction_get_resonance_flags

```

Return the quantum-numbers mask (or part of it)

<Interactions: interaction: TBP>+≡

```

  generic :: get_mask => get_mask_all, get_mask_slice
  procedure :: get_mask_all => interaction_get_mask_all
  procedure :: get_mask_slice => interaction_get_mask_slice

```

<Interactions: sub interfaces>+≡

```

  module function interaction_get_mask_all (int) result (mask)
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_mask_t), dimension(size(int%mask)) :: mask
  end function interaction_get_mask_all
  module function interaction_get_mask_slice (int, index) result (mask)
    class(interaction_t), intent(in) :: int
    integer, dimension(:), intent(in) :: index
    type(quantum_numbers_mask_t), dimension(size(index)) :: mask
  end function interaction_get_mask_slice

```

<Interactions: procedures>+≡

```

  module function interaction_get_mask_all (int) result (mask)
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_mask_t), dimension(size(int%mask)) :: mask
    mask = int%mask
  end function interaction_get_mask_all

  module function interaction_get_mask_slice (int, index) result (mask)
    class(interaction_t), intent(in) :: int
    integer, dimension(:), intent(in) :: index
    type(quantum_numbers_mask_t), dimension(size(index)) :: mask
    mask = int%mask(index)
  end function interaction_get_mask_slice

```

Compute the invariant mass squared of the incoming particles (if any, otherwise outgoing).

```

<Interactions: interaction: TBP>+≡
  procedure :: get_s => interaction_get_s

<Interactions: sub interfaces>+≡
  module function interaction_get_s (int) result (s)
    real(default) :: s
    class(interaction_t), intent(in) :: int
  end function interaction_get_s

<Interactions: procedures>+≡
  module function interaction_get_s (int) result (s)
    real(default) :: s
    class(interaction_t), intent(in) :: int
    if (int%n_in /= 0) then
      s = sum (int%p(:int%n_in)) ** 2
    else
      s = sum (int%p(int%n_vir + 1 : )) ** 2
    end if
  end function interaction_get_s

```

Compute the Lorentz transformation that transforms the incoming particles from the center-of-mass frame to the lab frame where they are given. If the c.m. mass squared is negative or zero, return the identity.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_cm_transformation => interaction_get_cm_transformation

<Interactions: sub interfaces>+≡
  module function interaction_get_cm_transformation (int) result (lt)
    type(lorentz_transformation_t) :: lt
    class(interaction_t), intent(in) :: int
  end function interaction_get_cm_transformation

<Interactions: procedures>+≡
  module function interaction_get_cm_transformation (int) result (lt)
    type(lorentz_transformation_t) :: lt
    class(interaction_t), intent(in) :: int
    type(vector4_t) :: p_cm
    real(default) :: s
    if (int%n_in /= 0) then
      p_cm = sum (int%p(:int%n_in))
    else
      p_cm = sum (int%p(int%n_vir+1:))
    end if
    s = p_cm ** 2
    if (s > 0) then
      lt = boost (p_cm, sqrt (s))
    else
      lt = identity
    end if
  end function interaction_get_cm_transformation

```

Return flavor, momentum, and position of the first outgoing unstable particle present in the interaction. Note that we need not iterate through the state matrix; if there is an unstable particle, it will be present in all state-matrix entries.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_unstable_particle => interaction_get_unstable_particle

<Interactions: sub interfaces>+≡
  module subroutine interaction_get_unstable_particle (int, flv, p, i)
    class(interaction_t), intent(in), target :: int
    type(flavor_t), intent(out) :: flv
    type(vector4_t), intent(out) :: p
    integer, intent(out) :: i
  end subroutine interaction_get_unstable_particle

<Interactions: procedures>+≡
  module subroutine interaction_get_unstable_particle (int, flv, p, i)
    class(interaction_t), intent(in), target :: int
    type(flavor_t), intent(out) :: flv
    type(vector4_t), intent(out) :: p
    integer, intent(out) :: i
    type(state_iterator_t) :: it
    type(flavor_t), dimension(int%n_tot) :: flv_array
    call it%init (int%state_matrix)
    flv_array = it%get_flavor ()
    do i = int%n_in + int%n_vir + 1, int%n_tot
      if (.not. flv_array(i)%is_stable ()) then
        flv = flv_array(i)
        p = int%p(i)
        return
      end if
    end do
  end subroutine interaction_get_unstable_particle

```

Return the complete set of *outgoing* flavors, assuming that the flavor quantum number is not suppressed.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_flv_out => interaction_get_flv_out

<Interactions: sub interfaces>+≡
  module subroutine interaction_get_flv_out (int, flv)
    class(interaction_t), intent(in), target :: int
    type(flavor_t), dimension(:, :), allocatable, intent(out) :: flv
  end subroutine interaction_get_flv_out

<Interactions: procedures>+≡
  module subroutine interaction_get_flv_out (int, flv)
    class(interaction_t), intent(in), target :: int
    type(flavor_t), dimension(:, :), allocatable, intent(out) :: flv
    type(state_iterator_t) :: it
    type(flavor_t), dimension(:, :), allocatable :: flv_state
    integer :: n_in, n_vir, n_out, n_tot, n_state, i
    n_in = int%get_n_in ()
    n_vir = int%get_n_vir ()
    n_out = int%get_n_out ()

```



```

n_tot = int%get_n_tot ()
n_state = int%get_n_matrix_elements ()
allocate (flv (n_out, n_state))
allocate (flv_state (n_tot))
i = 1
call it%init (int%get_state_matrix_ptr ())
do while (it%is_valid ())
  flv_state = it%get_flavor ()
  flv(:,i) = flv_state(n_in + n_vir + 1 : )
  i = i + 1
  call it%advance ()
end do
end subroutine interaction_get_flv_out

```

Determine the flavor content of the interaction. We analyze the state matrix for this, and we select the outgoing particles of the hard process only for the required mask, which indicates the particles that can appear in any order in a matching event record.

We have to assume that any radiated particles (beam remnants) appear at the beginning of the particles marked as outgoing.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_flv_content => interaction_get_flv_content

<Interactions: sub interfaces>+≡
  module subroutine interaction_get_flv_content (int, state_flv, n_out_hard)
    class(interaction_t), intent(in), target :: int
    type(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n_out_hard
  end subroutine interaction_get_flv_content

<Interactions: procedures>+≡
  module subroutine interaction_get_flv_content (int, state_flv, n_out_hard)
    class(interaction_t), intent(in), target :: int
    type(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n_out_hard
    logical, dimension(:), allocatable :: mask
    integer :: n_tot
    n_tot = int%get_n_tot ()
    allocate (mask (n_tot), source = .false.)
    mask(n_tot-n_out_hard + 1 : ) = .true.
    call state_flv%fill (int%get_state_matrix_ptr (), mask)
  end subroutine interaction_get_flv_content

```

12.2.6 Modifying contents

Set the quantum numbers mask.

```

<Interactions: interaction: TBP>+≡
  procedure :: set_mask => interaction_set_mask

<Interactions: sub interfaces>+≡
  module subroutine interaction_set_mask (int, mask)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
  end subroutine interaction_set_mask

```

(Interactions: procedures)+≡

```

module subroutine interaction_set_mask (int, mask)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
  if (size (int%mask) /= size (mask)) &
    call msg_fatal ("Attempting to set mask with unfitting size!")
  int%mask = mask
  int%update_state_matrix = .true.
end subroutine interaction_set_mask

```

Merge a particular mask entry, respecting a possible helicity lock for this entry. We apply an OR relation, which means that quantum numbers are summed over if either of the two masks requires it.

(Interactions: procedures)+≡

```

subroutine interaction_merge_mask_entry (int, i, mask)
  type(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(quantum_numbers_mask_t), intent(in) :: mask
  type(quantum_numbers_mask_t) :: mask_tmp
  integer :: ii
  ii = idx (int, i)
  if (int%mask(ii) .neqv. mask) then
    int%mask(ii) = int%mask(ii) .or. mask
    if (int%hel_lock(ii) /= 0) then
      call mask_tmp%assign (mask, helicity=.true.)
      int%mask(int%hel_lock(ii)) = int%mask(int%hel_lock(ii)) .or. mask_tmp
    end if
  end if
  int%update_state_matrix = .true.
end subroutine interaction_merge_mask_entry

```

Fill the momenta array, do not care about the quantum numbers of particles.

(Interactions: interaction: TBP)+≡

```

procedure :: reset_momenta => interaction_reset_momenta
procedure :: set_momenta => interaction_set_momenta
procedure :: set_momentum => interaction_set_momentum

```

(Interactions: sub interfaces)+≡

```

module subroutine interaction_reset_momenta (int)
  class(interaction_t), intent(inout) :: int
end subroutine interaction_reset_momenta
module subroutine interaction_set_momenta (int, p, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), dimension(:), intent(in) :: p
  logical, intent(in), optional :: outgoing
end subroutine interaction_set_momenta
module subroutine interaction_set_momentum (int, p, i, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), intent(in) :: p
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
end subroutine interaction_set_momentum

```

<Interactions: procedures>+≡

```

module subroutine interaction_reset_momenta (int)
  class(interaction_t), intent(inout) :: int
  int%p = vector4_null
  int%p_is_known = .true.
end subroutine interaction_reset_momenta

module subroutine interaction_set_momenta (int, p, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), dimension(:), intent(in) :: p
  logical, intent(in), optional :: outgoing
  integer :: i, index
  do i = 1, size (p)
    index = idx (int, i, outgoing)
    int%p(index) = p(i)
    int%p_is_known(index) = .true.
  end do
end subroutine interaction_set_momenta

module subroutine interaction_set_momentum (int, p, i, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), intent(in) :: p
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
  integer :: index
  index = idx (int, i, outgoing)
  int%p(index) = p
  int%p_is_known(index) = .true.
end subroutine interaction_set_momentum

```

This more sophisticated version of setting values is used for structure functions, in particular if nontrivial flavor, color, and helicity may be present: set values selectively for the given flavors. If there is more than one flavor, scan the interaction and check for a matching flavor at the specified particle location. If it matches, insert the value that corresponds to this flavor.

<Interactions: interaction: TBP>+≡

```

procedure :: set_flavored_values => interaction_set_flavored_values

```

<Interactions: sub interfaces>+≡

```

module subroutine interaction_set_flavored_values (int, value, flv_in, pos)
  class(interaction_t), intent(inout) :: int
  complex(default), dimension(:), intent(in) :: value
  type(flavor_t), dimension(:), intent(in) :: flv_in
  integer, intent(in) :: pos
end subroutine interaction_set_flavored_values

```

<Interactions: procedures>+≡

```

module subroutine interaction_set_flavored_values (int, value, flv_in, pos)
  class(interaction_t), intent(inout) :: int
  complex(default), dimension(:), intent(in) :: value
  type(flavor_t), dimension(:), intent(in) :: flv_in
  integer, intent(in) :: pos
  type(state_iterator_t) :: it
  type(flavor_t) :: flv

```

```

integer :: i
if (size (value) == 1) then
  call int%set_matrix_element (value(1))
else
  call it%init (int%state_matrix)
  do while (it%is_valid ())
    flv = it%get_flavor (pos)
    SCAN_FLV: do i = 1, size (value)
      if (flv == flv_in(i)) then
        call it%set_matrix_element (value(i))
        exit SCAN_FLV
      end if
    end do SCAN_FLV
    call it%advance ()
  end do
end if
end subroutine interaction_set_flavored_values

```

12.2.7 Handling Linked interactions

Store relations between corresponding particles within one interaction. The first particle is the parent, the second one the child. Links are established in both directions.

These relations have no effect on the propagation of momenta etc., they are rather used for mother-daughter relations in event output.

```

<Interactions: interaction: TBP>+≡
  procedure :: relate => interaction_relate

<Interactions: sub interfaces>+≡
  module subroutine interaction_relate (int, i1, i2)
    class(interaction_t), intent(inout), target :: int
    integer, intent(in) :: i1, i2
  end subroutine interaction_relate

<Interactions: procedures>+≡
  module subroutine interaction_relate (int, i1, i2)
    class(interaction_t), intent(inout), target :: int
    integer, intent(in) :: i1, i2
    if (i1 /= 0 .and. i2 /= 0) then
      call int%children(i1)%append (i2)
      call int%parents(i2)%append (i1)
    end if
  end subroutine interaction_relate

```

Transfer internal parent-child relations defined within interaction `int1` to a new interaction `int` where the particle indices are mapped to. Some particles in `int1` may have no image in `int`. In that case, a child entry maps to zero, and we skip this relation.

Also transfer resonance flags.

```

<Interactions: interaction: TBP>+≡
  procedure :: transfer_relations => interaction_transfer_relations

```

```

<Interactions: sub interfaces>+≡
  module subroutine interaction_transfer_relations (int1, int2, map)
    class(interaction_t), intent(in) :: int1
    class(interaction_t), intent(inout), target :: int2
    integer, dimension(:), intent(in) :: map
  end subroutine interaction_transfer_relations

<Interactions: procedures>+≡
  module subroutine interaction_transfer_relations (int1, int2, map)
    class(interaction_t), intent(in) :: int1
    class(interaction_t), intent(inout), target :: int2
    integer, dimension(:), intent(in) :: map
    integer :: i, j, k
    do i = 1, size (map)
      do j = 1, int1%parents(i)%get_length ()
        k = int1%parents(i)%get_link (j)
        call int2%relate (map(k), map(i))
      end do
      if (map(i) /= 0) then
        int2%resonant(map(i)) = int1%resonant(i)
      end if
    end do
  end subroutine interaction_transfer_relations

```

Make up internal parent-child relations for the particle(s) that are connected to a new interaction `int`.

If `resonant` is defined and true, the connections are marked as resonant in the result interaction. Also, the children of the resonant connections are untagged if they were tagged with hard-interaction flags previously.

```

<Interactions: interaction: TBP>+≡
  procedure :: relate_connections => interaction_relate_connections

<Interactions: sub interfaces>+≡
  module subroutine interaction_relate_connections &
    (int, int_in, connection_index, &
     map, map_connections, resonant)
    class(interaction_t), intent(inout), target :: int
    class(interaction_t), intent(in) :: int_in
    integer, dimension(:), intent(in) :: connection_index
    integer, dimension(:), intent(in) :: map, map_connections
    logical, intent(in), optional :: resonant
  end subroutine interaction_relate_connections

<Interactions: procedures>+≡
  module subroutine interaction_relate_connections &
    (int, int_in, connection_index, &
     map, map_connections, resonant)
    class(interaction_t), intent(inout), target :: int
    class(interaction_t), intent(in) :: int_in
    integer, dimension(:), intent(in) :: connection_index
    integer, dimension(:), intent(in) :: map, map_connections
    logical, intent(in), optional :: resonant
    logical :: reson
    integer :: i, j, i2, k2
    reson = .false.; if (present (resonant)) reson = resonant

```

```

do i = 1, size (map_connections)
  k2 = connection_index(i)
  do j = 1, int_in%children(k2)%get_length ()
    i2 = int_in%children(k2)%get_link (j)
    call int%relate (map_connections(i), map(i2))
    if (reson) call int%retag_hard_process (map(i2), .false.)
  end do
  int%resonant(map_connections(i)) = reson
end do
end subroutine interaction_relate_connections

```

Return the number of source/target links of the internal connections of particle i.

<Interactions: interaction: TBP>+≡

```

procedure :: get_n_children => interaction_get_n_children
procedure :: get_n_parents => interaction_get_n_parents

```

<Interactions: sub interfaces>+≡

```

module function interaction_get_n_children (int, i) result (n)
  integer :: n
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i
end function interaction_get_n_children
module function interaction_get_n_parents (int, i) result (n)
  integer :: n
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i
end function interaction_get_n_parents

```

<Interactions: procedures>+≡

```

module function interaction_get_n_children (int, i) result (n)
  integer :: n
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  n = int%children(i)%get_length ()
end function interaction_get_n_children

module function interaction_get_n_parents (int, i) result (n)
  integer :: n
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  n = int%parents(i)%get_length ()
end function interaction_get_n_parents

```

Return the source/target links of the internal connections of particle i as an array.

<Interactions: interaction: TBP>+≡

```

procedure :: get_children => interaction_get_children
procedure :: get_parents => interaction_get_parents

```

<Interactions: sub interfaces>+≡

```

module function interaction_get_children (int, i) result (idx)
  integer, dimension(:), allocatable :: idx
  class(interaction_t), intent(in) :: int

```

```

        integer, intent(in) :: i
    end function interaction_get_children
    module function interaction_get_parents (int, i) result (idx)
        integer, dimension(:), allocatable :: idx
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
    end function interaction_get_parents
<Interactions: procedures>+≡
    module function interaction_get_children (int, i) result (idx)
        integer, dimension(:), allocatable :: idx
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        integer :: k, l
        l = int%children(i)%get_length ()
        allocate (idx (l))
        do k = 1, l
            idx(k) = int%children(i)%get_link (k)
        end do
    end function interaction_get_children

    module function interaction_get_parents (int, i) result (idx)
        integer, dimension(:), allocatable :: idx
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        integer :: k, l
        l = int%parents(i)%get_length ()
        allocate (idx (l))
        do k = 1, l
            idx(k) = int%parents(i)%get_link (k)
        end do
    end function interaction_get_parents

```

Add a source link from an interaction to a corresponding particle within another interaction. These links affect the propagation of particles: the two linked particles are considered as the same particle, outgoing and incoming.

```

<Interactions: interaction: TBP>+≡
    procedure :: set_source_link => interaction_set_source_link
<Interactions: sub interfaces>+≡
    module subroutine interaction_set_source_link (int, i, int1, i1)
        class(interaction_t), intent(inout) :: int
        integer, intent(in) :: i
        class(interaction_t), intent(in), target :: int1
        integer, intent(in) :: i1
    end subroutine interaction_set_source_link
<Interactions: procedures>+≡
    module subroutine interaction_set_source_link (int, i, int1, i1)
        class(interaction_t), intent(inout) :: int
        integer, intent(in) :: i
        class(interaction_t), intent(in), target :: int1
        integer, intent(in) :: i1
        if (i /= 0) call external_link_set (int%source(i), int1, i1)
    end subroutine interaction_set_source_link

```

Reassign links to a new interaction (which is an image of the current interaction).

```

<Interactions: public>+≡
    public :: interaction_reassign_links

<Interactions: sub interfaces>+≡
    module subroutine interaction_reassign_links (int, int_src, int_target)
        type(interaction_t), intent(inout) :: int
        type(interaction_t), intent(in) :: int_src
        type(interaction_t), intent(in), target :: int_target
    end subroutine interaction_reassign_links

<Interactions: procedures>+≡
    module subroutine interaction_reassign_links (int, int_src, int_target)
        type(interaction_t), intent(inout) :: int
        type(interaction_t), intent(in) :: int_src
        type(interaction_t), intent(in), target :: int_target
        integer :: i
        if (allocated (int%source)) then
            do i = 1, size (int%source)
                call external_link_reassign (int%source(i), int_src, int_target)
            end do
        end if
    end subroutine interaction_reassign_links

```

Since links are one-directional, if we want to follow them backwards we have to scan all possibilities. This procedure returns the index of the particle within `int` which points to the particle `i1` within interaction `int1`. If unsuccessful, return zero.

```

<Interactions: public>+≡
    public :: interaction_find_link

<Interactions: sub interfaces>+≡
    module function interaction_find_link (int, int1, i1) result (i)
        integer :: i
        type(interaction_t), intent(in) :: int, int1
        integer, intent(in) :: i1
    end function interaction_find_link

<Interactions: procedures>+≡
    module function interaction_find_link (int, int1, i1) result (i)
        integer :: i
        type(interaction_t), intent(in) :: int, int1
        integer, intent(in) :: i1
        type(interaction_t), pointer :: int_tmp
        do i = 1, int%n_tot
            int_tmp => external_link_get_ptr (int%source(i))
            if (int_tmp%tag == int1%tag) then
                if (external_link_get_index (int%source(i)) == i1) return
            end if
        end do
        i = 0
    end function interaction_find_link

```


The inverse: return interaction pointer and index for the ultimate source of *i* within *int*.

```

<Interactions: interaction: TBP>+≡
    procedure :: find_source => interaction_find_source

<Interactions: sub interfaces>+≡
    module subroutine interaction_find_source (int, i, int1, i1)
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        type(interaction_t), intent(out), pointer :: int1
        integer, intent(out) :: i1
    end subroutine interaction_find_source

<Interactions: procedures>+≡
    module subroutine interaction_find_source (int, i, int1, i1)
        class(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        type(interaction_t), intent(out), pointer :: int1
        integer, intent(out) :: i1
        type(external_link_t) :: link
        link = interaction_get_ultimate_source (int, i)
        int1 => external_link_get_ptr (link)
        i1 = external_link_get_index (link)
    end subroutine interaction_find_source

```

Follow source links recursively to return the ultimate source of a particle.

```

<Interactions: sub interfaces>+≡
    module function interaction_get_ultimate_source (int, i) result (link)
        type(external_link_t) :: link
        type(interaction_t), intent(in) :: int
        integer, intent(in) :: i
    end function interaction_get_ultimate_source

<Interactions: procedures>+≡
    module function interaction_get_ultimate_source (int, i) result (link)
        type(external_link_t) :: link
        type(interaction_t), intent(in) :: int
        integer, intent(in) :: i
        type(interaction_t), pointer :: int_src
        integer :: i_src
        link = int%source(i)
        if (external_link_is_set (link)) then
            do
                int_src => external_link_get_ptr (link)
                i_src = external_link_get_index (link)
                if (external_link_is_set (int_src%source(i_src))) then
                    link = int_src%source(i_src)
                else
                    exit
                end if
            end do
        end if
    end function interaction_get_ultimate_source

```

Update mask entries by merging them with corresponding masks in interactions linked to the current one. The mask determines quantum numbers which are summed over.

Note that both the mask of the current interaction and the mask of the linked interaction are updated (side effect!). This ensures that both agree for the linked particle.

```

<Interactions: interaction: TBP>+≡
  procedure :: exchange_mask => interaction_exchange_mask

<Interactions: sub interfaces>+≡
  module subroutine interaction_exchange_mask (int)
    class(interaction_t), intent(inout) :: int
    end subroutine interaction_exchange_mask

<Interactions: procedures>+≡
  module subroutine interaction_exchange_mask (int)
    class(interaction_t), intent(inout) :: int
    integer :: i, index_link
    type(interaction_t), pointer :: int_link
    do i = 1, int%n_tot
      if (external_link_is_set (int%source(i))) then
        int_link => external_link_get_ptr (int%source(i))
        index_link = external_link_get_index (int%source(i))
        call interaction_merge_mask_entry &
          (int, i, int_link%mask(index_link))
        call interaction_merge_mask_entry &
          (int_link, index_link, int%mask(i))
      end if
    end do
    call int%freeze ()
  end subroutine interaction_exchange_mask

```

Copy momenta from interactions linked to the current one.

```

<Interactions: interaction: TBP>+≡
  procedure :: receive_momenta => interaction_receive_momenta

<Interactions: sub interfaces>+≡
  module subroutine interaction_receive_momenta (int)
    class(interaction_t), intent(inout) :: int
    end subroutine interaction_receive_momenta

<Interactions: procedures>+≡
  module subroutine interaction_receive_momenta (int)
    class(interaction_t), intent(inout) :: int
    integer :: i, index_link
    type(interaction_t), pointer :: int_link
    do i = 1, int%n_tot
      if (external_link_is_set (int%source(i))) then
        int_link => external_link_get_ptr (int%source(i))
        index_link = external_link_get_index (int%source(i))
        call int%set_momentum (int_link%p(index_link), i)
      end if
    end do
  end subroutine interaction_receive_momenta

```

The inverse operation: Copy momenta back to the interactions linked to the current one.

```

<Interactions: interaction: TBP>+≡
    procedure :: send_momenta => interaction_send_momenta

<Interactions: sub interfaces>+≡
    module subroutine interaction_send_momenta (int)
        class(interaction_t), intent(in) :: int
    end subroutine interaction_send_momenta

<Interactions: procedures>+≡
    module subroutine interaction_send_momenta (int)
        class(interaction_t), intent(in) :: int
        integer :: i, index_link
        type(interaction_t), pointer :: int_link
        do i = 1, int%n_tot
            if (external_link_is_set (int%source(i))) then
                int_link => external_link_get_ptr (int%source(i))
                index_link = external_link_get_index (int%source(i))
                call int_link%set_momentum (int%p(i), index_link)
            end if
        end do
    end subroutine interaction_send_momenta

```

For numerical comparisons: pacify all momenta in an interaction.

```

<Interactions: interaction: TBP>+≡
    procedure :: pacify_momenta => interaction_pacify_momenta

<Interactions: sub interfaces>+≡
    module subroutine interaction_pacify_momenta (int, acc)
        class(interaction_t), intent(inout) :: int
        real(default), intent(in) :: acc
    end subroutine interaction_pacify_momenta

<Interactions: procedures>+≡
    module subroutine interaction_pacify_momenta (int, acc)
        class(interaction_t), intent(inout) :: int
        real(default), intent(in) :: acc
        integer :: i
        do i = 1, int%n_tot
            call pacify (int%p(i), acc)
        end do
    end subroutine interaction_pacify_momenta

```

For each subtraction entry starting from SUB = 0, we duplicate the original state matrix entries as is.

```

<Interactions: interaction: TBP>+≡
    procedure :: declare_subtraction => interaction_declare_subtraction

<Interactions: sub interfaces>+≡
    module subroutine interaction_declare_subtraction (int, n_sub)
        class(interaction_t), intent(inout), target :: int
        integer, intent(in) :: n_sub
    end subroutine interaction_declare_subtraction

```

<Interactions: procedures>+≡

```

module subroutine interaction_declare_subtraction (int, n_sub)
  class(interaction_t), intent(inout), target :: int
  integer, intent(in) :: n_sub
  integer :: i_sub
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  type(state_matrix_t) :: state_matrix
  call state_matrix%init (store_values = .true.)
  allocate (qn (int%get_state_depth ()))
  do i_sub = 0, n_sub
    call it%init (int%state_matrix)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      call qn%set_subtraction_index (i_sub)
      call state_matrix%add_state (qn, value = it%get_matrix_element ())
      call it%advance ()
    end do
  end do
  call state_matrix%freeze ()
  call state_matrix%set_n_sub ()
  call int%state_matrix%final ()
  int%state_matrix = state_matrix
end subroutine interaction_declare_subtraction

```

12.2.8 Recovering connections

When creating an evaluator for two interactions, we have to know by which particles they are connected. The connection indices can be determined if we have two linked interactions. We assume that `int1` is the source and `int2` the target, so the connections of interest are stored within `int2`. A connection is found if either the source is `int1`, or the (ultimate) source of a particle within `int2` coincides with the (ultimate) source of a particle within `int1`. The result is an array of index pairs.

To make things simple, we scan the interaction twice, once for counting hits, then allocate the array, then scan again and store the connections.

The connections are scanned for `int2`, which has sources in `int1`. It may happen that the order of connections is interchanged (crossed). We require the indices in `int1` to be sorted, so we reorder both index arrays correspondingly before returning them. (After this, the indices in `int2` may be out of order.)

<Interactions: public>+≡

```

public :: find_connections

```

<Interactions: sub interfaces>+≡

```

module subroutine find_connections (int1, int2, n, connection_index)
  class(interaction_t), intent(in) :: int1, int2
  integer, intent(out) :: n
  integer, dimension(:,:), intent(out), allocatable :: connection_index
  integer, dimension(:,:), allocatable :: conn_index_tmp
  integer, dimension(:), allocatable :: ordering
end subroutine find_connections

```

(Interactions: procedures)+≡

```

module subroutine find_connections (int1, int2, n, connection_index)
  class(interaction_t), intent(in) :: int1, int2
  integer, intent(out) :: n
  integer, dimension(:,:), intent(out), allocatable :: connection_index
  integer, dimension(:,:), allocatable :: conn_index_tmp
  integer, dimension(:), allocatable :: ordering
  integer :: i, j, k
  type(external_link_t) :: link1, link2
  type(interaction_t), pointer :: int_link1, int_link2
  n = 0
  do i = 1, size (int2%source)
    link2 = interaction_get_ultimate_source (int2, i)
    if (external_link_is_set (link2)) then
      int_link2 => external_link_get_ptr (link2)
      if (int_link2%tag == int1%tag) then
        n = n + 1
      else
        k = external_link_get_index (link2)
        do j = 1, size (int1%source)
          link1 = interaction_get_ultimate_source (int1, j)
          if (external_link_is_set (link1)) then
            int_link1 => external_link_get_ptr (link1)
            if (int_link1%tag == int_link2%tag) then
              if (external_link_get_index (link1) == k) &
                n = n + 1
            end if
          end if
        end do
      end if
    end if
  end do
  allocate (conn_index_tmp (n, 2))
  n = 0
  do i = 1, size (int2%source)
    link2 = interaction_get_ultimate_source (int2, i)
    if (external_link_is_set (link2)) then
      int_link2 => external_link_get_ptr (link2)
      if (int_link2%tag == int1%tag) then
        n = n + 1
        conn_index_tmp(n,1) = external_link_get_index (int2%source(i))
        conn_index_tmp(n,2) = i
      else
        k = external_link_get_index (link2)
        do j = 1, size (int1%source)
          link1 = interaction_get_ultimate_source (int1, j)
          if (external_link_is_set (link1)) then
            int_link1 => external_link_get_ptr (link1)
            if (int_link1%tag == int_link2%tag) then
              if (external_link_get_index (link1) == k) then
                n = n + 1
                conn_index_tmp(n,1) = j
                conn_index_tmp(n,2) = i
              end if
            end if
          end if
        end do
      end if
    end if
  end do
end subroutine

```

```

                end if
            end if
        end do
    end if
end do
allocate (connection_index (n, 2))
if (n > 1) then
    allocate (ordering (n))
    ordering = order (conn_index_tmp(:,1))
    connection_index = conn_index_tmp(ordering,:)
else
    connection_index = conn_index_tmp
end if
end subroutine find_connections

```

12.2.9 Unit tests

Test module, followed by the corresponding implementation module.

```

<interactions_ut.f90>≡
  <File header>

  module interactions_ut
    use unit_tests
    use interactions_uti

    <Standard module head>

    <Interactions: public test>

    contains

    <Interactions: test driver>

  end module interactions_ut
<interactions_uti.f90>≡
  <File header>

  module interactions_uti

    <Use kinds>
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices

    use interactions

    <Standard module head>

```

<Interactions: test declarations>

contains

<Interactions: tests>

end module interactions_uti

API: driver for the unit tests below.

<Interactions: public test>≡

public :: interaction_test

<Interactions: test driver>≡

subroutine interaction_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Interactions: execute tests>

end subroutine interaction_test

Generate an interaction of a polarized virtual photon and a colored quark which may be either up or down. Remove the quark polarization. Generate another interaction for the quark radiating a photon and link this to the first interaction. The radiation ignores polarization; transfer this information to the first interaction to simplify it. Then, transfer the momentum to the radiating quark and perform a splitting.

<Interactions: execute tests>≡

call test (interaction_1, "interaction_1", &
"check interaction setup", &
u, results)

<Interactions: test declarations>≡

public :: interaction_1

<Interactions: tests>≡

subroutine interaction_1 (u)

integer, intent(in) :: u

type(interaction_t), target :: int, rad

type(vector4_t), dimension(3) :: p

type(quantum_numbers_mask_t), dimension(3) :: mask

p(2) = vector4_moving (500._default, 500._default, 1)

p(3) = vector4_moving (500._default,-500._default, 1)

p(1) = p(2) + p(3)

write (u, "(A)") " * Test output: interaction"

write (u, "(A)") " * Purpose: check routines for interactions"

write (u, "(A)")

call int%basic_init (1, 0, 2, set_relations=.true., &
store_values = .true.)

call int_set (int, 1, -1, 1, 1, &

cmplx (0.3_default, 0.1_default, kind=default))

call int_set (int, 1, -1,-1, 1, &

cmplx (0.5_default,-0.7_default, kind=default))

call int_set (int, 1, 1, 1, 1, &

cmplx (0.1_default, 0._default, kind=default))

```

call int_set (int, -1, 1, -1, 2, &
             cmplx (0.4_default, -0.1_default, kind=default))
call int_set (int, 1, 1, 1, 2, &
             cmplx (0.2_default, 0._default, kind=default))
call int%freeze ()
call int%set_momenta (p)
mask = quantum_numbers_mask (.false.,.false., [.true.,.true.,.true.])
call rad%basic_init (1, 0, 2, &
                    mask=mask, set_relations=.true., store_values = .true.)
call rad_set (1)
call rad_set (2)
call rad%set_source_link (1, int, 2)
call rad%exchange_mask ()
call rad%receive_momenta ()
p(1) = rad%get_momentum (1)
p(2) = 0.4_default * p(1)
p(3) = p(1) - p(2)
call rad%set_momenta (p(2:3), outgoing=.true.)
call int%freeze ()
call rad%freeze ()
call rad%set_matrix_element &
    (cmplx (0._default, 0._default, kind=default))
call int%basic_write (u)
write (u, "(A)")
call rad%basic_write (u)
write (u, "(A)")
write (u, "(A)")  "* Cleanup"
call int%final ()
call rad%final ()
write (u, "(A)")
write (u, "(A)")  "* Test interaction_1: successful."
contains
subroutine int_set (int, h1, h2, hq, q, val)
    type(interaction_t), target, intent(inout) :: int
    integer, intent(in) :: h1, h2, hq, q
    type(flavor_t), dimension(3) :: flv
    type(color_t), dimension(3) :: col
    type(helicity_t), dimension(3) :: hel
    type(quantum_numbers_t), dimension(3) :: qn
    complex(default), intent(in) :: val
    call flv%init ([21, q, -q])
    call col(2)%init_col_acl (5, 0)
    call col(3)%init_col_acl (0, 5)
    call hel%init ([h1, hq, -hq], [h2, hq, -hq])
    call qn%init (flv, col, hel)
    call int%add_state (qn)
    call int%set_matrix_element (val)
end subroutine int_set
subroutine rad_set (q)
    integer, intent(in) :: q
    type(flavor_t), dimension(3) :: flv
    type(quantum_numbers_t), dimension(3) :: qn
    call flv%init ([ q, q, 21 ])
    call qn%init (flv)

```



```

        call rad%add_state (qn)
    end subroutine rad_set
end subroutine interaction_1

```

12.3 Matrix element evaluation

The `evaluator_t` type is an extension of the `interaction_t` type. It represents either a density matrix as the square of a transition matrix element, or the product of two density matrices. Usually, some quantum numbers are summed over in the result.

The `interaction_t` subobject represents a multi-particle interaction with incoming, virtual, and outgoing particles and the associated (not necessarily diagonal) density matrix of quantum state. When the evaluator is initialized, this interaction is constructed from the input `interaction(s)`.

In addition, the initialization process sets up a multiplication table. For each matrix element of the result, it states which matrix elements are to be taken from the input `interaction(s)`, multiplied (optionally, with an additional weight factor) and summed over.

Eventually, to a processes we associate a chain of evaluators which are to be evaluated sequentially. The physical event and its matrix element value(s) can be extracted from the last evaluator in such a chain.

Evaluators are constructed only once (as long as this is possible) during an initialization step. Then, for each event, momenta are computed and transferred among evaluators using the links within the interaction subobject. The multiplication tables enable fast evaluation of the result without looking at quantum numbers anymore.

```

<evaluators.f90>≡
  <File header>

  module evaluators

    <Use kinds>
    <Use strings>
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices
    use interactions

    <Standard module head>

    <Evaluators: public>

    <Evaluators: parameters>

    <Evaluators: types>

    <Evaluators: interfaces>

```

```

        interface
        <Evaluators: sub interfaces>
        end interface

    end module evaluators

<evaluators_sub.f90>≡
    <File header>

    submodule (evaluators) evaluators_s

        use io_units
        use format_defs, only: FMT_19
        use physics_defs, only: n_beams_rescaled
        use diagnostics
        use lorentz

        implicit none

    contains

    <Evaluators: procedures>

    end submodule evaluators_s

```

12.3.1 Array of pairings

The evaluator contains an array of `pairing_array` objects. This makes up the multiplication table.

Each pairing array contains two lists of matrix element indices and a list of numerical factors. The matrix element indices correspond to the input interactions. The corresponding matrix elements are to be multiplied and optionally multiplied by a factor. The results are summed over to yield one specific matrix element of the result evaluator.

```

<Evaluators: types>≡
    type :: pairing_array_t
        integer, dimension(:), allocatable :: i1, i2
        complex(default), dimension(:), allocatable :: factor
    end type pairing_array_t

<Evaluators: sub interfaces>≡
    elemental module subroutine pairing_array_init (pa, n, has_i2, has_factor)
        type(pairing_array_t), intent(out) :: pa
        integer, intent(in) :: n
        logical, intent(in) :: has_i2, has_factor
    end subroutine pairing_array_init

<Evaluators: procedures>≡
    elemental module subroutine pairing_array_init (pa, n, has_i2, has_factor)
        type(pairing_array_t), intent(out) :: pa
        integer, intent(in) :: n
        logical, intent(in) :: has_i2, has_factor

```

```

        allocate (pa%i1 (n))
        if (has_i2) allocate (pa%i2 (n))
        if (has_factor) allocate (pa%factor (n))
    end subroutine pairing_array_init

    <Evaluators: public>≡
        public :: pairing_array_write

    <Evaluators: sub interfaces>+≡
        module subroutine pairing_array_write (pa, unit)
            type(pairing_array_t), intent(in) :: pa
            integer, intent(in), optional :: unit
        end subroutine pairing_array_write

    <Evaluators: procedures>+≡
        module subroutine pairing_array_write (pa, unit)
            type(pairing_array_t), intent(in) :: pa
            integer, intent(in), optional :: unit
            integer :: i, u
            u = given_output_unit (unit); if (u < 0) return
            write (u, "(A)", advance = "no") "["
            if (allocated (pa%i1)) then
                write (u, "(I0,A)", advance = "no") pa%i1, ","
            else
                write (u, "(A)", advance = "no") "x,"
            end if
            if (allocated (pa%i2)) then
                write (u, "(I0,A)", advance = "no") pa%i1, ","
            else
                write (u, "(A)", advance = "no") "x,"
            end if
            write (u, "(A)", advance = "no") "]"
            if (allocated (pa%factor)) then
                write (u, "(A,F5.4,A,F5.4,A)") ";(", &
                    real(pa%factor), ",", aimag(pa%factor), ")]"
            else
                write (u, "(A)") ""
            end if
        end subroutine pairing_array_write

```

12.3.2 The evaluator type

Possible variants of evaluators:

```

    <Evaluators: parameters>≡
        integer, parameter :: &
            EVAL_UNDEFINED = 0, &
            EVAL_PRODUCT = 1, &
            EVAL_SQUARED_FLOWS = 2, &
            EVAL_SQUARE_WITH_COLOR_FACTORS = 3, &
            EVAL_COLOR_CONTRACTION = 4, &
            EVAL_IDENTITY = 5, &
            EVAL_QN_SUM = 6

```

The evaluator type contains the result interaction and an array of pairing lists, one for each matrix element in the result interaction.

```

(Evaluators: public)+≡
    public :: evaluator_t

(Evaluators: types)+≡
    type, extends (interaction_t) :: evaluator_t
        private
            integer :: type = EVAL_UNDEFINED
            class(interaction_t), pointer :: int_in1 => null ()
            class(interaction_t), pointer :: int_in2 => null ()
            type(pairing_array_t), dimension(:), allocatable :: pairing_array
        contains
            (Evaluators: evaluator: TBP)
    end type evaluator_t

```

Output.

```

(Evaluators: evaluator: TBP)≡
    procedure :: write => evaluator_write

(Evaluators: sub interfaces)+≡
    module subroutine evaluator_write (eval, unit, &
        verbose, show_momentum_sum, show_mass, show_state, show_table, &
        col_verbose, testflag)
        class(evaluator_t), intent(in) :: eval
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, show_table, col_verbose
        logical, intent(in), optional :: testflag
    end subroutine evaluator_write

(Evaluators: procedures)+≡
    module subroutine evaluator_write (eval, unit, &
        verbose, show_momentum_sum, show_mass, show_state, show_table, &
        col_verbose, testflag)
        class(evaluator_t), intent(in) :: eval
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, show_table, col_verbose
        logical, intent(in), optional :: testflag
        logical :: conjugate, square, show_tab
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        show_tab = .true.; if (present (show_table)) show_tab = .false.
        call eval%basic_write &
            (unit, verbose, show_momentum_sum, show_mass, &
            show_state, col_verbose, testflag)
        if (show_tab) then
            write (u, "(1x,A)") "Matrix-element multiplication"
            write (u, "(2x,A)", advance="no") "Input interaction 1:"
            if (associated (eval%int_in1)) then
                write (u, "(1x,I0)") eval%int_in1%get_tag ()
            else
                write (u, "(A)") " [undefined]"
            end if
        end if
    end subroutine evaluator_write

```

```

write (u, "(2x,A)", advance="no") "Input interaction 2:"
if (associated (eval%int_in2)) then
  write (u, "(1x,I0)") eval%int_in2%get_tag ()
else
  write (u, "(A)") " [undefined]"
end if
select case (eval%type)
case (EVAL_SQUARED_FLOWS, EVAL_SQUARE_WITH_COLOR_FACTORS)
  conjugate = .true.
  square = .true.
case (EVAL_IDENTITY)
  write (u, "(1X,A)") "Identity evaluator, pairing array unused"
  return
case default
  conjugate = .false.
  square = .false.
end select
call eval%write_pairing_array (conjugate, square, u)
end if
end subroutine evaluator_write

```

(Evaluators: evaluator: TBP)+≡

```

procedure :: write_pairing_array => evaluator_write_pairing_array

```

(Evaluators: sub interfaces)+≡

```

module subroutine evaluator_write_pairing_array (eval, conjugate, square, unit)
  class(evaluator_t), intent(in) :: eval
  logical, intent(in) :: conjugate, square
  integer, intent(in), optional :: unit
end subroutine evaluator_write_pairing_array

```

(Evaluators: procedures)+≡

```

module subroutine evaluator_write_pairing_array (eval, conjugate, square, unit)
  class(evaluator_t), intent(in) :: eval
  logical, intent(in) :: conjugate, square
  integer, intent(in), optional :: unit
  integer :: u, i, j
  u = given_output_unit (unit); if (u < 0) return
  if (allocated (eval%pairing_array)) then
    do i = 1, size (eval%pairing_array)
      write (u, "(2x,A,I0,A)") "ME(", i, ") = "
      do j = 1, size (eval%pairing_array(i)%i1)
        write (u, "(4x,A)", advance="no") "+"
        if (allocated (eval%pairing_array(i)%i2)) then
          write (u, "(1x,A,I0,A)", advance="no") &
            "ME1(", eval%pairing_array(i)%i1(j), ")"
          if (conjugate) then
            write (u, "(A)", advance="no") "* x"
          else
            write (u, "(A)", advance="no") " x"
          end if
          write (u, "(1x,A,I0,A)", advance="no") &
            "ME2(", eval%pairing_array(i)%i2(j), ")"
        else if (square) then
          write (u, "(1x,A)", advance="no") "|"
        end if
      end do
    end do
  end if

```

```

        write (u, "(A,I0,A)", advance="no") &
            "ME1(", eval%pairing_array(i)%i1(j), ")"
        write (u, "(A)", advance="no") " |^2"
    else
        write (u, "(1x,A,I0,A)", advance="no") &
            "ME1(", eval%pairing_array(i)%i1(j), ")"
    end if
    if (allocated (eval%pairing_array(i)%factor)) then
        write (u, "(1x,A)", advance="no") "x"
        write (u, "(1x,'('," // FMT_19 // ",','," // FMT_19 // &
            ",')')") eval%pairing_array(i)%factor(j)
    else
        write (u, *)
    end if
end do
end do
end if
end subroutine evaluator_write_pairing_array

```

Assignment: Deep copy of the interaction component.

```

<Evaluators: public>+≡
    public :: assignment(=)

<Evaluators: interfaces>≡
    interface assignment(=)
        module procedure evaluator_assign
    end interface

<Evaluators: sub interfaces>+≡
    module subroutine evaluator_assign (eval_out, eval_in)
        type(evaluator_t), intent(out) :: eval_out
        type(evaluator_t), intent(in) :: eval_in
    end subroutine evaluator_assign

<Evaluators: procedures>+≡
    module subroutine evaluator_assign (eval_out, eval_in)
        type(evaluator_t), intent(out) :: eval_out
        type(evaluator_t), intent(in) :: eval_in
        eval_out%type = eval_in%type
        eval_out%int_in1 => eval_in%int_in1
        eval_out%int_in2 => eval_in%int_in2
        eval_out%interaction_t = eval_in%interaction_t
        if (allocated (eval_in%pairing_array)) then
            allocate (eval_out%pairing_array (size (eval_in%pairing_array)))
            eval_out%pairing_array = eval_in%pairing_array
        end if
    end subroutine evaluator_assign

```

12.3.3 Auxiliary structures for evaluator creation

Creating an evaluator that properly handles all quantum numbers requires some bookkeeping. In this section, we define several auxiliary types and methods that

organize and simplify this task. More structures are defined within the specific initializers (as local types and internal subroutines).

These types are currently implemented in a partial object-oriented way: We define some basic methods for initialization etc. here, but the evaluator routines below do access their internals as well. This simplifies some things such as index addressing using array slices, at the expense of losing some clarity.

Index mapping

Index mapping are abundant when constructing an evaluator. To have arrays of index mappings, we define this:

```

(Evaluators: types)+≡
    type :: index_map_t
        integer, dimension(:), allocatable :: entry
    end type index_map_t

(Evaluators: sub interfaces)+≡
    elemental module subroutine index_map_init (map, n)
        type(index_map_t), intent(out) :: map
        integer, intent(in) :: n
    end subroutine index_map_init

(Evaluators: procedures)+≡
    elemental module subroutine index_map_init (map, n)
        type(index_map_t), intent(out) :: map
        integer, intent(in) :: n
        allocate (map%entry (n))
        map%entry = 0
    end subroutine index_map_init

(Evaluators: procedures)+≡
    function index_map_exists (map) result (flag)
        logical :: flag
        type(index_map_t), intent(in) :: map
        flag = allocated (map%entry)
    end function index_map_exists

(Evaluators: interfaces)+≡
    interface size
        module procedure index_map_size
    end interface

(Evaluators: sub interfaces)+≡
    module function index_map_size (map) result (s)
        integer :: s
        type(index_map_t), intent(in) :: map
    end function index_map_size

(Evaluators: procedures)+≡
    module function index_map_size (map) result (s)
        integer :: s
        type(index_map_t), intent(in) :: map
        if (allocated (map%entry)) then

```

```

        s = size (map%entry)
    else
        s = 0
    end if
end function index_map_size

```

<Evaluators: interfaces>+≡

```

interface assignment(=)
    module procedure index_map_assign_int
    module procedure index_map_assign_array
end interface

```

<Evaluators: sub interfaces>+≡

```

    elemental module subroutine index_map_assign_int (map, ival)
        type(index_map_t), intent(inout) :: map
        integer, intent(in) :: ival
    end subroutine index_map_assign_int
    module subroutine index_map_assign_array (map, array)
        type(index_map_t), intent(inout) :: map
        integer, dimension(:), intent(in) :: array
    end subroutine index_map_assign_array

```

<Evaluators: procedures>+≡

```

    elemental module subroutine index_map_assign_int (map, ival)
        type(index_map_t), intent(inout) :: map
        integer, intent(in) :: ival
        map%entry = ival
    end subroutine index_map_assign_int

    module subroutine index_map_assign_array (map, array)
        type(index_map_t), intent(inout) :: map
        integer, dimension(:), intent(in) :: array
        map%entry = array
    end subroutine index_map_assign_array

```

<Evaluators: sub interfaces>+≡

```

    elemental module subroutine index_map_set_entry (map, i, ival)
        type(index_map_t), intent(inout) :: map
        integer, intent(in) :: i
        integer, intent(in) :: ival
    end subroutine index_map_set_entry

```

<Evaluators: procedures>+≡

```

    elemental module subroutine index_map_set_entry (map, i, ival)
        type(index_map_t), intent(inout) :: map
        integer, intent(in) :: i
        integer, intent(in) :: ival
        map%entry(i) = ival
    end subroutine index_map_set_entry

```

<Evaluators: sub interfaces>+≡

```

    elemental module function index_map_get_entry (map, i) result (ival)
        integer :: ival
        type(index_map_t), intent(in) :: map

```



```

        integer, intent(in) :: i
    end function index_map_get_entry
<Evaluators: procedures>+=
    elemental module function index_map_get_entry (map, i) result (ival)
        integer :: ival
        type(index_map_t), intent(in) :: map
        integer, intent(in) :: i
        ival = map%entry(i)
    end function index_map_get_entry

```

Index mapping (two-dimensional)

This is a variant with a square matrix instead of an array.

```

<Evaluators: types>+=
    type :: index_map2_t
        integer :: s = 0
        integer, dimension(:,:), allocatable :: entry
    end type index_map2_t

<Evaluators: procedures>+=
    elemental subroutine index_map2_init (map, n)
        type(index_map2_t), intent(out) :: map
        integer, intent(in) :: n
        map%s = n
        allocate (map%entry (n, n))
    end subroutine index_map2_init

<Evaluators: procedures>+=
    function index_map2_exists (map) result (flag)
        logical :: flag
        type(index_map2_t), intent(in) :: map
        flag = allocated (map%entry)
    end function index_map2_exists

<Evaluators: interfaces>+=
    interface size
        module procedure index_map2_size
    end interface

<Evaluators: sub interfaces>+=
    module function index_map2_size (map) result (s)
        integer :: s
        type(index_map2_t), intent(in) :: map
    end function index_map2_size

<Evaluators: procedures>+=
    module function index_map2_size (map) result (s)
        integer :: s
        type(index_map2_t), intent(in) :: map
        s = map%s
    end function index_map2_size

```

```

<Evaluators: interfaces>+≡
  interface assignment(=)
    module procedure index_map2_assign_int
  end interface

<Evaluators: sub interfaces>+≡
  elemental module subroutine index_map2_assign_int (map, ival)
    type(index_map2_t), intent(inout) :: map
    integer, intent(in) :: ival
  end subroutine index_map2_assign_int

<Evaluators: procedures>+≡
  elemental module subroutine index_map2_assign_int (map, ival)
    type(index_map2_t), intent(inout) :: map
    integer, intent(in) :: ival
    map%entry = ival
  end subroutine index_map2_assign_int

<Evaluators: procedures>+≡
  elemental subroutine index_map2_set_entry (map, i, j, ival)
    type(index_map2_t), intent(inout) :: map
    integer, intent(in) :: i, j
    integer, intent(in) :: ival
    map%entry(i,j) = ival
  end subroutine index_map2_set_entry

<Evaluators: procedures>+≡
  elemental function index_map2_get_entry (map, i, j) result (ival)
    integer :: ival
    type(index_map2_t), intent(in) :: map
    integer, intent(in) :: i, j
    ival = map%entry(i,j)
  end function index_map2_get_entry

```

Auxiliary structures: particle mask

This is a simple container of a logical array.

```

<Evaluators: types>+≡
  type :: prt_mask_t
    logical, dimension(:), allocatable :: entry
  end type prt_mask_t

<Evaluators: procedures>+≡
  subroutine prt_mask_init (mask, n)
    type(prt_mask_t), intent(out) :: mask
    integer, intent(in) :: n
    allocate (mask%entry (n))
  end subroutine prt_mask_init

```

```

<Evaluators: interfaces>+≡
  interface size
    module procedure prt_mask_size
  end interface

<Evaluators: sub interfaces>+≡
  module function prt_mask_size (mask) result (s)
    integer :: s
    type(prt_mask_t), intent(in) :: mask
  end function prt_mask_size

<Evaluators: procedures>+≡
  module function prt_mask_size (mask) result (s)
    integer :: s
    type(prt_mask_t), intent(in) :: mask
    s = size (mask%entry)
  end function prt_mask_size

```

Quantum number containers

Trivial transparent containers:

```

<Evaluators: types>+≡
  type :: qn_list_t
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  end type qn_list_t

  type :: qn_mask_array_t
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
  end type qn_mask_array_t

```

Auxiliary structures: connection entries

This type is used as intermediate storage when computing the product of two evaluators or the square of an evaluator. The quantum-number array **qn** corresponds to the particles common to both interactions, but irrelevant quantum numbers (color) masked out. The index arrays **index_in** determine the entries in the input interactions that contribute to this connection. **n_index** is the size of these arrays, and **count** is used while filling the entries. Finally, the quantum-number arrays **qn_in_list** are the actual entries in the input interaction that contribute. In the product case, they exclude the connected quantum numbers.

Each evaluator has its own **connection_table** which contains an array of **connection_entry** objects, but also has stuff that specifically applies to the evaluator type. Hence, we do not generalize the **connection_table_t** type.

The filling procedure **connection_entry_add_state** is specific to the various evaluator types.

```

<Evaluators: types>+≡
  type :: connection_entry_t
    type(quantum_numbers_t), dimension(:), allocatable :: qn_conn
    integer, dimension(:), allocatable :: n_index
    integer, dimension(:), allocatable :: count

```

```

        type(index_map_t), dimension(:), allocatable :: index_in
        type(qn_list_t), dimension(:), allocatable :: qn_in_list
    end type connection_entry_t

```

(Evaluators: procedures)+≡

```

subroutine connection_entry_init &
    (entry, n_count, n_map, qn_conn, count, n_rest)
    type(connection_entry_t), intent(out) :: entry
    integer, intent(in) :: n_count, n_map
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_conn
    integer, dimension(n_count), intent(in) :: count
    integer, dimension(n_count), intent(in) :: n_rest
    integer :: i
    allocate (entry%qn_conn (size (qn_conn)))
    allocate (entry%n_index (n_count))
    allocate (entry%count (n_count))
    allocate (entry%index_in (n_map))
    allocate (entry%qn_in_list (n_count))
    entry%qn_conn = qn_conn
    entry%n_index = count
    entry%count = 0
    if (size (entry%index_in) == size (count)) then
        call index_map_init (entry%index_in, count)
    else
        call index_map_init (entry%index_in, count(1))
    end if
    do i = 1, n_count
        allocate (entry%qn_in_list(i)%qn (n_rest(i), count(i)))
    end do
end subroutine connection_entry_init

```

(Evaluators: procedures)+≡

```

subroutine connection_entry_write (entry, unit)
    type(connection_entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    integer :: i, j
    integer :: u
    u = given_output_unit (unit)
    call quantum_numbers_write (entry%qn_conn, unit)
    write (u, *)
    do i = 1, size (entry%n_index)
        write (u, *) "Input interaction", i
        do j = 1, entry%n_index(i)
            if (size (entry%n_index) == size (entry%index_in)) then
                write (u, "(2x,I0,4x,I0,2x)", advance = "no") &
                    j, index_map_get_entry (entry%index_in(i), j)
            else
                write (u, "(2x,I0,4x,I0,2x,I0,2x)", advance = "no") &
                    j, index_map_get_entry (entry%index_in(1), j), &
                    index_map_get_entry (entry%index_in(2), j)
            end if
            call quantum_numbers_write (entry%qn_in_list(i)%qn(:,j), unit)
        end do
        write (u, *)
    end do

```

```

        end do
    end do
end subroutine connection_entry_write

```

These are the different connection tables for the three different cases of evaluators for matrix elements, squared diagonal and non-diagonal matrix elements, respectively.

(Evaluators: types)+≡

```

type :: connection_table_t
    integer :: n_conn = 0
    integer, dimension(2) :: n_rest = 0
    integer :: n_tot = 0
    integer :: n_me_conn = 0
    type(state_matrix_t) :: state
    type(index_map_t), dimension(:), allocatable :: index_conn
    type(connection_entry_t), dimension(:), allocatable :: entry
    type(index_map_t) :: index_result
end type connection_table_t

type :: connection_table_diag_t
    integer :: n_tot = 0
    integer :: n_me_conn = 0
    type(state_matrix_t) :: state
    type(index_map_t) :: index_conn
    type(connection_entry_t), dimension(:), allocatable :: entry
    type(index_map_t) :: index_result
end type connection_table_diag_t

type :: connection_table_nondiag_t
    integer :: n_tot = 0
    integer :: n_me_conn = 0
    type(state_matrix_t) :: state
    type(index_map2_t) :: index_conn
    type(connection_entry_t), dimension(:), allocatable :: entry
    type(index_map_t) :: index_result
end type connection_table_nondiag_t

```

Color handling

For managing color-factor computation, we introduce this local type. The `index` is the index in the color table that corresponds to a given matrix element index in the input interaction. The `col` array stores the color assignments in rows. The `factor` array associates a complex number with each pair of arrays in the color table. The `factor_is_known` array reveals whether a given factor is known already or still has to be computed.

(Evaluators: types)+≡

```

type :: color_table_t
    integer, dimension(:), allocatable :: index
    type(color_t), dimension(:,:), allocatable :: col
    logical, dimension(:,:), allocatable :: factor_is_known
    complex(default), dimension(:,:), allocatable :: factor

```

```
end type color_table_t
```

This is the initializer. We extract the color states from the given state matrices, establish index mappings between the two states (implemented by the array `me_index`), make an array of color states, and initialize the color-factor table. The latter is two-dimensional (includes interference) and not yet filled.

(*Evaluators: procedures*)+=≡

```
subroutine color_table_init (color_table, state, n_tot)
  type(color_table_t), intent(out) :: color_table
  type(state_matrix_t), intent(in) :: state
  integer, intent(in) :: n_tot
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  type(state_matrix_t) :: state_col
  integer :: index, n_col_state
  allocate (color_table%index (state%get_n_matrix_elements ()))
  color_table%index = 0
  allocate (qn (n_tot))
  call state_col%init ()
  call it%init (state)
  do while (it%is_valid ())
    index = it%get_me_index ()
    call qn%init (col = it%get_color ())
    call state_col%add_state (qn, me_index = color_table%index(index))
    call it%advance ()
  end do
  n_col_state = state_col%get_n_matrix_elements ()
  allocate (color_table%col (n_tot, n_col_state))
  call it%init (state_col)
  do while (it%is_valid ())
    index = it%get_me_index ()
    color_table%col(:,index) = it%get_color ()
    call it%advance ()
  end do
  call state_col%final ()
  allocate (color_table%factor_is_known (n_col_state, n_col_state))
  allocate (color_table%factor (n_col_state, n_col_state))
  color_table%factor_is_known = .false.
end subroutine color_table_init
```

Output (debugging use):

(*Evaluators: procedures*)+=≡

```
subroutine color_table_write (color_table, unit)
  type(color_table_t), intent(in) :: color_table
  integer, intent(in), optional :: unit
  integer :: i, j
  integer :: u
  u = given_output_unit (unit)
  write (u, *) "Color table:"
  if (allocated (color_table%index)) then
    write (u, *) " Index mapping state => color table:"
    do i = 1, size (color_table%index)
      write (u, "(3x,I0,2x,I0,2x)" i, color_table%index(i)
```

```

end do
write (u, *) " Color table:"
do i = 1, size (color_table%col, 2)
  write (u, "(3x,I0,2x)", advance = "no") i
  call color_write (color_table%col(:,i), unit)
  write (u, *)
end do
write (u, *) " Defined color factors:"
do i = 1, size (color_table%factor, 1)
  do j = 1, size (color_table%factor, 2)
    if (color_table%factor_is_known(i,j)) then
      write (u, *) i, j, color_table%factor(i,j)
    end if
  end do
end do
end if
end subroutine color_table_write

```

This subroutine sets color factors, based on information from the hard matrix element: the list of pairs of color-flow indices (in the basis of the matrix element code), the list of corresponding factors, and the list of mappings from the matrix element index in the input interaction to the color-flow index in the hard matrix element object.

We first determine the mapping of color-flow indices from the hard matrix element code to the current color table. The mapping could be nontrivial because the latter is derived from iterating over a state matrix, which may return states in non-canonical order. The translation table can be determined because we have, for the complete state matrix, both the mapping to the hard interaction (the input `col_index_hi`) and the mapping to the current color table (the component `color_table%index`).

Once this mapping is known, we scan the list of index pairs `color_flow_index` and translate them to valid color-table index pairs. For this pair, the color factor is set using the corresponding entry in the list `col_factor`.

(Evaluators: procedures)+≡

```

subroutine color_table_set_color_factors (color_table, &
  col_flow_index, col_factor, col_index_hi)
  type(color_table_t), intent(inout) :: color_table
  integer, dimension(:,:), intent(in) :: col_flow_index
  complex(default), dimension(:), intent(in) :: col_factor
  integer, dimension(:), intent(in) :: col_index_hi
  integer, dimension(:), allocatable :: hi_to_ct
  integer :: n_cflow
  integer :: hi_index, me_index, ct_index, cf_index
  integer, dimension(2) :: hi_index_pair, ct_index_pair
  n_cflow = size (col_index_hi)
  if (size (color_table%index) /= n_cflow) &
    call msg_bug ("Mismatch between hard matrix element and color table")
  allocate (hi_to_ct (n_cflow))
  do me_index = 1, size (color_table%index)
    ct_index = color_table%index(me_index)
    hi_index = col_index_hi(me_index)
    hi_to_ct(hi_index) = ct_index
  end do
end subroutine

```

```

end do
do cf_index = 1, size (col_flow_index, 2)
  hi_index_pair = col_flow_index(:,cf_index)
  ct_index_pair = hi_to_ct(hi_index_pair)
  color_table%factor(ct_index_pair(1), ct_index_pair(2)) = &
    col_factor(cf_index)
  color_table%factor_is_known(ct_index_pair(1), ct_index_pair(2)) = .true.
end do
end subroutine color_table_set_color_factors

```

This function returns a color factor, given two indices which point to the matrix elements of the initial state matrix. Internally, we can map them to the corresponding indices in the color table. As a side effect, we store the color factor in the color table for later lookup. (I.e., this function is impure.)

(Evaluators: procedures) +=

```

function color_table_get_color_factor (color_table, index1, index2, nc) &
  result (factor)
  real(default) :: factor
  type(color_table_t), intent(inout) :: color_table
  integer, intent(in) :: index1, index2
  integer, intent(in), optional :: nc
  integer :: i1, i2
  i1 = color_table%index(index1)
  i2 = color_table%index(index2)
  if (color_table%factor_is_known(i1,i2)) then
    factor = real(color_table%factor(i1,i2), kind=default)
  else
    factor = compute_color_factor &
      (color_table%col(:,i1), color_table%col(:,i2), nc)
    color_table%factor(i1,i2) = factor
    color_table%factor_is_known(i1,i2) = .true.
  end if
end function color_table_get_color_factor

```

12.3.4 Creating an evaluator: Matrix multiplication

The evaluator for matrix multiplication is the most complicated variant.

The initializer takes two input interactions and constructs the result evaluator, which consists of the interaction and the multiplication table for the product (or convolution) of the two. Normally, the input interactions are connected by one or more common particles (e.g., decay, structure function convolution).

In the result interaction, quantum numbers of the connections can be summed over. This is determined by the `qn_mask_conn` argument. The `qn_mask_rest` argument is its analog for the other particles within the result interaction. (E.g., for the trace of the state matrix, all quantum numbers are summed over.)

Finally, the `connections_are_resonant` argument tells whether the connecting particles should be marked as resonant in the final event record. If true, this also implies that the second interaction is not the hard process, so any corresponding tags should be removed from the outgoing particles. This applies to decays.

The algorithm consists of the following steps:

1. **find_connections**: Find the particles which are connected, i.e., common to both input interactions. Either they are directly linked, or both are linked to a common source.
2. **compute_index_bounds_and_mappings**: Compute the mappings of particle indices from the input interactions to the result interaction. There is a separate mapping for the connected particles.
3. **accumulate_connected_states**: Create an auxiliary state matrix which lists the possible quantum numbers for the connected particles. When building this matrix, count the number of times each assignment is contained in any of the input states and, for each of the input states, record the index of the matrix element within the new state matrix. For the connected particles, reassign color indices such that no color state is present twice in different color-index assignment. Note that helicity assignments of the connected state can be (and will be) off-diagonal, so no spin correlations are lost in decays.

Do this for both input interactions.

4. **allocate_connection_entries**: Allocate a table of connections. Each table row corresponds to one state in the auxiliary matrix, and to multiple states of the input interactions. It collects all states of the unconnected particles in the two input interactions that are associated with the particular state (quantum-number assignment) of the connected particles.
5. **fill_connection_table**: Fill the table of connections by scanning both input interactions. When copying states, reassign color indices for the unconnected particles such that they match between all involved particle sets (interaction 1, interaction 2, and connected particles).
6. **make_product_interaction**: Scan the table of connections we have just built. For each entry, construct all possible pairs of states of the unconnected particles and combine them with the specific connected-particle state. This is a possible quantum-number assignment of the result interaction. Now mask all quantum numbers that should be summed over, and append this to the result state matrix. Record the matrix element index of the result. We now have the result interaction.
7. **make_pairing_array**: First allocate the pairing array with the number of entries of the result interaction. Then scan the table of connections again. For each entry, record the indices of the matrix elements which have to be multiplied and summed over in order to compute this particular matrix element. This makes up the multiplication table.
8. **record_links**: Transfer all source pointers from the input interactions to the result interaction. Do the same for the internal parent-child relations and resonance assignments. For the connected particles, make up appropriate additional parent-child relations. This allows for fetching momenta from other interactions when a new event is filled, and to reconstruct the event history when the event is analyzed.

After all this is done, for each event, we just have to evaluate the pairing arrays (multiplication tables) in order to compute the result matrix elements in their proper positions. The quantum-number assignments remain fixed from now on.

```

(Evaluators: evaluator: TBP)+≡
  procedure :: init_product => evaluator_init_product

(Evaluators: sub interfaces)+≡
  module subroutine evaluator_init_product &
    (eval, int_in1, int_in2, qn_mask_conn, qn_filter_conn, qn_mask_rest, &
      connections_are_resonant, ignore_sub_for_qn)
    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), intent(in), target :: int_in1, int_in2
    type(quantum_numbers_mask_t), intent(in) :: qn_mask_conn
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
    type(quantum_numbers_mask_t), intent(in), optional :: qn_mask_rest
    logical, intent(in), optional :: connections_are_resonant
    logical, intent(in), optional :: ignore_sub_for_qn
  end subroutine evaluator_init_product

(Evaluators: procedures)+≡
  module subroutine evaluator_init_product &
    (eval, int_in1, int_in2, qn_mask_conn, qn_filter_conn, qn_mask_rest, &
      connections_are_resonant, ignore_sub_for_qn)

    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), intent(in), target :: int_in1, int_in2
    type(quantum_numbers_mask_t), intent(in) :: qn_mask_conn
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
    type(quantum_numbers_mask_t), intent(in), optional :: qn_mask_rest
    logical, intent(in), optional :: connections_are_resonant
    logical, intent(in), optional :: ignore_sub_for_qn

    type(qn_mask_array_t), dimension(2) :: qn_mask_in
    type(state_matrix_t), pointer :: state_in1, state_in2
    type(connection_table_t) :: connection_table

    integer :: n_in, n_vir, n_out, n_tot
    integer, dimension(2) :: n_rest
    integer :: n_conn

    integer, dimension(:,:), allocatable :: connection_index
    type(index_map_t), dimension(2) :: prt_map_in
    type(index_map_t) :: prt_map_conn
    type(prt_mask_t), dimension(2) :: prt_is_connected
    type(quantum_numbers_mask_t), dimension(:), allocatable :: &
      qn_mask_conn_initial, int_in1_mask, int_in2_mask

    integer :: i

    eval%type = EVAL_PRODUCT
    eval%int_in1 => int_in1
    eval%int_in2 => int_in2

    state_in1 => int_in1%get_state_matrix_ptr ()

```

```

state_in2 => int_in2%get_state_matrix_ptr ()

call find_connections (int_in1, int_in2, n_conn, connection_index)
if (n_conn == 0) then
    call msg_message ("First interaction:")
    call int_in1%basic_write (col_verbosity=.true.)
    call msg_message ("Second interaction:")
    call int_in2%basic_write (col_verbosity=.true.)
    call msg_fatal ("Evaluator product: no connections found between factors")
end if
call compute_index_bounds_and_mappings &
    (int_in1, int_in2, n_conn, &
    n_in, n_vir, n_out, n_tot, &
    n_rest, prt_map_in, prt_map_conn)

call prt_mask_init (prt_is_connected(1), int_in1%get_n_tot ())
call prt_mask_init (prt_is_connected(2), int_in2%get_n_tot ())
do i = 1, 2
    prt_is_connected(i)%entry = .true.
    prt_is_connected(i)%entry(connection_index(:,i)) = .false.
end do
allocate (qn_mask_conn_initial (n_conn), &
    int_in1_mask (n_conn), int_in2_mask (n_conn))
int_in1_mask = int_in1%get_mask (connection_index(:,1))
int_in2_mask = int_in2%get_mask (connection_index(:,2))
do i = 1, n_conn
    qn_mask_conn_initial(i) = int_in1_mask(i) .or. int_in2_mask(i)
end do
allocate (qn_mask_in(1)%mask (int_in1%get_n_tot ()))
allocate (qn_mask_in(2)%mask (int_in2%get_n_tot ()))
qn_mask_in(1)%mask = int_in1%get_mask ()
qn_mask_in(2)%mask = int_in2%get_mask ()
call connection_table_init (connection_table, &
    state_in1, state_in2, &
    qn_mask_conn_initial, &
    n_conn, connection_index, n_rest, &
    qn_filter_conn, ignore_sub_for_qn)
call connection_table_fill (connection_table, &
    state_in1, state_in2, &
    connection_index, prt_is_connected)
call make_product_interaction (eval%interaction_t, &
    n_in, n_vir, n_out, &
    connection_table, &
    prt_map_in, prt_is_connected, &
    qn_mask_in, qn_mask_conn_initial, &
    qn_mask_conn, qn_filter_conn, qn_mask_rest)
call make_pairing_array (eval%pairing_array, &
    eval%get_n_matrix_elements (), &
    connection_table)
call record_links (eval%interaction_t, &
    int_in1, int_in2, connection_index, prt_map_in, prt_map_conn, &
    prt_is_connected, connections_are_resonant)
call connection_table_final (connection_table)

```

```

if (eval%get_n_matrix_elements () == 0) then
  print *, "Evaluator product"
  print *, "First interaction"
  call int_in1%basic_write (col_verbosity=.true.)
  print *
  print *, "Second interaction"
  call int_in2%basic_write (col_verbosity=.true.)
  print *
  call msg_fatal ("Product of density matrices is empty", &
    [var_str (" -----"), &
      var_str ("This happens when two density matrices are convoluted "), &
      var_str ("but the processes they belong to (e.g., production "), &
      var_str ("and decay) do not match. This could happen if the "), &
      var_str ("beam specification does not match the hard "), &
      var_str ("process. Or it may indicate a WHIZARD bug.")])
end if

contains

subroutine compute_index_bounds_and_mappings &
  (int1, int2, n_conn, &
    n_in, n_vir, n_out, n_tot, &
    n_rest, prt_map_in, prt_map_conn)
class(interaction_t), intent(in) :: int1, int2
integer, intent(in) :: n_conn
integer, intent(out) :: n_in, n_vir, n_out, n_tot
integer, dimension(2), intent(out) :: n_rest
type(index_map_t), dimension(2), intent(out) :: prt_map_in
type(index_map_t), intent(out) :: prt_map_conn
integer, dimension(:), allocatable :: index
integer :: n_in1, n_vir1, n_out1
integer :: n_in2, n_vir2, n_out2
integer :: k
n_in1 = int1%get_n_in ()
n_vir1 = int1%get_n_vir ()
n_out1 = int1%get_n_out () - n_conn
n_rest(1) = n_in1 + n_vir1 + n_out1
n_in2 = int2%get_n_in () - n_conn
n_vir2 = int2%get_n_vir ()
n_out2 = int2%get_n_out ()
n_rest(2) = n_in2 + n_vir2 + n_out2
n_in = n_in1 + n_in2
n_vir = n_vir1 + n_vir2 + n_conn
n_out = n_out1 + n_out2
n_tot = n_in + n_vir + n_out
call index_map_init (prt_map_in, n_rest)
call index_map_init (prt_map_conn, n_conn)
allocate (index (n_tot))
index = [ (i, i = 1, n_tot) ]
prt_map_in(1)%entry(1 : n_in1) = index( 1 : n_in1)
k = n_in1
prt_map_in(2)%entry(1 : n_in2) = index(k + 1 : k + n_in2)
k = k + n_in2
prt_map_in(1)%entry(n_in1 + 1 : n_in1 + n_vir1) = index(k + 1 : k + n_vir1)

```

```

k = k + n_vir1
prt_map_in(2)%entry(n_in2 + 1 : n_in2 + n_vir2) = index(k + 1 : k + n_vir2)
k = k + n_vir2
prt_map_conn%entry = index(k + 1 : k + n_conn)
k = k + n_conn
prt_map_in(1)%entry(n_in1 + n_vir1 + 1 : n_rest(1)) = index(k + 1 : k + n_out1)
k = k + n_out1
prt_map_in(2)%entry(n_in2 + n_vir2 + 1 : n_rest(2)) = index(k + 1 : k + n_out2)
end subroutine compute_index_bounds_and_mappings

```

```

subroutine connection_table_init &
    (connection_table, state_in1, state_in2, qn_mask_conn, &
     n_conn, connection_index, n_rest, &
     qn_filter_conn, ignore_sub_for_qn_in)
type(connection_table_t), intent(out) :: connection_table
type(state_matrix_t), intent(in), target :: state_in1, state_in2
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_conn
integer, intent(in) :: n_conn
integer, dimension(:,:), intent(in) :: connection_index
integer, dimension(2), intent(in) :: n_rest
type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
logical, intent(in), optional :: ignore_sub_for_qn_in
integer, dimension(2) :: n_me_in
type(state_iterator_t) :: it
type(quantum_numbers_t), dimension(n_conn) :: qn
integer :: i, me_index_in, me_index_conn, n_me_conn
integer, dimension(2) :: me_count
logical :: ignore_sub_for_qn, has_sub_qn
integer :: i_beam_sub
connection_table%n_conn = n_conn
connection_table%n_rest = n_rest
n_me_in(1) = state_in1%get_n_matrix_elements ()
n_me_in(2) = state_in2%get_n_matrix_elements ()
allocate (connection_table%index_conn (2))
call index_map_init (connection_table%index_conn, n_me_in)
call connection_table%state%init (n_counters = 2)
do i = 1, 2
    select case (i)
    case (1); call it%init (state_in1)
    case (2); call it%init (state_in2)
    end select
    do while (it%is_valid ())
        qn = it%get_quantum_numbers (connection_index(:,i))
        call qn%undefine (qn_mask_conn)
        if (present (qn_filter_conn)) then
            if (.not. all (qn .match. qn_filter_conn)) then
                call it%advance (); cycle
            end if
        end if
        call quantum_numbers_canonicalize_color (qn)
        me_index_in = it%get_me_index ()
        ignore_sub_for_qn = .false.; if (present (ignore_sub_for_qn_in)) ignore_sub_for_qn = i
        has_sub_qn = .false.
        do i_beam_sub = 1, n_beams_rescaled

```

```

        has_sub_qn = has_sub_qn .or. any (qn%get_sub () == i_beam_sub)
    end do
    call connection_table%state%add_state (qn, &
        counter_index = i, &
        ignore_sub_for_qn = .not. (ignore_sub_for_qn .and. has_sub_qn), &
        me_index = me_index_conn)
    call index_map_set_entry (connection_table%index_conn(i), &
        me_index_in, me_index_conn)
    call it%advance ()
end do
end do
n_me_conn = connection_table%state%get_n_matrix_elements ()
connection_table%n_me_conn = n_me_conn
allocate (connection_table%entry (n_me_conn))
call it%init (connection_table%state)
do while (it%is_valid ())
    i = it%get_me_index ()
    me_count = it%get_me_count ()
    call connection_entry_init (connection_table%entry(i), 2, 2, &
        it%get_quantum_numbers (), me_count, n_rest)
    call it%advance ()
end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
    type(connection_table_t), intent(inout) :: connection_table
    call connection_table%state%final ()
end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
    type(connection_table_t), intent(in) :: connection_table
    integer, intent(in), optional :: unit
    integer :: i, j
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Connection table:"
    call connection_table%state%write (unit)
    if (allocated (connection_table%index_conn)) then
        write (u, *) "  Index mapping input => connection table:"
        do i = 1, size (connection_table%index_conn)
            write (u, *) "    Input state", i
            do j = 1, size (connection_table%index_conn(i))
                write (u, *)      j, &
                    index_map_get_entry (connection_table%index_conn(i), j)
            end do
        end do
    end if
    if (allocated (connection_table%entry)) then
        write (u, *) "  Connection table contents:"
        do i = 1, size (connection_table%entry)
            call connection_entry_write (connection_table%entry(i), unit)
        end do
    end if
    if (index_map_exists (connection_table%index_result)) then

```

```

        write (u, *) "   Index mapping connection table => output:"
        do i = 1, size (connection_table%index_result)
            write (u, *)   i, &
                index_map_get_entry (connection_table%index_result, i)
        end do
    end if
end subroutine connection_table_write

subroutine connection_table_fill &
    (connection_table, state_in1, state_in2, &
     connection_index, prt_is_connected)
type(connection_table_t), intent(inout) :: connection_table
type(state_matrix_t), intent(in), target :: state_in1, state_in2
integer, dimension(:, :), intent(in) :: connection_index
type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
type(state_iterator_t) :: it
integer :: index_in, index_conn
integer :: color_offset
integer :: n_result_entries
integer :: i, k
color_offset = connection_table%state%get_max_color_value ()
do i = 1, 2
    select case (i)
    case (1); call it%init (state_in1)
    case (2); call it%init (state_in2)
    end select
    do while (it%is_valid ())
        index_in = it%get_me_index ()
        index_conn = index_map_get_entry &
            (connection_table%index_conn(i), index_in)
        if (index_conn /= 0) then
            call connection_entry_add_state &
                (connection_table%entry(index_conn), i, &
                 index_in, it%get_quantum_numbers (), &
                 connection_index(:, i), prt_is_connected(i), &
                 color_offset)
        end if
        call it%advance ()
    end do
    color_offset = color_offset + state_in1%get_max_color_value ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + product (connection_table%entry(k)%n_index)
end do
call index_map_init (connection_table%index_result, n_result_entries)
end subroutine connection_table_fill

subroutine connection_entry_add_state &
    (entry, i, index_in, qn_in, connection_index, prt_is_connected, &
     color_offset)
type(connection_entry_t), intent(inout) :: entry
integer, intent(in) :: i

```

```

integer, intent(in) :: index_in
type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
integer, dimension(:), intent(in) :: connection_index
type(prt_mask_t), intent(in) :: prt_is_connected
integer, intent(in) :: color_offset
integer :: c
integer, dimension(:,:), allocatable :: color_map
entry%count(i) = entry%count(i) + 1
c = entry%count(i)
call make_color_map (color_map, &
    qn_in(connection_index), entry%qn_conn)
call index_map_set_entry (entry%index_in(i), c, index_in)
entry%qn_in_list(i)%qn(:,c) = pack (qn_in, prt_is_connected%entry)
call quantum_numbers_translate_color &
    (entry%qn_in_list(i)%qn(:,c), color_map, color_offset)
end subroutine connection_entry_add_state

subroutine make_product_interaction (int, &
    n_in, n_vir, n_out, &
    connection_table, &
    prt_map_in, prt_is_connected, &
    qn_mask_in, qn_mask_conn_initial, &
    qn_mask_conn, qn_filter_conn, qn_mask_rest)
type(interaction_t), intent(out), target :: int
integer, intent(in) :: n_in, n_vir, n_out
type(connection_table_t), intent(inout), target :: connection_table
type(index_map_t), dimension(2), intent(in) :: prt_map_in
type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
type(qn_mask_array_t), dimension(2), intent(in) :: qn_mask_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: &
    qn_mask_conn_initial
type(quantum_numbers_mask_t), intent(in) :: qn_mask_conn
type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
type(quantum_numbers_mask_t), intent(in), optional :: qn_mask_rest
type(index_map_t), dimension(2) :: prt_index_in
type(index_map_t) :: prt_index_conn
integer :: n_tot, n_conn
integer, dimension(2) :: n_rest
integer :: i, j, k, m
type(quantum_numbers_t), dimension(:), allocatable :: qn
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
type(connection_entry_t), pointer :: entry
integer :: result_index
n_conn = connection_table%n_conn
n_rest = connection_table%n_rest
n_tot = sum (n_rest) + n_conn
allocate (qn (n_tot), qn_mask (n_tot))
do i = 1, 2
    call index_map_init (prt_index_in(i), n_rest(i))
    prt_index_in(i)%entry = &
        prt_map_in(i)%entry ([ (j, j = 1, n_rest(i)) ])
end do
call index_map_init (prt_index_conn, n_conn)
prt_index_conn%entry = prt_map_conn%entry ([ (j, j = 1, n_conn) ])

```



```

do i = 1, 2
  if (present (qn_mask_rest)) then
    qn_mask(prt_index_in(i)%entry) = &
      pack (qn_mask_in(i)%mask, prt_is_connected(i)%entry) &
      .or. qn_mask_rest
  else
    qn_mask(prt_index_in(i)%entry) = &
      pack (qn_mask_in(i)%mask, prt_is_connected(i)%entry)
  end if
end do
qn_mask(prt_index_conn%entry) = qn_mask_conn_initial .or. qn_mask_conn
call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask = qn_mask)
m = 1
do i = 1, connection_table%n_me_conn
  entry => connection_table%entry(i)
  qn(prt_index_conn%entry) = &
    quantum_numbers_undefined (entry%qn_conn, qn_mask_conn)
  if (present (qn_filter_conn)) then
    if (.not. all (qn(prt_index_conn%entry) .match. qn_filter_conn)) &
      cycle
  end if
  do j = 1, entry%n_index(1)
    qn(prt_index_in(1)%entry) = entry%qn_in_list(1)%qn(:,j)
    do k = 1, entry%n_index(2)
      qn(prt_index_in(2)%entry) = entry%qn_in_list(2)%qn(:,k)
      call int%add_state (qn, me_index = result_index)
      call index_map_set_entry &
        (connection_table%index_result, m, result_index)
      m = m + 1
    end do
  end do
end do
call int%freeze ()
end subroutine make_product_interaction

subroutine make_pairing_array (pa, n_matrix_elements, connection_table)
  type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
  integer, intent(in) :: n_matrix_elements
  type(connection_table_t), intent(in), target :: connection_table
  type(connection_entry_t), pointer :: entry
  integer, dimension(:), allocatable :: n_entries
  integer :: i, j, k, m, r
  allocate (pa (n_matrix_elements))
  allocate (n_entries (n_matrix_elements))
  n_entries = 0
  do m = 1, size (connection_table%index_result)
    r = index_map_get_entry (connection_table%index_result, m)
    n_entries(r) = n_entries(r) + 1
  end do
  call pairing_array_init &
    (pa, n_entries, has_i2=.true., has_factor=.false.)
  m = 1
  n_entries = 0
  do i = 1, connection_table%n_me_conn

```

```

entry => connection_table%entry(i)
do j = 1, entry%n_index(1)
  do k = 1, entry%n_index(2)
    r = index_map_get_entry (connection_table%index_result, m)
    n_entries(r) = n_entries(r) + 1
    pa(r)%i1(n_entries(r)) = &
      index_map_get_entry (entry%index_in(1), j)
    pa(r)%i2(n_entries(r)) = &
      index_map_get_entry (entry%index_in(2), k)
    m = m + 1
  end do
end do
end do
end subroutine make_pairing_array

subroutine record_links (int, &
  int_in1, int_in2, connection_index, prt_map_in, prt_map_conn, &
  prt_is_connected, connections_are_resonant)
class(interaction_t), intent(inout) :: int
class(interaction_t), intent(in), target :: int_in1, int_in2
integer, dimension(:,:), intent(in) :: connection_index
type(index_map_t), dimension(2), intent(in) :: prt_map_in
type(index_map_t), intent(in) :: prt_map_conn
type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
logical, intent(in), optional :: connections_are_resonant
type(index_map_t), dimension(2) :: prt_map_all
integer :: i, j, k, ival
call index_map_init (prt_map_all(1), size (prt_is_connected(1)))
k = 0
j = 0
do i = 1, size (prt_is_connected(1))
  if (prt_is_connected(1)%entry(i)) then
    j = j + 1
    ival = index_map_get_entry (prt_map_in(1), j)
    call index_map_set_entry (prt_map_all(1), i, ival)
  else
    k = k + 1
    ival = index_map_get_entry (prt_map_conn, k)
    call index_map_set_entry (prt_map_all(1), i, ival)
  end if
  call int%set_source_link (ival, int_in1, i)
end do
call int_in1%transfer_relations (int, prt_map_all(1)%entry)
call index_map_init (prt_map_all(2), size (prt_is_connected(2)))
j = 0
do i = 1, size (prt_is_connected(2))
  if (prt_is_connected(2)%entry(i)) then
    j = j + 1
    ival = index_map_get_entry (prt_map_in(2), j)
    call index_map_set_entry (prt_map_all(2), i, ival)
    call int%set_source_link (ival, int_in2, i)
  else
    call index_map_set_entry (prt_map_all(2), i, 0)
  end if
end do

```

```

end do
call int_in2%transfer_relations (int, prt_map_all(2)%entry)
call int%relate_connections &
    (int_in2, connection_index(:,2), prt_map_all(2)%entry, &
    prt_map_conn%entry, connections_are_resonant)
end subroutine record_links

end subroutine evaluator_init_product

```

12.3.5 Creating an evaluator: square

The generic initializer for an evaluator that squares a matrix element. Depending on the provided mask, we select the appropriate specific initializer for either diagonal or non-diagonal helicity density matrices.

```

<Evaluators: evaluator: TBP>+≡
    procedure :: init_square => evaluator_init_square

<Evaluators: sub interfaces>+≡
    module subroutine evaluator_init_square (eval, int_in, qn_mask, &
        col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
        class(evaluator_t), intent(out), target :: eval
        class(interaction_t), intent(in), target :: int_in
        type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
        integer, dimension(:,:), intent(in), optional :: col_flow_index
        complex(default), dimension(:), intent(in), optional :: col_factor
        integer, dimension(:), intent(in), optional :: col_index_hi
        logical, intent(in), optional :: expand_color_flows
        integer, intent(in), optional :: nc
    end subroutine evaluator_init_square

<Evaluators: procedures>+≡
    module subroutine evaluator_init_square (eval, int_in, qn_mask, &
        col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
        class(evaluator_t), intent(out), target :: eval
        class(interaction_t), intent(in), target :: int_in
        type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
        integer, dimension(:,:), intent(in), optional :: col_flow_index
        complex(default), dimension(:), intent(in), optional :: col_factor
        integer, dimension(:), intent(in), optional :: col_index_hi
        logical, intent(in), optional :: expand_color_flows
        integer, intent(in), optional :: nc
        if (all (qn_mask%diagonal_helicity ())) then
            call eval%init_square_diag (int_in, qn_mask, &
                col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
        else
            call eval%init_square_nondiag (int_in, qn_mask, &
                col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
        end if
    end subroutine evaluator_init_square

```

Color-summed squared matrix (diagonal helicities)

The initializer for an evaluator that squares a matrix element, including color factors. The mask must be such that off-diagonal matrix elements are excluded.

If `color_flows` is set, the evaluator keeps color-flow entries separate and drops all interfering color structures. The color factors are set to unity in this case.

There is only one input interaction. The quantum-number mask is an array, one entry for each particle, so they can be treated individually. For academic purposes, we allow for the number of colors being different from three (but 3 is the default).

The algorithm is analogous to multiplication, with a few notable differences:

1. The connected particles are known, the correspondence is one-to-one. All particles are connected, and the mapping of indices is trivial, which simplifies the following steps.
2. `accumulate_connected_states`: The matrix of connected states encompasses all particles, but color indices are removed. However, ghost states are still kept separate from physical color states. No color-index reassignment is necessary.
3. The table of connections contains single index and quantum-number arrays instead of pairs of them. They are paired with themselves in all possible ways.
4. `make_squared_interaction`: Now apply the predefined quantum-numbers mask, which usually collects all color states (physical and ghosts), and possibly a helicity sum.
5. `make_pairing_array`: For each pair of input states, compute the color factor (including a potential ghost-parity sign) and store this in the pairing array together with the matrix-element indices for multiplication.
6. `record_links`: This is again trivial due to the one-to-one correspondence.

(Evaluators: evaluator: TBP)+≡

```
procedure :: init_square_diag => evaluator_init_square_diag
```

(Evaluators: sub interfaces)+≡

```
module subroutine evaluator_init_square_diag (eval, int_in, qn_mask, &
  col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), intent(in), target :: int_in
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  integer, dimension(:,:), intent(in), optional :: col_flow_index
  complex(default), dimension(:), intent(in), optional :: col_factor
  integer, dimension(:), intent(in), optional :: col_index_hi
  logical, intent(in), optional :: expand_color_flows
  integer, intent(in), optional :: nc
end subroutine evaluator_init_square_diag
```

(Evaluators: procedures) +=

```

module subroutine evaluator_init_square_diag (eval, int_in, qn_mask, &
      col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)

  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), intent(in), target :: int_in
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  integer, dimension(:,:), intent(in), optional :: col_flow_index
  complex(default), dimension(:), intent(in), optional :: col_factor
  integer, dimension(:), intent(in), optional :: col_index_hi
  logical, intent(in), optional :: expand_color_flows
  integer, intent(in), optional :: nc

  integer :: n_in, n_vir, n_out, n_tot
  type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask_initial
  type(state_matrix_t), pointer :: state_in
  type(connection_table_diag_t) :: connection_table

  logical :: sum_colors
  type(color_table_t) :: color_table

  if (present (expand_color_flows)) then
    sum_colors = .not. expand_color_flows
  else
    sum_colors = .true.
  end if

  if (sum_colors) then
    eval%type = EVAL_SQUARE_WITH_COLOR_FACTORS
  else
    eval%type = EVAL_SQUARED_FLOWS
  end if
  eval%int_in1 => int_in

  n_in = int_in%get_n_in ()
  n_vir = int_in%get_n_vir ()
  n_out = int_in%get_n_out ()
  n_tot = int_in%get_n_tot ()

  state_in => int_in%get_state_matrix_ptr ()

  allocate (qn_mask_initial (n_tot))
  qn_mask_initial = int_in%get_mask ()
  call qn_mask_initial%set_color (sum_colors, mask_cg=.false.)
  if (sum_colors) then
    call color_table_init (color_table, state_in, n_tot)
    if (present (col_flow_index) .and. present (col_factor) &
        .and. present (col_index_hi)) then
      call color_table_set_color_factors &
        (color_table, col_flow_index, col_factor, col_index_hi)
    end if
  end if

  call connection_table_init (connection_table, state_in, &

```

```

        qn_mask_initial, qn_mask, n_tot)
call connection_table_fill (connection_table, state_in)
call make_squared_interaction (eval%interaction_t, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask_initial .or. qn_mask)
call make_pairing_array (eval%pairing_array, &
    eval%get_n_matrix_elements (), &
    connection_table, sum_colors, color_table, n_in, n_tot, nc)
call record_links (eval, int_in, n_tot)
call connection_table_final (connection_table)

```

contains

```

subroutine connection_table_init &
    (connection_table, state_in, qn_mask_in, qn_mask, n_tot)
    type(connection_table_diag_t), intent(out) :: connection_table
    type(state_matrix_t), intent(in), target :: state_in
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    integer, intent(in) :: n_tot
    type(quantum_numbers_t), dimension(n_tot) :: qn
    type(state_iterator_t) :: it
    integer :: i, n_me_in, me_index_in
    integer :: me_index_conn, n_me_conn
    integer, dimension(1) :: me_count
    logical :: qn_passed
    connection_table%n_tot = n_tot
    n_me_in = state_in%get_n_matrix_elements ()
    call index_map_init (connection_table%index_conn, n_me_in)
    call connection_table%state%init (n_counters=1)
    call it%init (state_in)
    do while (it%is_valid ())
        qn = it%get_quantum_numbers ()
        if (all (quantum_numbers_are_physical (qn, qn_mask))) then
            call qn%undefine (qn_mask_in)
            qn_passed = .true.
            if (qn_passed) then
                me_index_in = it%get_me_index ()
                call connection_table%state%add_state (qn, &
                    counter_index = 1, me_index = me_index_conn)
                call index_map_set_entry (connection_table%index_conn, &
                    me_index_in, me_index_conn)
            end if
        end if
        call it%advance ()
    end do
    n_me_conn = connection_table%state%get_n_matrix_elements ()
    connection_table%n_me_conn = n_me_conn
    allocate (connection_table%entry (n_me_conn))
    call it%init (connection_table%state)
    do while (it%is_valid ())
        i = it%get_me_index ()
        me_count = it%get_me_count ()
        call connection_entry_init (connection_table%entry(i), 1, 2, &

```

```

        it%get_quantum_numbers (), me_count, [n_tot])
    call it%advance ()
end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
    type(connection_table_diag_t), intent(inout) :: connection_table
    call connection_table%state%final ()
end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
    type(connection_table_diag_t), intent(in) :: connection_table
    integer, intent(in), optional :: unit
    integer :: i
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Connection table:"
    call connection_table%state%write (unit)
    if (index_map_exists (connection_table%index_conn)) then
        write (u, *) " Index mapping input => connection table:"
        do i = 1, size (connection_table%index_conn)
            write (u, *) i, &
                index_map_get_entry (connection_table%index_conn, i)
        end do
    end if
    if (allocated (connection_table%entry)) then
        write (u, *) " Connection table contents"
        do i = 1, size (connection_table%entry)
            call connection_entry_write (connection_table%entry(i), unit)
        end do
    end if
    if (index_map_exists (connection_table%index_result)) then
        write (u, *) " Index mapping connection table => output"
        do i = 1, size (connection_table%index_result)
            write (u, *) i, &
                index_map_get_entry (connection_table%index_result, i)
        end do
    end if
end subroutine connection_table_write

subroutine connection_table_fill (connection_table, state)
    type(connection_table_diag_t), intent(inout) :: connection_table
    type(state_matrix_t), intent(in), target :: state
    integer :: index_in, index_conn, n_result_entries
    type(state_iterator_t) :: it
    integer :: k
    call it%init (state)
    do while (it%is_valid ())
        index_in = it%get_me_index ()
        index_conn = &
            index_map_get_entry (connection_table%index_conn, index_in)
        if (index_conn /= 0) then
            call connection_entry_add_state &
                (connection_table%entry(index_conn), &

```

```

        index_in, it%get_quantum_numbers ())
    end if
    call it%advance ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + connection_table%entry(k)%n_index(1) ** 2
end do
call index_map_init (connection_table%index_result, n_result_entries)
end subroutine connection_table_fill

subroutine connection_entry_add_state (entry, index_in, qn_in)
    type(connection_entry_t), intent(inout) :: entry
    integer, intent(in) :: index_in
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    integer :: c
    entry%count = entry%count + 1
    c = entry%count(1)
    call index_map_set_entry (entry%index_in(1), c, index_in)
    entry%qn_in_list(1)%qn(:,c) = qn_in
end subroutine connection_entry_add_state

subroutine make_squared_interaction (int, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(connection_table_diag_t), intent(inout), target :: connection_table
    logical, intent(in) :: sum_colors
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(connection_entry_t), pointer :: entry
    integer :: result_index, n_contrib
    integer :: i, m
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    m = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        qn = quantum_numbers_undefined (entry%qn_conn, qn_mask)
        if (.not. sum_colors) call qn(1:n_in)%invert_color ()
        call int%add_state (qn, me_index = result_index)
        n_contrib = entry%n_index(1) ** 2
        connection_table%index_result%entry(m+1:m+n_contrib) = result_index
        m = m + n_contrib
    end do
    call int%freeze ()
end subroutine make_squared_interaction

subroutine make_pairing_array (pa, &
    n_matrix_elements, connection_table, sum_colors, color_table, &
    n_in, n_tot, nc)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, intent(in) :: n_matrix_elements

```



```

type(connection_table_diag_t), intent(in), target :: connection_table
logical, intent(in) :: sum_colors
type(color_table_t), intent(inout) :: color_table
type(connection_entry_t), pointer :: entry
integer, intent(in) :: n_in, n_tot
integer, intent(in), optional :: nc
integer, dimension(:), allocatable :: n_entries
integer :: i, k, l, ks, ls, m, r
integer :: color_multiplicity_in
allocate (pa (n_matrix_elements))
allocate (n_entries (n_matrix_elements))
n_entries = 0
do m = 1, size (connection_table%index_result)
    r = index_map_get_entry (connection_table%index_result, m)
    n_entries(r) = n_entries(r) + 1
end do
call pairing_array_init &
    (pa, n_entries, has_i2 = sum_colors, has_factor = sum_colors)
m = 1
n_entries = 0
do i = 1, connection_table%n_me_conn
    entry => connection_table%entry(i)
    do k = 1, entry%n_index(1)
        if (sum_colors) then
            color_multiplicity_in = product (abs &
                (entry%qn_in_list(1)%qn(:n_in, k)%get_color_type ()))
            do l = 1, entry%n_index(1)
                r = index_map_get_entry (connection_table%index_result, m)
                n_entries(r) = n_entries(r) + 1
                ks = index_map_get_entry (entry%index_in(1), k)
                ls = index_map_get_entry (entry%index_in(1), l)
                pa(r)%i1(n_entries(r)) = ks
                pa(r)%i2(n_entries(r)) = ls
                pa(r)%factor(n_entries(r)) = &
                    color_table_get_color_factor (color_table, ks, ls, nc) &
                    / color_multiplicity_in
                m = m + 1
            end do
        else
            r = index_map_get_entry (connection_table%index_result, m)
            n_entries(r) = n_entries(r) + 1
            ks = index_map_get_entry (entry%index_in(1), k)
            pa(r)%i1(n_entries(r)) = ks
            m = m + 1
        end if
    end do
end do
end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
class(interaction_t), intent(inout) :: int
class(interaction_t), intent(in), target :: int_in
integer, intent(in) :: n_tot
integer, dimension(n_tot) :: map

```

```

integer :: i
do i = 1, n_tot
  call int%set_source_link (i, int_in, i)
end do
map = [ (i, i = 1, n_tot) ]
call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_square_diag

```

Color-summed squared matrix (support nodiagonal helicities)

The initializer for an evaluator that squares a matrix element, including color factors. Unless requested otherwise by the quantum-number mask, the result contains off-diagonal matrix elements. (The input interaction must be diagonal since it represents an amplitude, not a density matrix.)

There is only one input interaction. The quantum-number mask is an array, one entry for each particle, so they can be treated individually. For academic purposes, we allow for the number of colors being different from three (but 3 is the default).

The algorithm is analogous to the previous one, with some additional complications due to the necessity to loop over two helicity indices.

(Evaluators: evaluator: TBP)+≡

```

procedure :: init_square_nondiag => evaluator_init_square_nondiag

```

(Evaluators: sub interfaces)+≡

```

module subroutine evaluator_init_square_nondiag (eval, int_in, qn_mask, &
  col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), intent(in), target :: int_in
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  integer, dimension(:,:), intent(in), optional :: col_flow_index
  complex(default), dimension(:), intent(in), optional :: col_factor
  integer, dimension(:), intent(in), optional :: col_index_hi
  logical, intent(in), optional :: expand_color_flows
  integer, intent(in), optional :: nc
end subroutine evaluator_init_square_nondiag

```

(Evaluators: procedures)+≡

```

module subroutine evaluator_init_square_nondiag (eval, int_in, qn_mask, &
  col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)

```

```

  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), intent(in), target :: int_in
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  integer, dimension(:,:), intent(in), optional :: col_flow_index
  complex(default), dimension(:), intent(in), optional :: col_factor
  integer, dimension(:), intent(in), optional :: col_index_hi
  logical, intent(in), optional :: expand_color_flows
  integer, intent(in), optional :: nc

```

```

integer :: n_in, n_vir, n_out, n_tot
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask_initial

```

```

type(state_matrix_t), pointer :: state_in
type(connection_table_nondiag_t) :: connection_table

logical :: sum_colors
type(color_table_t) :: color_table

if (present (expand_color_flows)) then
    sum_colors = .not. expand_color_flows
else
    sum_colors = .true.
end if

if (sum_colors) then
    eval%type = EVAL_SQUARE_WITH_COLOR_FACTORS
else
    eval%type = EVAL_SQUARED_FLOWS
end if
eval%int_in1 => int_in

n_in = int_in%get_n_in ()
n_vir = int_in%get_n_vir ()
n_out = int_in%get_n_out ()
n_tot = int_in%get_n_tot ()

state_in => int_in%get_state_matrix_ptr ()

allocate (qn_mask_initial (n_tot))
qn_mask_initial = int_in%get_mask ()
call qn_mask_initial%set_color (sum_colors, mask_cg=.false.)
if (sum_colors) then
    call color_table_init (color_table, state_in, n_tot)
    if (present (col_flow_index) .and. present (col_factor) &
        .and. present (col_index_hi)) then
        call color_table_set_color_factors &
            (color_table, col_flow_index, col_factor, col_index_hi)
    end if
end if

call connection_table_init (connection_table, state_in, &
    qn_mask_initial, qn_mask, n_tot)
call connection_table_fill (connection_table, state_in)
call make_squared_interaction (eval%interaction_t, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask_initial .or. qn_mask)
call make_pairing_array (eval%pairing_array, &
    eval%get_n_matrix_elements (), &
    connection_table, sum_colors, color_table, n_in, n_tot, nc)
call record_links (eval, int_in, n_tot)
call connection_table_final (connection_table)

contains

subroutine connection_table_init &
    (connection_table, state_in, qn_mask_in, qn_mask, n_tot)

```

```

type(connection_table_nondiag_t), intent(out) :: connection_table
type(state_matrix_t), intent(in), target :: state_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
integer, intent(in) :: n_tot
type(quantum_numbers_t), dimension(n_tot) :: qn1, qn2, qn
type(state_iterator_t) :: it1, it2, it
integer :: i, n_me_in, me_index_in1, me_index_in2
integer :: me_index_conn, n_me_conn
integer, dimension(1) :: me_count
logical :: qn_passed
connection_table%n_tot = n_tot
n_me_in = state_in%get_n_matrix_elements ()
call index_map2_init (connection_table%index_conn, n_me_in)
connection_table%index_conn = 0
call connection_table%state%init (n_counters=1)
call it1%init (state_in)
do while (it1%is_valid ())
    qn1 = it1%get_quantum_numbers ()
    me_index_in1 = it1%get_me_index ()
    call it2%init (state_in)
    do while (it2%is_valid ())
        qn2 = it2%get_quantum_numbers ()
        if (all (quantum_numbers_are_compatible (qn1, qn2, qn_mask))) then
            qn = qn1 .merge. qn2
            call qn%undefine (qn_mask_in)
            qn_passed = .true.
            if (qn_passed) then
                me_index_in2 = it2%get_me_index ()
                call connection_table%state%add_state (qn, &
                    counter_index = 1, me_index = me_index_conn)
                call index_map2_set_entry (connection_table%index_conn, &
                    me_index_in1, me_index_in2, me_index_conn)
            end if
        end if
        call it2%advance ()
    end do
    call it1%advance ()
end do
n_me_conn = connection_table%state%get_n_matrix_elements ()
connection_table%n_me_conn = n_me_conn
allocate (connection_table%entry (n_me_conn))
call it%init (connection_table%state)
do while (it%is_valid ())
    i = it%get_me_index ()
    me_count = it%get_me_count ()
    call connection_entry_init (connection_table%entry(i), 1, 2, &
        it%get_quantum_numbers (), me_count, [n_tot])
    call it%advance ()
end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
    type(connection_table_nondiag_t), intent(inout) :: connection_table

```

```

    call connection_table%state%final ()
end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
    type(connection_table_nondiag_t), intent(in) :: connection_table
    integer, intent(in), optional :: unit
    integer :: i, j
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Connection table:"
    call connection_table%state%write (unit)
    if (index_map2_exists (connection_table%index_conn)) then
        write (u, *) "  Index mapping input => connection table:"
        do i = 1, size (connection_table%index_conn)
            do j = 1, size (connection_table%index_conn)
                write (u, *)  i, j, &
                    index_map2_get_entry (connection_table%index_conn, i, j)
            end do
        end do
    end if
    if (allocated (connection_table%entry)) then
        write (u, *) "  Connection table contents"
        do i = 1, size (connection_table%entry)
            call connection_entry_write (connection_table%entry(i), unit)
        end do
    end if
    if (index_map_exists (connection_table%index_result)) then
        write (u, *) "  Index mapping connection table => output"
        do i = 1, size (connection_table%index_result)
            write (u, *)  i, &
                index_map_get_entry (connection_table%index_result, i)
        end do
    end if
end subroutine connection_table_write

subroutine connection_table_fill (connection_table, state)
    type(connection_table_nondiag_t), intent(inout), target :: connection_table
    type(state_matrix_t), intent(in), target :: state
    integer :: index1_in, index2_in, index_conn, n_result_entries
    type(state_iterator_t) :: it1, it2
    integer :: k
    call it1%init (state)
    do while (it1%is_valid ())
        index1_in = it1%get_me_index ()
        call it2%init (state)
        do while (it2%is_valid ())
            index2_in = it2%get_me_index ()
            index_conn = index_map2_get_entry &
                (connection_table%index_conn, index1_in, index2_in)
            if (index_conn /= 0) then
                call connection_entry_add_state &
                    (connection_table%entry(index_conn), &
                     index1_in, index2_in, &
                     it1%get_quantum_numbers () &

```

```

        .merge. &
        it2%get_quantum_numbers ()
    end if
    call it2%advance ()
end do
call it1%advance ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + connection_table%entry(k)%n_index(1)
end do
call index_map_init (connection_table%index_result, n_result_entries)
end subroutine connection_table_fill

subroutine connection_entry_add_state (entry, index1_in, index2_in, qn_in)
    type(connection_entry_t), intent(inout) :: entry
    integer, intent(in) :: index1_in, index2_in
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    integer :: c
    entry%count = entry%count + 1
    c = entry%count(1)
    call index_map_set_entry (entry%index_in(1), c, index1_in)
    call index_map_set_entry (entry%index_in(2), c, index2_in)
    entry%qn_in_list(1)%qn(:,c) = qn_in
end subroutine connection_entry_add_state

subroutine make_squared_interaction (int, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(connection_table_nondiag_t), intent(inout), target :: connection_table
    logical, intent(in) :: sum_colors
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(connection_entry_t), pointer :: entry
    integer :: result_index
    integer :: i, k, m
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    m = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do k = 1, size (entry%qn_in_list(1)%qn, 2)
            qn = quantum_numbers_undefined &
                (entry%qn_in_list(1)%qn(:,k), qn_mask)
            if (.not. sum_colors) call qn(1:n_in)%invert_color ()
            call int%add_state (qn, me_index = result_index)
            call index_map_set_entry (connection_table%index_result, m + 1, &
                result_index)
            m = m + 1
        end do
    end do
    call int%freeze ()
end subroutine

```

```

end subroutine make_squared_interaction

subroutine make_pairing_array (pa, &
    n_matrix_elements, connection_table, sum_colors, color_table, &
    n_in, n_tot, nc)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, intent(in) :: n_matrix_elements
    type(connection_table_nondiag_t), intent(in), target :: connection_table
    logical, intent(in) :: sum_colors
    type(color_table_t), intent(inout) :: color_table
    type(connection_entry_t), pointer :: entry
    integer, intent(in) :: n_in, n_tot
    integer, intent(in), optional :: nc
    integer, dimension(:), allocatable :: n_entries
    integer :: i, k, k1s, k2s, m, r
    integer :: color_multiplicity_in
    allocate (pa (n_matrix_elements))
    allocate (n_entries (n_matrix_elements))
    n_entries = 0
    do m = 1, size (connection_table%index_result)
        r = index_map_get_entry (connection_table%index_result, m)
        n_entries(r) = n_entries(r) + 1
    end do
    call pairing_array_init &
        (pa, n_entries, has_i2 = sum_colors, has_factor = sum_colors)
    m = 1
    n_entries = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do k = 1, entry%n_index(1)
            r = index_map_get_entry (connection_table%index_result, m)
            n_entries(r) = n_entries(r) + 1
            if (sum_colors) then
                k1s = index_map_get_entry (entry%index_in(1), k)
                k2s = index_map_get_entry (entry%index_in(2), k)
                pa(r)%i1(n_entries(r)) = k1s
                pa(r)%i2(n_entries(r)) = k2s
                color_multiplicity_in = product (abs &
                    (entry%qn_in_list(1)%qn(:n_in, k)%get_color_type ()))
                pa(r)%factor(n_entries(r)) = &
                    color_table_get_color_factor (color_table, k1s, k2s, nc) &
                    / color_multiplicity_in
            else
                k1s = index_map_get_entry (entry%index_in(1), k)
                pa(r)%i1(n_entries(r)) = k1s
            end if
            m = m + 1
        end do
    end do
end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in), target :: int_in

```

```

integer, intent(in) :: n_tot
integer, dimension(n_tot) :: map
integer :: i
do i = 1, n_tot
    call int%set_source_link (i, int_in, i)
end do
map = [ (i, i = 1, n_tot) ]
call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_square_nondiag

```

Copy with additional contracted color states

This evaluator involves no square or multiplication, its matrix elements are just copies of the (single) input interaction. However, the state matrix of the interaction contains additional states that have color indices contracted. This is used for copies of the beam or structure-function interactions that need to match the hard interaction also in the case where its color indices coincide.

(Evaluators: evaluator: TBP)+≡

```
procedure :: init_color_contractions => evaluator_init_color_contractions
```

(Evaluators: sub interfaces)+≡

```

module subroutine evaluator_init_color_contractions (eval, int_in)
    class(evaluator_t), intent(out), target :: eval
    type(interaction_t), intent(in), target :: int_in
end subroutine evaluator_init_color_contractions

```

(Evaluators: procedures)+≡

```

module subroutine evaluator_init_color_contractions (eval, int_in)
    class(evaluator_t), intent(out), target :: eval
    type(interaction_t), intent(in), target :: int_in
    integer :: n_in, n_vir, n_out, n_tot
    type(state_matrix_t) :: state_with_contractions
    integer, dimension(:), allocatable :: me_index
    integer, dimension(:), allocatable :: result_index
    eval%type = EVAL_COLOR_CONTRACTION
    eval%int_in1 => int_in
    n_in = int_in%get_n_in ()
    n_vir = int_in%get_n_vir ()
    n_out = int_in%get_n_out ()
    n_tot = int_in%get_n_tot ()
    state_with_contractions = int_in%get_state_matrix_ptr ()
    call state_with_contractions%add_color_contractions ()
    call make_contracted_interaction (eval%interaction_t, &
        me_index, result_index, &
        n_in, n_vir, n_out, n_tot, &
        state_with_contractions, int_in%get_mask ())
    call make_pairing_array (eval%pairing_array, me_index, result_index)
    call record_links (eval, int_in, n_tot)
    call state_with_contractions%final ()

```

contains


```

subroutine make_contracted_interaction (int, &
    me_index, result_index, &
    n_in, n_vir, n_out, n_tot, state, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, dimension(:), intent(out), allocatable :: me_index
    integer, dimension(:), intent(out), allocatable :: result_index
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(state_matrix_t), intent(in) :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(state_iterator_t) :: it
    integer :: n_me, i
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call int%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    n_me = state%get_n_leaves ()
    allocate (me_index (n_me))
    allocate (result_index (n_me))
    call it%init (state)
    i = 0
    do while (it%is_valid ())
        i = i + 1
        me_index(i) = it%get_me_index ()
        qn = it%get_quantum_numbers ()
        call int%add_state (qn, me_index = result_index(i))
        call it%advance ()
    end do
    call int%freeze ()
end subroutine make_contracted_interaction

subroutine make_pairing_array (pa, me_index, result_index)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, dimension(:), intent(in) :: me_index, result_index
    integer, dimension(:), allocatable :: n_entries
    integer :: n_matrix_elements, r, i, k
    !!! The result indices of the appended color contracted states
    !!! start counting from 1 again. For the pairing array, we currently
    !!! only take the first part of ascending indices into account
    !!! excluding the color contracted states.
    n_matrix_elements = size (me_index)
    k = 0
    do i = 1, n_matrix_elements
        r = result_index(i)
        if (r < i) exit
        k = r
    end do
    allocate (pa (k))
    allocate (n_entries (k))
    n_entries = 1
    call pairing_array_init &
        (pa, n_entries, has_i2=.false., has_factor=.false.)
    do i = 1, k
        r = result_index(i)
        pa(r)%i1(1) = me_index(i)
    end do

```

```

end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
  class(interaction_t), intent(inout) :: int
  class(interaction_t), intent(in), target :: int_in
  integer, intent(in) :: n_tot
  integer, dimension(n_tot) :: map
  integer :: i
  do i = 1, n_tot
    call int%set_source_link (i, int_in, i)
  end do
  map = [ (i, i = 1, n_tot) ]
  call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_color_contractions

```

Auxiliary procedure for initialization

This will become a standard procedure in F2008. The result is true if the number of true values in the mask is odd. We use the function for determining the ghost parity of a quantum-number array.

[tho:] It's not used anymore and `mod (count (mask), 2) == 1` is a cooler implementation anyway.

```

<(UNUSED) Evaluators: procedures>≡
function parity (mask)
  logical :: parity
  logical, dimension(:) :: mask
  integer :: i
  parity = .false.
  do i = 1, size (mask)
    if (mask(i)) parity = .not. parity
  end do
end function parity

```

Reassign external source links from one to another.

```

<(Evaluators: public)+≡
public :: evaluator_reassign_links

<(Evaluators: interfaces)+≡
interface evaluator_reassign_links
  module procedure evaluator_reassign_links_eval
  module procedure evaluator_reassign_links_int
end interface

<(Evaluators: sub interfaces)+≡
module subroutine evaluator_reassign_links_eval (eval, eval_src, eval_target)
  type(evaluator_t), intent(inout) :: eval
  type(evaluator_t), intent(in) :: eval_src
  type(evaluator_t), intent(in), target :: eval_target
end subroutine evaluator_reassign_links_eval
module subroutine evaluator_reassign_links_int (eval, int_src, int_target)

```

```

        type(evaluator_t), intent(inout) :: eval
        type(interaction_t), intent(in) :: int_src
        type(interaction_t), intent(in), target :: int_target
    end subroutine evaluator_reassign_links_int

<Evaluators: procedures>+≡
    module subroutine evaluator_reassign_links_eval (eval, eval_src, eval_target)
        type(evaluator_t), intent(inout) :: eval
        type(evaluator_t), intent(in) :: eval_src
        type(evaluator_t), intent(in), target :: eval_target
        if (associated (eval%int_in1)) then
            if (eval%int_in1%get_tag () == eval_src%get_tag ()) then
                eval%int_in1 => eval_target%interaction_t
            end if
        end if
        if (associated (eval%int_in2)) then
            if (eval%int_in2%get_tag () == eval_src%get_tag ()) then
                eval%int_in2 => eval_target%interaction_t
            end if
        end if
        call interaction_reassign_links &
            (eval%interaction_t, eval_src%interaction_t, &
            eval_target%interaction_t)
    end subroutine evaluator_reassign_links_eval

    module subroutine evaluator_reassign_links_int (eval, int_src, int_target)
        type(evaluator_t), intent(inout) :: eval
        type(interaction_t), intent(in) :: int_src
        type(interaction_t), intent(in), target :: int_target
        if (associated (eval%int_in1)) then
            if (eval%int_in1%get_tag () == int_src%get_tag ()) then
                eval%int_in1 => int_target
            end if
        end if
        if (associated (eval%int_in2)) then
            if (eval%int_in2%get_tag () == int_src%get_tag ()) then
                eval%int_in2 => int_target
            end if
        end if
        call interaction_reassign_links (eval%interaction_t, int_src, int_target)
    end subroutine evaluator_reassign_links_int

<Evaluators: public>+≡
    public :: evaluator_get_int_in_ptr

<Evaluators: sub interfaces>+≡
    module function evaluator_get_int_in_ptr (eval, i) result (int_in)
        class(interaction_t), pointer :: int_in
        type(evaluator_t), intent(in), target :: eval
        integer, intent(in) :: i
    end function evaluator_get_int_in_ptr

<Evaluators: procedures>+≡
    module function evaluator_get_int_in_ptr (eval, i) result (int_in)
        class(interaction_t), pointer :: int_in

```

```

type(evaluator_t), intent(in), target :: eval
integer, intent(in) :: i
if (i == 1) then
    int_in => eval%int_in1
else if (i == 2) then
    int_in => eval%int_in2
else
    int_in => null ()
end if
end function evaluator_get_int_in_ptr

```

12.3.6 Creating an evaluator: identity

The identity evaluator creates a copy of the first input evaluator; the second input is not used.

All particles link back to the input evaluator and the internal relations are copied. As evaluation does take a shortcut by cloning the matrix elements, the pairing array is not used and does not have to be set up.

(Evaluators: evaluator: TBP)+≡

```

procedure :: init_identity => evaluator_init_identity

```

(Evaluators: sub interfaces)+≡

```

module subroutine evaluator_init_identity (eval, int)
    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), intent(in), target :: int
end subroutine evaluator_init_identity

```

(Evaluators: procedures)+≡

```

module subroutine evaluator_init_identity (eval, int)
    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), intent(in), target :: int
    integer :: n_in, n_out, n_vir, n_tot
    integer :: i
    integer, dimension(:), allocatable :: map
    type(state_matrix_t), pointer :: state
    type(state_iterator_t) :: it
    eval%type = EVAL_IDENTITY
    eval%int_in1 => int
    nullify (eval%int_in2)
    n_in = int%get_n_in ()
    n_out = int%get_n_out ()
    n_vir = int%get_n_vir ()
    n_tot = int%get_n_tot ()
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, &
        mask = int%get_mask (), &
        resonant = int%get_resonance_flags ())
    do i = 1, n_tot
        call eval%set_source_link (i, int, i)
    end do
    allocate (map(n_tot))
    map = [(i, i = 1, n_tot)]
    call int%transfer_relations (eval, map)
    state => int%get_state_matrix_ptr ()

```

```

call it%init (state)
do while (it%is_valid ())
  call eval%add_state (it%get_quantum_numbers (), &
    it%get_me_index ())
  call it%advance ()
end do
call eval%freeze ()

end subroutine evaluator_init_identity

```

12.3.7 Creating an evaluator: quantum number sum

This evaluator operates on the diagonal of a density matrix and sums over the quantum numbers specified by the mask. The optional argument **drop** allows to drop a particle from the resulting density matrix. The handling of virtuals is not completely sane, especially in connection with dropping particles.

When summing over matrix element entries, we keep the separation into entries and normalization (in the corresponding evaluation routine below).

(Evaluators: evaluator: TBP)+≡

```

procedure :: init_qn_sum => evaluator_init_qn_sum

```

(Evaluators: sub interfaces)+≡

```

module subroutine evaluator_init_qn_sum (eval, int, qn_mask, drop)
  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), target, intent(in) :: int
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  logical, intent(in), optional, dimension(:) :: drop
end subroutine evaluator_init_qn_sum

```

(Evaluators: procedures)+≡

```

module subroutine evaluator_init_qn_sum (eval, int, qn_mask, drop)
  class(evaluator_t), intent(out), target :: eval
  class(interaction_t), target, intent(in) :: int
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
  logical, intent(in), optional, dimension(:) :: drop
  type(state_iterator_t) :: it_old, it_new
  integer, dimension(:), allocatable :: pairing_size, pairing_target, i_new
  integer, dimension(:), allocatable :: map
  integer :: n_in, n_out, n_vir, n_tot, n_me_old, n_me_new
  integer :: i, j
  type(state_matrix_t), pointer :: state_new, state_old
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  logical :: matched
  logical, dimension(size (qn_mask)) :: dropped
  integer :: ndropped
  integer, dimension(:), allocatable :: inotdropped
  type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
  logical, dimension(:), allocatable :: resonant

  eval%type = EVAL_QN_SUM
  eval%int_in1 => int
  nullify (eval%int_in2)
  if (present (drop)) then

```

```

        dropped = drop
    else
        dropped = .false.
    end if
    ndropped = count (dropped)

    n_in = int%get_n_in ()
    n_out = int%get_n_out () - ndropped
    n_vir = int%get_n_vir ()
    n_tot = int%get_n_tot () - ndropped

    allocate (inotdropped (n_tot))
    i = 1
    do j = 1, n_tot + ndropped
        if (dropped (j)) cycle
        inotdropped(i) = j
        i = i + 1
    end do

    allocate (mask(n_tot + ndropped))
    mask = int%get_mask ()
    allocate (resonant(n_tot + ndropped))
    resonant = int%get_resonance_flags ()
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, &
        mask = mask(inotdropped) .or. qn_mask(inotdropped), &
        resonant = resonant(inotdropped))
    i = 1
    do j = 1, n_tot + ndropped
        if (dropped(j)) cycle
        call eval%set_source_link (i, int, j)
        i = i + 1
    end do
    allocate (map(n_tot + ndropped))
    i = 1
    do j = 1, n_tot + ndropped
        if (dropped (j)) then
            map(j) = 0
        else
            map(j) = i
            i = i + 1
        end if
    end do
    call int%transfer_relations (eval, map)

    n_me_old = int%get_n_matrix_elements ()
    allocate (pairing_size (n_me_old), source = 0)
    allocate (pairing_target (n_me_old), source = 0)
    pairing_size = 0
    state_old => int%get_state_matrix_ptr ()
    state_new => eval%get_state_matrix_ptr ()
    call it_old%init (state_old)
    allocate (qn(n_tot + ndropped))
    do while (it_old%is_valid ())
        qn = it_old%get_quantum_numbers ()
    end do

```

```

    if (.not. all (qn%are_diagonal ())) then
        call it_old%advance ()
        cycle
    end if
    matched = .false.
    call it_new%init (state_new)
    if (eval%get_n_matrix_elements () > 0) then
        do while (it_new%is_valid ())
            if (all (qn(inotdropped) .match. &
                it_new%get_quantum_numbers ())) &
            then
                matched = .true.
                i = it_new%get_me_index ()
                exit
            end if
            call it_new%advance ()
        end do
    end if
    if (.not. matched) then
        call eval%add_state (qn(inotdropped))
        i = eval%get_n_matrix_elements ()
    end if
    pairing_size(i) = pairing_size(i) + 1
    pairing_target(it_old%get_me_index ()) = i
    call it_old%advance ()
end do
call eval%freeze ()

n_me_new = eval%get_n_matrix_elements ()
allocate (eval%pairing_array (n_me_new))
do i = 1, n_me_new
    call pairing_array_init (eval%pairing_array(i), &
        pairing_size(i), .false., .false.)
end do

allocate (i_new (n_me_new), source = 0)
do i = 1, n_me_old
    j = pairing_target(i)
    if (j > 0) then
        i_new(j) = i_new(j) + 1
        eval%pairing_array(j)%i1(i_new(j)) = i
    end if
end do

end subroutine evaluator_init_qn_sum

```

12.3.8 Evaluation

When the input interactions (which are pointed to in the pairings stored within the evaluator) are filled with values, we can activate the evaluator, i.e., calculate the result values which are stored in the interaction.

The evaluation of matrix elements can be done in parallel. A `forall` con-

struct is not appropriate, however. We would need `do concurrent` here. Nevertheless, the evaluation functions are marked as `pure`.

(Evaluators: evaluator: TBP)+≡

```
procedure :: evaluate => evaluator_evaluate
```

(Evaluators: sub interfaces)+≡

```
module subroutine evaluator_evaluate (eval)
  class(evaluator_t), intent(inout), target :: eval
end subroutine evaluator_evaluate
```

(Evaluators: procedures)+≡

```
module subroutine evaluator_evaluate (eval)
  class(evaluator_t), intent(inout), target :: eval
  integer :: i
  select case (eval%type)
  case (EVAL_PRODUCT)
    do i = 1, size(eval%pairing_array)
      call eval%evaluate_product (i, &
        eval%int_in1, eval%int_in2, &
        eval%pairing_array(i)%i1, eval%pairing_array(i)%i2)
      if (debug2_active (D_QFT)) then
        print *, 'eval%pairing_array(i)%i1, eval%pairing_array(i)%i2 = ', &
          eval%pairing_array(i)%i1, eval%pairing_array(i)%i2
        print *, 'MEs = ', &
          eval%int_in1%get_matrix_element (eval%pairing_array(i)%i1), &
          eval%int_in2%get_matrix_element (eval%pairing_array(i)%i2)
      end if
    end do
  case (EVAL_SQUARE_WITH_COLOR_FACTORS)
    do i = 1, size(eval%pairing_array)
      call eval%evaluate_product_cf (i, &
        eval%int_in1, eval%int_in1, &
        eval%pairing_array(i)%i1, eval%pairing_array(i)%i2, &
        eval%pairing_array(i)%factor)
    end do
  case (EVAL_SQUARED_FLOWS)
    do i = 1, size(eval%pairing_array)
      call eval%evaluate_square_c (i, &
        eval%int_in1, &
        eval%pairing_array(i)%i1)
    end do
  case (EVAL_COLOR_CONTRACTION)
    do i = 1, size(eval%pairing_array)
      call eval%evaluate_sum (i, &
        eval%int_in1, &
        eval%pairing_array(i)%i1)
    end do
  case (EVAL_IDENTITY)
    call eval%set_matrix_element (eval%int_in1)
  case (EVAL_QN_SUM)
    do i = 1, size (eval%pairing_array)
      call eval%evaluate_me_sum (i, &
        eval%int_in1, eval%pairing_array(i)%i1)
      call eval%set_norm (eval%int_in1%get_norm ())
    end do
```



```

        end select
    end subroutine evaluator_evaluate

```

12.3.9 Unit tests

Test module, followed by the corresponding implementation module.

(evaluators_ut.f90)≡
(File header)

```

module evaluators_ut
    use unit_tests
    use evaluators_uti

```

(Standard module head)

(Evaluators: public test)

contains

(Evaluators: test driver)

```

end module evaluators_ut

```

(evaluators_uti.f90)≡
(File header)

```

module evaluators_uti

```

(Use kinds)

```

    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use interactions
    use model_data

```

```

    use evaluators

```

(Standard module head)

(Evaluators: test declarations)

contains

(Evaluators: tests)

```

end module evaluators_uti

```

API: driver for the unit tests below.

(Evaluators: public test)≡
 public :: evaluator_test

```

<Evaluators: test driver>≡
  subroutine evaluator_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Evaluators: execute tests>
  end subroutine evaluator_test

```

Test: Create two interactions. The interactions are twofold connected. The first connection has a helicity index that is kept, the second connection has a helicity index that is summed over. Concatenate the interactions in an evaluator, which thus contains a result interaction. Fill the input interactions with values, activate the evaluator and print the result.

```

<Evaluators: execute tests>≡
  call test (evaluator_1, "evaluator_1", &
    "check evaluators (1)", &
    u, results)

<Evaluators: test declarations>≡
  public :: evaluator_1

<Evaluators: tests>≡
  subroutine evaluator_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(interaction_t), target :: int_qqtt, int_tbw, int1, int2
    type(flavor_t), dimension(:), allocatable :: flv
    type(color_t), dimension(:), allocatable :: col
    type(helicity_t), dimension(:), allocatable :: hel
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: f, c, h1, h2, h3
    type(vector4_t), dimension(4) :: p
    type(vector4_t), dimension(2) :: q
    type(quantum_numbers_mask_t) :: qn_mask_conn
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask2
    type(evaluator_t), target :: eval, eval2, eval3

    call model%init_sm_test ()

    write (u, "(A)")   "*** Evaluator for matrix product"
    write (u, "(A)")   "***   Construct interaction for qq -> tt"
    write (u, "(A)")
    call int_qqtt%basic_init (2, 0, 2, set_relations=.true.)
    allocate (flv (4), col (4), hel (4), qn (4))
    allocate (qn_mask2 (4))
    do c = 1, 2
      select case (c)
      case (1)
        call col%init_col_acl ([1, 0, 1, 0], [0, 2, 0, 2])
      case (2)
        call col%init_col_acl ([1, 0, 2, 0], [0, 1, 0, 2])
      end select
    do f = 1, 2
      call flv%init ([f, -f, 6, -6], model)
      do h1 = -1, 1, 2

```

```

        call hel(3)%init (h1)
        do h2 = -1, 1, 2
            call hel(4)%init (h2)
            call qn%init (flv, col, hel)
            call int_qqtt%add_state (qn)
        end do
    end do
end do
call int_qqtt%freeze ()
deallocate (flv, col, hel, qn)
write (u, "(A)")  "**** Construct interaction for t -> bW"
call int_tbw%basic_init (1, 0, 2, set_relations=.true.)
allocate (flv (3), col (3), hel (3), qn (3))
call flv%init ([6, 5, 24], model)
call col%init_col_acl ([1, 1, 0], [0, 0, 0])
do h1 = -1, 1, 2
    call hel(1)%init (h1)
    do h2 = -1, 1, 2
        call hel(2)%init (h2)
        do h3 = -1, 1
            call hel(3)%init (h3)
            call qn%init (flv, col, hel)
            call int_tbw%add_state (qn)
        end do
    end do
end do
call int_tbw%freeze ()
deallocate (flv, col, hel, qn)
write (u, "(A)")  "**** Link interactions"
call int_tbw%set_source_link (1, int_qqtt, 3)
qn_mask_conn = quantum_numbers_mask (.false.,.false.,.true.)
write (u, "(A)")
write (u, "(A)")  "**** Show input"
call int_qqtt%basic_write (unit = u)
write (u, "(A)")
call int_tbw%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)")  "**** Evaluate product"
call eval%init_product (int_qqtt, int_tbw, qn_mask_conn)
call eval%write (unit = u)

call int1%basic_init (2, 0, 2, set_relations=.true.)
call int2%basic_init (1, 0, 2, set_relations=.true.)
p(1) = vector4_moving (1000._default, 1000._default, 3)
p(2) = vector4_moving (200._default, 200._default, 2)
p(3) = vector4_moving (100._default, 200._default, 1)
p(4) = p(1) - p(2) - p(3)
call int1%set_momenta (p)
q(1) = vector4_moving (50._default,-50._default, 3)
q(2) = p(2) + p(4) - q(1)
call int2%set_momenta (q, outgoing=.true.)
call int1%set_matrix_element ([ (2._default,0._default), &
    (4._default,1._default), (-3._default,0._default)])

```

```

call int2%set_matrix_element ([(-3._default,0._default), &
    (0._default,1._default), (1._default,2._default)])
call eval%receive_momenta ()
call eval%evaluate ()
call int1%basic_write (unit = u)
write (u, "(A)")
call int2%basic_write (unit = u)
write (u, "(A)")
call eval%write (unit = u)
write (u, "(A)")
call int1%final ()
call int2%final ()
call eval%final ()

write (u, "(A)")
write (u, "(A)")    "*** Evaluator for matrix square"
allocate (flv(4), col(4), qn(4))
call int1%basic_init (2, 0, 2, set_relations=.true.)
call flv%init ([1, -1, 21, 21], model)
call col(1)%init ([1])
call col(2)%init ([-2])
call col(3)%init ([2, -3])
call col(4)%init ([3, -1])
call qn%init (flv, col)
call int1%add_state (qn)
call col(3)%init ([3, -1])
call col(4)%init ([2, -3])
call qn%init (flv, col)
call int1%add_state (qn)
call col(3)%init ([2, -1])
call col(4)%init (.true.)
call qn%init (flv, col)
call int1%add_state (qn)
call int1%freeze ()
! [qn_mask2 not set since default is false]
call eval%init_square (int1, qn_mask2, nc=3)
call eval2%init_square_nondiag (int1, qn_mask2)
qn_mask2 = quantum_numbers_mask (.false., .true., .true.)
call eval3%init_square_diag (eval, qn_mask2)
call int1%set_matrix_element &
    ([ (2._default,0._default), &
        (4._default,1._default), (-3._default,0._default)])
call int1%set_momenta (p)
call int1%basic_write (unit = u)
write (u, "(A)")
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (unit = u)
write (u, "(A)")
call eval2%receive_momenta ()
call eval2%evaluate ()
call eval2%write (unit = u)
write (u, "(A)")
call eval3%receive_momenta ()

```

```

        call eval3%evaluate ()
        call eval3%write (unit = u)
        call int1%final ()
        call eval%final ()
        call eval2%final ()
        call eval3%final ()

        call model%final ()
    end subroutine evaluator_1

<Evaluators: execute tests>+≡
    call test (evaluator_2, "evaluator_2", &
        "check evaluators (2)", &
        u, results)

<Evaluators: test declarations>+≡
    public :: evaluator_2

<Evaluators: tests>+≡
    subroutine evaluator_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(interaction_t), target :: int
        integer :: h1, h2, h3, h4
        type(helicity_t), dimension(4) :: hel
        type(color_t), dimension(4) :: col
        type(flavor_t), dimension(4) :: flv
        type(quantum_numbers_t), dimension(4) :: qn
        type(vector4_t), dimension(4) :: p
        type(evaluator_t) :: eval
        integer :: i

        call model%init_sm_test ()

        write (u, "(A)") "*** Creating interaction for e+ e- -> W+ W-"
        write (u, "(A)")

        call flv%init ([11, -11, 24, -24], model)
        do i = 1, 4
            call col(i)%init ()
        end do
        call int%basic_init (2, 0, 2, set_relations=.true.)
        do h1 = -1, 1, 2
            call hel(1)%init (h1)
            do h2 = -1, 1, 2
                call hel(2)%init (h2)
                do h3 = -1, 1
                    call hel(3)%init (h3)
                    do h4 = -1, 1
                        call hel(4)%init (h4)
                        call qn%init (flv, col, hel)
                        call int%add_state (qn)
                    end do
                end do
            end do
        end do
    end do
end do

```

```

end do
call int%freeze ()
call int%set_matrix_element &
    [(cplx (i, kind=default), i = 1, 36)]
p(1) = vector4_moving (1000._default, 1000._default, 3)
p(2) = vector4_moving (1000._default, -1000._default, 3)
p(3) = vector4_moving (1000._default, &
    sqrt (1E6_default - 80._default**2), 3)
p(4) = p(1) + p(2) - p(3)
call int%set_momenta (p)
write (u, "(A)") "*** Setting up evaluator"
write (u, "(A)")

call eval%init_identity (int)
write (u, "(A)") "*** Transferring momenta and evaluating"
write (u, "(A)")

call eval%receive_momenta ()
call eval%evaluate ()
write (u, "(A)") "*****"
write (u, "(A)") "    Interaction dump"
write (u, "(A)") "*****"
call int%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)") "*****"
write (u, "(A)") "    Evaluator dump"
write (u, "(A)") "*****"
call eval%write (unit = u)
write (u, "(A)")
write (u, "(A)") "*** cleaning up"
call int%final ()
call eval%final ()

call model%final ()
end subroutine evaluator_2

```

(Evaluators: execute tests)+≡

```

call test (evaluator_3, "evaluator_3", &
    "check evaluators (3)", &
    u, results)

```

(Evaluators: test declarations)+≡

```

public :: evaluator_3

```

(Evaluators: tests)+≡

```

subroutine evaluator_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(interaction_t), target :: int
    integer :: h1, h2, h3, h4
    type(helicity_t), dimension(4) :: hel
    type(color_t), dimension(4) :: col
    type(flavor_t), dimension(4) :: flv1, flv2
    type(quantum_numbers_t), dimension(4) :: qn
    type(vector4_t), dimension(4) :: p

```

```

type(evaluator_t) :: eval1, eval2, eval3
type(quantum_numbers_mask_t), dimension(4) :: qn_mask
integer :: i

call model%init_sm_test ()

write (u, "(A)")  "*** Creating interaction for e+/mu+ e-/mu- -> W+ W-"
call flv1%init ([11, -11, 24, -24], model)
call flv2%init ([13, -13, 24, -24], model)
do i = 1, 4
    call col (i)%init ()
end do
call int%basic_init (2, 0, 2, set_relations=.true.)
do h1 = -1, 1, 2
    call hel(1)%init (h1)
    do h2 = -1, 1, 2
        call hel(2)%init (h2)
        do h3 = -1, 1
            call hel(3)%init (h3)
            do h4 = -1, 1
                call hel(4)%init (h4)
                call qn%init (flv1, col, hel)
                call int%add_state (qn)
                call qn%init (flv2, col, hel)
                call int%add_state (qn)
            end do
        end do
    end do
end do
call int%freeze ()
call int%set_matrix_element &
    [(cplx (1, kind=default), i = 1, 72)]
p(1) = vector4_moving (1000._default, 1000._default, 3)
p(2) = vector4_moving (1000._default, -1000._default, 3)
p(3) = vector4_moving (1000._default, &
    sqrt (1E6_default - 80._default**2), 3)
p(4) = p(1) + p(2) - p(3)
call int%set_momenta (p)
write (u, "(A)")  "*** Setting up evaluators"
call qn_mask%init (.false., .true., .true.)
call eval1%init_qn_sum (int, qn_mask)
call qn_mask%init (.true., .true., .true.)
call eval2%init_qn_sum (int, qn_mask)
call qn_mask%init (.false., .true., .false.)
call eval3%init_qn_sum (int, qn_mask, &
    [.false., .false., .false., .true.])
write (u, "(A)")  "*** Transferring momenta and evaluating"
call eval1%receive_momenta ()
call eval1%evaluate ()
call eval2%receive_momenta ()
call eval2%evaluate ()
call eval3%receive_momenta ()
call eval3%evaluate ()
write (u, "(A)")  "*****"

```

```

write (u, "(A)") "    Interaction dump"
write (u, "(A)") "*****"
call int%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)") "*****"
write (u, "(A)") "    Evaluator dump -- spin sum"
write (u, "(A)") "*****"
call eval1%write (unit = u)
call eval1%basic_write (unit = u)
write (u, "(A)") "*****"
write (u, "(A)") "    Evaluator dump -- spin / flavor sum"
write (u, "(A)") "*****"
call eval2%write (unit = u)
call eval2%basic_write (unit = u)
write (u, "(A)") "*****"
write (u, "(A)") "    Evaluator dump -- flavor sum, drop last W"
write (u, "(A)") "*****"
call eval3%write (unit = u)
call eval3%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)") "*** cleaning up"
call int%final ()
call eval1%final ()
call eval2%final ()
call eval3%final ()

call model%final ()
end subroutine evaluator_3

```

This test evaluates a product with different quantum-number masks and filters for the linked entry.

```

<Evaluators: execute tests>+≡
call test (evaluator_4, "evaluator_4", &
  "check evaluator product with filter", &
  u, results)

<Evaluators: test declarations>+≡
public :: evaluator_4

<Evaluators: tests>+≡
subroutine evaluator_4 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(interaction_t), target :: int1, int2
  integer :: h1, h2, h3
  type(helicity_t), dimension(3) :: hel
  type(color_t), dimension(3) :: col
  type(flavor_t), dimension(2) :: flv1, flv2
  type(flavor_t), dimension(3) :: flv3, flv4
  type(quantum_numbers_t), dimension(3) :: qn
  type(evaluator_t) :: eval1, eval2, eval3, eval4
  type(quantum_numbers_mask_t) :: qn_mask
  type(flavor_t) :: flv_filter
  type(helicity_t) :: hel_filter
  type(color_t) :: col_filter

```



```

type(quantum_numbers_t) :: qn_filter
integer :: i

write (u, "(A)")  "* Test output: evaluator_4"
write (u, "(A)")  "* Purpose: test evaluator products &
                  &with mask and filter"
write (u, "(A)")

call model%init_sm_test ()

write (u, "(A)")  "* Creating interaction for e- -> W+/Z"
write (u, "(A)")

call flv1%init ([11, 24], model)
call flv2%init ([11, 23], model)
do i = 1, 3
    call col(i)%init ()
end do
call int1%basic_init (1, 0, 1, set_relations=.true.)
do h1 = -1, 1, 2
    call hel(1)%init (h1)
    do h2 = -1, 1
        call hel(2)%init (h2)
        call qn(:2)%init (flv1, col(:2), hel(:2))
        call int1%add_state (qn(:2))
        call qn(:2)%init (flv2, col(:2), hel(:2))
        call int1%add_state (qn(:2))
    end do
end do
call int1%freeze ()
call int1%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Creating interaction for W+/Z -> u ubar/dbar"
write (u, "(A)")

call flv3%init ([24, 2, -1], model)
call flv4%init ([23, 2, -2], model)

call int2%basic_init (1, 0, 2, set_relations=.true.)
do h1 = -1, 1
    call hel(1)%init (h1)
    do h2 = -1, 1, 2
        call hel(2)%init (h2)
        do h3 = -1, 1, 2
            call hel(3)%init (h3)
            call qn(:3)%init (flv3, col(:3), hel(:3))
            call int2%add_state (qn(:3))
            call qn(:3)%init (flv4, col(:3), hel(:3))
            call int2%add_state (qn(:3))
        end do
    end do
end do
call int2%freeze ()

```

```

call int2%set_source_link (1, int1, 2)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Product evaluator"
write (u, "(A)")

call qn_mask%init (.false., .false., .false.)
call eval1%init_product (int1, int2, qn_mask_conn = qn_mask)
call eval1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product evaluator with helicity mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call eval2%init_product (int1, int2, qn_mask_conn = qn_mask)
call eval2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product with flavor filter and helicity mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call flv_filter%init (24, model)
call hel_filter%init ()
call col_filter%init ()
call qn_filter%init (flv_filter, col_filter, hel_filter)
call eval3%init_product (int1, int2, &
    qn_mask_conn = qn_mask, qn_filter_conn = qn_filter)
call eval3%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product with helicity filter and mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call flv_filter%init ()
call hel_filter%init (0)
call col_filter%init ()
call qn_filter%init (flv_filter, col_filter, hel_filter)
call eval4%init_product (int1, int2, &
    qn_mask_conn = qn_mask, qn_filter_conn = qn_filter)
call eval4%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eval1%final ()
call eval2%final ()
call eval3%final ()
call eval4%final ()

```

```
call int1%final ()
call int2%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: evaluator_4"

end subroutine evaluator_4
```

Chapter 13

Sindarin Built-In Types

Here, we define a couple of types and objects which are useful both internally for WHIZARD, and visible to the user, so they correspond to Sindarin types.

particle_specifiers Expressions for particles and particle alternatives, involving particle names.

pdg_arrays Integer (PDG) codes for particles. Useful for particle aliases (e.g., 'quark' for u, d, s etc.).

jets Define (pseudo)jets as objects. Functional only if the **fastjet** library is linked. (This may change in the future.)

subevents Particle collections built from event records, for use in analysis and other Sindarin expressions

analysis Observables, histograms, and plots.

13.1 Particle Specifiers

In this module we introduce a type for specifying a particle or particle alternative. In addition to the particle specifiers (strings separated by colons), the type contains an optional flag **polarized** and a string **decay**. If the **polarized** flag is set, particle polarization information should be kept when generating events for this process. If the **decay** string is set, it is the ID of a decay process which should be applied to this particle when generating events.

In input/output form, the **polarized** flag is indicated by an asterisk (*) in brackets, and the **decay** is indicated by its ID in brackets.

The **read** and **write** procedures in this module are not type-bound but generic procedures which handle scalar and array arguments.

```
<particle_specifiers.f90>≡  
  <File header>
```

```
  module particle_specifiers
```

```
    <Use strings>
```

```
    <Standard module head>
```

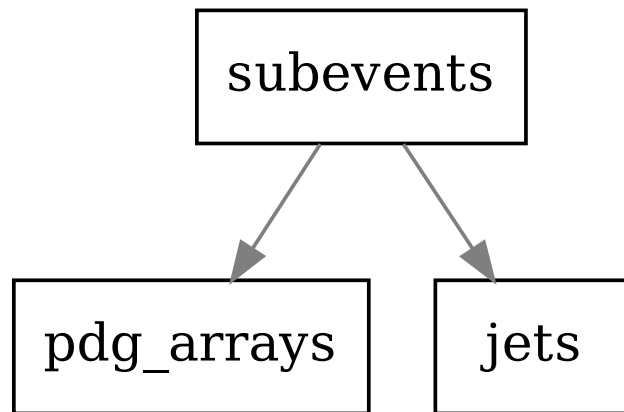


Figure 13.1: Module dependencies in `src/types`.

```

<Particle specifiers: public>

<Particle specifiers: types>

<Particle specifiers: interfaces>

  interface
<Particle specifiers: sub interfaces>
  end interface

contains

<Particle specifiers: main procedures>

end module particle_specifiers
<particle_specifiers_sub.f90>≡
<File header>

submodule (particle_specifiers) particle_specifiers_s

  use io_units
  use diagnostics

  implicit none

```

```
contains

⟨Particle specifiers: procedures⟩

end submodule particle_specifiers_s
```

13.1.1 Base type

This is an abstract type which can hold a single particle or an expression.

```
⟨Particle specifiers: types⟩≡
  type, abstract :: prt_spec_expr_t
  contains
  ⟨Particle specifiers: prt spec expr: TBP⟩
end type prt_spec_expr_t
```

Output, as a string.

```
⟨Particle specifiers: prt spec expr: TBP⟩≡
  procedure (prt_spec_expr_to_string), deferred :: to_string

⟨Particle specifiers: interfaces⟩≡
  abstract interface
    function prt_spec_expr_to_string (object) result (string)
    import
      class(prt_spec_expr_t), intent(in) :: object
      type(string_t) :: string
    end function prt_spec_expr_to_string
  end interface
```

Call an `expand` method for all enclosed subexpressions (before handling the current expression).

```
⟨Particle specifiers: prt spec expr: TBP⟩+≡
  procedure (prt_spec_expr_expand_sub), deferred :: expand_sub

⟨Particle specifiers: interfaces⟩+≡
  abstract interface
    subroutine prt_spec_expr_expand_sub (object)
    import
      class(prt_spec_expr_t), intent(inout) :: object
    end subroutine prt_spec_expr_expand_sub
  end interface
```

13.1.2 Wrapper type

This wrapper can hold a particle expression of any kind. We need it so we can make variadic arrays.

```
⟨Particle specifiers: public⟩≡
  public :: prt_expr_t
```

```

<Particle specifiers: types>+≡
  type :: prt_expr_t
    class(prt_spec_expr_t), allocatable :: x
    contains
    <Particle specifiers: prt expr: TBP>
  end type prt_expr_t

```

Output as a string: delegate.

```

<Particle specifiers: prt expr: TBP>≡
  procedure :: to_string => prt_expr_to_string

<Particle specifiers: sub interfaces>≡
  recursive module function prt_expr_to_string (object) result (string)
    class(prt_expr_t), intent(in) :: object
    type(string_t) :: string
  end function prt_expr_to_string

<Particle specifiers: procedures>≡
  recursive module function prt_expr_to_string (object) result (string)
    class(prt_expr_t), intent(in) :: object
    type(string_t) :: string
    if (allocated (object%x)) then
      string = object%x%to_string ()
    else
      string = ""
    end if
  end function prt_expr_to_string

```

Allocate the expression as a particle specifier and copy the value. Due to compiler bugs in gfortran 7-9 not in submodule.

```

<Particle specifiers: prt expr: TBP>+≡
  procedure :: init_spec => prt_expr_init_spec

<Particle specifiers: main procedures>≡
  subroutine prt_expr_init_spec (object, spec)
    class(prt_expr_t), intent(out) :: object
    type(prt_spec_t), intent(in) :: spec
    allocate (prt_spec_t :: object%x)
    select type (x => object%x)
    type is (prt_spec_t)
      x = spec
    end select
  end subroutine prt_expr_init_spec

```

Allocate as a list/sum and allocate for a given length Due to compiler bugs in gfortran 7-9 not in submodule.

```

<Particle specifiers: prt expr: TBP>+≡
  procedure :: init_list => prt_expr_init_list
  procedure :: init_sum => prt_expr_init_sum

<Particle specifiers: main procedures>+≡
  subroutine prt_expr_init_list (object, n)
    class(prt_expr_t), intent(out) :: object
    integer, intent(in) :: n

```

```

        allocate (prt_spec_list_t :: object%x)
        select type (x => object%x)
        type is (prt_spec_list_t)
            allocate (x%expr (n))
        end select
    end subroutine prt_expr_init_list

    subroutine prt_expr_init_sum (object, n)
        class(prt_expr_t), intent(out) :: object
        integer, intent(in) :: n
        allocate (prt_spec_sum_t :: object%x)
        select type (x => object%x)
        type is (prt_spec_sum_t)
            allocate (x%expr (n))
        end select
    end subroutine prt_expr_init_sum

```

Return the number of terms. This is unity, except if the expression is a sum.

(Particle specifiers: prt expr: TBP)+≡

```

    procedure :: get_n_terms => prt_expr_get_n_terms

```

(Particle specifiers: sub interfaces)+≡

```

    module function prt_expr_get_n_terms (object) result (n)
        class(prt_expr_t), intent(in) :: object
        integer :: n
    end function prt_expr_get_n_terms

```

(Particle specifiers: procedures)+≡

```

    module function prt_expr_get_n_terms (object) result (n)
        class(prt_expr_t), intent(in) :: object
        integer :: n
        if (allocated (object%x)) then
            select type (x => object%x)
            type is (prt_spec_sum_t)
                n = size (x%expr)
            class default
                n = 1
            end select
        else
            n = 0
        end if
    end function prt_expr_get_n_terms

```

Transform one of the terms, as returned by the previous method, to an array of particle specifiers. The array has more than one entry if the selected term is a list. This makes sense only if the expression has been completely expanded, so the list contains only atoms.

(Particle specifiers: prt expr: TBP)+≡

```

    procedure :: term_to_array => prt_expr_term_to_array

```

(Particle specifiers: sub interfaces)+≡

```

    recursive module subroutine prt_expr_term_to_array (object, array, i)
        class(prt_expr_t), intent(in) :: object
        type(prt_spec_t), dimension(:), intent(inout), allocatable :: array
    end subroutine prt_expr_term_to_array

```



```

        integer, intent(in) :: i
    end subroutine prt_expr_term_to_array
<Particle specifiers: procedures>+≡
recursive module subroutine prt_expr_term_to_array (object, array, i)
    class(prt_expr_t), intent(in) :: object
    type(prt_spec_t), dimension(:), intent(inout), allocatable :: array
    integer, intent(in) :: i
    integer :: j
    if (allocated (array)) deallocate (array)
    select type (x => object%x)
    type is (prt_spec_t)
        allocate (array (1))
        array(1) = x
    type is (prt_spec_list_t)
        allocate (array (size (x%expr)))
        do j = 1, size (array)
            select type (y => x%expr(j)%x)
            type is (prt_spec_t)
                array(j) = y
            end select
        end do
    type is (prt_spec_sum_t)
        call x%expr(i)%term_to_array (array, 1)
    end select
end subroutine prt_expr_term_to_array

```

13.1.3 The atomic type

The trivial case is a single particle, including optional decay and polarization attributes.

Definition

The particle is unstable if the `decay` array is allocated. The `polarized` flag and decays may not be set simultaneously.

```

<Particle specifiers: public>+≡
    public :: prt_spec_t
<Particle specifiers: types>+≡
    type, extends (prt_spec_expr_t) :: prt_spec_t
    private
    type(string_t) :: name
    logical :: polarized = .false.
    type(string_t), dimension(:), allocatable :: decay
    contains
    <Particle specifiers: prt spec: TBP>
end type prt_spec_t

```

I/O

Output. Old-style subroutines.

```
<Particle specifiers: public>+≡
    public :: prt_spec_write

<Particle specifiers: interfaces>+≡
    interface prt_spec_write
        module procedure prt_spec_write1
        module procedure prt_spec_write2
    end interface prt_spec_write

<Particle specifiers: sub interfaces>+≡
    module subroutine prt_spec_write1 (object, unit, advance)
        type(prt_spec_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(len=*), intent(in), optional :: advance
    end subroutine prt_spec_write1

<Particle specifiers: procedures>+≡
    module subroutine prt_spec_write1 (object, unit, advance)
        type(prt_spec_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(len=*), intent(in), optional :: advance
        character(3) :: adv
        integer :: u
        u = given_output_unit (unit)
        adv = "yes"; if (present (advance)) adv = advance
        write (u, "(A)", advance = adv) char (object%to_string ())
    end subroutine prt_spec_write1
```

Write an array as a list of particle specifiers.

```
<Particle specifiers: sub interfaces>+≡
    module subroutine prt_spec_write2 (prt_spec, unit, advance)
        type(prt_spec_t), dimension(:), intent(in) :: prt_spec
        integer, intent(in), optional :: unit
        character(len=*), intent(in), optional :: advance
    end subroutine prt_spec_write2

<Particle specifiers: procedures>+≡
    module subroutine prt_spec_write2 (prt_spec, unit, advance)
        type(prt_spec_t), dimension(:), intent(in) :: prt_spec
        integer, intent(in), optional :: unit
        character(len=*), intent(in), optional :: advance
        character(3) :: adv
        integer :: u, i
        u = given_output_unit (unit)
        adv = "yes"; if (present (advance)) adv = advance
        do i = 1, size (prt_spec)
            if (i > 1) write (u, "(A)", advance="no") " ", "
            call prt_spec_write (prt_spec(i), u, advance="no")
        end do
        write (u, "(A)", advance = adv)
    end subroutine prt_spec_write2
```

Read. Input may be string or array of strings.

(Particle specifiers: public)+≡

```
public :: prt_spec_read
```

(Particle specifiers: interfaces)+≡

```
interface prt_spec_read
  module procedure prt_spec_read1
  module procedure prt_spec_read2
end interface prt_spec_read
```

Read a single particle specifier

(Particle specifiers: sub interfaces)+≡

```
pure module subroutine prt_spec_read1 (prt_spec, string)
  type(prt_spec_t), intent(out) :: prt_spec
  type(string_t), intent(in) :: string
end subroutine prt_spec_read1
```

(Particle specifiers: procedures)+≡

```
pure module subroutine prt_spec_read1 (prt_spec, string)
  type(prt_spec_t), intent(out) :: prt_spec
  type(string_t), intent(in) :: string
  type(string_t) :: arg, buffer
  integer :: b1, b2, c, n, i
  b1 = scan (string, "(")
  b2 = scan (string, ")")
  if (b1 == 0) then
    prt_spec%name = trim (adjustl (string))
  else
    prt_spec%name = trim (adjustl (extract (string, 1, b1-1)))
    arg = trim (adjustl (extract (string, b1+1, b2-1)))
    if (arg == "*") then
      prt_spec%polarized = .true.
    else
      n = 0
      buffer = arg
      do
        if (verify (buffer, " ") == 0) exit
        n = n + 1
        c = scan (buffer, "+")
        if (c == 0) exit
        buffer = extract (buffer, c+1)
      end do
      allocate (prt_spec%decay (n))
      buffer = arg
      do i = 1, n
        c = scan (buffer, "+")
        if (c == 0) c = len (buffer) + 1
        prt_spec%decay(i) = trim (adjustl (extract (buffer, 1, c-1)))
        buffer = extract (buffer, c+1)
      end do
    end if
  end if
end subroutine prt_spec_read1
```

Read a particle specifier array, given as a single string. The array is allocated to the correct size.

```

<Particle specifiers: sub interfaces>+≡
    pure module subroutine prt_spec_read2 (prt_spec, string)
        type(prt_spec_t), dimension(:), intent(out), allocatable :: prt_spec
        type(string_t), intent(in) :: string
    end subroutine prt_spec_read2

<Particle specifiers: procedures>+≡
    pure module subroutine prt_spec_read2 (prt_spec, string)
        type(prt_spec_t), dimension(:), intent(out), allocatable :: prt_spec
        type(string_t), intent(in) :: string
        type(string_t) :: buffer
        integer :: c, i, n
        n = 0
        buffer = string
    do
        n = n + 1
        c = scan (buffer, ",")
        if (c == 0) exit
        buffer = extract (buffer, c+1)
    end do
    allocate (prt_spec (n))
    buffer = string
    do i = 1, size (prt_spec)
        c = scan (buffer, ",")
        if (c == 0) c = len (buffer) + 1
        call prt_spec_read (prt_spec(i), &
            trim (adjustl (extract (buffer, 1, c-1))))
        buffer = extract (buffer, c+1)
    end do
end subroutine prt_spec_read2

```

Constructor

Initialize a particle specifier.

```

<Particle specifiers: public>+≡
    public :: new_prt_spec

<Particle specifiers: interfaces>+≡
    interface new_prt_spec
        module procedure new_prt_spec_
        module procedure new_prt_spec_polarized
        module procedure new_prt_spec_unstable
    end interface new_prt_spec

<Particle specifiers: sub interfaces>+≡
    elemental module function new_prt_spec_ (name) result (prt_spec)
        type(string_t), intent(in) :: name
        type(prt_spec_t) :: prt_spec
    end function new_prt_spec_
    elemental module function new_prt_spec_polarized (name, polarized) result (prt_spec)
        type(string_t), intent(in) :: name
        logical, intent(in) :: polarized

```

```

        type(prt_spec_t) :: prt_spec
    end function new_prt_spec_polarized
    pure module function new_prt_spec_unstable (name, decay) result (prt_spec)
        type(string_t), intent(in) :: name
        type(string_t), dimension(:), intent(in) :: decay
        type(prt_spec_t) :: prt_spec
    end function new_prt_spec_unstable
<Particle specifiers: procedures>+≡
    elemental module function new_prt_spec_ (name) result (prt_spec)
        type(string_t), intent(in) :: name
        type(prt_spec_t) :: prt_spec
        prt_spec%name = name
    end function new_prt_spec_

    elemental module function new_prt_spec_polarized (name, polarized) result (prt_spec)
        type(string_t), intent(in) :: name
        logical, intent(in) :: polarized
        type(prt_spec_t) :: prt_spec
        prt_spec%name = name
        prt_spec%polarized = polarized
    end function new_prt_spec_polarized

    pure module function new_prt_spec_unstable (name, decay) result (prt_spec)
        type(string_t), intent(in) :: name
        type(string_t), dimension(:), intent(in) :: decay
        type(prt_spec_t) :: prt_spec
        prt_spec%name = name
        allocate (prt_spec%decay (size (decay)))
        prt_spec%decay = decay
    end function new_prt_spec_unstable

```

Access Methods

Return the particle name without qualifiers

```

<Particle specifiers: prt spec: TBP>≡
    procedure :: get_name => prt_spec_get_name

<Particle specifiers: sub interfaces>+≡
    elemental module function prt_spec_get_name (prt_spec) result (name)
        class(prt_spec_t), intent(in) :: prt_spec
        type(string_t) :: name
    end function prt_spec_get_name

<Particle specifiers: procedures>+≡
    elemental module function prt_spec_get_name (prt_spec) result (name)
        class(prt_spec_t), intent(in) :: prt_spec
        type(string_t) :: name
        name = prt_spec%name
    end function prt_spec_get_name

```

Return the name with qualifiers

```

<Particle specifiers: prt spec: TBP>+≡
    procedure :: to_string => prt_spec_to_string

```

<Particle specifiers: sub interfaces>+≡

```
module function prt_spec_to_string (object) result (string)
  class(prt_spec_t), intent(in) :: object
  type(string_t) :: string
end function prt_spec_to_string
```

<Particle specifiers: procedures>+≡

```
module function prt_spec_to_string (object) result (string)
  class(prt_spec_t), intent(in) :: object
  type(string_t) :: string
  integer :: i
  string = object%name
  if (allocated (object%decay)) then
    string = string // "("
    do i = 1, size (object%decay)
      if (i > 1) string = string // " + "
      string = string // object%decay(i)
    end do
    string = string // ")"
  else if (object%polarized) then
    string = string // "(*)"
  end if
end function prt_spec_to_string
```

Return the polarization flag

<Particle specifiers: prt spec: TBP>+≡

```
procedure :: is_polarized => prt_spec_is_polarized
```

<Particle specifiers: sub interfaces>+≡

```
elemental module function prt_spec_is_polarized (prt_spec) result (flag)
  class(prt_spec_t), intent(in) :: prt_spec
  logical :: flag
end function prt_spec_is_polarized
```

<Particle specifiers: procedures>+≡

```
elemental module function prt_spec_is_polarized (prt_spec) result (flag)
  class(prt_spec_t), intent(in) :: prt_spec
  logical :: flag
  flag = prt_spec%polarized
end function prt_spec_is_polarized
```

The particle is unstable if there is a decay array.

<Particle specifiers: prt spec: TBP>+≡

```
procedure :: is_unstable => prt_spec_is_unstable
```

<Particle specifiers: sub interfaces>+≡

```
elemental module function prt_spec_is_unstable (prt_spec) result (flag)
  class(prt_spec_t), intent(in) :: prt_spec
  logical :: flag
end function prt_spec_is_unstable
```

<Particle specifiers: procedures>+≡

```
elemental module function prt_spec_is_unstable (prt_spec) result (flag)
  class(prt_spec_t), intent(in) :: prt_spec
  logical :: flag
```

```

        flag = allocated (prt_spec%decay)
    end function prt_spec_is_unstable

```

Return the number of decay channels

```

<Particle specifiers: prt spec: TBP>+≡
    procedure :: get_n_decays => prt_spec_get_n_decays

<Particle specifiers: sub interfaces>+≡
    elemental module function prt_spec_get_n_decays (prt_spec) result (n)
        class(prt_spec_t), intent(in) :: prt_spec
        integer :: n
    end function prt_spec_get_n_decays

<Particle specifiers: procedures>+≡
    elemental module function prt_spec_get_n_decays (prt_spec) result (n)
        class(prt_spec_t), intent(in) :: prt_spec
        integer :: n
        if (allocated (prt_spec%decay)) then
            n = size (prt_spec%decay)
        else
            n = 0
        end if
    end function prt_spec_get_n_decays

```

Return the decay channels

```

<Particle specifiers: prt spec: TBP>+≡
    procedure :: get_decays => prt_spec_get_decays

<Particle specifiers: sub interfaces>+≡
    module subroutine prt_spec_get_decays (prt_spec, decay)
        class(prt_spec_t), intent(in) :: prt_spec
        type(string_t), dimension(:), allocatable, intent(out) :: decay
    end subroutine prt_spec_get_decays

<Particle specifiers: procedures>+≡
    module subroutine prt_spec_get_decays (prt_spec, decay)
        class(prt_spec_t), intent(in) :: prt_spec
        type(string_t), dimension(:), allocatable, intent(out) :: decay
        if (allocated (prt_spec%decay)) then
            allocate (decay (size (prt_spec%decay)))
            decay = prt_spec%decay
        else
            allocate (decay (0))
        end if
    end subroutine prt_spec_get_decays

```

Miscellaneous

There is nothing to expand here:

```

<Particle specifiers: prt spec: TBP>+≡
    procedure :: expand_sub => prt_spec_expand_sub

```

```

<Particle specifiers: sub interfaces>+≡
  module subroutine prt_spec_expand_sub (object)
    class(prt_spec_t), intent(inout) :: object
    end subroutine prt_spec_expand_sub

<Particle specifiers: procedures>+≡
  module subroutine prt_spec_expand_sub (object)
    class(prt_spec_t), intent(inout) :: object
    end subroutine prt_spec_expand_sub

```

13.1.4 List

A list of particle specifiers, indicating, e.g., the final state of a process.

```

<Particle specifiers: public>+≡
  public :: prt_spec_list_t

<Particle specifiers: types>+≡
  type, extends (prt_spec_expr_t) :: prt_spec_list_t
    type(prt_spec_expr_t), dimension(:), allocatable :: expr
    contains
    <Particle specifiers: prt spec list: TBP>
  end type prt_spec_list_t

```

Output: Concatenate the components. Insert brackets if the component is also a list. The components of the `expr` array, if any, should all be filled.

```

<Particle specifiers: prt spec list: TBP>≡
  procedure :: to_string => prt_spec_list_to_string

<Particle specifiers: sub interfaces>+≡
  recursive module function prt_spec_list_to_string (object) result (string)
    class(prt_spec_list_t), intent(in) :: object
    type(string_t) :: string
    end function prt_spec_list_to_string

<Particle specifiers: procedures>+≡
  recursive module function prt_spec_list_to_string (object) result (string)
    class(prt_spec_list_t), intent(in) :: object
    type(string_t) :: string
    integer :: i
    string = ""
    if (allocated (object%expr)) then
      do i = 1, size (object%expr)
        if (i > 1) string = string // ", "
        select type (x => object%expr(i)%x)
          type is (prt_spec_list_t)
            string = string // "(" // x%to_string () // ")"
          class default
            string = string // x%to_string ()
        end select
      end do
    end if
  end function prt_spec_list_to_string

```


Flatten: if there is a subexpression which is also a list, include the components as direct members of the current list.

```

(Particle specifiers: prt_spec_list: TBP)+≡
  procedure :: flatten => prt_spec_list_flatten

(Particle specifiers: sub interfaces)+≡
  module subroutine prt_spec_list_flatten (object)
    class(prt_spec_list_t), intent(inout) :: object
  end subroutine prt_spec_list_flatten

(Particle specifiers: procedures)+≡
  module subroutine prt_spec_list_flatten (object)
    class(prt_spec_list_t), intent(inout) :: object
    type(prt_expr_t), dimension(:), allocatable :: tmp_expr
    integer :: i, n_flat, i_flat
    n_flat = 0
    do i = 1, size (object%expr)
      select type (y => object%expr(i)%x)
        type is (prt_spec_list_t)
          n_flat = n_flat + size (y%expr)
        class default
          n_flat = n_flat + 1
      end select
    end do
    if (n_flat > size (object%expr)) then
      allocate (tmp_expr (n_flat))
      i_flat = 0
      do i = 1, size (object%expr)
        select type (y => object%expr(i)%x)
          type is (prt_spec_list_t)
            tmp_expr (i_flat + 1 : i_flat + size (y%expr)) = y%expr
            i_flat = i_flat + size (y%expr)
          class default
            tmp_expr (i_flat + 1) = object%expr(i)
            i_flat = i_flat + 1
        end select
      end do
    end if
    if (allocated (tmp_expr)) &
      call move_alloc (from = tmp_expr, to = object%expr)
  end subroutine prt_spec_list_flatten

```

Convert a list of sums into a sum of lists. (Subexpressions which are not sums are left untouched.) Due to compiler bug in gfortran 7-9 not in submodule.

```

(Particle specifiers: main procedures)+≡
  subroutine distribute_prt_spec_list (object)
    class(prt_spec_expr_t), intent(inout), allocatable :: object
    class(prt_spec_expr_t), allocatable :: new_object
    integer, dimension(:), allocatable :: n, ii
    integer :: k, n_expr, n_terms, i_term
    select type (object)
      type is (prt_spec_list_t)
        n_expr = size (object%expr)
        allocate (n (n_expr), source = 1)

```

```

allocate (ii (n_expr), source = 1)
do k = 1, size (object%expr)
  select type (y => object%expr(k)%x)
  type is (prt_spec_sum_t)
    n(k) = size (y%expr)
  end select
end do
n_terms = product (n)
if (n_terms > 1) then
  allocate (prt_spec_sum_t :: new_object)
  select type (new_object)
  type is (prt_spec_sum_t)
    allocate (new_object%expr (n_terms))
    do i_term = 1, n_terms
      allocate (prt_spec_list_t :: new_object%expr(i_term)%x)
      select type (x => new_object%expr(i_term)%x)
      type is (prt_spec_list_t)
        allocate (x%expr (n_expr))
        do k = 1, n_expr
          select type (y => object%expr(k)%x)
          type is (prt_spec_sum_t)
            x%expr(k) = y%expr(ii(k))
          class default
            x%expr(k) = object%expr(k)
          end select
        end do
      end select
      INCR_INDEX: do k = n_expr, 1, -1
        if (ii(k) < n(k)) then
          ii(k) = ii(k) + 1
          exit INCR_INDEX
        else
          ii(k) = 1
        end if
      end do INCR_INDEX
    end do
  end select
end if
end select
if (allocated (new_object)) call move_alloc (from = new_object, to = object)
end subroutine distribute_prt_spec_list

```

Apply expand to all components of the list.

(Particle specifiers: prt spec list: TBP)+≡

```
procedure :: expand_sub => prt_spec_list_expand_sub
```

(Particle specifiers: sub interfaces)+≡

```

recursive module subroutine prt_spec_list_expand_sub (object)
  class(prt_spec_list_t), intent(inout) :: object
end subroutine prt_spec_list_expand_sub

```

(Particle specifiers: procedures)+≡

```

recursive module subroutine prt_spec_list_expand_sub (object)
  class(prt_spec_list_t), intent(inout) :: object
  integer :: i

```

```

    if (allocated (object%expr)) then
        do i = 1, size (object%expr)
            call object%expr(i)%expand ()
        end do
    end if
end subroutine prt_spec_list_expand_sub

```

13.1.5 Sum

A sum of particle specifiers, indicating, e.g., a sum of final states.

```

<Particle specifiers: public>+≡
    public :: prt_spec_sum_t

<Particle specifiers: types>+≡
    type, extends (prt_spec_expr_t) :: prt_spec_sum_t
        type(prt_spec_expr_t), dimension(:), allocatable :: expr
    contains
        <Particle specifiers: prt spec sum: TBP>
    end type prt_spec_sum_t

```

Output: Concatenate the components. Insert brackets if the component is a list or also a sum. The components of the `expr` array, if any, should all be filled.

```

<Particle specifiers: prt spec sum: TBP>≡
    procedure :: to_string => prt_spec_sum_to_string

<Particle specifiers: sub interfaces>+≡
    recursive module function prt_spec_sum_to_string (object) result (string)
        class(prt_spec_sum_t), intent(in) :: object
        type(string_t) :: string
    end function prt_spec_sum_to_string

<Particle specifiers: procedures>+≡
    recursive module function prt_spec_sum_to_string (object) result (string)
        class(prt_spec_sum_t), intent(in) :: object
        type(string_t) :: string
        integer :: i
        string = ""
        if (allocated (object%expr)) then
            do i = 1, size (object%expr)
                if (i > 1) string = string // " + "
                select type (x => object%expr(i)%x)
                    type is (prt_spec_list_t)
                        string = string // "(" // x%to_string () // ")"
                    type is (prt_spec_sum_t)
                        string = string // "(" // x%to_string () // ")"
                    class default
                        string = string // x%to_string ()
                end select
            end do
        end if
    end function prt_spec_sum_to_string

```

Flatten: if there is a subexpression which is also a sum, include the components as direct members of the current sum.

This is identical to `prt_spec_list_flatten` above, except for the type.

```

(Particle specifiers: prt spec sum: TBP)+≡
  procedure :: flatten => prt_spec_sum_flatten

(Particle specifiers: sub interfaces)+≡
  module subroutine prt_spec_sum_flatten (object)
    class(prt_spec_sum_t), intent(inout) :: object
  end subroutine prt_spec_sum_flatten

(Particle specifiers: procedures)+≡
  module subroutine prt_spec_sum_flatten (object)
    class(prt_spec_sum_t), intent(inout) :: object
    type(prt_expr_t), dimension(:), allocatable :: tmp_expr
    integer :: i, n_flat, i_flat
    n_flat = 0
    do i = 1, size (object%expr)
      select type (y => object%expr(i)%x)
        type is (prt_spec_sum_t)
          n_flat = n_flat + size (y%expr)
        class default
          n_flat = n_flat + 1
      end select
    end do
    if (n_flat > size (object%expr)) then
      allocate (tmp_expr (n_flat))
      i_flat = 0
      do i = 1, size (object%expr)
        select type (y => object%expr(i)%x)
          type is (prt_spec_sum_t)
            tmp_expr (i_flat + 1 : i_flat + size (y%expr)) = y%expr
            i_flat = i_flat + size (y%expr)
          class default
            tmp_expr (i_flat + 1) = object%expr(i)
            i_flat = i_flat + 1
        end select
      end do
    end if
    if (allocated (tmp_expr)) &
      call move_alloc (from = tmp_expr, to = object%expr)
  end subroutine prt_spec_sum_flatten

```

Apply `expand` to all terms in the sum.

```

(Particle specifiers: prt spec sum: TBP)+≡
  procedure :: expand_sub => prt_spec_sum_expand_sub

(Particle specifiers: sub interfaces)+≡
  recursive module subroutine prt_spec_sum_expand_sub (object)
    class(prt_spec_sum_t), intent(inout) :: object
  end subroutine prt_spec_sum_expand_sub

(Particle specifiers: procedures)+≡
  recursive module subroutine prt_spec_sum_expand_sub (object)
    class(prt_spec_sum_t), intent(inout) :: object

```

```

integer :: i
if (allocated (object%expr)) then
  do i = 1, size (object%expr)
    call object%expr(i)%expand ()
  end do
end if
end subroutine prt_spec_sum_expand_sub

```

13.1.6 Expression Expansion

The `expand` method transforms each particle specifier expression into a sum of lists, according to the rules

$$a, (b, c) \rightarrow a, b, c \quad (13.1)$$

$$a + (b + c) \rightarrow a + b + c \quad (13.2)$$

$$a, b + c \rightarrow (a, b) + (a, c) \quad (13.3)$$

Note that the precedence of comma and plus are opposite to this expansion, so the parentheses in the final expression are necessary.

We assume that subexpressions are filled, i.e., arrays are allocated. Do to compiler bug in gfortran 7-9 not in submodule.

```

⟨Particle specifiers: prt expr: TBP⟩+≡
  procedure :: expand => prt_expr_expand

⟨Particle specifiers: main procedures⟩+≡
  recursive subroutine prt_expr_expand (expr)
    class(prt_expr_t), intent(inout) :: expr
    if (allocated (expr%x)) then
      call distribute_prt_spec_list (expr%x)
      call expr%x%expand_sub ()
      select type (x => expr%x)
        type is (prt_spec_list_t)
          call x%flatten ()
        type is (prt_spec_sum_t)
          call x%flatten ()
      end select
    end if
  end subroutine prt_expr_expand

```

13.1.7 Unit Tests

Test module, followed by the corresponding implementation module.

```

⟨particle_specifiers_ut.f90⟩≡
  ⟨File header⟩

  module particle_specifiers_ut
    use unit_tests
    use particle_specifiers_ut

  ⟨Standard module head⟩

```

```

    <Particle specifiers: public test>

contains

    <Particle specifiers: test driver>

end module particle_specifiers_ut
<particle_specifiers_uti.f90>≡
    <File header>

module particle_specifiers_uti

    <Use strings>

    use particle_specifiers

    <Standard module head>

    <Particle specifiers: test declarations>

contains

    <Particle specifiers: tests>

end module particle_specifiers_uti
API: driver for the unit tests below.
<Particle specifiers: public test>≡
    public :: particle_specifiers_test
<Particle specifiers: test driver>≡
    subroutine particle_specifiers_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Particle specifiers: execute tests>
    end subroutine particle_specifiers_test

```

Particle specifier array

Define, read and write an array of particle specifiers.

```

<Particle specifiers: execute tests>≡
    call test (particle_specifiers_1, "particle_specifiers_1", &
        "Handle particle specifiers", &
        u, results)
<Particle specifiers: test declarations>≡
    public :: particle_specifiers_1
<Particle specifiers: tests>≡
    subroutine particle_specifiers_1 (u)
        integer, intent(in) :: u
        type(prt_spec_t), dimension(:), allocatable :: prt_spec
        type(string_t), dimension(:), allocatable :: decay

```

```

type(string_t), dimension(0) :: no_decay
integer :: i, j

write (u, "(A)")  "* Test output: particle_specifiers_1"
write (u, "(A)")  "* Purpose: Read and write a particle specifier array"
write (u, "(A)")

allocate (prt_spec (5))
prt_spec = [ &
    new_prt_spec (var_str ("a")), &
    new_prt_spec (var_str ("b"), .true.), &
    new_prt_spec (var_str ("c"), [var_str ("dec1")]), &
    new_prt_spec (var_str ("d"), [var_str ("dec1"), var_str ("dec2")]), &
    new_prt_spec (var_str ("e"), no_decay) &
]
do i = 1, size (prt_spec)
    write (u, "(A)") char (prt_spec(i)%to_string ())
end do
write (u, "(A)")

call prt_spec_read (prt_spec, &
    var_str (" a, b( *), c( dec1), d (dec1 + dec2 ), e()"))
call prt_spec_write (prt_spec, u)

do i = 1, size (prt_spec)
    write (u, "(A)")
    write (u, "(A,A)") char (prt_spec(i)%get_name ()), ":"
    write (u, "(A,L1)") "polarized = ", prt_spec(i)%is_polarized ()
    write (u, "(A,L1)") "unstable = ", prt_spec(i)%is_unstable ()
    write (u, "(A,I0)") "n_decays = ", prt_spec(i)%get_n_decays ()
    call prt_spec(i)%get_decays (decay)
    write (u, "(A)", advance="no") "decays   ="
    do j = 1, size (decay)
        write (u, "(1x,A)", advance="no") char (decay(j))
    end do
    write (u, "(A)")
end do

write (u, "(A)")
write (u, "(A)")  "* Test output end: particle_specifiers_1"
end subroutine particle_specifiers_1

```

Particle specifier expressions

Nested expressions (only basic particles, no decay specs).

(Particle specifiers: execute tests)+≡

```

call test (particle_specifiers_2, "particle_specifiers_2", &
    "Particle specifier expressions", &
    u, results)

```

(Particle specifiers: test declarations)+≡

```

public :: particle_specifiers_2

```

(Particle specifiers: tests)+≡

```

subroutine particle_specifiers_2 (u)
  integer, intent(in) :: u
  type(prt_spec_t) :: a, b, c, d, e, f
  type(prt_expr_t) :: pe1, pe2, pe3
  type(prt_expr_t) :: pe4, pe5, pe6, pe7, pe8, pe9
  integer :: i
  type(prt_spec_t), dimension(:), allocatable :: pa

  write (u, "(A)")  "* Test output: particle_specifiers_2"
  write (u, "(A)")  "* Purpose: Create and display particle expressions"
  write (u, "(A)")

  write (u, "(A)")  "* Basic expressions"
  write (u, *)

  a = new_prt_spec (var_str ("a"))
  b = new_prt_spec (var_str ("b"))
  c = new_prt_spec (var_str ("c"))
  d = new_prt_spec (var_str ("d"))
  e = new_prt_spec (var_str ("e"))
  f = new_prt_spec (var_str ("f"))

  call pe1%init_spec (a)
  write (u, "(A)")  char (pe1%to_string ())

  call pe2%init_sum (2)
  select type (x => pe2%x)
  type is (prt_spec_sum_t)
    call x%expr(1)%init_spec (a)
    call x%expr(2)%init_spec (b)
  end select
  write (u, "(A)")  char (pe2%to_string ())

  call pe3%init_list (2)
  select type (x => pe3%x)
  type is (prt_spec_list_t)
    call x%expr(1)%init_spec (a)
    call x%expr(2)%init_spec (b)
  end select
  write (u, "(A)")  char (pe3%to_string ())

  write (u, *)
  write (u, "(A)")  "* Nested expressions"
  write (u, *)

  call pe4%init_list (2)
  select type (x => pe4%x)
  type is (prt_spec_list_t)
    call x%expr(1)%init_sum (2)
    select type (y => x%expr(1)%x)
    type is (prt_spec_sum_t)
      call y%expr(1)%init_spec (a)
      call y%expr(2)%init_spec (b)
    end select
  end select

```



```

        end select
        call x%expr(2)%init_spec (c)
    end select
    write (u, "(A)")  char (pe4%to_string ())

    call pe5%init_list (2)
    select type (x => pe5%x)
    type is (prt_spec_list_t)
        call x%expr(1)%init_list (2)
        select type (y => x%expr(1)%x)
        type is (prt_spec_list_t)
            call y%expr(1)%init_spec (a)
            call y%expr(2)%init_spec (b)
        end select
        call x%expr(2)%init_spec (c)
    end select
    write (u, "(A)")  char (pe5%to_string ())

    call pe6%init_sum (2)
    select type (x => pe6%x)
    type is (prt_spec_sum_t)
        call x%expr(1)%init_spec (a)
        call x%expr(2)%init_sum (2)
        select type (y => x%expr(2)%x)
        type is (prt_spec_sum_t)
            call y%expr(1)%init_spec (b)
            call y%expr(2)%init_spec (c)
        end select
    end select
    write (u, "(A)")  char (pe6%to_string ())

    call pe7%init_list (2)
    select type (x => pe7%x)
    type is (prt_spec_list_t)
        call x%expr(1)%init_sum (2)
        select type (y => x%expr(1)%x)
        type is (prt_spec_sum_t)
            call y%expr(1)%init_spec (a)
            call y%expr(2)%init_list (2)
            select type (z => y%expr(2)%x)
            type is (prt_spec_list_t)
                call z%expr(1)%init_spec (b)
                call z%expr(2)%init_spec (c)
            end select
        end select
        call x%expr(2)%init_spec (d)
    end select
    write (u, "(A)")  char (pe7%to_string ())

    call pe8%init_sum (2)
    select type (x => pe8%x)
    type is (prt_spec_sum_t)
        call x%expr(1)%init_list (2)
        select type (y => x%expr(1)%x)

```

```

    type is (prt_spec_list_t)
      call y%expr(1)%init_spec (a)
      call y%expr(2)%init_spec (b)
    end select
    call x%expr(2)%init_list (2)
    select type (y => x%expr(2)%x)
    type is (prt_spec_list_t)
      call y%expr(1)%init_spec (c)
      call y%expr(2)%init_spec (d)
    end select
  end select
write (u, "(A)") char (pe8%to_string ())

call pe9%init_list (3)
select type (x => pe9%x)
type is (prt_spec_list_t)
  call x%expr(1)%init_sum (2)
  select type (y => x%expr(1)%x)
  type is (prt_spec_sum_t)
    call y%expr(1)%init_spec (a)
    call y%expr(2)%init_spec (b)
  end select
  call x%expr(2)%init_spec (c)
  call x%expr(3)%init_sum (3)
  select type (y => x%expr(3)%x)
  type is (prt_spec_sum_t)
    call y%expr(1)%init_spec (d)
    call y%expr(2)%init_spec (e)
    call y%expr(3)%init_spec (f)
  end select
end select
write (u, "(A)") char (pe9%to_string ())

write (u, *)
write (u, "(A)")  "* Expand as sum"
write (u, *)

call pe1%expand ()
write (u, "(A)") char (pe1%to_string ())

call pe4%expand ()
write (u, "(A)") char (pe4%to_string ())

call pe5%expand ()
write (u, "(A)") char (pe5%to_string ())

call pe6%expand ()
write (u, "(A)") char (pe6%to_string ())

call pe7%expand ()
write (u, "(A)") char (pe7%to_string ())

call pe8%expand ()
write (u, "(A)") char (pe8%to_string ())

```

```

call pe9%expand ()
write (u, "(A)") char (pe9%to_string ())

write (u, *)
write (u, "(A)")  "* Transform to arrays:"

write (u, "(A)")  "* Atomic specifier"
do i = 1, pe1%get_n_terms ()
  call pe1%term_to_array (pa, i)
  call prt_spec_write (pa, u)
end do

write (u, *)
write (u, "(A)")  "* List"
do i = 1, pe5%get_n_terms ()
  call pe5%term_to_array (pa, i)
  call prt_spec_write (pa, u)
end do

write (u, *)
write (u, "(A)")  "* Sum of atoms"
do i = 1, pe6%get_n_terms ()
  call pe6%term_to_array (pa, i)
  call prt_spec_write (pa, u)
end do

write (u, *)
write (u, "(A)")  "* Sum of lists"
do i = 1, pe9%get_n_terms ()
  call pe9%term_to_array (pa, i)
  call prt_spec_write (pa, u)
end do

write (u, "(A)")
write (u, "(A)")  "* Test output end: particle_specifiers_2"
end subroutine particle_specifiers_2

```

13.2 PDG arrays

For defining aliases, we introduce a special type which holds a set of (integer) PDG codes.

`<pdg_arrays.f90>`≡
<File header>

`module pdg_arrays`

<Standard module head>

<PDG arrays: public>

```

    <PDG arrays: types>

    <PDG arrays: interfaces>

    interface
    <PDG arrays: sub interfaces>
    end interface

end module pdg_arrays

<pdg_arrays_sub.f90>≡
<File header>

submodule (pdg_arrays) pdg_arrays_s

    use io_units
    use sorting
    use physics_defs

    implicit none

contains

    <PDG arrays: procedures>

end submodule pdg_arrays_s

```

13.2.1 Type definition

Using an allocatable array eliminates the need for initializer and/or finalizer.

```

<PDG arrays: public>≡
    public :: pdg_array_t

<PDG arrays: types>≡
    type :: pdg_array_t
    private
        integer, dimension(:), allocatable :: pdg
    contains
        <PDG arrays: pdg array: TBP>
    end type pdg_array_t

```

Output.

```

<PDG arrays: pdg array: TBP>≡
    procedure :: write => pdg_array_write

<PDG arrays: sub interfaces>≡
    module subroutine pdg_array_write (aval, unit)
        class(pdg_array_t), intent(in) :: aval
        integer, intent(in), optional :: unit
    end subroutine pdg_array_write

```

```

(PDG arrays: procedures)≡
module subroutine pdg_array_write (aval, unit)
  class(pdg_array_t), intent(in) :: aval
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)", advance="no") "PDG("
  if (allocated (aval%pdg)) then
    do i = 1, size (aval%pdg)
      if (i > 1) write (u, "(A)", advance="no") ", "
      write (u, "(I0)", advance="no") aval%pdg(i)
    end do
  end if
  write (u, "(A)", advance="no") ")"
end subroutine pdg_array_write

```

```

(PDG arrays: public)+≡
public :: pdg_array_write_set

```

```

(PDG arrays: sub interfaces)+≡
module subroutine pdg_array_write_set (aval, unit)
  type(pdg_array_t), intent(in), dimension(:) :: aval
  integer, intent(in), optional :: unit
end subroutine pdg_array_write_set

```

```

(PDG arrays: procedures)+≡
module subroutine pdg_array_write_set (aval, unit)
  type(pdg_array_t), intent(in), dimension(:) :: aval
  integer, intent(in), optional :: unit
  integer :: i
  do i = 1, size (aval)
    call aval(i)%write (unit)
    print *, "
  end do
end subroutine pdg_array_write_set

```

13.2.2 Basic operations

Assignment. We define assignment from and to an integer array. Note that the integer array, if it is the l.h.s., must be declared allocatable by the caller.

```

(PDG arrays: public)+≡
public :: assignment(=)
(PDG arrays: interfaces)≡
interface assignment(=)
  module procedure pdg_array_from_int_array
  module procedure pdg_array_from_int
  module procedure int_array_from_pdg_array
end interface

```

```

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_array_from_int_array (aval, iarray)
    type(pdg_array_t), intent(out) :: aval
    integer, dimension(:), intent(in) :: iarray
  end subroutine pdg_array_from_int_array
  elemental module subroutine pdg_array_from_int (aval, int)
    type(pdg_array_t), intent(out) :: aval
    integer, intent(in) :: int
  end subroutine pdg_array_from_int
  module subroutine int_array_from_pdg_array (iarray, aval)
    integer, dimension(:), allocatable, intent(out) :: iarray
    type(pdg_array_t), intent(in) :: aval
  end subroutine int_array_from_pdg_array

(PDG arrays: procedures)+≡
  module subroutine pdg_array_from_int_array (aval, iarray)
    type(pdg_array_t), intent(out) :: aval
    integer, dimension(:), intent(in) :: iarray
    allocate (aval%pdg (size (iarray)))
    aval%pdg = iarray
  end subroutine pdg_array_from_int_array

  elemental module subroutine pdg_array_from_int (aval, int)
    type(pdg_array_t), intent(out) :: aval
    integer, intent(in) :: int
    allocate (aval%pdg (1))
    aval%pdg = int
  end subroutine pdg_array_from_int

  module subroutine int_array_from_pdg_array (iarray, aval)
    integer, dimension(:), allocatable, intent(out) :: iarray
    type(pdg_array_t), intent(in) :: aval
    if (allocated (aval%pdg)) then
      allocate (iarray (size (aval%pdg)))
      iarray = aval%pdg
    else
      allocate (iarray (0))
    end if
  end subroutine int_array_from_pdg_array

```

Allocate space for a PDG array

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: init => pdg_array_init

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_array_init (aval, n_elements)
    class(pdg_array_t), intent(inout) :: aval
    integer, intent(in) :: n_elements
  end subroutine pdg_array_init

(PDG arrays: procedures)+≡
  module subroutine pdg_array_init (aval, n_elements)
    class(pdg_array_t), intent(inout) :: aval
    integer, intent(in) :: n_elements
    allocate(aval%pdg(n_elements))

```

```
end subroutine pdg_array_init
```

Deallocate a previously allocated pdg array

```
<PDG arrays: pdg array: TBP>+≡
  procedure :: delete => pdg_array_delete

<PDG arrays: sub interfaces>+≡
  module subroutine pdg_array_delete (aval)
    class(pdg_array_t), intent(inout) :: aval
  end subroutine pdg_array_delete

<PDG arrays: procedures>+≡
  module subroutine pdg_array_delete (aval)
    class(pdg_array_t), intent(inout) :: aval
    if (allocated (aval%pdg)) deallocate (aval%pdg)
  end subroutine pdg_array_delete
```

Merge two pdg arrays, i.e. append a particle string to another leaving out doublettes

```
<PDG arrays: pdg array: TBP>+≡
  procedure :: merge => pdg_array_merge

<PDG arrays: sub interfaces>+≡
  module subroutine pdg_array_merge (aval1, aval2)
    class(pdg_array_t), intent(inout) :: aval1
    type(pdg_array_t), intent(in) :: aval2
  end subroutine pdg_array_merge

<PDG arrays: procedures>+≡
  module subroutine pdg_array_merge (aval1, aval2)
    class(pdg_array_t), intent(inout) :: aval1
    type(pdg_array_t), intent(in) :: aval2
    type(pdg_array_t) :: aval
    if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
      if (.not. any (aval1%pdg == aval2%pdg)) aval = aval1 // aval2
    else if (allocated (aval1%pdg)) then
      aval = aval1
    else if (allocated (aval2%pdg)) then
      aval = aval2
    end if
    call pdg_array_delete (aval1)
    call pdg_array_from_int_array (aval1, aval%pdg)
  end subroutine pdg_array_merge
```

Length of the array.

```
<PDG arrays: pdg array: TBP>+≡
  procedure :: get_length => pdg_array_get_length

<PDG arrays: sub interfaces>+≡
  elemental module function pdg_array_get_length (aval) result (n)
    class(pdg_array_t), intent(in) :: aval
    integer :: n
  end function pdg_array_get_length
```

```

(PDG arrays: procedures)+≡
  elemental module function pdg_array_get_length (aval) result (n)
    class(pdg_array_t), intent(in) :: aval
    integer :: n
    if (allocated (aval%pdg)) then
      n = size (aval%pdg)
    else
      n = 0
    end if
  end function pdg_array_get_length

```

Return the element with index i.

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: get => pdg_array_get

(PDG arrays: sub interfaces)+≡
  elemental module function pdg_array_get (aval, i) result (pdg)
    class(pdg_array_t), intent(in) :: aval
    integer, intent(in), optional :: i
    integer :: pdg
  end function pdg_array_get

(PDG arrays: procedures)+≡
  elemental module function pdg_array_get (aval, i) result (pdg)
    class(pdg_array_t), intent(in) :: aval
    integer, intent(in), optional :: i
    integer :: pdg
    if (present (i)) then
      pdg = aval%pdg(i)
    else
      pdg = aval%pdg(1)
    end if
  end function pdg_array_get

```

Explicitly set the element with index i.

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: set => pdg_array_set

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_array_set (aval, i, pdg)
    class(pdg_array_t), intent(inout) :: aval
    integer, intent(in) :: i
    integer, intent(in) :: pdg
  end subroutine pdg_array_set

(PDG arrays: procedures)+≡
  module subroutine pdg_array_set (aval, i, pdg)
    class(pdg_array_t), intent(inout) :: aval
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    aval%pdg(i) = pdg
  end subroutine pdg_array_set

```

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: add => pdg_array_add

```



```

(PDG arrays: sub interfaces)+≡
  module function pdg_array_add (aval, aval_add) result (aval_out)
    type(pdg_array_t) :: aval_out
    class(pdg_array_t), intent(in) :: aval
    type(pdg_array_t), intent(in) :: aval_add
  end function pdg_array_add

```

```

(PDG arrays: procedures)+≡
  module function pdg_array_add (aval, aval_add) result (aval_out)
    type(pdg_array_t) :: aval_out
    class(pdg_array_t), intent(in) :: aval
    type(pdg_array_t), intent(in) :: aval_add
    integer :: n, n_add, i
    n = size (aval%pdg)
    n_add = size (aval_add%pdg)
    allocate (aval_out%pdg (n + n_add))
    aval_out%pdg(1:n) = aval%pdg
    do i = 1, n_add
      aval_out%pdg(n+i) = aval_add%pdg(i)
    end do
  end function pdg_array_add

```

Replace element with index i by a new array of elements.

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: replace => pdg_array_replace

(PDG arrays: sub interfaces)+≡
  module function pdg_array_replace (aval, i, pdg_new) result (aval_new)
    class(pdg_array_t), intent(in) :: aval
    integer, intent(in) :: i
    integer, dimension(:), intent(in) :: pdg_new
    type(pdg_array_t) :: aval_new
  end function pdg_array_replace

```

```

(PDG arrays: procedures)+≡
  module function pdg_array_replace (aval, i, pdg_new) result (aval_new)
    class(pdg_array_t), intent(in) :: aval
    integer, intent(in) :: i
    integer, dimension(:), intent(in) :: pdg_new
    type(pdg_array_t) :: aval_new
    integer :: n, l
    n = size (aval%pdg)
    l = size (pdg_new)
    allocate (aval_new%pdg (n + l - 1))
    aval_new%pdg(:i-1) = aval%pdg(:i-1)
    aval_new%pdg(i:i+l-1) = pdg_new
    aval_new%pdg(i+l:) = aval%pdg(i+1:)
  end function pdg_array_replace

```

Concatenate two PDG arrays

```

(PDG arrays: public)+≡
  public :: operator(//)

(PDG arrays: interfaces)+≡
  interface operator(//)

```

```

        module procedure concat_pdg_arrays
    end interface

    <PDG arrays: sub interfaces>+≡
        module function concat_pdg_arrays (aval1, aval2) result (aval)
            type(pdg_array_t) :: aval
            type(pdg_array_t), intent(in) :: aval1, aval2
        end function concat_pdg_arrays

    <PDG arrays: procedures>+≡
        module function concat_pdg_arrays (aval1, aval2) result (aval)
            type(pdg_array_t) :: aval
            type(pdg_array_t), intent(in) :: aval1, aval2
            integer :: n1, n2
            if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
                n1 = size (aval1%pdg)
                n2 = size (aval2%pdg)
                allocate (aval%pdg (n1 + n2))
                aval%pdg(:n1) = aval1%pdg
                aval%pdg(n1+1:) = aval2%pdg
            else if (allocated (aval1%pdg)) then
                aval = aval1
            else if (allocated (aval2%pdg)) then
                aval = aval2
            end if
        end function concat_pdg_arrays

```

13.2.3 Matching

A PDG array matches a given PDG code if the code is present within the array. If either one is zero (UNDEFINED), the match also succeeds.

```

    <PDG arrays: public>+≡
        public :: operator(.match.)

    <PDG arrays: interfaces>+≡
        interface operator(.match.)
            module procedure pdg_array_match_integer
            module procedure pdg_array_match_pdg_array
        end interface

```

Match a single code against the array.

```

    <PDG arrays: sub interfaces>+≡
        elemental module function pdg_array_match_integer (aval, pdg) result (flag)
            logical :: flag
            type(pdg_array_t), intent(in) :: aval
            integer, intent(in) :: pdg
        end function pdg_array_match_integer

    <PDG arrays: procedures>+≡
        elemental module function pdg_array_match_integer (aval, pdg) result (flag)
            logical :: flag
            type(pdg_array_t), intent(in) :: aval
            integer, intent(in) :: pdg

```

```

    if (allocated (aval%pdg)) then
        flag = pdg == UNDEFINED &
            .or. any (aval%pdg == UNDEFINED) &
            .or. any (aval%pdg == pdg)
    else
        flag = .false.
    end if
end function pdg_array_match_integer

```

Check if the pdg-number corresponds to a quark

```

<PDG arrays: public>+≡
    public :: is_quark

<PDG arrays: sub interfaces>+≡
    elemental module function is_quark (pdg_nr)
        logical :: is_quark
        integer, intent(in) :: pdg_nr
    end function is_quark

<PDG arrays: procedures>+≡
    elemental module function is_quark (pdg_nr)
        logical :: is_quark
        integer, intent(in) :: pdg_nr
        if (abs (pdg_nr) >= 1 .and. abs (pdg_nr) <= 6) then
            is_quark = .true.
        else
            is_quark = .false.
        end if
    end function is_quark

```

Check if pdg-number corresponds to a gluon

```

<PDG arrays: public>+≡
    public :: is_gluon

<PDG arrays: sub interfaces>+≡
    elemental module function is_gluon (pdg_nr)
        logical :: is_gluon
        integer, intent(in) :: pdg_nr
    end function is_gluon

<PDG arrays: procedures>+≡
    elemental module function is_gluon (pdg_nr)
        logical :: is_gluon
        integer, intent(in) :: pdg_nr
        if (pdg_nr == GLUON) then
            is_gluon = .true.
        else
            is_gluon = .false.
        end if
    end function is_gluon

```

Check if pdg-number corresponds to a photon

```

<PDG arrays: public>+≡
    public :: is_photon

```

```

(PDG arrays: sub interfaces)+≡
  elemental module function is_photon (pdg_nr)
    logical :: is_photon
    integer, intent(in) :: pdg_nr
  end function is_photon

```

```

(PDG arrays: procedures)+≡
  elemental module function is_photon (pdg_nr)
    logical :: is_photon
    integer, intent(in) :: pdg_nr
    if (pdg_nr == PHOTON) then
      is_photon = .true.
    else
      is_photon = .false.
    end if
  end function is_photon

```

Check if pdg-number corresponds to a colored particle

```

(PDG arrays: public)+≡
  public :: is_colored

(PDG arrays: sub interfaces)+≡
  elemental module function is_colored (pdg_nr)
    logical :: is_colored
    integer, intent(in) :: pdg_nr
  end function is_colored

(PDG arrays: procedures)+≡
  elemental module function is_colored (pdg_nr)
    logical :: is_colored
    integer, intent(in) :: pdg_nr
    is_colored = is_quark (pdg_nr) .or. is_gluon (pdg_nr)
  end function is_colored

```

Check if the pdg-number corresponds to a lepton

```

(PDG arrays: public)+≡
  public :: is_lepton

(PDG arrays: sub interfaces)+≡
  elemental module function is_lepton (pdg_nr)
    logical :: is_lepton
    integer, intent(in) :: pdg_nr
  end function is_lepton

(PDG arrays: procedures)+≡
  elemental module function is_lepton (pdg_nr)
    logical :: is_lepton
    integer, intent(in) :: pdg_nr
    if (abs (pdg_nr) >= ELECTRON .and. &
        abs (pdg_nr) <= TAU_NEUTRINO) then
      is_lepton = .true.
    else
      is_lepton = .false.
    end if
  end function is_lepton

```

Check if the pdg-number corresponds to a charged lepton

```
<PDG arrays: public>+≡
    public :: is_charged_lepton

<PDG arrays: sub interfaces>+≡
    elemental module function is_charged_lepton (pdg_nr)
        logical :: is_charged_lepton
        integer, intent(in) :: pdg_nr
    end function is_charged_lepton

<PDG arrays: procedures>+≡
    elemental module function is_charged_lepton (pdg_nr)
        logical :: is_charged_lepton
        integer, intent(in) :: pdg_nr
        if (abs (pdg_nr) == ELECTRON .or. &
            abs (pdg_nr) == MUON .or. &
            abs (pdg_nr) == TAU) then
            is_charged_lepton = .true.
        else
            is_charged_lepton = .false.
        end if
    end function is_charged_lepton

<PDG arrays: public>+≡
    public :: is_fermion

<PDG arrays: sub interfaces>+≡
    elemental module function is_fermion (pdg_nr)
        logical :: is_fermion
        integer, intent(in) :: pdg_nr
    end function is_fermion

<PDG arrays: procedures>+≡
    elemental module function is_fermion (pdg_nr)
        logical :: is_fermion
        integer, intent(in) :: pdg_nr
        is_fermion = is_lepton(pdg_nr) .or. is_quark(pdg_nr)
    end function is_fermion
```

Check if the pdg-number corresponds to a massless vector boson

```
<PDG arrays: public>+≡
    public :: is_massless_vector

<PDG arrays: sub interfaces>+≡
    elemental module function is_massless_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massless_vector
    end function is_massless_vector

<PDG arrays: procedures>+≡
    elemental module function is_massless_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massless_vector
        if (pdg_nr == GLUON .or. pdg_nr == PHOTON) then
            is_massless_vector = .true.
        else
            is_massless_vector = .false.
        end if
    end function is_massless_vector
```

```

        end if
    end function is_massless_vector

```

Check if pdg-number corresponds to a massive vector boson

```

(PDG arrays: public)+≡
    public :: is_massive_vector

(PDG arrays: sub interfaces)+≡
    elemental module function is_massive_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massive_vector
    end function is_massive_vector

(PDG arrays: procedures)+≡
    elemental module function is_massive_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massive_vector
        if (abs (pdg_nr) == Z_BOSON .or. abs (pdg_nr) == W_BOSON) then
            is_massive_vector = .true.
        else
            is_massive_vector = .false.
        end if
    end function is_massive_vector

```

Check if pdg-number corresponds to a vector boson

```

(PDG arrays: public)+≡
    public :: is_vector

(PDG arrays: sub interfaces)+≡
    elemental module function is_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_vector
    end function is_vector

(PDG arrays: procedures)+≡
    elemental module function is_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_vector
        if (is_massless_vector (pdg_nr) .or. is_massive_vector (pdg_nr)) then
            is_vector = .true.
        else
            is_vector = .false.
        end if
    end function is_vector

```

Check if particle is elementary.

```

(PDG arrays: public)+≡
    public :: is_elementary

(PDG arrays: sub interfaces)+≡
    elemental module function is_elementary (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_elementary
    end function is_elementary

```

```

(PDG arrays: procedures)+≡
  elemental module function is_elementary (pdg_nr)
    integer, intent(in) :: pdg_nr
    logical :: is_elementary
    if (is_vector (pdg_nr) .or. is_fermion (pdg_nr) .or. pdg_nr == 25) then
      is_elementary = .true.
    else
      is_elementary = .false.
    end if
  end function is_elementary

```

Check if particle is an EW boson or scalar.

```

(PDG arrays: public)+≡
  public :: is_ew_boson_scalar

```

```

(PDG arrays: sub interfaces)+≡
  elemental module function is_ew_boson_scalar (pdg_nr)
    integer, intent(in) :: pdg_nr
    logical :: is_ew_boson_scalar
  end function is_ew_boson_scalar

```

```

(PDG arrays: procedures)+≡
  elemental module function is_ew_boson_scalar (pdg_nr)
    integer, intent(in) :: pdg_nr
    logical :: is_ew_boson_scalar
    if (is_photon (pdg_nr) .or. is_massive_vector (pdg_nr) .or. pdg_nr == 25) then
      is_ew_boson_scalar = .true.
    else
      is_ew_boson_scalar = .false.
    end if
  end function is_ew_boson_scalar

```

Check if particle is strongly interacting

```

(PDG arrays: pdg array: TBP)+≡
  procedure :: has_colored_particles => pdg_array_has_colored_particles

```

```

(PDG arrays: sub interfaces)+≡
  module function pdg_array_has_colored_particles (pdg) result (colored)
    class(pdg_array_t), intent(in) :: pdg
    logical :: colored
  end function pdg_array_has_colored_particles

```

```

(PDG arrays: procedures)+≡
  module function pdg_array_has_colored_particles (pdg) result (colored)
    class(pdg_array_t), intent(in) :: pdg
    logical :: colored
    integer :: i, pdg_nr
    colored = .false.
    do i = 1, size (pdg%pdg)
      pdg_nr = pdg%pdg(i)
      if (is_quark (pdg_nr) .or. is_gluon (pdg_nr)) then
        colored = .true.
        exit
      end if
    end do
  end function

```

```
end function pdg_array_has_colored_particles
```

This function is a convenience function for the determination of possible compatibility of flavor structures of processes with certain orders of QCD and QED/EW coupling constants. It assumes the Standard Model (SM) as underlying physics model. The function is based on a naive counting of external particles which are connected to the process by the specific kind of couplings depending on the underlying theory (QCD and/or QED/EW) of which the corresponding particle is a part of. It is constructed in a way that the exclusion of coupling power combinations is well-defined.

(PDG arrays: public)+≡

```
public :: query_coupling_powers
```

(PDG arrays: sub interfaces)+≡

```
module function query_coupling_powers (flv, a_power, as_power) result (valid)
  integer, intent(in), dimension(:) :: flv
  integer, intent(in) :: a_power, as_power
  logical :: valid
end function query_coupling_powers
```

(PDG arrays: procedures)+≡

```
module function query_coupling_powers (flv, a_power, as_power) result (valid)
  integer, intent(in), dimension(:) :: flv
  integer, dimension(:, :), allocatable :: power_pair_array
  integer, dimension(2) :: power_pair_ref
  integer, intent(in) :: a_power, as_power
  integer :: i, n_legs, n_gluons, n_quarks, n_gamWZH, n_leptons
  logical, dimension(:), allocatable :: pairs_included
  logical :: valid
  integer :: n_bound
  power_pair_ref = [a_power, as_power]
  n_legs = size (flv)
  allocate (power_pair_array (2, n_legs - 1))
  do i = 1, n_legs - 1
    power_pair_array (1, i) = n_legs - 1 - i
    power_pair_array (2, i) = i - 1
  end do
  allocate (pairs_included (n_legs - 1))
  pairs_included = .true.
  n_gluons = count (is_gluon (flv))
  n_gamWZH = count (is_ew_boson_scalar (flv))
  n_quarks = count (is_quark (flv))
  n_leptons = count (is_lepton (flv))
  if (n_gluons >= 1 .and. n_gluons <= 3) then
    do i = 1, n_gluons
      pairs_included (i) = .false.
    end do
  else if (n_gluons > 2 .and. n_quarks <= 2 .and. n_gluons + n_quarks == n_legs) then
    do i = 1, n_legs - 2
      pairs_included (i) = .false.
    end do
  end if
  n_bound = 0
  if (n_gamWZH + n_leptons == n_legs) then
```



```

        n_bound = n_gamWZH + n_leptons - 2
    else if (n_quarks == 2 .and. n_leptons + n_quarks + n_gamWZH == n_legs) then
        n_bound = n_legs - 2
    else if (n_gamWZH + n_leptons > 0) then
        n_bound = n_leptons/2 + n_gamWZH
    end if
    if (n_bound > 0) then
        do i = 1, n_bound
            pairs_included (n_legs - i) = .false.
        end do
    end if
    if (n_quarks == 4 .and. .not. qcd_ew_interferences (flv)) then
        do i = 1, 2
            pairs_included (n_legs - i) = .false.
        end do
    end if
    valid = .false.
    do i = 1, n_legs - 1
        if (all (power_pair_array (:, i) == power_pair_ref) .and. pairs_included (i)) then
            valid = .true.
            exit
        end if
    end do
end function query_coupling_powers

```

This functions checks if there is a flavor structure which possibly can induce QCD-EW interference amplitudes. It evaluates to `true` if there are at least 2 quark pairs whereby the quarks of at least one quark pair must have the same flavor.

(PDG arrays: public)+≡

```
public :: qcd_ew_interferences
```

(PDG arrays: sub interfaces)+≡

```

module function qcd_ew_interferences (flv) result (valid)
    integer, intent(in), dimension(:) :: flv
    logical :: valid
end function qcd_ew_interferences

```

(PDG arrays: procedures)+≡

```

module function qcd_ew_interferences (flv) result (valid)
    integer, intent(in), dimension(:) :: flv
    integer :: i, n_pairs
    logical :: valid, qqbar_pair
    n_pairs = 0
    valid = .false.
    qqbar_pair = .false.
    if (count (is_quark (flv)) >= 4) then
        do i = DOWN_Q, TOP_Q
            qqbar_pair = count (abs (flv) == i) >= 2
            if (qqbar_pair) n_pairs = n_pairs + 1
            if (n_pairs > 0) then
                valid = .true.
                exit
            end if
        end do
    end if
end function

```

```

        end do
    end if
end function qcd_ew_interferences

```

Assign equivalent cut expression class to PDG code.

```

(PDG arrays: public)+≡
    public :: flv_eqv_expr_class

(PDG arrays: sub interfaces)+≡
    module function flv_eqv_expr_class (flv) result (assign_qgA)
        integer, intent(in) :: flv
        logical, dimension(3) :: assign_qgA
    end function flv_eqv_expr_class

(PDG arrays: procedures)+≡
    module function flv_eqv_expr_class (flv) result (assign_qgA)
        integer, intent(in) :: flv
        logical, dimension(3) :: assign_qgA
        assign_qgA = [is_quark (flv), is_gluon (flv), is_photon (flv)]
    end function flv_eqv_expr_class

```

Match two arrays. Succeeds if any pair of entries matches.

```

(PDG arrays: sub interfaces)+≡
    module function pdg_array_match_pdg_array (aval1, aval2) result (flag)
        logical :: flag
        type(pdg_array_t), intent(in) :: aval1, aval2
    end function pdg_array_match_pdg_array

(PDG arrays: procedures)+≡
    module function pdg_array_match_pdg_array (aval1, aval2) result (flag)
        logical :: flag
        type(pdg_array_t), intent(in) :: aval1, aval2
        if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
            flag = any (aval1 .match. aval2%pdg)
        else
            flag = .false.
        end if
    end function pdg_array_match_pdg_array

```

Comparison. Here, we take the PDG arrays as-is, assuming that they are sorted.

The ordering is a bit odd: first, we look only at the absolute values of the PDG codes. If they all match, the particle comes before the antiparticle, scanning from left to right.

```

(PDG arrays: public)+≡
    public :: operator(<)
    public :: operator(>)
    public :: operator(<=)
    public :: operator(>=)
    public :: operator(==)
    public :: operator(/=)

```

```

(PDG arrays: interfaces)+≡
  interface operator(<)
    module procedure pdg_array_lt
  end interface
  interface operator(>)
    module procedure pdg_array_gt
  end interface
  interface operator(<=)
    module procedure pdg_array_le
  end interface
  interface operator(>=)
    module procedure pdg_array_ge
  end interface
  interface operator(==)
    module procedure pdg_array_eq
  end interface
  interface operator(/=)
    module procedure pdg_array_ne
  end interface

(PDG arrays: sub interfaces)+≡
  elemental module function pdg_array_lt (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_lt
  elemental module function pdg_array_gt (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_gt
  elemental module function pdg_array_le (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_le
  elemental module function pdg_array_ge (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_ge
  elemental module function pdg_array_eq (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_eq
  elemental module function pdg_array_ne (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
  end function pdg_array_ne

(PDG arrays: procedures)+≡
  elemental module function pdg_array_lt (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
    integer :: i
    if (size (aval1%pdg) /= size (aval2%pdg)) then
      flag = size (aval1%pdg) < size (aval2%pdg)
    else

```

```

do i = 1, size (aval1%pdg)
  if (abs (aval1%pdg(i)) /= abs (aval2%pdg(i))) then
    flag = abs (aval1%pdg(i)) < abs (aval2%pdg(i))
    return
  end if
end do
do i = 1, size (aval1%pdg)
  if (aval1%pdg(i) /= aval2%pdg(i)) then
    flag = aval1%pdg(i) > aval2%pdg(i)
    return
  end if
end do
flag = .false.
end if
end function pdg_array_lt

elemental module function pdg_array_gt (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = .not. (aval1 < aval2 .or. aval1 == aval2)
end function pdg_array_gt

elemental module function pdg_array_le (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = aval1 < aval2 .or. aval1 == aval2
end function pdg_array_le

elemental module function pdg_array_ge (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = .not. (aval1 < aval2)
end function pdg_array_ge

elemental module function pdg_array_eq (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  if (size (aval1%pdg) /= size (aval2%pdg)) then
    flag = .false.
  else
    flag = all (aval1%pdg == aval2%pdg)
  end if
end function pdg_array_eq

elemental module function pdg_array_ne (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = .not. (aval1 == aval2)
end function pdg_array_ne

```

Equivalence. Two PDG arrays are equivalent if either one contains UNDEFINED or if each element of array 1 is present in array 2, and vice versa.

(PDG arrays: public)+≡

```

public :: operator(.eqv.)
public :: operator(.neqv.)

(PDG arrays: interfaces)+≡
interface operator(.eqv.)
  module procedure pdg_array_equivalent
end interface
interface operator(.neqv.)
  module procedure pdg_array_inequivalent
end interface

(PDG arrays: sub interfaces)+≡
  elemental module function pdg_array_equivalent (aval1, aval2) result (eq)
    logical :: eq
    type(pdg_array_t), intent(in) :: aval1, aval2
  end function pdg_array_equivalent
  elemental module function pdg_array_inequivalent (aval1, aval2) result (neq)
    logical :: neq
    type(pdg_array_t), intent(in) :: aval1, aval2
  end function pdg_array_inequivalent

(PDG arrays: procedures)+≡
  elemental module function pdg_array_equivalent (aval1, aval2) result (eq)
    logical :: eq
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical, dimension(:), allocatable :: match1, match2
    integer :: i
    if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
      eq = any (aval1%pdg == UNDEFINED) &
        .or. any (aval2%pdg == UNDEFINED)
    if (.not. eq) then
      allocate (match1 (size (aval1%pdg)))
      allocate (match2 (size (aval2%pdg)))
      match1 = .false.
      match2 = .false.
      do i = 1, size (aval1%pdg)
        match2 = match2 .or. aval1%pdg(i) == aval2%pdg
      end do
      do i = 1, size (aval2%pdg)
        match1 = match1 .or. aval2%pdg(i) == aval1%pdg
      end do
      eq = all (match1) .and. all (match2)
    end if
  else
    eq = .false.
  end if
end function pdg_array_equivalent

  elemental module function pdg_array_inequivalent (aval1, aval2) result (neq)
    logical :: neq
    type(pdg_array_t), intent(in) :: aval1, aval2
    neq = .not. pdg_array_equivalent (aval1, aval2)
  end function pdg_array_inequivalent

```

13.2.4 Sorting

Sort a PDG array by absolute value, particle before antiparticle. After sorting, we eliminate double entries.

```
<PDG arrays: public>+≡
    public :: sort_abs

<PDG arrays: interfaces>+≡
    interface sort_abs
        module procedure pdg_array_sort_abs
    end interface

<PDG arrays: pdg array: TBP>+≡
    procedure :: sort_abs => pdg_array_sort_abs

<PDG arrays: sub interfaces>+≡
    module function pdg_array_sort_abs (aval1, unique) result (aval2)
        class(pdg_array_t), intent(in) :: aval1
        logical, intent(in), optional :: unique
        type(pdg_array_t) :: aval2
    end function pdg_array_sort_abs

<PDG arrays: procedures>+≡
    module function pdg_array_sort_abs (aval1, unique) result (aval2)
        class(pdg_array_t), intent(in) :: aval1
        logical, intent(in), optional :: unique
        type(pdg_array_t) :: aval2
        integer, dimension(:), allocatable :: tmp
        logical, dimension(:), allocatable :: mask
        integer :: i, n
        logical :: uni
        uni = .false.; if (present (unique)) uni = unique
        n = size (aval1%pdg)
        if (uni) then
            allocate (tmp (n), mask(n))
            tmp = sort_abs (aval1%pdg)
            mask(1) = .true.
            do i = 2, n
                mask(i) = tmp(i) /= tmp(i-1)
            end do
            allocate (aval2%pdg (count (mask)))
            aval2%pdg = pack (tmp, mask)
        else
            allocate (aval2%pdg (n))
            aval2%pdg = sort_abs (aval1%pdg)
        end if
    end function pdg_array_sort_abs

<PDG arrays: pdg array: TBP>+≡
    procedure :: intersect => pdg_array_intersect

<PDG arrays: sub interfaces>+≡
    module function pdg_array_intersect (aval1, match) result (aval2)
        class(pdg_array_t), intent(in) :: aval1
        integer, dimension(:) :: match
```

```

        type(pdg_array_t) :: aval2
    end function pdg_array_intersect

<PDG arrays: procedures>+=
module function pdg_array_intersect (aval1, match) result (aval2)
    class(pdg_array_t), intent(in) :: aval1
    integer, dimension(:) :: match
    type(pdg_array_t) :: aval2
    integer, dimension(:), allocatable :: isec
    integer :: i
    isec = pack (aval1%pdg, [(any(aval1%pdg(i) == match), i=1,size(aval1%pdg))])
    call pdg_array_from_int_array (aval2, isec)
end function pdg_array_intersect

<PDG arrays: pdg array: TBP>+=
procedure :: search_for_particle => pdg_array_search_for_particle

<PDG arrays: sub interfaces>+=
    elemental module function pdg_array_search_for_particle (pdg, i_part) result (found)
        class(pdg_array_t), intent(in) :: pdg
        integer, intent(in) :: i_part
        logical :: found
    end function pdg_array_search_for_particle

<PDG arrays: procedures>+=
    elemental module function pdg_array_search_for_particle (pdg, i_part) result (found)
        class(pdg_array_t), intent(in) :: pdg
        integer, intent(in) :: i_part
        logical :: found
        found = any (pdg%pdg == i_part)
    end function pdg_array_search_for_particle

<PDG arrays: pdg array: TBP>+=
procedure :: invert => pdg_array_invert

<PDG arrays: sub interfaces>+=
    module function pdg_array_invert (pdg) result (pdg_inverse)
        class(pdg_array_t), intent(in) :: pdg
        type(pdg_array_t) :: pdg_inverse
    end function pdg_array_invert

<PDG arrays: procedures>+=
    module function pdg_array_invert (pdg) result (pdg_inverse)
        class(pdg_array_t), intent(in) :: pdg
        type(pdg_array_t) :: pdg_inverse
        integer :: i, n
        n = size (pdg%pdg)
        allocate (pdg_inverse%pdg (n))
        do i = 1, n
            select case (pdg%pdg(i))
            case (GLUON, PHOTON, Z_BOSON, 25)
                pdg_inverse%pdg(i) = pdg%pdg(i)
            case default
                pdg_inverse%pdg(i) = -pdg%pdg(i)
            end select
        end do
    end function
end do

```

```
end function pdg_array_invert
```

13.2.5 PDG array list

A PDG array list, or PDG list, is an array of PDG-array objects with some convenience methods.

```
<PDG arrays: public>+≡
    public :: pdg_list_t

<PDG arrays: types>+≡
    type :: pdg_list_t
        type(pdg_array_t), dimension(:), allocatable :: a
        contains
        <PDG arrays: pdg list: TBP>
    end type pdg_list_t
```

Output, as a comma-separated list without advancing I/O.

```
<PDG arrays: pdg list: TBP>≡
    procedure :: write => pdg_list_write

<PDG arrays: sub interfaces>+≡
    module subroutine pdg_list_write (object, unit)
        class(pdg_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine pdg_list_write

<PDG arrays: procedures>+≡
    module subroutine pdg_list_write (object, unit)
        class(pdg_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        if (allocated (object%a)) then
            do i = 1, size (object%a)
                if (i > 1) write (u, "(A)", advance="no") ", "
                call object%a(i)%write (u)
            end do
        end if
    end subroutine pdg_list_write
```

Initialize for a certain size. The entries are initially empty PDG arrays.

```
<PDG arrays: pdg list: TBP>+≡
    generic :: init => pdg_list_init_size
    procedure, private :: pdg_list_init_size

<PDG arrays: sub interfaces>+≡
    module subroutine pdg_list_init_size (pl, n)
        class(pdg_list_t), intent(out) :: pl
        integer, intent(in) :: n
    end subroutine pdg_list_init_size
```



```

(PDG arrays: procedures)+≡
module subroutine pdg_list_init_size (pl, n)
  class(pdg_list_t), intent(out) :: pl
  integer, intent(in) :: n
  allocate (pl%a (n))
end subroutine pdg_list_init_size

```

Initialize with a definite array of PDG codes. That is, each entry in the list becomes a single-particle PDG array.

```

(PDG arrays: pdg list: TBP)+≡
  generic :: init => pdg_list_init_int_array
  procedure, private :: pdg_list_init_int_array

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_list_init_int_array (pl, pdg)
    class(pdg_list_t), intent(out) :: pl
    integer, dimension(:), intent(in) :: pdg
  end subroutine pdg_list_init_int_array

(PDG arrays: procedures)+≡
module subroutine pdg_list_init_int_array (pl, pdg)
  class(pdg_list_t), intent(out) :: pl
  integer, dimension(:), intent(in) :: pdg
  integer :: i
  allocate (pl%a (size (pdg)))
  do i = 1, size (pdg)
    call pdg_array_from_int (pl%a(i), pdg(i))
  end do
end subroutine pdg_list_init_int_array

```

Set one of the entries. No bounds-check.

```

(PDG arrays: pdg list: TBP)+≡
  generic :: set => pdg_list_set_int
  generic :: set => pdg_list_set_int_array
  generic :: set => pdg_list_set_pdg_array
  procedure, private :: pdg_list_set_int
  procedure, private :: pdg_list_set_int_array
  procedure, private :: pdg_list_set_pdg_array

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_list_set_int (pl, i, pdg)
    class(pdg_list_t), intent(inout) :: pl
    integer, intent(in) :: i
    integer, intent(in) :: pdg
  end subroutine pdg_list_set_int
  module subroutine pdg_list_set_int_array (pl, i, pdg)
    class(pdg_list_t), intent(inout) :: pl
    integer, intent(in) :: i
    integer, dimension(:), intent(in) :: pdg
  end subroutine pdg_list_set_int_array
  module subroutine pdg_list_set_pdg_array (pl, i, pa)
    class(pdg_list_t), intent(inout) :: pl
    integer, intent(in) :: i
    type(pdg_array_t), intent(in) :: pa
  end subroutine pdg_list_set_pdg_array

```

```

(PDG arrays: procedures)+≡
module subroutine pdg_list_set_int (pl, i, pdg)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  integer, intent(in) :: pdg
  call pdg_array_from_int (pl%a(i), pdg)
end subroutine pdg_list_set_int

module subroutine pdg_list_set_int_array (pl, i, pdg)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  integer, dimension(:), intent(in) :: pdg
  call pdg_array_from_int_array (pl%a(i), pdg)
end subroutine pdg_list_set_int_array

module subroutine pdg_list_set_pdg_array (pl, i, pa)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  type(pdg_array_t), intent(in) :: pa
  pl%a(i) = pa
end subroutine pdg_list_set_pdg_array

```

Array size, not the length of individual entries

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: get_size => pdg_list_get_size

(PDG arrays: sub interfaces)+≡
  module function pdg_list_get_size (pl) result (n)
    class(pdg_list_t), intent(in) :: pl
    integer :: n
  end function pdg_list_get_size

(PDG arrays: procedures)+≡
module function pdg_list_get_size (pl) result (n)
  class(pdg_list_t), intent(in) :: pl
  integer :: n
  if (allocated (pl%a)) then
    n = size (pl%a)
  else
    n = 0
  end if
end function pdg_list_get_size

```

Return an entry, as a PDG array.

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: get => pdg_list_get

(PDG arrays: sub interfaces)+≡
  module function pdg_list_get (pl, i) result (pa)
    type(pdg_array_t) :: pa
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: i
  end function pdg_list_get

```

```

(PDG arrays: procedures)+≡
module function pdg_list_get (pl, i) result (pa)
  type(pdg_array_t) :: pa
  class(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: i
  pa = pl%a(i)
end function pdg_list_get

```

Check if the list entries are all either mutually disjoint or identical. The individual entries (PDG arrays) should already be sorted, so we can test for equality.

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: is_regular => pdg_list_is_regular

(PDG arrays: sub interfaces)+≡
  module function pdg_list_is_regular (pl) result (flag)
    class(pdg_list_t), intent(in) :: pl
    logical :: flag
  end function pdg_list_is_regular

(PDG arrays: procedures)+≡
module function pdg_list_is_regular (pl) result (flag)
  class(pdg_list_t), intent(in) :: pl
  logical :: flag
  integer :: i, j, s
  s = pl%get_size ()
  flag = .true.
  do i = 1, s
    do j = i + 1, s
      if (pl%a(i) .match. pl%a(j)) then
        if (pl%a(i) /= pl%a(j)) then
          flag = .false.
          return
        end if
      end if
    end do
  end do
end function pdg_list_is_regular

```

Sort the list. First, each entry gets sorted, including elimination of doublers. Then, we sort the list, using the first member of each PDG array as the marker. No removal of doublers at this stage.

If `n_in` is supplied, we do not reorder the first `n_in` particle entries.

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: sort_abs => pdg_list_sort_abs

(PDG arrays: sub interfaces)+≡
  module function pdg_list_sort_abs (pl, n_in) result (pl_sorted)
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in), optional :: n_in
    type(pdg_list_t) :: pl_sorted
  end function pdg_list_sort_abs

(PDG arrays: procedures)+≡
  module function pdg_list_sort_abs (pl, n_in) result (pl_sorted)
    class(pdg_list_t), intent(in) :: pl

```

```

integer, intent(in), optional :: n_in
type(pdg_list_t) :: pl_sorted
type(pdg_array_t), dimension(:), allocatable :: pa
integer, dimension(:), allocatable :: pdg, map
integer :: i, n0
call pl_sorted%init (pl%get_size ())
if (allocated (pl%a)) then
  allocate (pa (size (pl%a)))
  do i = 1, size (pl%a)
    pa(i) = pl%a(i)%sort_abs (unique = .true.)
  end do
  allocate (pdg (size (pa)), source = 0)
  do i = 1, size (pa)
    if (allocated (pa(i)%pdg)) then
      if (size (pa(i)%pdg) > 0) then
        pdg(i) = pa(i)%pdg(1)
      end if
    end if
  end do
  if (present (n_in)) then
    n0 = n_in
  else
    n0 = 0
  end if
  allocate (map (size (pdg)))
  map(:n0) = [(i, i = 1, n0)]
  map(n0+1:) = n0 + order_abs (pdg(n0+1:))
  do i = 1, size (pa)
    call pl_sorted%set (i, pa(map(i)))
  end do
end if
end function pdg_list_sort_abs

```

Compare sorted lists: equality. The result is undefined if some entries are not allocated.

```

(PDG arrays: pdg list: TBP)+≡
  generic :: operator (==) => pdg_list_eq
  procedure, private :: pdg_list_eq

(PDG arrays: sub interfaces)+≡
  module function pdg_list_eq (pl1, pl2) result (flag)
    class(pdg_list_t), intent(in) :: pl1, pl2
    logical :: flag
  end function pdg_list_eq

(PDG arrays: procedures)+≡
  module function pdg_list_eq (pl1, pl2) result (flag)
    class(pdg_list_t), intent(in) :: pl1, pl2
    logical :: flag
    integer :: i
    flag = .false.
    if (allocated (pl1%a) .and. allocated (pl2%a)) then
      if (size (pl1%a) == size (pl2%a)) then
        do i = 1, size (pl1%a)
          associate (a1 => pl1%a(i), a2 => pl2%a(i))

```

```

        if (allocated (a1%pdg) .and. allocated (a2%pdg)) then
            if (size (a1%pdg) == size (a2%pdg)) then
                if (size (a1%pdg) > 0) then
                    if (a1%pdg(1) /= a2%pdg(1)) return
                end if
            else
                return
            end if
        else
            return
        end if
    end associate
end do
flag = .true.
end if
end if
end function pdg_list_eq

```

Compare sorted lists. The result is undefined if some entries are not allocated.

The ordering is quite complicated. First, a shorter list comes before a longer list. Comparing entry by entry, a shorter entry comes first. Next, we check the first PDG code within corresponding entries. This is compared by absolute value. If equal, particle comes before antiparticle. Finally, if all is equal, the result is false.

```

(PDG arrays: pdg list: TBP)+≡
    generic :: operator (<) => pdg_list_lt
    procedure, private :: pdg_list_lt

(PDG arrays: sub interfaces)+≡
    module function pdg_list_lt (p1, p2) result (flag)
        class(pdg_list_t), intent(in) :: p1, p2
        logical :: flag
    end function pdg_list_lt

(PDG arrays: procedures)+≡
    module function pdg_list_lt (p1, p2) result (flag)
        class(pdg_list_t), intent(in) :: p1, p2
        logical :: flag
        integer :: i
        flag = .false.
        if (allocated (p1%a) .and. allocated (p2%a)) then
            if (size (p1%a) < size (p2%a)) then
                flag = .true.; return
            else if (size (p1%a) > size (p2%a)) then
                return
            else
                do i = 1, size (p1%a)
                    associate (a1 => p1%a(i), a2 => p2%a(i))
                        if (allocated (a1%pdg) .and. allocated (a2%pdg)) then
                            if (size (a1%pdg) < size (a2%pdg)) then
                                flag = .true.; return
                            else if (size (a1%pdg) > size (a2%pdg)) then
                                return
                            else

```

```

        if (size (a1%pdg) > 0) then
            if (abs (a1%pdg(1)) < abs (a2%pdg(1))) then
                flag = .true.; return
            else if (abs (a1%pdg(1)) > abs (a2%pdg(1))) then
                return
            else if (a1%pdg(1) > 0 .and. a2%pdg(1) < 0) then
                flag = .true.; return
            else if (a1%pdg(1) < 0 .and. a2%pdg(1) > 0) then
                return
            end if
        end if
    end if
else
    return
end if
end associate
end do
flag = .false.
end if
end if
end function pdg_list_lt

```

Replace an entry. In the result, the entry #i is replaced by the contents of the second argument. The result is not sorted.

If n_in is also set and i is less or equal to n_in, replace #i only by the first entry of pl_insert, and insert the remainder after entry n_in.

(PDG arrays: pdg list: TBP)+≡

```

    procedure :: replace => pdg_list_replace

```

(PDG arrays: sub interfaces)+≡

```

    module function pdg_list_replace (pl, i, pl_insert, n_in) result (pl_out)
        type(pdg_list_t) :: pl_out
        class(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: i
        class(pdg_list_t), intent(in) :: pl_insert
        integer, intent(in), optional :: n_in
    end function pdg_list_replace

```

(PDG arrays: procedures)+≡

```

    module function pdg_list_replace (pl, i, pl_insert, n_in) result (pl_out)
        type(pdg_list_t) :: pl_out
        class(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: i
        class(pdg_list_t), intent(in) :: pl_insert
        integer, intent(in), optional :: n_in
        integer :: n, n_insert, n_out, k
        n = pl%get_size ()
        n_insert = pl_insert%get_size ()
        n_out = n + n_insert - 1
        call pl_out%init (n_out)
!       if (allocated (pl%a)) then
            do k = 1, i - 1
                pl_out%a(k) = pl%a(k)
            end do

```

```

!   end if
  if (present (n_in)) then
    pl_out%a(i) = pl_insert%a(1)
    do k = i + 1, n_in
      pl_out%a(k) = pl%a(k)
    end do
    do k = 1, n_insert - 1
      pl_out%a(n_in+k) = pl_insert%a(1+k)
    end do
    do k = 1, n - n_in
      pl_out%a(n_in+k+n_insert-1) = pl%a(n_in+k)
    end do
  else
!   if (allocated (pl_insert%a)) then
      do k = 1, n_insert
        pl_out%a(i-1+k) = pl_insert%a(k)
      end do
!   end if
!   if (allocated (pl%a)) then
      do k = 1, n - i
        pl_out%a(i+n_insert-1+k) = pl%a(i+k)
      end do
    end if
!   end if
  end function pdg_list_replace

```

(PDG arrays: pdg list: TBP)+≡

```

  procedure :: fusion => pdg_list_fusion

```

(PDG arrays: sub interfaces)+≡

```

  module function pdg_list_fusion (pl, pl_insert, i, check_if_existing) result (pl_out)
    type(pdg_list_t) :: pl_out
    class(pdg_list_t), intent(in) :: pl
    type(pdg_list_t), intent(in) :: pl_insert
    integer, intent(in) :: i
    logical, intent(in) :: check_if_existing
  end function pdg_list_fusion

```

(PDG arrays: procedures)+≡

```

  module function pdg_list_fusion (pl, pl_insert, i, check_if_existing) result (pl_out)
    type(pdg_list_t) :: pl_out
    class(pdg_list_t), intent(in) :: pl
    type(pdg_list_t), intent(in) :: pl_insert
    integer, intent(in) :: i
    logical, intent(in) :: check_if_existing
    integer :: n, n_insert, k, n_out
    logical :: new_pdg
    n = pl%get_size ()
    n_insert = pl_insert%get_size ()
    new_pdg = .not. check_if_existing .or. &
      (.not. any (pl%search_for_particle (pl_insert%a(1)%pdg)))
    call pl_out%init (n + n_insert - 1)
    do k = 1, n
      if (new_pdg .and. k == i) then
        pl_out%a(k) = pl%a(k)%add (pl_insert%a(1))
      end if
    end do
  end function pdg_list_fusion

```

```

        else
            pl_out%a(k) = pl%a(k)
        end if
    end do
    do k = n + 1, n + n_insert - 1
        pl_out%a(k) = pl_insert%a(k-n)
    end do
end function pdg_list_fusion

```

```

(PDG arrays: pdg list: TBP)+≡
    procedure :: get_pdg_sizes => pdg_list_get_pdg_sizes

(PDG arrays: sub interfaces)+≡
    module function pdg_list_get_pdg_sizes (pl) result (i_size)
        integer, dimension(:), allocatable :: i_size
        class(pdg_list_t), intent(in) :: pl
    end function pdg_list_get_pdg_sizes

(PDG arrays: procedures)+≡
    module function pdg_list_get_pdg_sizes (pl) result (i_size)
        integer, dimension(:), allocatable :: i_size
        class(pdg_list_t), intent(in) :: pl
        integer :: i, n
        n = pl%get_size ()
        allocate (i_size (n))
        do i = 1, n
            i_size(i) = size (pl%a(i)%pdg)
        end do
    end function pdg_list_get_pdg_sizes

```

Replace the entries of `pl` by the matching entries of `pl_match`, one by one. This is done in-place. If there is no match, return failure.

```

(PDG arrays: pdg list: TBP)+≡
    procedure :: match_replace => pdg_list_match_replace

(PDG arrays: sub interfaces)+≡
    module subroutine pdg_list_match_replace (pl, pl_match, success)
        class(pdg_list_t), intent(inout) :: pl
        class(pdg_list_t), intent(in) :: pl_match
        logical, intent(out) :: success
    end subroutine pdg_list_match_replace

(PDG arrays: procedures)+≡
    module subroutine pdg_list_match_replace (pl, pl_match, success)
        class(pdg_list_t), intent(inout) :: pl
        class(pdg_list_t), intent(in) :: pl_match
        logical, intent(out) :: success
        integer :: i, j
        success = .true.
        SCAN_ENTRIES: do i = 1, size (pl%a)
            do j = 1, size (pl_match%a)
                if (pl%a(i) .match. pl_match%a(j)) then
                    pl%a(i) = pl_match%a(j)
                    cycle SCAN_ENTRIES
                end if
            end do
        end do
    end subroutine pdg_list_match_replace

```



```

        end do
        success = .false.
        return
    end do SCAN_ENTRIES
end subroutine pdg_list_match_replace

```

Just check if a PDG array matches any entry in the PDG list. The second version returns the position of the match within the list. An optional mask indicates the list elements that should be checked.

```

(PDG arrays: pdg list: TBP)+≡
generic :: operator (.match.) => pdg_list_match_pdg_array
procedure, private :: pdg_list_match_pdg_array
procedure :: find_match => pdg_list_find_match_pdg_array

(PDG arrays: sub interfaces)+≡
module function pdg_list_match_pdg_array (pl, pa) result (flag)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical :: flag
end function pdg_list_match_pdg_array
module function pdg_list_find_match_pdg_array (pl, pa, mask) result (i)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical, dimension(:), intent(in), optional :: mask
    integer :: i
end function pdg_list_find_match_pdg_array

(PDG arrays: procedures)+≡
module function pdg_list_match_pdg_array (pl, pa) result (flag)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical :: flag
    flag = pl%find_match (pa) /= 0
end function pdg_list_match_pdg_array

module function pdg_list_find_match_pdg_array (pl, pa, mask) result (i)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical, dimension(:), intent(in), optional :: mask
    integer :: i
    do i = 1, size (pl%a)
        if (present (mask)) then
            if (.not. mask(i)) cycle
        end if
        if (pl%a(i) .match. pa) return
    end do
    i = 0
end function pdg_list_find_match_pdg_array

```

Some old compilers have problems with allocatable arrays as intent(out) or as function result, so be conservative here:

```

(PDG arrays: pdg list: TBP)+≡
procedure :: create_pdg_array => pdg_list_create_pdg_array

```

```

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_list_create_pdg_array (pl, pdg)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), dimension(:), intent(inout), allocatable :: pdg
  end subroutine pdg_list_create_pdg_array

(PDG arrays: procedures)+≡
  module subroutine pdg_list_create_pdg_array (pl, pdg)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), dimension(:), intent(inout), allocatable :: pdg
    integer :: n_elements
    integer :: i
    associate (a => pl%a)
      n_elements = size (a)
      if (allocated (pdg)) deallocate (pdg)
      allocate (pdg (n_elements))
      do i = 1, n_elements
        pdg(i) = a(i)
      end do
    end associate
  end subroutine pdg_list_create_pdg_array

(PDG arrays: pdg list: TBP)+≡
  procedure :: create_antiparticles => pdg_list_create_antiparticles

(PDG arrays: sub interfaces)+≡
  module subroutine pdg_list_create_antiparticles (pl, pl_anti, n_new_particles)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_list_t), intent(out) :: pl_anti
    integer, intent(out) :: n_new_particles
  end subroutine pdg_list_create_antiparticles

(PDG arrays: procedures)+≡
  module subroutine pdg_list_create_antiparticles (pl, pl_anti, n_new_particles)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_list_t), intent(out) :: pl_anti
    integer, intent(out) :: n_new_particles
    type(pdg_list_t) :: pl_inverse
    integer :: i, n
    integer :: n_identical
    logical, dimension(:), allocatable :: collect
    n = pl%get_size (); n_identical = 0
    allocate (collect (n)); collect = .true.
    call pl_inverse%init (n)
    do i = 1, n
      pl_inverse%a(i) = pl%a(i)%invert()
    end do
    do i = 1, n
      if (any (pl_inverse%a(i) == pl%a)) then
        collect(i) = .false.
        n_identical = n_identical + 1
      end if
    end do
    n_new_particles = n - n_identical
    if (n_new_particles > 0) then

```

```

        call pl_anti%init (n_new_particles)
        do i = 1, n
            if (collect (i)) pl_anti%a(i) = pl_inverse%a(i)
        end do
    end if
end subroutine pdg_list_create_antiparticles

<PDG arrays: pdg list: TBP>+≡
    procedure :: search_for_particle => pdg_list_search_for_particle

<PDG arrays: sub interfaces>+≡
    elemental module function pdg_list_search_for_particle (pl, i_part) result (found)
        logical :: found
        class(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: i_part
    end function pdg_list_search_for_particle

<PDG arrays: procedures>+≡
    elemental module function pdg_list_search_for_particle (pl, i_part) result (found)
        logical :: found
        class(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: i_part
        integer :: i_pl
        do i_pl = 1, size (pl%a)
            found = pl%a(i_pl)%search_for_particle (i_part)
            if (found) return
        end do
    end function pdg_list_search_for_particle

<PDG arrays: pdg list: TBP>+≡
    procedure :: contains_colored_particles => pdg_list_contains_colored_particles

<PDG arrays: sub interfaces>+≡
    module function pdg_list_contains_colored_particles (pl) result (colored)
        class(pdg_list_t), intent(in) :: pl
        logical :: colored
    end function pdg_list_contains_colored_particles

<PDG arrays: procedures>+≡
    module function pdg_list_contains_colored_particles (pl) result (colored)
        class(pdg_list_t), intent(in) :: pl
        logical :: colored
        integer :: i
        colored = .false.
        do i = 1, size (pl%a)
            if (pl%a(i)%has_colored_particles()) then
                colored = .true.
                exit
            end if
        end do
    end function pdg_list_contains_colored_particles

```

13.2.6 Unit tests

Test module, followed by the corresponding implementation module.

<pdg_arrays_ut.f90>≡
<File header>

```
module pdg_arrays_ut
  use unit_tests
  use pdg_arrays_uti
```

<Standard module head>

<PDG arrays: public test>

contains

<PDG arrays: test driver>

```
end module pdg_arrays_ut
```

<pdg_arrays_uti.f90>≡
<File header>

```
module pdg_arrays_uti
```

```
  use pdg_arrays
```

<Standard module head>

<PDG arrays: test declarations>

contains

<PDG arrays: tests>

```
end module pdg_arrays_uti
```

API: driver for the unit tests below.

<PDG arrays: public test>≡
public :: pdg_arrays_test

<PDG arrays: test driver>≡
subroutine pdg_arrays_test (u, results)
 integer, intent(in) :: u
 type (test_results_t), intent(inout) :: results
<PDG arrays: execute tests>
end subroutine pdg_arrays_test

Basic functionality.

<PDG arrays: execute tests>≡
call test (pdg_arrays_1, "pdg_arrays_1", &
 "create and sort PDG array", &
 u, results)

<PDG arrays: test declarations>≡
public :: pdg_arrays_1

```

<PDG arrays: tests>≡
subroutine pdg_arrays_1 (u)
  integer, intent(in) :: u

  type(pdg_array_t) :: pa, pa1, pa2, pa3, pa4, pa5, pa6
  integer, dimension(:), allocatable :: pdg

  write (u, "(A)")  "* Test output: pdg_arrays_1"
  write (u, "(A)")  "* Purpose: create and sort PDG arrays"
  write (u, "(A)")

  write (u, "(A)")  "* Assignment"
  write (u, "(A)")

  call pa%write (u)
  write (u, *)
  write (u, "(A,I0)") "length = ", pa%get_length ()
  pdg = pa
  write (u, "(A,3(1x,I0))") "contents = ", pdg

  write (u, *)
  pa = 1
  call pa%write (u)
  write (u, *)
  write (u, "(A,I0)") "length = ", pa%get_length ()
  pdg = pa
  write (u, "(A,3(1x,I0))") "contents = ", pdg

  write (u, *)
  pa = [1, 2, 3]
  call pa%write (u)
  write (u, *)
  write (u, "(A,I0)") "length = ", pa%get_length ()
  pdg = pa
  write (u, "(A,3(1x,I0))") "contents = ", pdg
  write (u, "(A,I0)") "element #2 = ", pa%get (2)

  write (u, *)
  write (u, "(A)")  "* Replace"
  write (u, *)

  pa = pa%replace (2, [-5, 5, -7])
  call pa%write (u)
  write (u, *)

  write (u, *)
  write (u, "(A)")  "* Sort"
  write (u, *)

  pa = [1, -7, 3, -5, 5, 3]
  call pa%write (u)
  write (u, *)
  pa1 = pa%sort_abs ()
  pa2 = pa%sort_abs (unique = .true.)

```

```

call pa1%write (u)
write (u, *)
call pa2%write (u)
write (u, *)

write (u, *)
write (u, "(A)")  "* Compare"
write (u, *)

pa1 = [1, 3]
pa2 = [1, 2, -2]
pa3 = [1, 2, 4]
pa4 = [1, 2, 4]
pa5 = [1, 2, -4]
pa6 = [1, 2, -3]

write (u, "(A,6(1x,L1))") "< ", &
    pa1 < pa2, pa2 < pa3, pa3 < pa4, pa4 < pa5, pa5 < pa6, pa6 < pa1
write (u, "(A,6(1x,L1))") "> ", &
    pa1 > pa2, pa2 > pa3, pa3 > pa4, pa4 > pa5, pa5 > pa6, pa6 > pa1
write (u, "(A,6(1x,L1))") "<=", &
    pa1 <= pa2, pa2 <= pa3, pa3 <= pa4, pa4 <= pa5, pa5 <= pa6, pa6 <= pa1
write (u, "(A,6(1x,L1))") ">=", &
    pa1 >= pa2, pa2 >= pa3, pa3 >= pa4, pa4 >= pa5, pa5 >= pa6, pa6 >= pa1
write (u, "(A,6(1x,L1))") "==", &
    pa1 == pa2, pa2 == pa3, pa3 == pa4, pa4 == pa5, pa5 == pa6, pa6 == pa1
write (u, "(A,6(1x,L1))") "/=", &
    pa1 /= pa2, pa2 /= pa3, pa3 /= pa4, pa4 /= pa5, pa5 /= pa6, pa6 /= pa1

write (u, *)
pa1 = [0]
pa2 = [1, 2]
pa3 = [1, -2]

write (u, "(A,6(1x,L1))") ".eqv ", &
    pa1 .eqv. pa1, pa1 .eqv. pa2, &
    pa2 .eqv. pa2, pa2 .eqv. pa3

write (u, "(A,6(1x,L1))") ".neqv", &
    pa1 .neqv. pa1, pa1 .neqv. pa2, &
    pa2 .neqv. pa2, pa2 .neqv. pa3

write (u, *)
write (u, "(A,6(1x,L1))") ".match", &
    pa1 .match. 0, pa1 .match. 1, &
    pa2 .match. 0, pa2 .match. 1, pa2 .match. 3

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_1"

end subroutine pdg_arrays_1

```

PDG array list, i.e., arrays of arrays.

```

(PDG arrays: execute tests)+≡
    call test (pdg_arrays_2, "pdg_arrays_2", &
        "create and sort PDG lists", &
        u, results)

(PDG arrays: test declarations)+≡
    public :: pdg_arrays_2

(PDG arrays: tests)+≡
    subroutine pdg_arrays_2 (u)
        integer, intent(in) :: u

        type(pdg_array_t) :: pa
        type(pdg_list_t) :: pl, pl1

        write (u, "(A)")  "* Test output: pdg_arrays_2"
        write (u, "(A)")  "* Purpose: create and sort PDG lists"
        write (u, "(A)")

        write (u, "(A)")  "* Assignment"
        write (u, "(A)")

        call pl%init (3)
        call pl%set (1, 42)
        call pl%set (2, [3, 2])
        pa = [5, -5]
        call pl%set (3, pa)
        call pl%write (u)
        write (u, *)
        write (u, "(A,I0)") "size = ", pl%get_size ()

        write (u, "(A)")
        write (u, "(A)")  "* Sort"
        write (u, "(A)")

        pl = pl%sort_abs ()
        call pl%write (u)
        write (u, *)

        write (u, "(A)")
        write (u, "(A)")  "* Extract item #3"
        write (u, "(A)")

        pa = pl%get (3)
        call pa%write (u)
        write (u, *)

        write (u, "(A)")
        write (u, "(A)")  "* Replace item #3"
        write (u, "(A)")

        call pl1%init (2)
        call pl1%set (1, [2, 4])
        call pl1%set (2, -7)

```

```

pl = pl%replace (3, pl1)
call pl%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_2"

end subroutine pdg_arrays_2

```

Check if a (sorted) PDG array lists is regular. The entries (PDG arrays) must not overlap, unless they are identical.

```

<PDG arrays: execute tests>+≡
  call test (pdg_arrays_3, "pdg_arrays_3", &
    "check PDG lists", &
    u, results)

<PDG arrays: test declarations>+≡
  public :: pdg_arrays_3

<PDG arrays: tests>+≡
  subroutine pdg_arrays_3 (u)
    integer, intent(in) :: u

    type(pdg_list_t) :: pl

    write (u, "(A)")  "* Test output: pdg_arrays_3"
    write (u, "(A)")  "* Purpose: check for regular PDG lists"
    write (u, "(A)")

    write (u, "(A)")  "* Regular list"
    write (u, "(A)")

    call pl%init (4)
    call pl%set (1, [1, 2])
    call pl%set (2, [1, 2])
    call pl%set (3, [5, -5])
    call pl%set (4, 42)
    call pl%write (u)
    write (u, *)
    write (u, "(L1)") pl%is_regular ()

    write (u, "(A)")
    write (u, "(A)")  "* Irregular list"
    write (u, "(A)")

    call pl%init (4)
    call pl%set (1, [1, 2])
    call pl%set (2, [1, 2])
    call pl%set (3, [2, 5, -5])
    call pl%set (4, 42)
    call pl%write (u)
    write (u, *)
    write (u, "(L1)") pl%is_regular ()

    write (u, "(A)")

```



```

write (u, "(A)")  "* Test output end: pdg_arrays_3"

end subroutine pdg_arrays_3

```

Compare PDG array lists. The lists must be regular, i.e., sorted and with non-overlapping (or identical) entries.

```

(PDG arrays: execute tests)+≡
call test (pdg_arrays_4, "pdg_arrays_4", &
  "compare PDG lists", &
  u, results)

(PDG arrays: test declarations)+≡
public :: pdg_arrays_4

(PDG arrays: tests)+≡
subroutine pdg_arrays_4 (u)
  integer, intent(in) :: u

  type(pdg_list_t) :: pl1, pl2, pl3

  write (u, "(A)")  "* Test output: pdg_arrays_4"
  write (u, "(A)")  "* Purpose: check for regular PDG lists"
  write (u, "(A)")

  write (u, "(A)")  "* Create lists"
  write (u, "(A)")

  call pl1%init (4)
  call pl1%set (1, [1, 2])
  call pl1%set (2, [1, 2])
  call pl1%set (3, [5, -5])
  call pl1%set (4, 42)
  write (u, "(I1,1x)", advance = "no")  1
  call pl1%write (u)
  write (u, *)

  call pl2%init (2)
  call pl2%set (1, 3)
  call pl2%set (2, [5, -5])
  write (u, "(I1,1x)", advance = "no")  2
  call pl2%write (u)
  write (u, *)

  call pl3%init (2)
  call pl3%set (1, 4)
  call pl3%set (2, [5, -5])
  write (u, "(I1,1x)", advance = "no")  3
  call pl3%write (u)
  write (u, *)

  write (u, "(A)")
  write (u, "(A)")  "* a == b"
  write (u, "(A)")

  write (u, "(2x,A)")  "123"

```

```

write (u, *)
write (u, "(I1,1x,4L1)") 1, p11 == p11, p11 == p12, p11 == p13
write (u, "(I1,1x,4L1)") 2, p12 == p11, p12 == p12, p12 == p13
write (u, "(I1,1x,4L1)") 3, p13 == p11, p13 == p12, p13 == p13

write (u, "(A)")
write (u, "(A)")  "*" a < b"
write (u, "(A)")

write (u, "(2x,A)")  "123"
write (u, *)
write (u, "(I1,1x,4L1)") 1, p11 < p11, p11 < p12, p11 < p13
write (u, "(I1,1x,4L1)") 2, p12 < p11, p12 < p12, p12 < p13
write (u, "(I1,1x,4L1)") 3, p13 < p11, p13 < p12, p13 < p13

write (u, "(A)")
write (u, "(A)")  "*" Test output end: pdg_arrays_4"

end subroutine pdg_arrays_4

```

Match-replace: translate all entries in the first list into the matching entries of the second list, if there is a match.

```

<PDG arrays: execute tests>+≡
  call test (pdg_arrays_5, "pdg_arrays_5", &
    "match PDG lists", &
    u, results)

<PDG arrays: test declarations>+≡
  public :: pdg_arrays_5

<PDG arrays: tests>+≡
  subroutine pdg_arrays_5 (u)
    integer, intent(in) :: u

    type(pdg_list_t) :: p11, p12, p13
    logical :: success

    write (u, "(A)")  "*" Test output: pdg_arrays_5"
    write (u, "(A)")  "*" Purpose: match-replace"
    write (u, "(A)")

    write (u, "(A)")  "*" Create lists"
    write (u, "(A)")

    call p11%init (2)
    call p11%set (1, [1, 2])
    call p11%set (2, 42)
    call p11%write (u)
    write (u, *)
    call p13%init (2)
    call p13%set (1, [42, -42])
    call p13%set (2, [1, 2, 3, 4])
    call p11%match_replace (p13, success)
    call p13%write (u)
    write (u, "(1x,A,1x,L1,':',1x)", advance="no")  "=>", success

```

```

call pl1%write (u)
write (u, *)

write (u, *)

call pl2%init (2)
call pl2%set (1, 9)
call pl2%set (2, 42)
call pl2%write (u)
write (u, *)
call pl2%match_replace (pl3, success)
call pl3%write (u)
write (u, "(1x,A,1x,L1,':',1x)", advance="no")  "=>", success
call pl2%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_5"

end subroutine pdg_arrays_5

```

13.3 Jets

The FastJet library is linked externally, if available. The wrapper code is also in a separate directory. Here, we define WHIZARD-specific procedures and tests.

```
<jets.f90>≡  
  <File header>  
  
  module jets  
  
    use fastjet !NODEP!  
  
    <Standard module head>  
  
    <Jets: public>  
  
    contains  
  
    <Jets: procedures>  
  
  end module jets
```

13.3.1 Re-exported symbols

We use this module as a proxy for the FastJet interface, therefore we re-export some symbols.

```
<Jets: public>≡  
  public :: fastjet_available  
  public :: fastjet_init  
  public :: jet_definition_t  
  public :: pseudojet_t  
  public :: pseudojet_vector_t  
  public :: cluster_sequence_t  
  public :: assignment (=)
```

The initialization routine prints the banner.

```
<Jets: procedures>≡  
  subroutine fastjet_init ()  
    call print_banner ()  
  end subroutine fastjet_init
```

The jet algorithm codes (actually, integers)

```
<Jets: public>+≡  
  public :: kt_algorithm  
  public :: cambridge_algorithm  
  public :: antikt_algorithm  
  public :: genkt_algorithm  
  public :: cambridge_for_passive_algorithm  
  public :: genkt_for_passive_algorithm  
  public :: ee_kt_algorithm  
  public :: ee_genkt_algorithm  
  public :: plugin_algorithm  
  public :: undefined_jet_algorithm
```

13.3.2 Unit tests

Test module, followed by the corresponding implementation module.

<jets_ut.f90>≡
<File header>

```
module jets_ut
  use unit_tests
  use jets_uti
```

<Standard module head>

<Jets: public test>

contains

<Jets: test driver>

```
end module jets_ut
```

<jets_uti.f90>≡
<File header>

```
module jets_uti
```

<Use kinds>
 use fastjet !NODEP!

```
  use jets
```

<Standard module head>

<Jets: test declarations>

contains

<Jets: tests>

```
end module jets_uti
```

API: driver for the unit tests below.

<Jets: public test>≡
 public :: jets_test

<Jets: test driver>≡
 subroutine jets_test (u, results)
 integer, intent(in) :: u
 type (test_results_t), intent(inout) :: results
 <Jets: execute tests>
 end subroutine jets_test

This test is actually the minimal example from the FastJet manual, translated to Fortran.

Note that FastJet creates pseudojet vectors, which we mirror in the `pseudojet_vector_t`, but immediately assign to pseudojet arrays. Without automatic finalization available in the compilers, we should avoid this in actual code and rather introduce intermediate variables for those objects, which we can finalize explicitly.

```

<Jets: execute tests>≡
  call test (jets_1, "jets_1", &
    "basic FastJet functionality", &
    u, results)

<Jets: test declarations>≡
  public :: jets_1

<Jets: tests>≡
  subroutine jets_1 (u)
    integer, intent(in) :: u

    type(pseudojet_t), dimension(:), allocatable :: prt, jets, constituents
    type(jet_definition_t) :: jet_def
    type(cluster_sequence_t) :: cs

    integer, parameter :: dp = default
    integer :: i, j

    write (u, "(A)")  "* Test output: jets_1"
    write (u, "(A)")  "* Purpose: test basic FastJet functionality"
    write (u, "(A)")

    write (u, "(A)")  "* Print banner"
    call print_banner ()

    write (u, *)
    write (u, "(A)")  "* Prepare input particles"
    allocate (prt (3))
    call prt(1)%init ( 99._dp, 0.1_dp, 0._dp, 100._dp)
    call prt(2)%init (  4._dp,-0.1_dp, 0._dp,  5._dp)
    call prt(3)%init (-99._dp, 0._dp,  0._dp,  99._dp)

    write (u, *)
    write (u, "(A)")  "* Define jet algorithm"
    call jet_def%init (antikt_algorithm, 0.7_dp)

    write (u, *)
    write (u, "(A)")  "* Cluster particles according to jet algorithm"

    write (u, *)
    write (u, "(A,A)") "Clustering with ", jet_def%description ()
    call cs%init (pseudojet_vector (prt), jet_def)

    write (u, *)
    write (u, "(A)")  "* Sort output jets"
    jets = sorted_by_pt (cs%inclusive_jets ())

    write (u, *)

```

```

write (u, "(A)")  "* Print jet observables and constituents"
write (u, *)
write (u, "(4x,3(7x,A3))") "pt", "y", "phi"
do i = 1, size (jets)
  write (u, "(A,1x,I0,A,3(1x,F9.5))") &
    "jet", i, ":", jets(i)%perp (), jets(i)%rap (), jets(i)%phi ()
  constituents = jets(i)%constituents ()
  do j = 1, size (constituents)
    write (u, "(4x,A,1x,I0,A,F9.5)") &
      "constituent", j, "'s pt:", constituents(j)%perp ()
  end do
  do j = 1, size (constituents)
    call constituents(j)%final ()
  end do
end do

write (u, *)
write (u, "(A)")  "* Cleanup"

do i = 1, size (prt)
  call prt(i)%final ()
end do
do i = 1, size (jets)
  call jets(i)%final ()
end do
call jet_def%final ()
call cs%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: jets_1"

end subroutine jets_1

```

13.4 Subevents

The purpose of subevents is to store the relevant part of the physical event (either partonic or hadronic), and to hold particle selections and combinations which are constructed in cut or analysis expressions.

```
<subevents.f90>≡
  <File header>

  module subevents

    use, intrinsic :: iso_c_binding !NODEP!

    <Use kinds>
    use numeric_utils, only: pacify
    use c_particles
    use lorentz
    use pdg_arrays
    use jets

    <Standard module head>

    <Subevents: public>

    <Subevents: parameters>

    <Subevents: types>

    <Subevents: interfaces>

    interface
    <Subevents: sub interfaces>
    end interface

  end module subevents

<subevents_sub.f90>≡
  <File header>

  submodule (subevents) subevents_s

    use io_units
    use format_defs, only: FMT_14, FMT_19
    use format_utils, only: pac_fmt
    use physics_defs
    use sorting

    implicit none

  contains

    <Subevents: procedures>

  end submodule subevents_s
```


13.4.1 Particles

For the purpose of this module, a particle has a type which can indicate a beam, incoming, outgoing, or composite particle, flavor and helicity codes (integer, undefined for composite), four-momentum and invariant mass squared. (Other particles types are used in extended event types, but also defined here.) Furthermore, each particle has an allocatable array of ancestors – particle indices which indicate the building blocks of a composite particle. For an incoming/outgoing particle, the array contains only the index of the particle itself.

For incoming particles, the momentum is inverted before storing it in the particle object.

```
<Subevents: parameters>≡
  integer, parameter, public :: PRT_UNDEFINED = 0
  integer, parameter, public :: PRT_BEAM = -9
  integer, parameter, public :: PRT_INCOMING = 1
  integer, parameter, public :: PRT_OUTGOING = 2
  integer, parameter, public :: PRT_COMPOSITE = 3
  integer, parameter, public :: PRT_VIRTUAL = 4
  integer, parameter, public :: PRT_RESONANT = 5
  integer, parameter, public :: PRT_BEAM_REMNANT = 9
```

The type

We initialize only the type here and mark as unpolarized. The initializers below do the rest. The logicals `is_b_jet` and `is_c_jet` are true only if `prt_t` comes out of the `subevt_cluster` routine and fulfils the correct flavor content.

```
<Subevents: public>≡
  public :: prt_t

<Subevents: types>≡
  type :: prt_t
    private
    integer :: type = PRT_UNDEFINED
    integer :: pdg
    logical :: polarized = .false.
    logical :: colorized = .false.
    logical :: clustered = .false.
    logical :: is_b_jet = .false.
    logical :: is_c_jet = .false.
    integer :: h
    type(vector4_t) :: p
    real(default) :: p2
    integer, dimension(:), allocatable :: src
    integer, dimension(:), allocatable :: col
    integer, dimension(:), allocatable :: acl
  end type prt_t
```

Initializers. Polarization is set separately. Finalizers are not needed.

```
<Subevents: procedures>≡
  subroutine prt_init_beam (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
```

```

    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_BEAM
    call prt_set (prt, pdg, - p, p2, src)
end subroutine prt_init_beam

subroutine prt_init_incoming (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_INCOMING
    call prt_set (prt, pdg, - p, p2, src)
end subroutine prt_init_incoming

subroutine prt_init_outgoing (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_OUTGOING
    call prt_set (prt, pdg, p, p2, src)
end subroutine prt_init_outgoing

subroutine prt_init_composite (prt, p, src)
    type(prt_t), intent(out) :: prt
    type(vector4_t), intent(in) :: p
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_COMPOSITE
    call prt_set (prt, 0, p, p**2, src)
end subroutine prt_init_composite

```

This version is for temporary particle objects, so the `src` array is not set.

<Subevents: public>+≡

```
public :: prt_init_combine
```

<Subevents: sub interfaces>≡

```

module subroutine prt_init_combine (prt, prt1, prt2)
    type(prt_t), intent(out) :: prt
    type(prt_t), intent(in) :: prt1, prt2
end subroutine prt_init_combine

```

<Subevents: procedures>+≡

```

module subroutine prt_init_combine (prt, prt1, prt2)
    type(prt_t), intent(out) :: prt
    type(prt_t), intent(in) :: prt1, prt2
    type(vector4_t) :: p
    integer, dimension(0) :: src
    prt%type = PRT_COMPOSITE
    p = prt1%p + prt2%p
    call prt_set (prt, 0, p, p**2, src)
end subroutine prt_init_combine

```

Init from a pseudojet object.

```
<Subevents: procedures>+≡
  subroutine prt_init_pseudojet (prt, jet, src, pdg, is_b_jet, is_c_jet)
    type(prt_t), intent(out) :: prt
    type(pseudojet_t), intent(in) :: jet
    integer, dimension(:), intent(in) :: src
    integer, intent(in) :: pdg
    logical, intent(in) :: is_b_jet, is_c_jet
    type(vector4_t) :: p
    prt%type = PRT_COMPOSITE
    p = vector4_moving (jet%e(), &
      vector3_moving ([jet%px(), jet%py(), jet%pz()]))
    call prt_set (prt, pdg, p, p**2, src)
    prt%is_b_jet = is_b_jet
    prt%is_c_jet = is_c_jet
    prt%clustered = .true.
  end subroutine prt_init_pseudojet
```

Accessing contents

```
<Subevents: public>+≡
  public :: prt_get_pdg

<Subevents: sub interfaces>+≡
  elemental module function prt_get_pdg (prt) result (pdg)
    integer :: pdg
    type(prt_t), intent(in) :: prt
  end function prt_get_pdg

<Subevents: procedures>+≡
  elemental module function prt_get_pdg (prt) result (pdg)
    integer :: pdg
    type(prt_t), intent(in) :: prt
    pdg = prt%pdg
  end function prt_get_pdg

<Subevents: public>+≡
  public :: prt_get_momentum

<Subevents: sub interfaces>+≡
  elemental module function prt_get_momentum (prt) result (p)
    type(vector4_t) :: p
    type(prt_t), intent(in) :: prt
  end function prt_get_momentum

<Subevents: procedures>+≡
  elemental module function prt_get_momentum (prt) result (p)
    type(vector4_t) :: p
    type(prt_t), intent(in) :: prt
    p = prt%p
  end function prt_get_momentum
```

```

<Subevents: public>+≡
    public :: prt_get_msq

<Subevents: sub interfaces>+≡
    elemental module function prt_get_msq (prt) result (msq)
        real(default) :: msq
        type(prt_t), intent(in) :: prt
    end function prt_get_msq

<Subevents: procedures>+≡
    elemental module function prt_get_msq (prt) result (msq)
        real(default) :: msq
        type(prt_t), intent(in) :: prt
        msq = prt%p2
    end function prt_get_msq

<Subevents: public>+≡
    public :: prt_is_polarized

<Subevents: sub interfaces>+≡
    elemental module function prt_is_polarized (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_polarized

<Subevents: procedures>+≡
    elemental module function prt_is_polarized (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%polarized
    end function prt_is_polarized

<Subevents: public>+≡
    public :: prt_get_helicity

<Subevents: sub interfaces>+≡
    elemental module function prt_get_helicity (prt) result (h)
        integer :: h
        type(prt_t), intent(in) :: prt
    end function prt_get_helicity

<Subevents: procedures>+≡
    elemental module function prt_get_helicity (prt) result (h)
        integer :: h
        type(prt_t), intent(in) :: prt
        h = prt%h
    end function prt_get_helicity

<Subevents: public>+≡
    public :: prt_is_colorized

<Subevents: sub interfaces>+≡
    elemental module function prt_is_colorized (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_colorized

```

```

<Subevents: procedures>+≡
  elemental module function prt_is_colorized (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
    flag = prt%colorized
  end function prt_is_colorized

<Subevents: public>+≡
  public :: prt_is_clustered

<Subevents: sub interfaces>+≡
  elemental module function prt_is_clustered (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
  end function prt_is_clustered

<Subevents: procedures>+≡
  elemental module function prt_is_clustered (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
    flag = prt%clustered
  end function prt_is_clustered

<Subevents: public>+≡
  public :: prt_is_recombinable

<Subevents: sub interfaces>+≡
  elemental module function prt_is_recombinable (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
  end function prt_is_recombinable

<Subevents: procedures>+≡
  elemental module function prt_is_recombinable (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
    flag = prt_is_parton (prt) .or. &
      abs(prt%pdg) == TOP_Q .or. &
      prt_is_lepton (prt) .or. &
      prt_is_photon (prt)
  end function prt_is_recombinable

<Subevents: public>+≡
  public :: prt_is_photon

<Subevents: sub interfaces>+≡
  elemental module function prt_is_photon (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
  end function prt_is_photon

<Subevents: procedures>+≡
  elemental module function prt_is_photon (prt) result (flag)
    logical :: flag
    type(prt_t), intent(in) :: prt
    flag = prt%pdg == PHOTON
  end function prt_is_photon

```

We do not take the top quark into account here.

```

<Subevents: public>+≡
    public :: prt_is_parton

<Subevents: sub interfaces>+≡
    elemental module function prt_is_parton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_parton

<Subevents: procedures>+≡
    elemental module function prt_is_parton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = abs(prt%pdg) == DOWN_Q .or. &
               abs(prt%pdg) == UP_Q .or. &
               abs(prt%pdg) == STRANGE_Q .or. &
               abs(prt%pdg) == CHARM_Q .or. &
               abs(prt%pdg) == BOTTOM_Q .or. &
               prt%pdg == GLUON
    end function prt_is_parton

<Subevents: public>+≡
    public :: prt_is_lepton

<Subevents: sub interfaces>+≡
    elemental module function prt_is_lepton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_lepton

<Subevents: procedures>+≡
    elemental module function prt_is_lepton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = abs(prt%pdg) == ELECTRON .or. &
               abs(prt%pdg) == MUON .or. &
               abs(prt%pdg) == TAU
    end function prt_is_lepton

<Subevents: public>+≡
    public :: prt_is_b_jet

<Subevents: sub interfaces>+≡
    elemental module function prt_is_b_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_b_jet

<Subevents: procedures>+≡
    elemental module function prt_is_b_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%is_b_jet
    end function prt_is_b_jet

```

```

<Subevents: public>+≡
    public :: prt_is_c_jet

<Subevents: sub interfaces>+≡
    elemental module function prt_is_c_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
    end function prt_is_c_jet

<Subevents: procedures>+≡
    elemental module function prt_is_c_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%is_c_jet
    end function prt_is_c_jet

```

The number of open color (anticolor) lines. We inspect the list of color (anticolor) lines and count the entries that do not appear in the list of anticolors (colors). (There is no check against duplicates; we assume that color line indices are unique.)

```

<Subevents: public>+≡
    public :: prt_get_n_col
    public :: prt_get_n_acl

<Subevents: sub interfaces>+≡
    elemental module function prt_get_n_col (prt) result (n)
        integer :: n
        type(prt_t), intent(in) :: prt
    end function prt_get_n_col
    elemental module function prt_get_n_acl (prt) result (n)
        integer :: n
        type(prt_t), intent(in) :: prt
    end function prt_get_n_acl

<Subevents: procedures>+≡
    elemental module function prt_get_n_col (prt) result (n)
        integer :: n
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable :: col, acl
        integer :: i
        n = 0
        if (prt%colorized) then
            do i = 1, size (prt%col)
                if (all (prt%col(i) /= prt%acl)) n = n + 1
            end do
        end if
    end function prt_get_n_col

    elemental module function prt_get_n_acl (prt) result (n)
        integer :: n
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable :: col, acl
        integer :: i
        n = 0
        if (prt%colorized) then

```

```

        do i = 1, size (prt%acl)
            if (all (prt%acl(i) /= prt%col)) n = n + 1
        end do
    end if
end function prt_get_n_acl

```

Return the color and anticolor-flow line indices explicitly.

```

<Subevents: public>+≡
    public :: prt_get_color_indices

<Subevents: sub interfaces>+≡
    module subroutine prt_get_color_indices (prt, col, acl)
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable, intent(out) :: col, acl
    end subroutine prt_get_color_indices

<Subevents: procedures>+≡
    module subroutine prt_get_color_indices (prt, col, acl)
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable, intent(out) :: col, acl
        if (prt%colorized) then
            col = prt%col
            acl = prt%acl
        else
            col = [integer::]
            acl = [integer::]
        end if
    end subroutine prt_get_color_indices

```

Setting data

Set the PDG, momentum and momentum squared, and ancestors. If allocation-assignment is available, this can be simplified.

```

<Subevents: procedures>+≡
    subroutine prt_set (prt, pdg, p, p2, src)
        type(prt_t), intent(inout) :: prt
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: p2
        integer, dimension(:), intent(in) :: src
        prt%pdg = pdg
        prt%p = p
        prt%p2 = p2
        if (allocated (prt%src)) then
            if (size (src) /= size (prt%src)) then
                deallocate (prt%src)
                allocate (prt%src (size (src)))
            end if
        else
            allocate (prt%src (size (src)))
        end if
        prt%src = src
    end subroutine prt_set

```


Set the particle PDG code separately.

```
<Subevents: procedures>+≡  
  elemental subroutine prt_set_pdg (prt, pdg)  
    type(prt_t), intent(inout) :: prt  
    integer, intent(in) :: pdg  
    prt%pdg = pdg  
  end subroutine prt_set_pdg
```

Set the momentum separately.

```
<Subevents: procedures>+≡  
  elemental subroutine prt_set_p (prt, p)  
    type(prt_t), intent(inout) :: prt  
    type(vector4_t), intent(in) :: p  
    prt%p = p  
  end subroutine prt_set_p
```

Set the squared invariant mass separately.

```
<Subevents: procedures>+≡  
  elemental subroutine prt_set_p2 (prt, p2)  
    type(prt_t), intent(inout) :: prt  
    real(default), intent(in) :: p2  
    prt%p2 = p2  
  end subroutine prt_set_p2
```

Set helicity (optional).

```
<Subevents: procedures>+≡  
  subroutine prt_polarize (prt, h)  
    type(prt_t), intent(inout) :: prt  
    integer, intent(in) :: h  
    prt%polarized = .true.  
    prt%h = h  
  end subroutine prt_polarize
```

Set color-flow indices (optional).

```
<Subevents: procedures>+≡  
  subroutine prt_colorize (prt, col, acl)  
    type(prt_t), intent(inout) :: prt  
    integer, dimension(:), intent(in) :: col, acl  
    prt%colorized = .true.  
    prt%col = col  
    prt%acl = acl  
  end subroutine prt_colorize
```

Conversion

Transform a `prt_t` object into a `c_prt_t` object.

```
<Subevents: public>+≡  
  public :: c_prt
```

```

<Subevents: interfaces>≡
  interface c_prt
    module procedure c_prt_from_prt
  end interface

<Subevents: sub interfaces>+≡
  elemental module function c_prt_from_prt (prt) result (c_prt)
    type(c_prt_t) :: c_prt
    type(prt_t), intent(in) :: prt
  end function c_prt_from_prt

<Subevents: procedures>+≡
  elemental module function c_prt_from_prt (prt) result (c_prt)
    type(c_prt_t) :: c_prt
    type(prt_t), intent(in) :: prt
    c_prt = prt%p
    c_prt%type = prt%type
    c_prt%pdg = prt%pdg
    if (prt%polarized) then
      c_prt%polarized = 1
    else
      c_prt%polarized = 0
    end if
    c_prt%h = prt%h
  end function c_prt_from_prt

```

Output

```

<Subevents: public>+≡
  public :: prt_write

<Subevents: sub interfaces>+≡
  module subroutine prt_write (prt, unit, testflag)
    type(prt_t), intent(in) :: prt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine prt_write

<Subevents: procedures>+≡
  module subroutine prt_write (prt, unit, testflag)
    type(prt_t), intent(in) :: prt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    logical :: pacified
    type(prt_t) :: tmp
    character(len=7) :: fmt
    integer :: u, i
    call pac_fmt (fmt, FMT_19, FMT_14, testflag)
    u = given_output_unit (unit); if (u < 0) return
    pacified = .false.; if (present (testflag)) pacified = testflag
    tmp = prt
    if (pacified) call pacify (tmp)
    write (u, "(1x,A)", advance="no") "prt("
    select case (prt%type)

```

```

case (PRT_UNDEFINED);      write (u, "('?)", advance="no")
case (PRT_BEAM);           write (u, "('b:)", advance="no")
case (PRT_INCOMING);       write (u, "('i:)", advance="no")
case (PRT_OUTGOING);       write (u, "('o:)", advance="no")
case (PRT_COMPOSITE);      write (u, "('c:)", advance="no")
end select
select case (prt%type)
case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING)
  if (prt%polarized) then
    write (u, "(I0,'/',I0,'|')", advance="no") prt%pdg, prt%h
  else
    write (u, "(I0,'|')", advance="no") prt%pdg
  end if
end select
select case (prt%type)
case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING, PRT_COMPOSITE)
  if (prt%colorized) then
    write (u, "(*I0,:',',')", advance="no") prt%col
    write (u, "('/',)", advance="no")
    write (u, "(*I0,:',',')", advance="no") prt%acl
    write (u, "('/',)", advance="no")
  end if
end select
select case (prt%type)
case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING, PRT_COMPOSITE)
  write (u, "(" // FMT_14 // ",',';"," // FMT_14 // ",',',", " // &
    FMT_14 // ",',',", " // FMT_14 // ")", advance="no") tmp%p
  write (u, "('|',", " // fmt // ")", advance="no") tmp%p2
end select
if (allocated (prt%src)) then
  write (u, "('|')", advance="no")
  do i = 1, size (prt%src)
    write (u, "(1x,I0)", advance="no") prt%src(i)
  end do
end if
if (prt%is_b_jet) then
  write (u, "('|b jet')", advance="no")
end if
if (prt%is_c_jet) then
  write (u, "('|c jet')", advance="no")
end if
write (u, "(A)"  ")")
end subroutine prt_write

```

Tools

Two particles match if their src arrays are the same.

```

<Subevents: public>+≡
  public :: operator(.match.)

<Subevents: interfaces>+≡
  interface operator(.match.)
    module procedure prt_match

```

```
end interface
```

```

<Subevents: sub interfaces>+≡
    elemental module function prt_match (prt1, prt2) result (match)
        logical :: match
        type(prt_t), intent(in) :: prt1, prt2
    end function prt_match

<Subevents: procedures>+≡
    elemental module function prt_match (prt1, prt2) result (match)
        logical :: match
        type(prt_t), intent(in) :: prt1, prt2
        if (size (prt1%src) == size (prt2%src)) then
            match = all (prt1%src == prt2%src)
        else
            match = .false.
        end if
    end function prt_match

```

The combine operation makes a pseudoparticle whose momentum is the result of adding (the momenta of) the pair of input particles. We trace the particles from which a particle is built by storing a `src` array. Each particle entry in the `src` list contains a list of indices which indicates its building blocks. The indices refer to an original list of particles. Index lists are sorted, and they contain no element more than once.

We thus require that in a given pseudoparticle, each original particle occurs at most once.

The result is `intent(inout)`, so it will not be initialized when the subroutine is entered.

If the particles carry color, we recall that the combined particle is a composite which is understood as outgoing. If one of the arguments is an incoming particle, its color entries must be reversed.

```

<Subevents: procedures>+≡
    subroutine prt_combine (prt, prt_in1, prt_in2, ok)
        type(prt_t), intent(inout) :: prt
        type(prt_t), intent(in) :: prt_in1, prt_in2
        logical :: ok
        integer, dimension(:), allocatable :: src
        integer, dimension(:), allocatable :: col1, ac11, col2, ac12
        call combine_index_lists (src, prt_in1%src, prt_in2%src)
        ok = allocated (src)
        if (ok) then
            call prt_init_composite (prt, prt_in1%p + prt_in2%p, src)
            if (prt_in1%colorized .or. prt_in2%colorized) then
                select case (prt_in1%type)
                case default
                    call prt_get_color_indices (prt_in1, col1, ac11)
                case (PRT_BEAM, PRT_INCOMING)
                    call prt_get_color_indices (prt_in1, ac11, col1)
                end select
                select case (prt_in2%type)
                case default

```

```

        call prt_get_color_indices (prt_in2, col2, ac12)
      case (PRT_BEAM, PRT_INCOMING)
        call prt_get_color_indices (prt_in2, ac12, col2)
      end select
      call prt_colorize (prt, [col1, col2], [ac11, ac12])
    end if
  end if
end subroutine prt_combine

```

This variant does not produce the combined particle, it just checks whether the combination is valid (no common src entry).

<Subevents: public>+≡

```
public :: are_disjoint
```

<Subevents: sub interfaces>+≡

```

module function are_disjoint (prt_in1, prt_in2) result (flag)
  logical :: flag
  type(prt_t), intent(in) :: prt_in1, prt_in2
end function are_disjoint

```

<Subevents: procedures>+≡

```

module function are_disjoint (prt_in1, prt_in2) result (flag)
  logical :: flag
  type(prt_t), intent(in) :: prt_in1, prt_in2
  flag = index_lists_are_disjoint (prt_in1%src, prt_in2%src)
end function are_disjoint

```

src Lists with length > 1 are built by a combine operation which merges the lists in a sorted manner. If the result would have a duplicate entry, it is discarded, and the result is unallocated.

<Subevents: procedures>+≡

```

subroutine combine_index_lists (res, src1, src2)
  integer, dimension(:), intent(in) :: src1, src2
  integer, dimension(:), allocatable :: res
  integer :: i1, i2, i
  allocate (res (size (src1) + size (src2)))
  if (size (src1) == 0) then
    res = src2
    return
  else if (size (src2) == 0) then
    res = src1
    return
  end if
  i1 = 1
  i2 = 1
  LOOP: do i = 1, size (res)
    if (src1(i1) < src2(i2)) then
      res(i) = src1(i1); i1 = i1 + 1
      if (i1 > size (src1)) then
        res(i+1:) = src2(i2:)
        exit LOOP
      end if
    else if (src1(i1) > src2(i2)) then
      res(i) = src2(i2); i2 = i2 + 1
    end if
  end do
end subroutine combine_index_lists

```

```

        if (i2 > size (src2)) then
            res(i+1:) = src1(i1:)
            exit LOOP
        end if
    else
        deallocate (res)
        exit LOOP
    end if
end do LOOP
end subroutine combine_index_lists

```

This function is similar, but it does not actually merge the list, it just checks whether they are disjoint (no common `src` entry).

<Subevents: procedures>+≡

```

function index_lists_are_disjoint (src1, src2) result (flag)
    logical :: flag
    integer, dimension(:), intent(in) :: src1, src2
    integer :: i1, i2, i
    flag = .true.
    i1 = 1
    i2 = 1
    LOOP: do i = 1, size (src1) + size (src2)
        if (src1(i1) < src2(i2)) then
            i1 = i1 + 1
            if (i1 > size (src1)) then
                exit LOOP
            end if
        else if (src1(i1) > src2(i2)) then
            i2 = i2 + 1
            if (i2 > size (src2)) then
                exit LOOP
            end if
        else
            flag = .false.
            exit LOOP
        end if
    end do LOOP
end function index_lists_are_disjoint

```

13.4.2 subevents

Particles are collected in subevents. This type is implemented as a dynamically allocated array, which need not be completely filled. The value `n_active` determines the number of meaningful entries.

Type definition

<Subevents: public>+≡

```

public :: subevt_t

```

<Subevents: types>+≡

```

type :: subevt_t

```

```

    private
    integer :: n_active = 0
    type(prt_t), dimension(:), allocatable :: prt
contains
  <Subevents: subevt: TBP>
end type subevt_t

```

Initialize, allocating with size zero (default) or given size. The number of contained particles is set equal to the size.

```

<Subevents: public>+≡
  public :: subevt_init

<Subevents: sub interfaces>+≡
  module subroutine subevt_init (subevt, n_active)
    type(subevt_t), intent(out) :: subevt
    integer, intent(in), optional :: n_active
  end subroutine subevt_init

<Subevents: procedures>+≡
  module subroutine subevt_init (subevt, n_active)
    type(subevt_t), intent(out) :: subevt
    integer, intent(in), optional :: n_active
    if (present (n_active)) subevt%n_active = n_active
    allocate (subevt%prt (subevt%n_active))
  end subroutine subevt_init

```

(Re-)allocate the subevent with some given size. If the size is greater than the previous one, do a real reallocation. Otherwise, just reset the recorded size. Contents are untouched, but become invalid.

```

<Subevents: subevt: TBP>≡
  procedure :: reset => subevt_reset

<Subevents: sub interfaces>+≡
  module subroutine subevt_reset (subevt, n_active)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: n_active
  end subroutine subevt_reset

<Subevents: procedures>+≡
  module subroutine subevt_reset (subevt, n_active)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: n_active
    subevt%n_active = n_active
    if (subevt%n_active > size (subevt%prt)) then
      deallocate (subevt%prt)
      allocate (subevt%prt (subevt%n_active))
    end if
  end subroutine subevt_reset

```

Output. No prefix for the headline 'subevt', because this will usually be printed appending to a previous line.

```

<Subevents: subevt: TBP>+≡
  procedure :: write => subevt_write

```

<Subevents: sub interfaces>+≡

```

module subroutine subevt_write (object, unit, prefix, pacified)
  class(subevt_t), intent(in) :: object
  integer, intent(in), optional :: unit
  character(*), intent(in), optional :: prefix
  logical, intent(in), optional :: pacified
end subroutine subevt_write

```

<Subevents: procedures>+≡

```

module subroutine subevt_write (object, unit, prefix, pacified)
  class(subevt_t), intent(in) :: object
  integer, intent(in), optional :: unit
  character(*), intent(in), optional :: prefix
  logical, intent(in), optional :: pacified
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "subevent:"
  do i = 1, object%n_active
    if (present (prefix)) write (u, "(A)", advance="no") prefix
    write (u, "(1x,I0)", advance="no") i
    call prt_write (object%prt(i), unit = unit, testflag = pacified)
  end do
end subroutine subevt_write

```

Defined assignment: transfer only meaningful entries. This is a deep copy (as would be default assignment).

<Subevents: interfaces>+≡

```

interface assignment(=)
  module procedure subevt_assign
end interface

```

<Subevents: sub interfaces>+≡

```

module subroutine subevt_assign (subevt, subevt_in)
  type(subevt_t), intent(inout) :: subevt
  type(subevt_t), intent(in) :: subevt_in
end subroutine subevt_assign

```

<Subevents: procedures>+≡

```

module subroutine subevt_assign (subevt, subevt_in)
  type(subevt_t), intent(inout) :: subevt
  type(subevt_t), intent(in) :: subevt_in
  if (.not. allocated (subevt%prt)) then
    call subevt_init (subevt, subevt_in%n_active)
  else
    call subevt%reset (subevt_in%n_active)
  end if
  subevt%prt(:subevt%n_active) = subevt_in%prt(:subevt%n_active)
end subroutine subevt_assign

```

Fill contents

Store incoming/outgoing particles which are completely defined.

<Subevents: public>+≡


```

<Subevents: subevt: TBP>+≡
  procedure :: set_beam => subevt_set_beam
  procedure :: set_composite => subevt_set_composite
  procedure :: set_incoming => subevt_set_incoming
  procedure :: set_outgoing => subevt_set_outgoing

<Subevents: sub interfaces>+≡
  module subroutine subevt_set_beam (subevt, i, pdg, p, p2, src)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
  end subroutine subevt_set_beam
  module subroutine subevt_set_incoming (subevt, i, pdg, p, p2, src)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
  end subroutine subevt_set_incoming
  module subroutine subevt_set_outgoing (subevt, i, pdg, p, p2, src)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
  end subroutine subevt_set_outgoing
  module subroutine subevt_set_composite (subevt, i, p, src)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    integer, dimension(:), intent(in) :: src
  end subroutine subevt_set_composite

<Subevents: procedures>+≡
  module subroutine subevt_set_beam (subevt, i, pdg, p, p2, src)
    class(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
    if (present (src)) then
      call prt_init_beam (subevt%prt(i), pdg, p, p2, src)
    else
      call prt_init_beam (subevt%prt(i), pdg, p, p2, [i])
    end if
  end subroutine subevt_set_beam

  module subroutine subevt_set_incoming (subevt, i, pdg, p, p2, src)
    class(subevt_t), intent(inout) :: subevt

```

```

integer, intent(in) :: i
integer, intent(in) :: pdg
type(vector4_t), intent(in) :: p
real(default), intent(in) :: p2
integer, dimension(:), intent(in), optional :: src
if (present (src)) then
    call prt_init_incoming (subevt%prt(i), pdg, p, p2, src)
else
    call prt_init_incoming (subevt%prt(i), pdg, p, p2, [i])
end if
end subroutine subevt_set_incoming

module subroutine subevt_set_outgoing (subevt, i, pdg, p, p2, src)
class(subevt_t), intent(inout) :: subevt
integer, intent(in) :: i
integer, intent(in) :: pdg
type(vector4_t), intent(in) :: p
real(default), intent(in) :: p2
integer, dimension(:), intent(in), optional :: src
if (present (src)) then
    call prt_init_outgoing (subevt%prt(i), pdg, p, p2, src)
else
    call prt_init_outgoing (subevt%prt(i), pdg, p, p2, [i])
end if
end subroutine subevt_set_outgoing

module subroutine subevt_set_composite (subevt, i, p, src)
class(subevt_t), intent(inout) :: subevt
integer, intent(in) :: i
type(vector4_t), intent(in) :: p
integer, dimension(:), intent(in) :: src
call prt_init_composite (subevt%prt(i), p, src)
end subroutine subevt_set_composite

```

Separately assign flavors, simultaneously for all incoming/outgoing particles.

```

⟨Subevents: subevt: TBP⟩+≡
    procedure :: set_pdg_beam => subevt_set_pdg_beam
    procedure :: set_pdg_incoming => subevt_set_pdg_incoming
    procedure :: set_pdg_outgoing => subevt_set_pdg_outgoing

⟨Subevents: sub interfaces⟩+≡
    module subroutine subevt_set_pdg_beam (subevt, pdg)
        class(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
    end subroutine subevt_set_pdg_beam
    module subroutine subevt_set_pdg_incoming (subevt, pdg)
        class(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
    end subroutine subevt_set_pdg_incoming
    module subroutine subevt_set_pdg_outgoing (subevt, pdg)
        class(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
    end subroutine subevt_set_pdg_outgoing

⟨Subevents: procedures⟩+≡

```

```

module subroutine subevt_set_pdg_beam (subevt, pdg)
  class(subevt_t), intent(inout) :: subevt
  integer, dimension(:), intent(in) :: pdg
  integer :: i, j
  j = 1
  do i = 1, subevt%n_active
    if (subevt%prt(i)%type == PRT_BEAM) then
      call prt_set_pdg (subevt%prt(i), pdg(j))
      j = j + 1
      if (j > size (pdg)) exit
    end if
  end do
end subroutine subevt_set_pdg_beam

module subroutine subevt_set_pdg_incoming (subevt, pdg)
  class(subevt_t), intent(inout) :: subevt
  integer, dimension(:), intent(in) :: pdg
  integer :: i, j
  j = 1
  do i = 1, subevt%n_active
    if (subevt%prt(i)%type == PRT_INCOMING) then
      call prt_set_pdg (subevt%prt(i), pdg(j))
      j = j + 1
      if (j > size (pdg)) exit
    end if
  end do
end subroutine subevt_set_pdg_incoming

module subroutine subevt_set_pdg_outgoing (subevt, pdg)
  class(subevt_t), intent(inout) :: subevt
  integer, dimension(:), intent(in) :: pdg
  integer :: i, j
  j = 1
  do i = 1, subevt%n_active
    if (subevt%prt(i)%type == PRT_OUTGOING) then
      call prt_set_pdg (subevt%prt(i), pdg(j))
      j = j + 1
      if (j > size (pdg)) exit
    end if
  end do
end subroutine subevt_set_pdg_outgoing

```

Separately assign momenta, simultaneously for all incoming/outgoing particles.

```

⟨Subevents: subevt: TBP⟩+≡
  procedure :: set_p_beam => subevt_set_p_beam
  procedure :: set_p_incoming => subevt_set_p_incoming
  procedure :: set_p_outgoing => subevt_set_p_outgoing

⟨Subevents: sub interfaces⟩+≡
  module subroutine subevt_set_p_beam (subevt, p)
    class(subevt_t), intent(inout) :: subevt
    type(vector4_t), dimension(:), intent(in) :: p
  end subroutine subevt_set_p_beam
  module subroutine subevt_set_p_incoming (subevt, p)

```

```

        class(subevt_t), intent(inout) :: subevt
        type(vector4_t), dimension(:), intent(in) :: p
    end subroutine subevt_set_p_incoming
module subroutine subevt_set_p_outgoing (subevt, p)
    class(subevt_t), intent(inout) :: subevt
    type(vector4_t), dimension(:), intent(in) :: p
end subroutine subevt_set_p_outgoing
<Subevents: procedures>+≡
module subroutine subevt_set_p_beam (subevt, p)
    class(subevt_t), intent(inout) :: subevt
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_BEAM) then
            call prt_set_p (subevt%prt(i), p(j))
            j = j + 1
            if (j > size (p)) exit
        end if
    end do
end subroutine subevt_set_p_beam

module subroutine subevt_set_p_incoming (subevt, p)
    class(subevt_t), intent(inout) :: subevt
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_INCOMING) then
            call prt_set_p (subevt%prt(i), p(j))
            j = j + 1
            if (j > size (p)) exit
        end if
    end do
end subroutine subevt_set_p_incoming

module subroutine subevt_set_p_outgoing (subevt, p)
    class(subevt_t), intent(inout) :: subevt
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_OUTGOING) then
            call prt_set_p (subevt%prt(i), p(j))
            j = j + 1
            if (j > size (p)) exit
        end if
    end do
end subroutine subevt_set_p_outgoing

```

Separately assign the squared invariant mass, simultaneously for all incoming/outgoing particles.

<Subevents: subevt: TBP>+≡

```

procedure :: set_p2_beam => subevt_set_p2_beam
procedure :: set_p2_incoming => subevt_set_p2_incoming
procedure :: set_p2_outgoing => subevt_set_p2_outgoing

<Subevents: sub interfaces>+≡
  module subroutine subevt_set_p2_beam (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
  end subroutine subevt_set_p2_beam
  module subroutine subevt_set_p2_incoming (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
  end subroutine subevt_set_p2_incoming
  module subroutine subevt_set_p2_outgoing (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
  end subroutine subevt_set_p2_outgoing

<Subevents: procedures>+≡
  module subroutine subevt_set_p2_beam (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
      if (subevt%prt(i)%type == PRT_BEAM) then
        call prt_set_p2 (subevt%prt(i), p2(j))
        j = j + 1
        if (j > size (p2)) exit
      end if
    end do
  end subroutine subevt_set_p2_beam

  module subroutine subevt_set_p2_incoming (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
      if (subevt%prt(i)%type == PRT_INCOMING) then
        call prt_set_p2 (subevt%prt(i), p2(j))
        j = j + 1
        if (j > size (p2)) exit
      end if
    end do
  end subroutine subevt_set_p2_incoming

  module subroutine subevt_set_p2_outgoing (subevt, p2)
    class(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
      if (subevt%prt(i)%type == PRT_OUTGOING) then
        call prt_set_p2 (subevt%prt(i), p2(j))

```

```

        j = j + 1
        if (j > size (p2)) exit
    end if
end do
end subroutine subevt_set_p2_outgoing

```

Set polarization for an entry

```

<Subevents: public>+≡
    public :: subevt_polarize

<Subevents: sub interfaces>+≡
    module subroutine subevt_polarize (subevt, i, h)
        type(subevt_t), intent(inout) :: subevt
        integer, intent(in) :: i, h
    end subroutine subevt_polarize

<Subevents: procedures>+≡
    module subroutine subevt_polarize (subevt, i, h)
        type(subevt_t), intent(inout) :: subevt
        integer, intent(in) :: i, h
        call prt_polarize (subevt%prt(i), h)
    end subroutine subevt_polarize

```

Set color-flow indices for an entry

```

<Subevents: public>+≡
    public :: subevt_colorize

<Subevents: sub interfaces>+≡
    module subroutine subevt_colorize (subevt, i, col, acl)
        type(subevt_t), intent(inout) :: subevt
        integer, intent(in) :: i, col, acl
    end subroutine subevt_colorize

<Subevents: procedures>+≡
    module subroutine subevt_colorize (subevt, i, col, acl)
        type(subevt_t), intent(inout) :: subevt
        integer, intent(in) :: i, col, acl
        if (col > 0 .and. acl > 0) then
            call prt_colorize (subevt%prt(i), [col], [acl])
        else if (col > 0) then
            call prt_colorize (subevt%prt(i), [col], [integer ::])
        else if (acl > 0) then
            call prt_colorize (subevt%prt(i), [integer ::], [acl])
        else
            call prt_colorize (subevt%prt(i), [integer ::], [integer ::])
        end if
    end subroutine subevt_colorize

```

Accessing contents

Return true if the subevent has entries.

```

<Subevents: subevt: TBP>+≡
    procedure :: is_nonempty => subevt_is_nonempty

```

```

<Subevents: sub interfaces>+≡
  module function subvt_is_nonempty (subvt) result (flag)
    logical :: flag
    class(subvt_t), intent(in) :: subvt
  end function subvt_is_nonempty

```

```

<Subevents: procedures>+≡
  module function subvt_is_nonempty (subvt) result (flag)
    logical :: flag
    class(subvt_t), intent(in) :: subvt
    flag = subvt%n_active /= 0
  end function subvt_is_nonempty

```

Return the number of entries

```

<Subevents: subvt: TBP>+≡
  procedure :: get_length => subvt_get_length

<Subevents: sub interfaces>+≡
  module function subvt_get_length (subvt) result (length)
    integer :: length
    class(subvt_t), intent(in) :: subvt
  end function subvt_get_length

<Subevents: procedures>+≡
  module function subvt_get_length (subvt) result (length)
    integer :: length
    class(subvt_t), intent(in) :: subvt
    length = subvt%n_active
  end function subvt_get_length

```

Return a specific particle. The index is not checked for validity.

```

<Subevents: subvt: TBP>+≡
  procedure :: get_prt => subvt_get_prt

<Subevents: sub interfaces>+≡
  module function subvt_get_prt (subvt, i) result (prt)
    type(prt_t) :: prt
    class(subvt_t), intent(in) :: subvt
    integer, intent(in) :: i
  end function subvt_get_prt

<Subevents: procedures>+≡
  module function subvt_get_prt (subvt, i) result (prt)
    type(prt_t) :: prt
    class(subvt_t), intent(in) :: subvt
    integer, intent(in) :: i
    prt = subvt%prt(i)
  end function subvt_get_prt

```

Return the partonic energy squared. We take the particles with flag PRT_INCOMING and compute their total invariant mass.

```

<Subevents: subvt: TBP>+≡
  procedure :: get_sqrts_hat => subvt_get_sqrts_hat

```

```

<Subevents: sub interfaces>+≡
  module function subevt_get_sqrts_hat (subevt) result (sqrts_hat)
    class(subevt_t), intent(in) :: subevt
    real(default) :: sqrts_hat
  end function subevt_get_sqrts_hat

```

```

<Subevents: procedures>+≡
  module function subevt_get_sqrts_hat (subevt) result (sqrts_hat)
    class(subevt_t), intent(in) :: subevt
    real(default) :: sqrts_hat
    type(vector4_t) :: p
    integer :: i
    do i = 1, subevt%n_active
      if (subevt%prt(i)%type == PRT_INCOMING) then
        p = p + prt_get_momentum (subevt%prt(i))
      end if
    end do
    sqrts_hat = p ** 1
  end function subevt_get_sqrts_hat

```

Return the number of incoming (outgoing) particles, respectively. Beam particles or composites are not counted.

```

<Subevents: subevt: TBP>+≡
  procedure :: get_n_in => subevt_get_n_in
  procedure :: get_n_out => subevt_get_n_out

```

```

<Subevents: sub interfaces>+≡
  module function subevt_get_n_in (subevt) result (n_in)
    class(subevt_t), intent(in) :: subevt
    integer :: n_in
  end function subevt_get_n_in
  module function subevt_get_n_out (subevt) result (n_out)
    class(subevt_t), intent(in) :: subevt
    integer :: n_out
  end function subevt_get_n_out

```

```

<Subevents: procedures>+≡
  module function subevt_get_n_in (subevt) result (n_in)
    class(subevt_t), intent(in) :: subevt
    integer :: n_in
    n_in = count (subevt%prt(:subevt%n_active)%type == PRT_INCOMING)
  end function subevt_get_n_in

  module function subevt_get_n_out (subevt) result (n_out)
    class(subevt_t), intent(in) :: subevt
    integer :: n_out
    n_out = count (subevt%prt(:subevt%n_active)%type == PRT_OUTGOING)
  end function subevt_get_n_out

```

```

<Subevents: interfaces>+≡
  interface c_prt
    module procedure c_prt_from_subevt
    module procedure c_prt_array_from_subevt
  end interface

```



```

<Subevents: sub interfaces>+≡
  module function c_prt_from_subevt (subevt, i) result (c_prt)
    type(c_prt_t) :: c_prt
    type(subevt_t), intent(in) :: subevt
    integer, intent(in) :: i
  end function c_prt_from_subevt
  module function c_prt_array_from_subevt (subevt) result (c_prt_array)
    type(subevt_t), intent(in) :: subevt
    type(c_prt_t), dimension(subevt%n_active) :: c_prt_array
  end function c_prt_array_from_subevt

<Subevents: procedures>+≡
  module function c_prt_from_subevt (subevt, i) result (c_prt)
    type(c_prt_t) :: c_prt
    type(subevt_t), intent(in) :: subevt
    integer, intent(in) :: i
    c_prt = c_prt_from_prt (subevt%prt(i))
  end function c_prt_from_subevt

  module function c_prt_array_from_subevt (subevt) result (c_prt_array)
    type(subevt_t), intent(in) :: subevt
    type(c_prt_t), dimension(subevt%n_active) :: c_prt_array
    c_prt_array = c_prt_from_prt (subevt%prt(1:subevt%n_active))
  end function c_prt_array_from_subevt

```

Operations with subevents

The join operation joins two subevents. When appending the elements of the second list, we check for each particle whether it is already in the first list. If yes, it is discarded. The result list should be initialized already.

If a mask is present, it refers to the second subevent. Particles where the mask is not set are discarded.

```

<Subevents: public>+≡
  public :: subevt_join

<Subevents: sub interfaces>+≡
  module subroutine subevt_join (subevt, pl1, pl2, mask2)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1, pl2
    logical, dimension(:), intent(in), optional :: mask2
  end subroutine subevt_join

<Subevents: procedures>+≡
  module subroutine subevt_join (subevt, pl1, pl2, mask2)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1, pl2
    logical, dimension(:), intent(in), optional :: mask2
    integer :: n1, n2, i, n
    n1 = pl1%n_active
    n2 = pl2%n_active
    call subevt%reset (n1 + n2)
    subevt%prt(:n1) = pl1%prt(:n1)
    n = n1
    if (present (mask2)) then

```

```

do i = 1, pl2%n_active
  if (mask2(i)) then
    if (disjoint (i)) then
      n = n + 1
      subevt%prt(n) = pl2%prt(i)
    end if
  end if
end do
else
  do i = 1, pl2%n_active
    if (disjoint (i)) then
      n = n + 1
      subevt%prt(n) = pl2%prt(i)
    end if
  end do
end if
subevt%n_active = n
contains
function disjoint (i) result (flag)
  integer, intent(in) :: i
  logical :: flag
  integer :: j
  do j = 1, pl1%n_active
    if (.not. are_disjoint (pl1%prt(j), pl2%prt(i))) then
      flag = .false.
      return
    end if
  end do
  flag = .true.
end function disjoint
end subroutine subevt_join

```

The combine operation makes a subevent whose entries are the result of adding (the momenta of) each pair of particles in the input lists. We trace the particles from which a particle is built by storing a `src` array. Each particle entry in the `src` list contains a list of indices which indicates its building blocks. The indices refer to an original list of particles. Index lists are sorted, and they contain no element more than once.

We thus require that in a given pseudoparticle, each original particle occurs at most once.

```

<Subevents: public>+≡
  public :: subevt_combine

<Subevents: sub interfaces>+≡
  module subroutine subevt_combine (subevt, pl1, pl2, mask12)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1, pl2
    logical, dimension(:,:), intent(in), optional :: mask12
  end subroutine subevt_combine

<Subevents: procedures>+≡
  module subroutine subevt_combine (subevt, pl1, pl2, mask12)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1, pl2

```

```

logical, dimension(:,:), intent(in), optional :: mask12
integer :: n1, n2, i1, i2, n, j
logical :: ok
n1 = pl1%n_active
n2 = pl2%n_active
call subevt%reset (n1 * n2)
n = 1
do i1 = 1, n1
  do i2 = 1, n2
    if (present (mask12)) then
      ok = mask12(i1,i2)
    else
      ok = .true.
    end if
    if (ok) call prt_combine &
      (subevt%prt(n), pl1%prt(i1), pl2%prt(i2), ok)
    if (ok) then
      CHECK_DOUBLES: do j = 1, n - 1
        if (subevt%prt(n) .match. subevt%prt(j)) then
          ok = .false.; exit CHECK_DOUBLES
        end if
      end do CHECK_DOUBLES
      if (ok) n = n + 1
    end if
  end do
end do
subevt%n_active = n - 1
end subroutine subevt_combine

```

The collect operation makes a single-entry subevent which results from combining (the momenta of) all particles in the input list. As above, the result does not contain an original particle more than once; this is checked for each particle when it is collected. Furthermore, each entry has a mask; where the mask is false, the entry is dropped.

(Thus, if the input particles are already composite, there is some chance that the result depends on the order of the input list and is not as expected. This situation should be avoided.)

```

<Subevents: public>+≡
  public :: subevt_collect

<Subevents: sub interfaces>+≡
  module subroutine subevt_collect (subevt, pl1, mask1)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1
    logical, dimension(:), intent(in) :: mask1
  end subroutine subevt_collect

<Subevents: procedures>+≡
  module subroutine subevt_collect (subevt, pl1, mask1)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1
    logical, dimension(:), intent(in) :: mask1
    type(prt_t) :: prt
    integer :: i

```

```

logical :: ok
call subevt%reset (1)
subevt%n_active = 0
do i = 1, pl1%n_active
  if (mask1(i)) then
    if (subevt%n_active == 0) then
      subevt%n_active = 1
      subevt%prt(1) = pl1%prt(i)
    else
      call prt_combine (prt, subevt%prt(1), pl1%prt(i), ok)
      if (ok) subevt%prt(1) = prt
    end if
  end if
end do
end subroutine subevt_collect

```

The cluster operation is similar to `collect`, but applies a jet algorithm. The result is a subevent consisting of jets and, possibly, unclustered extra particles. As above, the result does not contain an original particle more than once; this is checked for each particle when it is collected. Furthermore, each entry has a mask; where the mask is false, the entry is dropped.

The algorithm: first determine the (pseudo)particles that participate in the clustering. They should not overlap, and the mask entry must be set. We then cluster the particles, using the given jet definition. The result particles are retrieved from the cluster sequence. We still have to determine the source indices for each jet: for each input particle, we get the jet index. Accumulating the source entries for all particles that are part of a given jet, we derive the jet source entries. Finally, we delete the C structures that have been constructed by FastJet and its interface.

```

<Subevents: public>+≡
  public :: subevt_cluster

<Subevents: sub interfaces>+≡
  module subroutine subevt_cluster (subevt, pl1, dcut, mask1, jet_def, &
    keep_jets, exclusive)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1
    real(default), intent(in) :: dcut
    logical, dimension(:), intent(in) :: mask1
    type(jet_definition_t), intent(in) :: jet_def
    logical, intent(in) :: keep_jets, exclusive
  end subroutine subevt_cluster

<Subevents: procedures>+≡
  module subroutine subevt_cluster (subevt, pl1, dcut, mask1, jet_def, &
    keep_jets, exclusive)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1
    real(default), intent(in) :: dcut
    logical, dimension(:), intent(in) :: mask1
    type(jet_definition_t), intent(in) :: jet_def
    logical, intent(in) :: keep_jets, exclusive
    integer, dimension(:), allocatable :: map, jet_index
    type(pseudojet_t), dimension(:), allocatable :: jet_in, jet_out

```

```

type(pseudojet_vector_t) :: jv_in, jv_out
type(cluster_sequence_t) :: cs
integer :: i, n_src, n_active
call map_prt_index (pl1, mask1, n_src, map)
n_active = count (map /= 0)
allocate (jet_in (n_active))
allocate (jet_index (n_active))
do i = 1, n_active
    call jet_in(i)%init (prt_get_momentum (pl1%prt(map(i))))
end do
call jv_in%init (jet_in)
call cs%init (jv_in, jet_def)
if (exclusive) then
    jv_out = cs%exclusive_jets (dcut)
else
    jv_out = cs%inclusive_jets ()
end if
call cs%assign_jet_indices (jv_out, jet_index)
allocate (jet_out (jv_out%size ()))
jet_out = jv_out
call fill_pseudojet (subevt, pl1, jet_out, jet_index, n_src, map)
do i = 1, size (jet_out)
    call jet_out(i)%final ()
end do
call jv_out%final ()
call cs%final ()
call jv_in%final ()
do i = 1, size (jet_in)
    call jet_in(i)%final ()
end do
contains
! Uniquely combine sources and add map those new indices to the old ones
subroutine map_prt_index (pl1, mask1, n_src, map)
    type(subevt_t), intent(in) :: pl1
    logical, dimension(:), intent(in) :: mask1
    integer, intent(out) :: n_src
    integer, dimension(:), allocatable, intent(out) :: map
    integer, dimension(:), allocatable :: src, src_tmp
    integer :: i
    allocate (src(0))
    allocate (map (pl1%n_active), source = 0)
    n_active = 0
    do i = 1, pl1%n_active
        if (.not. mask1(i)) cycle
        call combine_index_lists (src_tmp, src, pl1%prt(i)%src)
        if (.not. allocated (src_tmp)) cycle
        call move_alloc (from=src_tmp, to=src)
        n_active = n_active + 1
        map(n_active) = i
    end do
    n_src = size (src)
end subroutine map_prt_index
! Retrieve source(s) of a jet and fill corresponding subevent
subroutine fill_pseudojet (subevt, pl1, jet_out, jet_index, n_src, map)

```

```

type(subevt_t), intent(inout) :: subevt
type(subevt_t), intent(in) :: pl1
type(pseudojet_t), dimension(:), intent(in) :: jet_out
integer, dimension(:), intent(in) :: jet_index
integer, dimension(:), intent(in) :: map
integer, intent(in) :: n_src
integer, dimension(n_src) :: src_fill
integer :: i, jet, k, combined_pdg, pdg, n_quarks, n_src_fill
logical :: is_b, is_c
call subevt%reset (size (jet_out))
do jet = 1, size (jet_out)
  pdg = 0; src_fill = 0; n_src_fill = 0; combined_pdg = 0; n_quarks = 0
  is_b = .false.; is_c = .false.
  PARTICLE: do i = 1, size (jet_index)
    if (jet_index(i) /= jet) cycle PARTICLE
    associate (prt => pl1%prt(map(i)), n_src_prt => size(pl1%prt(map(i))%src))
      do k = 1, n_src_prt
        src_fill(n_src_fill + k) = prt%src(k)
      end do
      n_src_fill = n_src_fill + n_src_prt
      if (is_quark (prt%pdg)) then
        n_quarks = n_quarks + 1
        if (.not. is_b) then
          if (abs (prt%pdg) == 5) then
            is_b = .true.
            is_c = .false.
          else if (abs (prt%pdg) == 4) then
            is_c = .true.
          end if
        end if
      end if
      if (combined_pdg == 0) combined_pdg = prt%pdg
    end if
  end associate
end do PARTICLE
if (keep_jets .and. n_quarks == 1) pdg = combined_pdg
call prt_init_pseudojet (subevt%prt(jet), jet_out(jet), &
  src_fill(:n_src_fill), pdg, is_b, is_c)
end do
end subroutine fill_pseudojet
end subroutine subevt_cluster

```

Do recombination. The incoming subevent `pl` is left unchanged if it either does not contain photons at all, or consists just of a single photon and nothing else or the photon does have a larger $R > R_0$ distance to the nearest other particle or does not fulfill the `mask1` condition. Otherwise, the subevent is one entry shorter and contains a single recombined particle whose original flavor is kept depending on the setting `keep_flv`. When this subroutine is called, it is explicitly assumed that there is only one photon. For the moment, we take here the first photon from the subevent to possibly recombine and leave this open for generalization.

```

⟨Subevents: public⟩+≡
  public :: subevt_recombine
⟨Subevents: sub interfaces⟩+≡

```

```

module subroutine subevt_recombine (subevt, pl, mask1, reco_r0, keep_flg)
  type(subevt_t), intent(inout) :: subevt
  type(subevt_t), intent(in) :: pl
  logical, dimension(:), intent(in) :: mask1
  logical, intent(in) :: keep_flg
  real(default), intent(in) :: reco_r0
end subroutine subevt_recombine

```

<Subevents: procedures>+≡

```

module subroutine subevt_recombine (subevt, pl, mask1, reco_r0, keep_flg)
  type(subevt_t), intent(inout) :: subevt
  type(subevt_t), intent(in) :: pl
  type(prt_t), dimension(:), allocatable :: prt_rec
  logical, dimension(:), intent(in) :: mask1
  logical, intent(in) :: keep_flg
  real(default), intent(in) :: reco_r0
  real(default), dimension(:), allocatable :: del_rij
  integer, dimension(:), allocatable :: i_sortr
  type(prt_t) :: prt_gam, prt_comb
  logical :: recombine, ok
  integer :: i, n, i_gam, n_gam, n_rec, pdg_orig
  n = pl%get_length ()
  n_gam = 0
  FIND_FIRST_PHOTON: do i = 1, n
    if (prt_is_photon (pl%prt (i))) then
      n_gam = n_gam + 1
      prt_gam = pl%prt (i)
      i_gam = i
      exit FIND_FIRST_PHOTON
    end if
  end do FIND_FIRST_PHOTON
  n_rec = n - n_gam
  if (n_gam == 0) then
    subevt = pl
  else
    if (n_rec > 0) then
      allocate (prt_rec (n_rec))
      do i = 1, n_rec
        if (i == i_gam) cycle
        if (i < i_gam) then
          prt_rec(i) = pl%prt(i)
        else
          prt_rec(i) = pl%prt(i+n_gam)
        end if
      end do
      allocate (del_rij (n_rec), i_sortr (n_rec))
      del_rij(1:n_rec) = eta_phi_distance(prt_get_momentum (prt_gam), &
        prt_get_momentum (prt_rec(1:n_rec)))
      i_sortr = order (del_rij)
      recombine = del_rij (i_sortr (1)) <= reco_r0 .and. mask1(i_gam)
      if (recombine) then
        call subevt%reset (pl%n_active-n_gam)
        do i = 1, n_rec
          if (i == i_sortr(1)) then
            pdg_orig = prt_get_pdg (prt_rec(i_sortr (1)))

```

```

        call prt_combine (prt_comb, prt_gam, prt_rec(i_sortr (1)), ok)
        if (ok) then
            subevt%prt(i_sortr (1)) = prt_comb
            if (keep_flg) call prt_set_pdg &
                (subevt%prt(i_sortr (1)), pdg_orig)
        end if
    else
        subevt%prt(i) = prt_rec(i)
    end if
end do
else
    subevt = pl
end if
else
    subevt = pl
end if
end if
end subroutine subevt_recombine

```

Return a list of all particles for which the mask is true.

```

<Subevents: public>+≡
    public :: subevt_select

<Subevents: sub interfaces>+≡
    module subroutine subevt_select (subevt, pl, mask1)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        logical, dimension(:), intent(in) :: mask1
    end subroutine subevt_select

<Subevents: procedures>+≡
    module subroutine subevt_select (subevt, pl, mask1)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        logical, dimension(:), intent(in) :: mask1
        integer :: i, n
        call subevt%reset (pl%n_active)
        n = 0
        do i = 1, pl%n_active
            if (mask1(i)) then
                n = n + 1
                subevt%prt(n) = pl%prt(i)
            end if
        end do
        subevt%n_active = n
    end subroutine subevt_select

```

Return a subevent which consists of the single particle with specified `index`. If `index` is negative, count from the end. If it is out of bounds, return an empty list.

```

<Subevents: public>+≡
    public :: subevt_extract

```



```

<Subevents: sub interfaces>+≡
    module subroutine subevt_extract (subevt, pl, index)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        integer, intent(in) :: index
    end subroutine subevt_extract

<Subevents: procedures>+≡
    module subroutine subevt_extract (subevt, pl, index)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        integer, intent(in) :: index
        if (index > 0) then
            if (index <= pl%n_active) then
                call subevt%reset (1)
                subevt%prt(1) = pl%prt(index)
            else
                call subevt%reset (0)
            end if
        else if (index < 0) then
            if (abs (index) <= pl%n_active) then
                call subevt%reset (1)
                subevt%prt(1) = pl%prt(pl%n_active + 1 + index)
            else
                call subevt%reset (0)
            end if
        else
            call subevt%reset (0)
        end if
    end subroutine subevt_extract

```

Return the list of particles sorted according to increasing values of the provided integer or real array. If no array is given, sort by PDG value.

```

<Subevents: public>+≡
    public :: subevt_sort

<Subevents: interfaces>+≡
    interface subevt_sort
        module procedure subevt_sort_pdg
        module procedure subevt_sort_int
        module procedure subevt_sort_real
    end interface

<Subevents: sub interfaces>+≡
    module subroutine subevt_sort_pdg (subevt, pl)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
    end subroutine subevt_sort_pdg
    module subroutine subevt_sort_int (subevt, pl, ival)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        integer, dimension(:), intent(in) :: ival
    end subroutine subevt_sort_int
    module subroutine subevt_sort_real (subevt, pl, rval)

```

```

        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        real(default), dimension(:), intent(in) :: rval
    end subroutine subevt_sort_real
<Subevents: procedures>+≡
    module subroutine subevt_sort_pdg (subevt, pl)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        integer :: n
        n = subevt%n_active
        call subevt_sort_int (subevt, pl, abs (3 * subevt%prt(:n)%pdg - 1))
    end subroutine subevt_sort_pdg

    module subroutine subevt_sort_int (subevt, pl, ival)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        integer, dimension(:), intent(in) :: ival
        call subevt%reset (pl%n_active)
        subevt%n_active = pl%n_active
        subevt%prt = pl%prt( order (ival) )
    end subroutine subevt_sort_int

    module subroutine subevt_sort_real (subevt, pl, rval)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        real(default), dimension(:), intent(in) :: rval
        integer :: i
        integer, dimension(size(rval)) :: idx
        call subevt%reset (pl%n_active)
        subevt%n_active = pl%n_active
        if (allocated (subevt%prt)) deallocate (subevt%prt)
        allocate (subevt%prt (size(pl%prt)))
        idx = order (rval)
        do i = 1, size (idx)
            subevt%prt(i) = pl%prt (idx(i))
        end do
    end subroutine subevt_sort_real

```

Return the list of particles which have any of the specified PDG codes (and optionally particle type: beam, incoming, outgoing).

```

<Subevents: public>+≡
    public :: subevt_select_pdg_code
<Subevents: sub interfaces>+≡
    module subroutine subevt_select_pdg_code (subevt, aval, subevt_in, prt_type)
        type(subevt_t), intent(inout) :: subevt
        type(pdg_array_t), intent(in) :: aval
        type(subevt_t), intent(in) :: subevt_in
        integer, intent(in), optional :: prt_type
    end subroutine subevt_select_pdg_code
<Subevents: procedures>+≡
    module subroutine subevt_select_pdg_code (subevt, aval, subevt_in, prt_type)
        type(subevt_t), intent(inout) :: subevt

```

```

type(pdg_array_t), intent(in) :: aval
type(subevt_t), intent(in) :: subevt_in
integer, intent(in), optional :: prt_type
integer :: n_active, n_match
logical, dimension(:), allocatable :: mask
integer :: i, j
n_active = subevt_in%n_active
allocate (mask (n_active))
forall (i = 1:n_active) &
    mask(i) = aval .match. subevt_in%prt(i)%pdg
if (present (prt_type)) &
    mask = mask .and. subevt_in%prt(:n_active)%type == prt_type
n_match = count (mask)
call subevt%reset (n_match)
j = 0
do i = 1, n_active
    if (mask(i)) then
        j = j + 1
        subevt%prt(j) = subevt_in%prt(i)
    end if
end do
end subroutine subevt_select_pdg_code

```

13.4.3 Eliminate numerical noise

This is useful for testing purposes: set entries to zero that are smaller in absolute values than a given tolerance parameter.

Note: instead of setting the tolerance in terms of EPSILON (kind-dependent), we fix it to 10^{-16} , which is the typical value for double precision. The reason is that there are situations where intermediate representations (external libraries, files) are limited to double precision, even if the main program uses higher precision.

```

<Subevents: public>+≡
    public :: pacify

<Subevents: interfaces>+≡
    interface pacify
        module procedure pacify_prt
        module procedure pacify_subevt
    end interface pacify

<Subevents: sub interfaces>+≡
    module subroutine pacify_prt (prt)
        class(prt_t), intent(inout) :: prt
    end subroutine pacify_prt
    module subroutine pacify_subevt (subevt)
        class(subevt_t), intent(inout) :: subevt
    end subroutine pacify_subevt

<Subevents: procedures>+≡
    module subroutine pacify_prt (prt)
        class(prt_t), intent(inout) :: prt

```

```

real(default) :: e
e = max (1E-10_default * energy (prt%p), 1E-13_default)
call pacify (prt%p, e)
call pacify (prt%p2, 1E3_default * e)
end subroutine pacify_prt

module subroutine pacify_subevt (subevt)
  class(subevt_t), intent(inout) :: subevt
  integer :: i
  do i = 1, subevt%n_active
    call pacify (subevt%prt(i))
  end do
end subroutine pacify_subevt

```

13.5 Analysis tools

This module defines structures useful for data analysis. These include observables, histograms, and plots.

Observables are quantities that are calculated and summed up event by event. At the end, one can compute the average and error.

Histograms have their bins in addition to the observable properties. Histograms are usually written out in tables and displayed graphically.

In plots, each record creates its own entry in a table. This can be used for scatter plots if called event by event, or for plotting dependencies on parameters if called once per integration run.

Graphs are container for histograms and plots, which carry their own graphics options.

The type layout is still somewhat obfuscated. This would become much simpler if type extension could be used.

```
<analysis.f90>≡
  <File header>

  module analysis

    <Use kinds>
    <Use strings>
    use os_interface

    <Standard module head>

    <Analysis: public>

    <Analysis: parameters>

    <Analysis: types>

    <Analysis: interfaces>

    <Analysis: variables>

    interface
    <Analysis: sub interfaces>
    end interface

  end module analysis

<analysis_sub.f90>≡
  <File header>

  submodule (analysis) analysis_s

    use io_units
    use format_utils, only: quote_underscore, tex_format
    use system_defs, only: TAB
    use diagnostics
    use ifiles
```

```

        implicit none

contains

  <Analysis: procedures>

end submodule analysis_s

```

13.5.1 Output formats

These formats share a common field width (alignment).

```

<Analysis: parameters>≡
  character(*), parameter, public :: HISTOGRAM_HEAD_FORMAT = "1x,A15,3x"
  character(*), parameter, public :: HISTOGRAM_INTG_FORMAT = "3x,I9,3x"
  character(*), parameter, public :: HISTOGRAM_DATA_FORMAT = "ES19.12"

```

13.5.2 Graph options

These parameters are used for displaying data. They apply to a whole graph, which may contain more than one plot element.

The GAMELAN code chunks are part of both `graph_options` and `drawing_options`. The `drawing_options` copy is used in histograms and plots, also as graph elements. The `graph_options` copy is used for `graph` objects as a whole. Both copies are usually identical.

```

<Analysis: public>≡
  public :: graph_options_t

<Analysis: types>≡
  type :: graph_options_t
  private
    type(string_t) :: id
    type(string_t) :: title
    type(string_t) :: description
    type(string_t) :: x_label
    type(string_t) :: y_label
    integer :: width_mm = 130
    integer :: height_mm = 90
    logical :: x_log = .false.
    logical :: y_log = .false.
    real(default) :: x_min = 0
    real(default) :: x_max = 1
    real(default) :: y_min = 0
    real(default) :: y_max = 1
    logical :: x_min_set = .false.
    logical :: x_max_set = .false.
    logical :: y_min_set = .false.
    logical :: y_max_set = .false.
    type(string_t) :: gmlcode_bg
    type(string_t) :: gmlcode_fg
  contains
    <Analysis: graph options: TBP>

```

```
end type graph_options_t
```

Initialize the record, all strings are empty. The limits are undefined.

<Analysis: graph options: TBP>≡

```
procedure :: init => graph_options_init
```

<Analysis: sub interfaces>≡

```
module subroutine graph_options_init (graph_options)
  class(graph_options_t), intent(out) :: graph_options
end subroutine graph_options_init
```

<Analysis: procedures>≡

```
module subroutine graph_options_init (graph_options)
  class(graph_options_t), intent(out) :: graph_options
  graph_options%id = ""
  graph_options%title = ""
  graph_options%description = ""
  graph_options%x_label = ""
  graph_options%y_label = ""
  graph_options%gmlcode_bg = ""
  graph_options%gmlcode_fg = ""
end subroutine graph_options_init
```

Set individual options.

<Analysis: graph options: TBP>+≡

```
procedure :: set => graph_options_set
```

<Analysis: sub interfaces>+≡

```
module subroutine graph_options_set (graph_options, id, &
  title, description, x_label, y_label, width_mm, height_mm, &
  x_log, y_log, x_min, x_max, y_min, y_max, &
  gmlcode_bg, gmlcode_fg)
  class(graph_options_t), intent(inout) :: graph_options
  type(string_t), intent(in), optional :: id
  type(string_t), intent(in), optional :: title
  type(string_t), intent(in), optional :: description
  type(string_t), intent(in), optional :: x_label, y_label
  integer, intent(in), optional :: width_mm, height_mm
  logical, intent(in), optional :: x_log, y_log
  real(default), intent(in), optional :: x_min, x_max, y_min, y_max
  type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg
end subroutine graph_options_set
```

<Analysis: procedures>+≡

```
module subroutine graph_options_set (graph_options, id, &
  title, description, x_label, y_label, width_mm, height_mm, &
  x_log, y_log, x_min, x_max, y_min, y_max, &
  gmlcode_bg, gmlcode_fg)
  class(graph_options_t), intent(inout) :: graph_options
  type(string_t), intent(in), optional :: id
  type(string_t), intent(in), optional :: title
  type(string_t), intent(in), optional :: description
  type(string_t), intent(in), optional :: x_label, y_label
  integer, intent(in), optional :: width_mm, height_mm
  logical, intent(in), optional :: x_log, y_log
```

```

real(default), intent(in), optional :: x_min, x_max, y_min, y_max
type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg
if (present (id)) graph_options%id = id
if (present (title)) graph_options%title = title
if (present (description)) graph_options%description = description
if (present (x_label)) graph_options%x_label = x_label
if (present (y_label)) graph_options%y_label = y_label
if (present (width_mm)) graph_options%width_mm = width_mm
if (present (height_mm)) graph_options%height_mm = height_mm
if (present (x_log)) graph_options%x_log = x_log
if (present (y_log)) graph_options%y_log = y_log
if (present (x_min)) graph_options%x_min = x_min
if (present (x_max)) graph_options%x_max = x_max
if (present (y_min)) graph_options%y_min = y_min
if (present (y_max)) graph_options%y_max = y_max
if (present (x_min)) graph_options%x_min_set = .true.
if (present (x_max)) graph_options%x_max_set = .true.
if (present (y_min)) graph_options%y_min_set = .true.
if (present (y_max)) graph_options%y_max_set = .true.
if (present (gmlcode_bg)) graph_options%gmlcode_bg = gmlcode_bg
if (present (gmlcode_fg)) graph_options%gmlcode_fg = gmlcode_fg
end subroutine graph_options_set

```

Write a simple account of all options.

<Analysis: graph options: TBP>+≡

```

procedure :: write => graph_options_write

```

<Analysis: sub interfaces>+≡

```

module subroutine graph_options_write (gro, unit)
  class(graph_options_t), intent(in) :: gro
  integer, intent(in), optional :: unit
end subroutine graph_options_write

```

<Analysis: procedures>+≡

```

module subroutine graph_options_write (gro, unit)
  class(graph_options_t), intent(in) :: gro
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
1  format (A,1x,"",A,"")
2  format (A,1x,L1)
3  format (A,1x,ES19.12)
4  format (A,1x,IO)
5  format (A,1x,'[undefined]')
  write (u, 1) "title      =", char (gro%title)
  write (u, 1) "description =", char (gro%description)
  write (u, 1) "x_label    =", char (gro%x_label)
  write (u, 1) "y_label    =", char (gro%y_label)
  write (u, 2) "x_log      =", gro%x_log
  write (u, 2) "y_log      =", gro%y_log
  if (gro%x_min_set) then
    write (u, 3) "x_min      =", gro%x_min
  else
    write (u, 5) "x_min      ="
  end if
end if

```



```

if (gro%x_max_set) then
  write (u, 3) "x_max      =", gro%x_max
else
  write (u, 5) "x_max      ="
end if
if (gro%y_min_set) then
  write (u, 3) "y_min      =", gro%y_min
else
  write (u, 5) "y_min      ="
end if
if (gro%y_max_set) then
  write (u, 3) "y_max      =", gro%y_max
else
  write (u, 5) "y_max      ="
end if
write (u, 4) "width_mm    =", gro%width_mm
write (u, 4) "height_mm   =", gro%height_mm
write (u, 1) "gmlcode_bg  =", char (gro%gmlcode_bg)
write (u, 1) "gmlcode_fg  =", char (gro%gmlcode_fg)
end subroutine graph_options_write

```

Write a L^AT_EX header/footer for the analysis file.

<Analysis: procedures>+≡

```

subroutine graph_options_write_tex_header (gro, unit)
  type(graph_options_t), intent(in) :: gro
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  if (gro%title /= "") then
    write (u, "(A)")
    write (u, "(A)") "\section{" // char (gro%title) // "}"
  else
    write (u, "(A)") "\section{" // char (quote_underscore (gro%id)) // "}"
  end if
  if (gro%description /= "") then
    write (u, "(A)") char (gro%description)
    write (u, *)
    write (u, "(A)") "\vspace*{\baselineskip}"
  end if
  write (u, "(A)") "\vspace*{\baselineskip}"
  write (u, "(A)") "\unitlength 1mm"
  write (u, "(A,IO,',',IO,A)") &
    "\begin{gmlgraph*}(", &
    gro%width_mm, gro%height_mm, &
    ")[dat]"
end subroutine graph_options_write_tex_header

subroutine graph_options_write_tex_footer (gro, unit)
  type(graph_options_t), intent(in) :: gro
  integer, intent(in), optional :: unit
  integer :: u, width, height
  width = gro%width_mm - 10
  height = gro%height_mm - 10

```

```

u = given_output_unit (unit)
write (u, "(A)" " begingmleps ""Whizard-Logo.eps"";"
write (u, "(A,IO,A,IO,A)" &
      " base := (" width, "*unitlength", height, "*unitlength");"
write (u, "(A)" " height := 9.6*unitlength;"
write (u, "(A)" " width := 11.2*unitlength;"
write (u, "(A)" " endgmleps;"
write (u, "(A)" "\end{gmlgraph*}"
end subroutine graph_options_write_tex_footer

```

Return the analysis object ID.

```

<Analysis: procedures>+≡
function graph_options_get_id (gro) result (id)
  type(string_t) :: id
  type(graph_options_t), intent(in) :: gro
  id = gro%id
end function graph_options_get_id

```

Create an appropriate `setup` command (linear/log).

```

<Analysis: procedures>+≡
function graph_options_get_gml_setup (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  type(string_t) :: x_str, y_str
  if (gro%x_log) then
    x_str = "log"
  else
    x_str = "linear"
  end if
  if (gro%y_log) then
    y_str = "log"
  else
    y_str = "linear"
  end if
  cmd = "setup (" // x_str // ", " // y_str // ");"
end function graph_options_get_gml_setup

```

Return the labels in GAMELAN form.

```

<Analysis: procedures>+≡
function graph_options_get_gml_x_label (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = 'label.bot (<' // '<' // gro%x_label // '>' // '>', out);'
end function graph_options_get_gml_x_label

function graph_options_get_gml_y_label (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = 'label.ulft (<' // '<' // gro%y_label // '>' // '>', out);'
end function graph_options_get_gml_y_label

```

Create an appropriate **graphrange** statement for the given graph options. Where the graph options are not set, use the supplied arguments, if any, otherwise set the undefined value.

(Analysis: procedures)+≡

```
function graph_options_get_gml_graphrange &
  (gro, x_min, x_max, y_min, y_max) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  real(default), intent(in), optional :: x_min, x_max, y_min, y_max
  type(string_t) :: x_min_str, x_max_str, y_min_str, y_max_str
  character(*), parameter :: fmt = "(ES15.8)"
  if (gro%x_min_set) then
    x_min_str = "#" // trim (adjustl (real2string (gro%x_min, fmt)))
  else if (present (x_min)) then
    x_min_str = "#" // trim (adjustl (real2string (x_min, fmt)))
  else
    x_min_str = "???"
  end if
  if (gro%x_max_set) then
    x_max_str = "#" // trim (adjustl (real2string (gro%x_max, fmt)))
  else if (present (x_max)) then
    x_max_str = "#" // trim (adjustl (real2string (x_max, fmt)))
  else
    x_max_str = "???"
  end if
  if (gro%y_min_set) then
    y_min_str = "#" // trim (adjustl (real2string (gro%y_min, fmt)))
  else if (present (y_min)) then
    y_min_str = "#" // trim (adjustl (real2string (y_min, fmt)))
  else
    y_min_str = "???"
  end if
  if (gro%y_max_set) then
    y_max_str = "#" // trim (adjustl (real2string (gro%y_max, fmt)))
  else if (present (y_max)) then
    y_max_str = "#" // trim (adjustl (real2string (y_max, fmt)))
  else
    y_max_str = "???"
  end if
  cmd = "graphrange (" // x_min_str // ", " // y_min_str // ")", " &
    // "(" // x_max_str // ", " // y_max_str // ");"
end function graph_options_get_gml_graphrange
```

Get extra GAMELAN code to be executed before and after the usual drawing commands.

(Analysis: procedures)+≡

```
function graph_options_get_gml_bg_command (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = gro%gmlcode_bg
end function graph_options_get_gml_bg_command

function graph_options_get_gml_fg_command (gro) result (cmd)
```

```

type(string_t) :: cmd
type(graph_options_t), intent(in) :: gro
cmd = gro%gmlcode_fg
end function graph_options_get_gml_fg_command

```

Append the header for generic data output in ifile format. We print only labels, not graphics parameters.

```

<Analysis: procedures>+≡
subroutine graph_options_get_header (pl, header, comment)
type(graph_options_t), intent(in) :: pl
type(ifile_t), intent(inout) :: header
type(string_t), intent(in), optional :: comment
type(string_t) :: c
if (present (comment)) then
c = comment
else
c = ""
end if
call ifile_append (header, &
c // "ID: " // pl%id)
call ifile_append (header, &
c // "title: " // pl%title)
call ifile_append (header, &
c // "description: " // pl%description)
call ifile_append (header, &
c // "x axis label: " // pl%x_label)
call ifile_append (header, &
c // "y axis label: " // pl%y_label)
end subroutine graph_options_get_header

```

13.5.3 Drawing options

These options apply to an individual graph element (histogram or plot).

```

<Analysis: public>+≡
public :: drawing_options_t

<Analysis: types>+≡
type :: drawing_options_t
type(string_t) :: dataset
logical :: with_hbars = .false.
logical :: with_base = .false.
logical :: piecewise = .false.
logical :: fill = .false.
logical :: draw = .false.
logical :: err = .false.
logical :: symbols = .false.
type(string_t) :: fill_options
type(string_t) :: draw_options
type(string_t) :: err_options
type(string_t) :: symbol
type(string_t) :: gmlcode_bg
type(string_t) :: gmlcode_fg

```

```

contains
  <Analysis: drawing options: TBP>≡
end type drawing_options_t

```

Write a simple account of all options.

```

<Analysis: drawing options: TBP>≡
  procedure :: write => drawing_options_write

<Analysis: sub interfaces>+≡
  module subroutine drawing_options_write (dro, unit)
    class(drawing_options_t), intent(in) :: dro
    integer, intent(in), optional :: unit
  end subroutine drawing_options_write

<Analysis: procedures>+≡
  module subroutine drawing_options_write (dro, unit)
    class(drawing_options_t), intent(in) :: dro
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
1   format (A,1x,'',A,'')
2   format (A,1x,L1)
    write (u, 2) "with_hbars =", dro%with_hbars
    write (u, 2) "with_base  =", dro%with_base
    write (u, 2) "piecewise  =", dro%piecewise
    write (u, 2) "fill       =", dro%fill
    write (u, 2) "draw       =", dro%draw
    write (u, 2) "err        =", dro%err
    write (u, 2) "symbols    =", dro%symbols
    write (u, 1) "fill_options=", char (dro%fill_options)
    write (u, 1) "draw_options=", char (dro%draw_options)
    write (u, 1) "err_options =", char (dro%err_options)
    write (u, 1) "symbol     =", char (dro%symbol)
    write (u, 1) "gmlcode_bg  =", char (dro%gmlcode_bg)
    write (u, 1) "gmlcode_fg  =", char (dro%gmlcode_fg)
  end subroutine drawing_options_write

```

Init with empty strings and default options, appropriate for either histogram or plot.

```

<Analysis: drawing options: TBP>+≡
  procedure :: init_histogram => drawing_options_init_histogram
  procedure :: init_plot     => drawing_options_init_plot

<Analysis: sub interfaces>+≡
  module subroutine drawing_options_init_histogram (dro)
    class(drawing_options_t), intent(out) :: dro
  end subroutine drawing_options_init_histogram
  module subroutine drawing_options_init_plot (dro)
    class(drawing_options_t), intent(out) :: dro
  end subroutine drawing_options_init_plot

<Analysis: procedures>+≡
  module subroutine drawing_options_init_histogram (dro)
    class(drawing_options_t), intent(out) :: dro
    dro%dataset = "dat"

```

```

dro%with_hbars = .true.
dro%with_base = .true.
dro%piecewise = .true.
dro%fill = .true.
dro%draw = .true.
dro%fill_options = "withcolor col.default"
dro%draw_options = ""
dro%err_options = ""
dro%symbol = "fshape(circle scaled 1mm())"
dro%gmlcode_bg = ""
dro%gmlcode_fg = ""
end subroutine drawing_options_init_histogram

```

```

module subroutine drawing_options_init_plot (dro)
  class(drawing_options_t), intent(out) :: dro
  dro%dataset = "dat"
  dro%draw = .true.
  dro%fill_options = "withcolor col.default"
  dro%draw_options = ""
  dro%err_options = ""
  dro%symbol = "fshape(circle scaled 1mm())"
  dro%gmlcode_bg = ""
  dro%gmlcode_fg = ""
end subroutine drawing_options_init_plot

```

Set individual options.

<Analysis: drawing options: TBP>+≡

```

procedure :: set => drawing_options_set

```

<Analysis: sub interfaces>+≡

```

module subroutine drawing_options_set (dro, dataset, &
  with_hbars, with_base, piecewise, fill, draw, err, symbols, &
  fill_options, draw_options, err_options, symbol, &
  gmlcode_bg, gmlcode_fg)
  class(drawing_options_t), intent(inout) :: dro
  type(string_t), intent(in), optional :: dataset
  logical, intent(in), optional :: with_hbars, with_base, piecewise
  logical, intent(in), optional :: fill, draw, err, symbols
  type(string_t), intent(in), optional :: fill_options, draw_options
  type(string_t), intent(in), optional :: err_options, symbol
  type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg
end subroutine drawing_options_set

```

<Analysis: procedures>+≡

```

module subroutine drawing_options_set (dro, dataset, &
  with_hbars, with_base, piecewise, fill, draw, err, symbols, &
  fill_options, draw_options, err_options, symbol, &
  gmlcode_bg, gmlcode_fg)
  class(drawing_options_t), intent(inout) :: dro
  type(string_t), intent(in), optional :: dataset
  logical, intent(in), optional :: with_hbars, with_base, piecewise
  logical, intent(in), optional :: fill, draw, err, symbols
  type(string_t), intent(in), optional :: fill_options, draw_options
  type(string_t), intent(in), optional :: err_options, symbol
  type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg

```

```

if (present (dataset)) dro%dataset = dataset
if (present (with_hbars)) dro%with_hbars = with_hbars
if (present (with_base)) dro%with_base = with_base
if (present (piecewise)) dro%piecewise = piecewise
if (present (fill)) dro%fill = fill
if (present (draw)) dro%draw = draw
if (present (err)) dro%err = err
if (present (symbols)) dro%symbols = symbols
if (present (fill_options)) dro%fill_options = fill_options
if (present (draw_options)) dro%draw_options = draw_options
if (present (err_options)) dro%err_options = err_options
if (present (symbol)) dro%symbol = symbol
if (present (gmlcode_bg)) dro%gmlcode_bg = gmlcode_bg
if (present (gmlcode_fg)) dro%gmlcode_fg = gmlcode_fg
end subroutine drawing_options_set

```

There are separate commands for drawing the curve and for drawing errors. The symbols are applied to the latter. First of all, we may have to compute a baseline:

```

<Analysis: procedures>+≡
function drawing_options_get_calc_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  if (dro%with_base) then
    cmd = "calculate " // dro%dataset // ".base (" // dro%dataset // ") " &
      // "(x, #0);"
  else
    cmd = ""
  end if
end function drawing_options_get_calc_command

```

Return the drawing command.

```

<Analysis: procedures>+≡
function drawing_options_get_draw_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  if (dro%fill) then
    cmd = "fill"
  else if (dro%draw) then
    cmd = "draw"
  else
    cmd = ""
  end if
  if (dro%fill .or. dro%draw) then
    if (dro%piecewise) cmd = cmd // " piecewise"
    if (dro%draw .and. dro%with_base) cmd = cmd // " cyclic"
    cmd = cmd // " from (" // dro%dataset
    if (dro%with_base) then
      if (dro%piecewise) then
        cmd = cmd // ", " // dro%dataset // ".base\" ! "
      else
        cmd = cmd // " ~ " // dro%dataset // ".base\" ! "
      end if
    end if
  end if

```

```

        end if
        cmd = cmd // ")"
        if (dro%fill) then
            cmd = cmd // " " // dro%fill_options
            if (dro%draw) cmd = cmd // " outlined"
        end if
        if (dro%draw) cmd = cmd // " " // dro%draw_options
        cmd = cmd // ";"
    end if
end function drawing_options_get_draw_command

```

The error command draws error bars, if any.

```

<Analysis: procedures>+≡
function drawing_options_get_err_command (dro) result (cmd)
    type(string_t) :: cmd
    type(drawing_options_t), intent(in) :: dro
    if (dro%err) then
        cmd = "draw piecewise " &
            // "from (" // dro%dataset // ".err)" &
            // " " // dro%err_options // ";"
    else
        cmd = ""
    end if
end function drawing_options_get_err_command

```

The symbol command draws symbols, if any.

```

<Analysis: procedures>+≡
function drawing_options_get_symb_command (dro) result (cmd)
    type(string_t) :: cmd
    type(drawing_options_t), intent(in) :: dro
    if (dro%symbols) then
        cmd = "phantom" &
            // " from (" // dro%dataset // ")" &
            // " withsymbol (" // dro%symbol // ");"
    else
        cmd = ""
    end if
end function drawing_options_get_symb_command

```

Get extra GAMELAN code to be executed before and after the usual drawing commands.

```

<Analysis: procedures>+≡
function drawing_options_get_gml_bg_command (dro) result (cmd)
    type(string_t) :: cmd
    type(drawing_options_t), intent(in) :: dro
    cmd = dro%gmlcode_bg
end function drawing_options_get_gml_bg_command

function drawing_options_get_gml_fg_command (dro) result (cmd)
    type(string_t) :: cmd
    type(drawing_options_t), intent(in) :: dro
    cmd = dro%gmlcode_fg

```



```
end function drawing_options_get_gml_fg_command
```

13.5.4 Observables

The observable type holds the accumulated observable values and weight sums which are necessary for proper averaging.

(Analysis: types)+≡

```
type :: observable_t
  private
  real(default) :: sum_values = 0
  real(default) :: sum_squared_values = 0
  real(default) :: sum_weights = 0
  real(default) :: sum_squared_weights = 0
  integer :: count = 0
  type(string_t) :: obs_label
  type(string_t) :: obs_unit
  type(graph_options_t) :: graph_options
end type observable_t
```

Initialize with defined properties

(Analysis: procedures)+≡

```
subroutine observable_init (obs, obs_label, obs_unit, graph_options)
  type(observable_t), intent(out) :: obs
  type(string_t), intent(in), optional :: obs_label, obs_unit
  type(graph_options_t), intent(in), optional :: graph_options
  if (present (obs_label)) then
    obs%obs_label = obs_label
  else
    obs%obs_label = ""
  end if
  if (present (obs_unit)) then
    obs%obs_unit = obs_unit
  else
    obs%obs_unit = ""
  end if
  if (present (graph_options)) then
    obs%graph_options = graph_options
  else
    call obs%graph_options%init ()
  end if
end subroutine observable_init
```

Reset all numeric entries.

(Analysis: procedures)+≡

```
subroutine observable_clear (obs)
  type(observable_t), intent(inout) :: obs
  obs%sum_values = 0
  obs%sum_squared_values = 0
  obs%sum_weights = 0
  obs%sum_squared_weights = 0
  obs%count = 0
```

```
end subroutine observable_clear
```

Record a value. Always successful for observables.

<Analysis: interfaces>≡

```
interface observable_record_value
  module procedure observable_record_value_unweighted
  module procedure observable_record_value_weighted
end interface
```

<Analysis: sub interfaces>+≡

```
module subroutine observable_record_value_unweighted (obs, value, success)
  type(observable_t), intent(inout) :: obs
  real(default), intent(in) :: value
  logical, intent(out), optional :: success
end subroutine observable_record_value_unweighted
module subroutine observable_record_value_weighted (obs, value, weight, success)
  type(observable_t), intent(inout) :: obs
  real(default), intent(in) :: value, weight
  logical, intent(out), optional :: success
end subroutine observable_record_value_weighted
```

<Analysis: procedures>+≡

```
module subroutine observable_record_value_unweighted (obs, value, success)
  type(observable_t), intent(inout) :: obs
  real(default), intent(in) :: value
  logical, intent(out), optional :: success
  obs%sum_values = obs%sum_values + value
  obs%sum_squared_values = obs%sum_squared_values + value**2
  obs%sum_weights = obs%sum_weights + 1
  obs%sum_squared_weights = obs%sum_squared_weights + 1
  obs%count = obs%count + 1
  if (present (success)) success = .true.
end subroutine observable_record_value_unweighted

module subroutine observable_record_value_weighted (obs, value, weight, success)
  type(observable_t), intent(inout) :: obs
  real(default), intent(in) :: value, weight
  logical, intent(out), optional :: success
  obs%sum_values = obs%sum_values + value * weight
  obs%sum_squared_values = obs%sum_squared_values + value**2 * weight
  obs%sum_weights = obs%sum_weights + weight
  obs%sum_squared_weights = obs%sum_squared_weights + weight**2
  obs%count = obs%count + 1
  if (present (success)) success = .true.
end subroutine observable_record_value_weighted
```

Here are the statistics formulas:

1. Unweighted case: Given a sample of n values x_i , the average is

$$\langle x \rangle = \frac{\sum x_i}{n} \quad (13.4)$$

and the error estimate

$$\Delta x = \sqrt{\frac{1}{n-1} \langle \sum (x_i - \langle x \rangle)^2 \rangle} \quad (13.5)$$

$$= \sqrt{\frac{1}{n-1} \left(\frac{\sum x_i^2}{n} - \frac{(\sum x_i)^2}{n^2} \right)} \quad (13.6)$$

2. Weighted case: Instead of weight 1, each event comes with weight w_i .

$$\langle x \rangle = \frac{\sum x_i w_i}{\sum w_i} \quad (13.7)$$

and

$$\Delta x = \sqrt{\frac{1}{n-1} \left(\frac{\sum x_i^2 w_i}{\sum w_i} - \frac{(\sum x_i w_i)^2}{(\sum w_i)^2} \right)} \quad (13.8)$$

For $w_i = 1$, this specializes to the previous formula.

<Analysis: procedures>+≡

```
function observable_get_n_entries (obs) result (n)
  integer :: n
  type(observable_t), intent(in) :: obs
  n = obs%count
end function observable_get_n_entries

function observable_get_average (obs) result (avg)
  real(default) :: avg
  type(observable_t), intent(in) :: obs
  if (obs%sum_weights /= 0) then
    avg = obs%sum_values / obs%sum_weights
  else
    avg = 0
  end if
end function observable_get_average

function observable_get_error (obs) result (err)
  real(default) :: err
  type(observable_t), intent(in) :: obs
  real(default) :: var, n
  if (obs%sum_weights /= 0) then
    select case (obs%count)
      case (0:1)
        err = 0
      case default
        n = obs%count
        var = obs%sum_squared_values / obs%sum_weights &
              - (obs%sum_values / obs%sum_weights) ** 2
        err = sqrt (max (var, 0._default) / (n - 1))
    end select
  else
    err = 0
  end if
end function observable_get_error
```

Write label and/or physical unit to a string.

<Analysis: procedures>+≡

```
function observable_get_label (obs, wl, wu) result (string)
  type(string_t) :: string
  type(observable_t), intent(in) :: obs
  logical, intent(in) :: wl, wu
  type(string_t) :: obs_label, obs_unit
  if (wl) then
    if (obs%obs_label /= "") then
      obs_label = obs%obs_label
    else
      obs_label = "\textrm{Observable}"
    end if
  else
    obs_label = ""
  end if
  if (wu) then
    if (obs%obs_unit /= "") then
      if (wl) then
        obs_unit = "\;[" // obs%obs_unit // "]"
      else
        obs_unit = obs%obs_unit
      end if
    else
      obs_unit = ""
    end if
  else
    obs_unit = ""
  end if
  string = obs_label // obs_unit
end function observable_get_label
```

13.5.5 Output

<Analysis: procedures>+≡

```
subroutine observable_write (obs, unit)
  type(observable_t), intent(in) :: obs
  integer, intent(in), optional :: unit
  real(default) :: avg, err, relerr
  integer :: n
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  avg = observable_get_average (obs)
  err = observable_get_error (obs)
  if (avg /= 0) then
    relerr = err / abs (avg)
  else
    relerr = 0
  end if
  n = observable_get_n_entries (obs)
  if (obs%graph_options%title /= "") then
    write (u, "(A,1x,3A)") &
```

```

        "title      =", "'", char (obs%graph_options%title), '''
end if
if (obs%graph_options%title /= "") then
    write (u, "(A,1x,3A)" &
        "description =", "'", char (obs%graph_options%description), '''
end if
write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ")", advance = "no") &
    "average      =", avg
call write_unit ()
write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ")", advance = "no") &
    "error[abs]   =", err
call write_unit ()
write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ")") &
    "error[rel]   =", relerr
write (u, "(A,1x,I0)" &
    "n_entries   =", n
contains
subroutine write_unit ()
    if (obs%obs_unit /= "") then
        write (u, "(1x,A)" char (obs%obs_unit)
    else
        write (u, *)
    end if
end subroutine write_unit
end subroutine observable_write

```

L^AT_EX output.

<Analysis: procedures>+≡

```

subroutine observable_write_driver (obs, unit, write_heading)
    type(observable_t), intent(in) :: obs
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: write_heading
    real(default) :: avg, err
    integer :: n_digits
    logical :: heading
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    heading = .true.; if (present (write_heading)) heading = write_heading
    avg = observable_get_average (obs)
    err = observable_get_error (obs)
    if (avg /= 0 .and. err /= 0) then
        n_digits = max (2, 2 - int (log10 (abs (err / real (avg, default)))))
    else if (avg /= 0) then
        n_digits = 100
    else
        n_digits = 1
    end if
    if (heading) then
        write (u, "(A)")
        if (obs%graph_options%title /= "") then
            write (u, "(A)" " \section{" // char (obs%graph_options%title) &
                // "}")
        else

```

```

        write (u, "(A)") "\section{Observable}"
    end if
    if (obs%graph_options%description /= "") then
        write (u, "(A)") char (obs%graph_options%description)
        write (u, *)
    end if
    write (u, "(A)") "\begin{flushleft}"
end if
write (u, "(A)", advance="no") " \$\langle{" ! $ sign
write (u, "(A)", advance="no") char (observable_get_label (obs, wl=.true., wu=.false.))
write (u, "(A)", advance="no") "}\rangle = "
write (u, "(A)", advance="no") char (tex_format (avg, n_digits))
write (u, "(A)", advance="no") "\pm"
write (u, "(A)", advance="no") char (tex_format (err, 2))
write (u, "(A)", advance="no") "\;{"
write (u, "(A)", advance="no") char (observable_get_label (obs, wl=.false., wu=.true.))
write (u, "(A)") "}"
write (u, "(A)", advance="no") " \quad[n_{\text{entries}}] = "
write (u, "(IO)", advance="no") observable_get_n_entries (obs)
write (u, "(A)") "]"$ " ! $ fool Emacs' noweb mode
if (heading) then
    write (u, "(A)") "\end{flushleft}"
end if
end subroutine observable_write_driver

```

13.5.6 Histograms

Bins

<Analysis: types>+≡

```

type :: bin_t
private
real(default) :: midpoint = 0
real(default) :: width = 0
real(default) :: sum_weights = 0
real(default) :: sum_squared_weights = 0
real(default) :: sum_excess_weights = 0
integer :: count = 0
end type bin_t

```

<Analysis: procedures>+≡

```

subroutine bin_init (bin, midpoint, width)
type(bin_t), intent(out) :: bin
real(default), intent(in) :: midpoint, width
bin%midpoint = midpoint
bin%width = width
end subroutine bin_init

```

<Analysis: procedures>+≡

```

elemental subroutine bin_clear (bin)
type(bin_t), intent(inout) :: bin
bin%sum_weights = 0

```

```

    bin%sum_squared_weights = 0
    bin%sum_excess_weights = 0
    bin%count = 0
end subroutine bin_clear

```

<Analysis: procedures>+≡

```

subroutine bin_record_value (bin, normalize, weight, excess)
  type(bin_t), intent(inout) :: bin
  logical, intent(in) :: normalize
  real(default), intent(in) :: weight
  real(default), intent(in), optional :: excess
  real(default) :: w, e
  if (normalize) then
    if (bin%width /= 0) then
      w = weight / bin%width
      if (present (excess)) e = excess / bin%width
    else
      w = 0
      if (present (excess)) e = 0
    end if
  else
    w = weight
    if (present (excess)) e = excess
  end if
  bin%sum_weights = bin%sum_weights + w
  bin%sum_squared_weights = bin%sum_squared_weights + w ** 2
  if (present (excess)) &
    bin%sum_excess_weights = bin%sum_excess_weights + abs (e)
  bin%count = bin%count + 1
end subroutine bin_record_value

```

<Analysis: procedures>+≡

```

function bin_get_midpoint (bin) result (x)
  real(default) :: x
  type(bin_t), intent(in) :: bin
  x = bin%midpoint
end function bin_get_midpoint

function bin_get_width (bin) result (w)
  real(default) :: w
  type(bin_t), intent(in) :: bin
  w = bin%width
end function bin_get_width

function bin_get_n_entries (bin) result (n)
  integer :: n
  type(bin_t), intent(in) :: bin
  n = bin%count
end function bin_get_n_entries

function bin_get_sum (bin) result (s)
  real(default) :: s
  type(bin_t), intent(in) :: bin

```

```

    s = bin%sum_weights
end function bin_get_sum

function bin_get_error (bin) result (err)
    real(default) :: err
    type(bin_t), intent(in) :: bin
    err = sqrt (bin%sum_squared_weights)
end function bin_get_error

function bin_get_excess (bin) result (excess)
    real(default) :: excess
    type(bin_t), intent(in) :: bin
    excess = bin%sum_excess_weights
end function bin_get_excess

```

<Analysis: procedures>+≡

```

subroutine bin_write_header (unit)
    integer, intent(in), optional :: unit
    character(120) :: buffer
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (buffer, "(A,4(1x," //HISTOGRAM_HEAD_FORMAT // "),2x,A)") &
        "#", "bin midpoint", "value      ", "error      ", &
        "excess      ", "n"
    write (u, "(A)") trim (buffer)
end subroutine bin_write_header

subroutine bin_write (bin, unit)
    type(bin_t), intent(in) :: bin
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,4(1x," // HISTOGRAM_DATA_FORMAT // "),2x,IO)") &
        bin_get_midpoint (bin), &
        bin_get_sum (bin), &
        bin_get_error (bin), &
        bin_get_excess (bin), &
        bin_get_n_entries (bin)
end subroutine bin_write

```

Histograms

<Analysis: types>+≡

```

type :: histogram_t
    private
    real(default) :: lower_bound = 0
    real(default) :: upper_bound = 0
    real(default) :: width = 0
    integer :: n_bins = 0
    logical :: normalize_bins = .false.
    type(observable_t) :: obs
    type(observable_t) :: obs_within_bounds

```



```

type(bin_t) :: underflow
type(bin_t), dimension(:), allocatable :: bin
type(bin_t) :: overflow
type(graph_options_t) :: graph_options
type(drawing_options_t) :: drawing_options
end type histogram_t

```

Initializer/finalizer

Initialize a histogram. We may provide either the bin width or the number of bins. A finalizer is not needed, since the histogram contains no pointer (sub)components.

(Analysis: interfaces)+≡

```

interface histogram_init
  module procedure histogram_init_n_bins
  module procedure histogram_init_bin_width
end interface

```

(Analysis: sub interfaces)+≡

```

module subroutine histogram_init_n_bins (h, id, &
  lower_bound, upper_bound, n_bins, normalize_bins, &
  obs_label, obs_unit, graph_options, drawing_options)
  type(histogram_t), intent(out) :: h
  type(string_t), intent(in) :: id
  real(default), intent(in) :: lower_bound, upper_bound
  integer, intent(in) :: n_bins
  logical, intent(in) :: normalize_bins
  type(string_t), intent(in), optional :: obs_label, obs_unit
  type(graph_options_t), intent(in), optional :: graph_options
  type(drawing_options_t), intent(in), optional :: drawing_options
end subroutine histogram_init_n_bins
module subroutine histogram_init_bin_width (h, id, &
  lower_bound, upper_bound, bin_width, normalize_bins, &
  obs_label, obs_unit, graph_options, drawing_options)
  type(histogram_t), intent(out) :: h
  type(string_t), intent(in) :: id
  real(default), intent(in) :: lower_bound, upper_bound, bin_width
  logical, intent(in) :: normalize_bins
  type(string_t), intent(in), optional :: obs_label, obs_unit
  type(graph_options_t), intent(in), optional :: graph_options
  type(drawing_options_t), intent(in), optional :: drawing_options
end subroutine histogram_init_bin_width

```

(Analysis: procedures)+≡

```

module subroutine histogram_init_n_bins (h, id, &
  lower_bound, upper_bound, n_bins, normalize_bins, &
  obs_label, obs_unit, graph_options, drawing_options)
  type(histogram_t), intent(out) :: h
  type(string_t), intent(in) :: id
  real(default), intent(in) :: lower_bound, upper_bound
  integer, intent(in) :: n_bins
  logical, intent(in) :: normalize_bins

```

```

type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
real(default) :: bin_width
integer :: i
call observable_init (h%obs_within_bounds, obs_label, obs_unit)
call observable_init (h%obs, obs_label, obs_unit)
h%lower_bound = lower_bound
h%upper_bound = upper_bound
h%n_bins = max (n_bins, 1)
h%width = h%upper_bound - h%lower_bound
h%normalize_bins = normalize_bins
bin_width = h%width / h%n_bins
allocate (h%bin (h%n_bins))
call bin_init (h%underflow, h%lower_bound, 0._default)
do i = 1, h%n_bins
    call bin_init (h%bin(i), &
        h%lower_bound - bin_width/2 + i * bin_width, bin_width)
end do
call bin_init (h%overflow, h%upper_bound, 0._default)
if (present (graph_options)) then
    h%graph_options = graph_options
else
    call h%graph_options%init ()
end if
call graph_options_set (h%graph_options, id = id)
if (present (drawing_options)) then
    h%drawing_options = drawing_options
else
    call h%drawing_options%init_histogram ()
end if
end subroutine histogram_init_n_bins

module subroutine histogram_init_bin_width (h, id, &
    lower_bound, upper_bound, bin_width, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)
type(histogram_t), intent(out) :: h
type(string_t), intent(in) :: id
real(default), intent(in) :: lower_bound, upper_bound, bin_width
logical, intent(in) :: normalize_bins
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
integer :: n_bins
if (bin_width /= 0) then
    n_bins = nint ((upper_bound - lower_bound) / bin_width)
else
    n_bins = 1
end if
call histogram_init_n_bins (h, id, &
    lower_bound, upper_bound, n_bins, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)
end subroutine histogram_init_bin_width

```

Initialize a histogram by copying another one.

Since `h` has no pointer (sub)components, intrinsic assignment is sufficient. Optionally, we replace the drawing options.

```

<Analysis: procedures>+≡
subroutine histogram_init_histogram (h, h_in, drawing_options)
  type(histogram_t), intent(out) :: h
  type(histogram_t), intent(in) :: h_in
  type(drawing_options_t), intent(in), optional :: drawing_options
  h = h_in
  if (present (drawing_options)) then
    h%drawing_options = drawing_options
  end if
end subroutine histogram_init_histogram

```

Fill histograms

Clear the histogram contents, but do not modify the structure.

```

<Analysis: procedures>+≡
subroutine histogram_clear (h)
  type(histogram_t), intent(inout) :: h
  call observable_clear (h%obs)
  call observable_clear (h%obs_within_bounds)
  call bin_clear (h%underflow)
  if (allocated (h%bin)) call bin_clear (h%bin)
  call bin_clear (h%overflow)
end subroutine histogram_clear

```

Record a value. Successful if the value is within bounds, otherwise it is recorded as under-/overflow. Optionally, we may provide an excess weight that could be returned by the unweighting procedure.

```

<Analysis: procedures>+≡
subroutine histogram_record_value_unweighted (h, value, excess, success)
  type(histogram_t), intent(inout) :: h
  real(default), intent(in) :: value
  real(default), intent(in), optional :: excess
  logical, intent(out), optional :: success
  integer :: i_bin
  call observable_record_value (h%obs, value)
  if (h%width /= 0) then
    i_bin = floor (((value - h%lower_bound) / h%width) * h%n_bins) + 1
  else
    i_bin = 0
  end if
  if (i_bin <= 0) then
    call bin_record_value (h%underflow, .false., 1._default, excess)
    if (present (success)) success = .false.
  else if (i_bin <= h%n_bins) then
    call observable_record_value (h%obs_within_bounds, value)
    call bin_record_value &
      (h%bin(i_bin), h%normalize_bins, 1._default, excess)
    if (present (success)) success = .true.
  end if
end subroutine histogram_record_value_unweighted

```

```

else
  call bin_record_value (h%overflow, .false., 1._default, excess)
  if (present (success)) success = .false.
end if
end subroutine histogram_record_value_unweighted

```

Weighted events: analogous, but no excess weight.

(Analysis: procedures)+≡

```

subroutine histogram_record_value_weighted (h, value, weight, success)
  type(histogram_t), intent(inout) :: h
  real(default), intent(in) :: value, weight
  logical, intent(out), optional :: success
  integer :: i_bin
  call observable_record_value (h%obs, value, weight)
  if (h%width /= 0) then
    i_bin = floor (((value - h%lower_bound) / h%width) * h%n_bins) + 1
  else
    i_bin = 0
  end if
  if (i_bin <= 0) then
    call bin_record_value (h%underflow, .false., weight)
    if (present (success)) success = .false.
  else if (i_bin <= h%n_bins) then
    call observable_record_value (h%obs_within_bounds, value, weight)
    call bin_record_value (h%bin(i_bin), h%normalize_bins, weight)
    if (present (success)) success = .true.
  else
    call bin_record_value (h%overflow, .false., weight)
    if (present (success)) success = .false.
  end if
end subroutine histogram_record_value_weighted

```

Access contents

Inherited from the observable component (all-over average etc.)

(Analysis: procedures)+≡

```

function histogram_get_n_entries (h) result (n)
  integer :: n
  type(histogram_t), intent(in) :: h
  n = observable_get_n_entries (h%obs)
end function histogram_get_n_entries

function histogram_get_average (h) result (avg)
  real(default) :: avg
  type(histogram_t), intent(in) :: h
  avg = observable_get_average (h%obs)
end function histogram_get_average

function histogram_get_error (h) result (err)
  real(default) :: err
  type(histogram_t), intent(in) :: h
  err = observable_get_error (h%obs)

```

```
end function histogram_get_error
```

Analogous, but applied only to events within bounds.

<Analysis: procedures>+≡

```
function histogram_get_n_entries_within_bounds (h) result (n)
  integer :: n
  type(histogram_t), intent(in) :: h
  n = observable_get_n_entries (h%obs_within_bounds)
end function histogram_get_n_entries_within_bounds

function histogram_get_average_within_bounds (h) result (avg)
  real(default) :: avg
  type(histogram_t), intent(in) :: h
  avg = observable_get_average (h%obs_within_bounds)
end function histogram_get_average_within_bounds

function histogram_get_error_within_bounds (h) result (err)
  real(default) :: err
  type(histogram_t), intent(in) :: h
  err = observable_get_error (h%obs_within_bounds)
end function histogram_get_error_within_bounds
```

Get the number of bins

<Analysis: procedures>+≡

```
function histogram_get_n_bins (h) result (n)
  type(histogram_t), intent(in) :: h
  integer :: n
  n = h%n_bins
end function histogram_get_n_bins
```

Check bins. If the index is zero or above the limit, return the results for under-flow or overflow, respectively.

<Analysis: procedures>+≡

```
function histogram_get_n_entries_for_bin (h, i) result (n)
  integer :: n
  type(histogram_t), intent(in) :: h
  integer, intent(in) :: i
  if (i <= 0) then
    n = bin_get_n_entries (h%underflow)
  else if (i <= h%n_bins) then
    n = bin_get_n_entries (h%bin(i))
  else
    n = bin_get_n_entries (h%overflow)
  end if
end function histogram_get_n_entries_for_bin

function histogram_get_sum_for_bin (h, i) result (avg)
  real(default) :: avg
  type(histogram_t), intent(in) :: h
  integer, intent(in) :: i
  if (i <= 0) then
    avg = bin_get_sum (h%underflow)
  end if
end function histogram_get_sum_for_bin
```

```

        else if (i <= h%n_bins) then
            avg = bin_get_sum (h%bin(i))
        else
            avg = bin_get_sum (h%overflow)
        end if
    end function histogram_get_sum_for_bin

function histogram_get_error_for_bin (h, i) result (err)
    real(default) :: err
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i
    if (i <= 0) then
        err = bin_get_error (h%underflow)
    else if (i <= h%n_bins) then
        err = bin_get_error (h%bin(i))
    else
        err = bin_get_error (h%overflow)
    end if
end function histogram_get_error_for_bin

function histogram_get_excess_for_bin (h, i) result (err)
    real(default) :: err
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i
    if (i <= 0) then
        err = bin_get_excess (h%underflow)
    else if (i <= h%n_bins) then
        err = bin_get_excess (h%bin(i))
    else
        err = bin_get_excess (h%overflow)
    end if
end function histogram_get_excess_for_bin

```

Return a pointer to the graph options.

<Analysis: procedures>+≡

```

function histogram_get_graph_options_ptr (h) result (ptr)
    type(graph_options_t), pointer :: ptr
    type(histogram_t), intent(in), target :: h
    ptr => h%graph_options
end function histogram_get_graph_options_ptr

```

Return a pointer to the drawing options.

<Analysis: procedures>+≡

```

function histogram_get_drawing_options_ptr (h) result (ptr)
    type(drawing_options_t), pointer :: ptr
    type(histogram_t), intent(in), target :: h
    ptr => h%drawing_options
end function histogram_get_drawing_options_ptr

```

Output

<Analysis: procedures>+≡

```

subroutine histogram_write (h, unit)
  type(histogram_t), intent(in) :: h
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call bin_write_header (u)
  if (allocated (h%bin)) then
    do i = 1, h%n_bins
      call bin_write (h%bin(i), u)
    end do
  end if
  write (u, "(A)")
  write (u, "(A,1x,A)" "#", "Underflow:")
  call bin_write (h%underflow, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" "#", "Overflow:")
  call bin_write (h%overflow, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" "#", "Summary: data within bounds")
  call observable_write (h%obs_within_bounds, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" "#", "Summary: all data")
  call observable_write (h%obs, u)
  write (u, "(A)")
end subroutine histogram_write

```

Write the GAMELAN reader for histogram contents.

<Analysis: procedures>+≡

```

subroutine histogram_write_gml_reader (h, filename, unit)
  type(histogram_t), intent(in) :: h
  type(string_t), intent(in) :: filename
  integer, intent(in), optional :: unit
  character(*), parameter :: fmt = "(ES15.8)"
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(2x,A)" 'fromfile "' // char (filename) // '":'
  write (u, "(4x,A)" 'key "# Histogram:");'
  write (u, "(4x,A)" 'dx := #' &
    // real2char (h%width / h%n_bins / 2, fmt) // ';'
  write (u, "(4x,A)" 'for i withinblock:')
  write (u, "(6x,A)" 'get x, y, y.d, y.n, y.e;')
  if (h%drawing_options%with_hbars) then
    write (u, "(6x,A)" 'plot (' // char (h%drawing_options%dataset) &
      // ') (x,y) hbar dx;')
  else
    write (u, "(6x,A)" 'plot (' // char (h%drawing_options%dataset) &
      // ') (x,y);')
  end if
  if (h%drawing_options%err) then
    write (u, "(6x,A)" 'plot (' // char (h%drawing_options%dataset) &
      // '.err) ' &
      // '(x,y) vbar y.d;')
  end if
end if

```

```

!!! Future excess options for plots
! write (u, "(6x,A)") 'if show_excess: ' // &
!           & 'plot(dat.e)(x, y plus y.e) hbar dx; fi'
write (u, "(4x,A)") 'endfor'
write (u, "(2x,A)") 'endfrom'
end subroutine histogram_write_gml_reader

```

L^AT_EX and GAMELAN output.

(Analysis: procedures)+≡

```

subroutine histogram_write_gml_driver (h, filename, unit)
  type(histogram_t), intent(in) :: h
  type(string_t), intent(in) :: filename
  integer, intent(in), optional :: unit
  type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call graph_options_write_tex_header (h%graph_options, unit)
  write (u, "(2x,A)") char (graph_options_get_gml_setup (h%graph_options))
  write (u, "(2x,A)") char (graph_options_get_gml_graphrange &
    (h%graph_options, x_min=h%lower_bound, x_max=h%upper_bound))
  call histogram_write_gml_reader (h, filename, unit)
  calc_cmd = drawing_options_get_calc_command (h%drawing_options)
  if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
  bg_cmd = drawing_options_get_gml_bg_command (h%drawing_options)
  if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
  draw_cmd = drawing_options_get_draw_command (h%drawing_options)
  if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
  err_cmd = drawing_options_get_err_command (h%drawing_options)
  if (err_cmd /= "") write (u, "(2x,A)") char (err_cmd)
  symb_cmd = drawing_options_get_symb_command (h%drawing_options)
  if (symb_cmd /= "") write (u, "(2x,A)") char (symb_cmd)
  fg_cmd = drawing_options_get_gml_fg_command (h%drawing_options)
  if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
  write (u, "(2x,A)") char (graph_options_get_gml_x_label (h%graph_options))
  write (u, "(2x,A)") char (graph_options_get_gml_y_label (h%graph_options))
  call graph_options_write_tex_footer (h%graph_options, unit)
  write (u, "(A)") "\vspace*{2\baselineskip}"
  write (u, "(A)") "\begin{flushleft}"
  write (u, "(A)") "\textbf{Data within bounds:} \\"
  call observable_write_driver (h%obs_within_bounds, unit, &
    write_heading=.false.)
  write (u, "(A)") "\\[0.5\baselineskip]"
  write (u, "(A)") "\textbf{All data:} \\"
  call observable_write_driver (h%obs, unit, write_heading=.false.)
  write (u, "(A)") "\end{flushleft}"
end subroutine histogram_write_gml_driver

```

Return the header for generic data output as an ifile.

(Analysis: procedures)+≡

```

subroutine histogram_get_header (h, header, comment)
  type(histogram_t), intent(in) :: h
  type(ifile_t), intent(inout) :: header
  type(string_t), intent(in), optional :: comment

```



```

type(string_t) :: c
if (present (comment)) then
    c = comment
else
    c = ""
end if
call ifile_append (header, c // "WHIZARD histogram data")
call graph_options_get_header (h%graph_options, header, comment)
call ifile_append (header, &
    c // "range: " // real2string (h%lower_bound) &
    // " - " // real2string (h%upper_bound))
call ifile_append (header, &
    c // "counts total: " &
    // int2char (histogram_get_n_entries_within_bounds (h)))
call ifile_append (header, &
    c // "total average: " &
    // real2string (histogram_get_average_within_bounds (h)) // " +- " &
    // real2string (histogram_get_error_within_bounds (h)))
end subroutine histogram_get_header

```

13.5.7 Plots

Points

<Analysis: types>+≡

```

type :: point_t
private
real(default) :: x = 0
real(default) :: y = 0
real(default) :: yerr = 0
real(default) :: xerr = 0
type(point_t), pointer :: next => null ()
end type point_t

```

<Analysis: interfaces>+≡

```

interface point_init
    module procedure point_init_contents
    module procedure point_init_point
end interface

```

<Analysis: sub interfaces>+≡

```

module subroutine point_init_contents (point, x, y, yerr, xerr)
    type(point_t), intent(out) :: point
    real(default), intent(in) :: x, y
    real(default), intent(in), optional :: yerr, xerr
end subroutine point_init_contents
module subroutine point_init_point (point, point_in)
    type(point_t), intent(out) :: point
    type(point_t), intent(in) :: point_in
end subroutine point_init_point

```

<Analysis: procedures>+≡

```

module subroutine point_init_contents (point, x, y, yerr, xerr)
    type(point_t), intent(out) :: point

```

```

real(default), intent(in) :: x, y
real(default), intent(in), optional :: yerr, xerr
point%x = x
point%y = y
if (present (yerr)) point%yerr = yerr
if (present (xerr)) point%xerr = xerr
end subroutine point_init_contents

module subroutine point_init_point (point, point_in)
  type(point_t), intent(out) :: point
  type(point_t), intent(in) :: point_in
  point%x = point_in%x
  point%y = point_in%y
  point%yerr = point_in%yerr
  point%xerr = point_in%xerr
end subroutine point_init_point

```

<Analysis: procedures>+≡

```

function point_get_x (point) result (x)
  real(default) :: x
  type(point_t), intent(in) :: point
  x = point%x
end function point_get_x

function point_get_y (point) result (y)
  real(default) :: y
  type(point_t), intent(in) :: point
  y = point%y
end function point_get_y

function point_get_xerr (point) result (xerr)
  real(default) :: xerr
  type(point_t), intent(in) :: point
  xerr = point%xerr
end function point_get_xerr

function point_get_yerr (point) result (yerr)
  real(default) :: yerr
  type(point_t), intent(in) :: point
  yerr = point%yerr
end function point_get_yerr

```

<Analysis: procedures>+≡

```

subroutine point_write_header (unit)
  integer, intent(in) :: unit
  character(120) :: buffer
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (buffer, "(A,4(1x," // HISTOGRAM_HEAD_FORMAT // "))" &
    "#", "x", "y", "yerr", "xerr"
  write (u, "(A)") trim (buffer)
end subroutine point_write_header

```

```

subroutine point_write (point, unit)
  type(point_t), intent(in) :: point
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,4(1x," // HISTOGRAM_DATA_FORMAT // "))" ) &
    point_get_x (point), &
    point_get_y (point), &
    point_get_yerr (point), &
    point_get_xerr (point)
end subroutine point_write

```

Plots

```

<Analysis: types>+≡
  type :: plot_t
  private
  type(point_t), pointer :: first => null ()
  type(point_t), pointer :: last => null ()
  integer :: count = 0
  type(graph_options_t) :: graph_options
  type(drawing_options_t) :: drawing_options
end type plot_t

```

Initializer/finalizer

Initialize a plot. We provide the lower and upper bound in the x direction.

```

<Analysis: interfaces>+≡
  interface plot_init
    module procedure plot_init_empty
    module procedure plot_init_plot
  end interface

<Analysis: sub interfaces>+≡
  module subroutine plot_init_empty (p, id, graph_options, drawing_options)
    type(plot_t), intent(out) :: p
    type(string_t), intent(in) :: id
    type(graph_options_t), intent(in), optional :: graph_options
    type(drawing_options_t), intent(in), optional :: drawing_options
  end subroutine plot_init_empty

<Analysis: procedures>+≡
  module subroutine plot_init_empty (p, id, graph_options, drawing_options)
    type(plot_t), intent(out) :: p
    type(string_t), intent(in) :: id
    type(graph_options_t), intent(in), optional :: graph_options
    type(drawing_options_t), intent(in), optional :: drawing_options
    if (present (graph_options)) then
      p%graph_options = graph_options
    else
      call p%graph_options%init ()
    end if
  end subroutine plot_init_empty

```

```

    call p%graph_options%set (id = id)
    if (present (drawing_options)) then
        p%drawing_options = drawing_options
    else
        call p%drawing_options%init_plot ()
    end if
end subroutine plot_init_empty

```

Initialize a plot by copying another one, optionally merging in a new set of drawing options.

Since `p` has pointer (sub)components, we have to explicitly deep-copy the original.

(Analysis: sub interfaces)+≡

```

module subroutine plot_init_plot (p, p_in, drawing_options)
    type(plot_t), intent(out) :: p
    type(plot_t), intent(in) :: p_in
    type(drawing_options_t), intent(in), optional :: drawing_options
end subroutine plot_init_plot

```

(Analysis: procedures)+≡

```

module subroutine plot_init_plot (p, p_in, drawing_options)
    type(plot_t), intent(out) :: p
    type(plot_t), intent(in) :: p_in
    type(drawing_options_t), intent(in), optional :: drawing_options
    type(point_t), pointer :: current, new
    current => p_in%first
    do while (associated (current))
        allocate (new)
        call point_init (new, current)
        if (associated (p%last)) then
            p%last%next => new
        else
            p%first => new
        end if
        p%last => new
        current => current%next
    end do
    p%count = p_in%count
    p%graph_options = p_in%graph_options
    if (present (drawing_options)) then
        p%drawing_options = drawing_options
    else
        p%drawing_options = p_in%drawing_options
    end if
end subroutine plot_init_plot

```

Finalize the plot by deallocating the list of points.

(Analysis: procedures)+≡

```

subroutine plot_final (plot)
    type(plot_t), intent(inout) :: plot
    type(point_t), pointer :: current
    do while (associated (plot%first))
        current => plot%first
    end do

```

```

        plot%first => current%next
        deallocate (current)
    end do
    plot%last => null ()
end subroutine plot_final

```

Fill plots

Clear the plot contents, but do not modify the structure.

<Analysis: procedures>+≡

```

subroutine plot_clear (plot)
    type(plot_t), intent(inout) :: plot
    plot%count = 0
    call plot_final (plot)
end subroutine plot_clear

```

Record a value. Successful if the value is within bounds, otherwise it is recorded as under-/overflow.

<Analysis: procedures>+≡

```

subroutine plot_record_value (plot, x, y, yerr, xerr, success)
    type(plot_t), intent(inout) :: plot
    real(default), intent(in) :: x, y
    real(default), intent(in), optional :: yerr, xerr
    logical, intent(out), optional :: success
    type(point_t), pointer :: point
    plot%count = plot%count + 1
    allocate (point)
    call point_init (point, x, y, yerr, xerr)
    if (associated (plot%first)) then
        plot%last%next => point
    else
        plot%first => point
    end if
    plot%last => point
    if (present (success)) success = .true.
end subroutine plot_record_value

```

Access contents

The number of points.

<Analysis: procedures>+≡

```

function plot_get_n_entries (plot) result (n)
    integer :: n
    type(plot_t), intent(in) :: plot
    n = plot%count
end function plot_get_n_entries

```

Return a pointer to the graph options.

```
<Analysis: procedures>+≡  
function plot_get_graph_options_ptr (p) result (ptr)  
  type(graph_options_t), pointer :: ptr  
  type(plot_t), intent(in), target :: p  
  ptr => p%graph_options  
end function plot_get_graph_options_ptr
```

Return a pointer to the drawing options.

```
<Analysis: procedures>+≡  
function plot_get_drawing_options_ptr (p) result (ptr)  
  type(drawing_options_t), pointer :: ptr  
  type(plot_t), intent(in), target :: p  
  ptr => p%drawing_options  
end function plot_get_drawing_options_ptr
```

Output

This output format is used by the GAMELAN driver below.

```
<Analysis: procedures>+≡  
subroutine plot_write (plot, unit)  
  type(plot_t), intent(in) :: plot  
  integer, intent(in), optional :: unit  
  type(point_t), pointer :: point  
  integer :: u  
  u = given_output_unit (unit); if (u < 0) return  
  call point_write_header (u)  
  point => plot%first  
  do while (associated (point))  
    call point_write (point, unit)  
    point => point%next  
  end do  
  write (u, *)  
  write (u, "(A,1x,A)" ) "#", "Summary:"  
  write (u, "(A,1x,I0)" ) &  
    "n_entries =", plot_get_n_entries (plot)  
  write (u, *)  
end subroutine plot_write
```

Write the GAMELAN reader for plot contents.

```
<Analysis: procedures>+≡  
subroutine plot_write_gml_reader (p, filename, unit)  
  type(plot_t), intent(in) :: p  
  type(string_t), intent(in) :: filename  
  integer, intent(in), optional :: unit  
  integer :: u  
  u = given_output_unit (unit); if (u < 0) return  
  write (u, "(2x,A)" ) 'fromfile "' // char (filename) // '" :'  
  write (u, "(4x,A)" ) 'key "# Plot:" ;'  
  write (u, "(4x,A)" ) 'for i withinblock :'  
  write (u, "(6x,A)" ) 'get x, y, y.err, x.err ;'
```

```

write (u, "(6x,A)") 'plot (' // char (p%drawing_options%dataset) &
// ') (x,y);'
if (p%drawing_options%err) then
write (u, "(6x,A)") 'plot (' // char (p%drawing_options%dataset) &
// '.err) (x,y) vbar y.err hbar x.err;'
end if
write (u, "(4x,A)") 'endfor'
write (u, "(2x,A)") 'endfrom'
end subroutine plot_write_gml_reader

```

L^AT_EX and GAMELAN output. Analogous to histogram output.

(Analysis: procedures)+≡

```

subroutine plot_write_gml_driver (p, filename, unit)
type(plot_t), intent(in) :: p
type(string_t), intent(in) :: filename
integer, intent(in), optional :: unit
type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
integer :: u
u = given_output_unit (unit); if (u < 0) return
call graph_options_write_tex_header (p%graph_options, unit)
write (u, "(2x,A)") &
char (graph_options_get_gml_setup (p%graph_options))
write (u, "(2x,A)") &
char (graph_options_get_gml_graphrange (p%graph_options))
call plot_write_gml_reader (p, filename, unit)
calc_cmd = drawing_options_get_calc_command (p%drawing_options)
if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
bg_cmd = drawing_options_get_gml_bg_command (p%drawing_options)
if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
draw_cmd = drawing_options_get_draw_command (p%drawing_options)
if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
err_cmd = drawing_options_get_err_command (p%drawing_options)
if (err_cmd /= "") write (u, "(2x,A)") char (err_cmd)
symb_cmd = drawing_options_get_symb_command (p%drawing_options)
if (symb_cmd /= "") write (u, "(2x,A)") char (symb_cmd)
fg_cmd = drawing_options_get_gml_fg_command (p%drawing_options)
if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
write (u, "(2x,A)") char (graph_options_get_gml_x_label (p%graph_options))
write (u, "(2x,A)") char (graph_options_get_gml_y_label (p%graph_options))
call graph_options_write_tex_footer (p%graph_options, unit)
end subroutine plot_write_gml_driver

```

Append header for generic data output in ifile format.

(Analysis: procedures)+≡

```

subroutine plot_get_header (plot, header, comment)
type(plot_t), intent(in) :: plot
type(ifile_t), intent(inout) :: header
type(string_t), intent(in), optional :: comment
type(string_t) :: c
if (present (comment)) then
c = comment
else
c = ""

```

```

end if
call ifile_append (header, c // "WHIZARD plot data")
call graph_options_get_header (plot%graph_options, header, comment)
call ifile_append (header, &
    c // "number of points: " &
    // int2char (plot_get_n_entries (plot)))
end subroutine plot_get_header

```

13.5.8 Graphs

A graph is a container for several graph elements. Each graph element is either a plot or a histogram. There is an appropriate base type below (the `analysis_object_t`), but to avoid recursion, we define a separate base type here. Note that there is no actual recursion: a graph is an analysis object, but a graph cannot contain graphs.

(If we could use type extension, the implementation would be much more transparent.)

Graph elements

Graph elements cannot be filled by the `record` command directly. The contents are always copied from elementary histograms or plots.

<Analysis: types>+≡

```

type :: graph_element_t
private
integer :: type = AN_UNDEFINED
type(histogram_t), pointer :: h => null ()
type(plot_t), pointer :: p => null ()
end type graph_element_t

```

<Analysis: procedures>+≡

```

subroutine graph_element_final (el)
type(graph_element_t), intent(inout) :: el
select case (el%type)
case (AN_HISTOGRAM)
deallocate (el%h)
case (AN_PLOT)
call plot_final(el%p)
deallocate (el%p)
end select
el%type = AN_UNDEFINED
end subroutine graph_element_final

```

Return the number of entries in the graph element:

<Analysis: procedures>+≡

```

function graph_element_get_n_entries (el) result (n)
integer :: n
type(graph_element_t), intent(in) :: el
select case (el%type)
case (AN_HISTOGRAM); n = histogram_get_n_entries (el%h)

```



```

        case (AN_PLOT);          n = plot_get_n_entries (el%p)
        case default;           n = 0
    end select
end function graph_element_get_n_entries

```

Return a pointer to the graph / drawing options.

<Analysis: procedures>+≡

```

function graph_element_get_graph_options_ptr (el) result (ptr)
    type(graph_options_t), pointer :: ptr
    type(graph_element_t), intent(in) :: el
    select case (el%type)
        case (AN_HISTOGRAM); ptr => histogram_get_graph_options_ptr (el%h)
        case (AN_PLOT);      ptr => plot_get_graph_options_ptr (el%p)
        case default;        ptr => null ()
    end select
end function graph_element_get_graph_options_ptr

function graph_element_get_drawing_options_ptr (el) result (ptr)
    type(drawing_options_t), pointer :: ptr
    type(graph_element_t), intent(in) :: el
    select case (el%type)
        case (AN_HISTOGRAM); ptr => histogram_get_drawing_options_ptr (el%h)
        case (AN_PLOT);      ptr => plot_get_drawing_options_ptr (el%p)
        case default;        ptr => null ()
    end select
end function graph_element_get_drawing_options_ptr

```

Output, simple wrapper for the plot/histogram writer.

<Analysis: procedures>+≡

```

subroutine graph_element_write (el, unit)
    type(graph_element_t), intent(in) :: el
    integer, intent(in), optional :: unit
    type(graph_options_t), pointer :: gro
    type(string_t) :: id
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    gro => graph_element_get_graph_options_ptr (el)
    id = graph_options_get_id (gro)
    write (u, "(A,A)" ' #', repeat (" ", 78))
    select case (el%type)
        case (AN_HISTOGRAM)
            write (u, "(A)", advance="no") "# Histogram: "
            write (u, "(1x,A)" char (id)
            call histogram_write (el%h, unit)
        case (AN_PLOT)
            write (u, "(A)", advance="no") "# Plot: "
            write (u, "(1x,A)" char (id)
            call plot_write (el%p, unit)
    end select
end subroutine graph_element_write

```

<Analysis: procedures>+≡

```

subroutine graph_element_write_gml_reader (el, filename, unit)

```

```

    type(graph_element_t), intent(in) :: el
    type(string_t), intent(in) :: filename
    integer, intent(in), optional :: unit
    select case (el%type)
    case (AN_HISTOGRAM); call histogram_write_gml_reader (el%h, filename, unit)
    case (AN_PLOT);      call plot_write_gml_reader (el%p, filename, unit)
    end select
end subroutine graph_element_write_gml_reader

```

The graph type

The actual graph type contains its own `graph_options`, which override the individual settings. The `drawing_options` are set in the graph elements. This distinction motivates the separation of the two types.

(Analysis: types) +=

```

    type :: graph_t
    private
    type(graph_element_t), dimension(:), allocatable :: el
    type(graph_options_t) :: graph_options
end type graph_t

```

Initializer/finalizer

The graph is created with a definite number of elements. The elements are filled one by one, optionally with modified drawing options.

(Analysis: procedures) +=

```

subroutine graph_init (g, id, n_elements, graph_options)
    type(graph_t), intent(out) :: g
    type(string_t), intent(in) :: id
    integer, intent(in) :: n_elements
    type(graph_options_t), intent(in), optional :: graph_options
    allocate (g%el (n_elements))
    if (present (graph_options)) then
        g%graph_options = graph_options
    else
        call g%graph_options%init ()
    end if
    call g%graph_options%set (id = id)
end subroutine graph_init

```

(Analysis: procedures) +=

```

subroutine graph_insert_histogram (g, i, h, drawing_options)
    type(graph_t), intent(inout), target :: g
    integer, intent(in) :: i
    type(histogram_t), intent(in) :: h
    type(drawing_options_t), intent(in), optional :: drawing_options
    type(graph_options_t), pointer :: gro
    type(drawing_options_t), pointer :: dro
    type(string_t) :: id
    g%el(i)%type = AN_HISTOGRAM

```

```

allocate (g%el(i)%h)
call histogram_init_histogram (g%el(i)%h, h, drawing_options)
gro => histogram_get_graph_options_ptr (g%el(i)%h)
dro => histogram_get_drawing_options_ptr (g%el(i)%h)
id = graph_options_get_id (gro)
call dro%set (dataset = "dat." // id)
end subroutine graph_insert_histogram

```

<Analysis: procedures>+≡

```

subroutine graph_insert_plot (g, i, p, drawing_options)
  type(graph_t), intent(inout) :: g
  integer, intent(in) :: i
  type(plot_t), intent(in) :: p
  type(drawing_options_t), intent(in), optional :: drawing_options
  type(graph_options_t), pointer :: gro
  type(drawing_options_t), pointer :: dro
  type(string_t) :: id
  g%el(i)%type = AN_PLOT
  allocate (g%el(i)%p)
  call plot_init_plot (g%el(i)%p, p, drawing_options)
  gro => plot_get_graph_options_ptr (g%el(i)%p)
  dro => plot_get_drawing_options_ptr (g%el(i)%p)
  id = graph_options_get_id (gro)
  call dro%set (dataset = "dat." // id)
end subroutine graph_insert_plot

```

Finalizer.

<Analysis: procedures>+≡

```

subroutine graph_final (g)
  type(graph_t), intent(inout) :: g
  integer :: i
  do i = 1, size (g%el)
    call graph_element_final (g%el(i))
  end do
  deallocate (g%el)
end subroutine graph_final

```

Access contents

The number of elements.

<Analysis: procedures>+≡

```

function graph_get_n_elements (graph) result (n)
  integer :: n
  type(graph_t), intent(in) :: graph
  n = size (graph%el)
end function graph_get_n_elements

```

Retrieve a pointer to the drawing options of an element, so they can be modified. (The `target` attribute is not actually needed because the components are pointers.)

<Analysis: procedures>+≡

```

function graph_get_drawing_options_ptr (g, i) result (ptr)
  type(drawing_options_t), pointer :: ptr
  type(graph_t), intent(in), target :: g
  integer, intent(in) :: i
  ptr => graph_element_get_drawing_options_ptr (g%el(i))
end function graph_get_drawing_options_ptr

```

Output

The default output format just writes histogram and plot data.

<Analysis: procedures>+≡

```

subroutine graph_write (graph, unit)
  type(graph_t), intent(in) :: graph
  integer, intent(in), optional :: unit
  integer :: i
  do i = 1, size (graph%el)
    call graph_element_write (graph%el(i), unit)
  end do
end subroutine graph_write

```

The GAMELAN driver is not a simple wrapper, but it writes the plot/histogram contents embedded the complete graph. First, data are read in, global background commands next, then individual elements, then global foreground commands.

<Analysis: procedures>+≡

```

subroutine graph_write_gml_driver (g, filename, unit)
  type(graph_t), intent(in) :: g
  type(string_t), intent(in) :: filename
  type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
  integer, intent(in), optional :: unit
  type(drawing_options_t), pointer :: dro
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call graph_options_write_tex_header (g%graph_options, unit)
  write (u, "(2x,A)") &
    char (graph_options_get_gml_setup (g%graph_options))
  write (u, "(2x,A)") &
    char (graph_options_get_gml_graphrange (g%graph_options))
  do i = 1, size (g%el)
    call graph_element_write_gml_reader (g%el(i), filename, unit)
    calc_cmd = drawing_options_get_calc_command &
      (graph_element_get_drawing_options_ptr (g%el(i)))
    if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
  end do
  bg_cmd = graph_options_get_gml_bg_command (g%graph_options)
  if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
  do i = 1, size (g%el)
    dro => graph_element_get_drawing_options_ptr (g%el(i))
    bg_cmd = drawing_options_get_gml_bg_command (dro)
    if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
    draw_cmd = drawing_options_get_draw_command (dro)
    if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
  end do
end subroutine graph_write_gml_driver

```

```

err_cmd = drawing_options_get_err_command (dro)
if (err_cmd /= "") write (u, "(2x,A)" char (err_cmd)
symb_cmd = drawing_options_get_symb_command (dro)
if (symb_cmd /= "") write (u, "(2x,A)" char (symb_cmd)
fg_cmd = drawing_options_get_gml_fg_command (dro)
if (fg_cmd /= "") write (u, "(2x,A)" char (fg_cmd)
end do
fg_cmd = graph_options_get_gml_fg_command (g%graph_options)
if (fg_cmd /= "") write (u, "(2x,A)" char (fg_cmd)
write (u, "(2x,A)" char (graph_options_get_gml_x_label (g%graph_options))
write (u, "(2x,A)" char (graph_options_get_gml_y_label (g%graph_options))
call graph_options_write_tex_footer (g%graph_options, unit)
end subroutine graph_write_gml_driver

```

Append header for generic data output in ifile format.

<Analysis: procedures>+≡

```

subroutine graph_get_header (graph, header, comment)
type(graph_t), intent(in) :: graph
type(ifile_t), intent(inout) :: header
type(string_t), intent(in), optional :: comment
type(string_t) :: c
if (present (comment)) then
c = comment
else
c = ""
end if
call ifile_append (header, c // "WHIZARD graph data")
call graph_options_get_header (graph%graph_options, header, comment)
call ifile_append (header, &
c // "number of graph elements: " &
// int2char (graph_get_n_elements (graph)))
end subroutine graph_get_header

```

13.5.9 Analysis objects

This data structure holds all observables, histograms and such that are currently active. We have one global store; individual items are identified by their ID strings.

(This should rather be coded by type extension.)

<Analysis: parameters>+≡

```

integer, parameter :: AN_UNDEFINED = 0
integer, parameter :: AN_OBSERVABLE = 1
integer, parameter :: AN_HISTOGRAM = 2
integer, parameter :: AN_PLOT = 3
integer, parameter :: AN_GRAPH = 4

```

<Analysis: public>+≡

```

public :: AN_UNDEFINED, AN_HISTOGRAM, AN_OBSERVABLE, AN_PLOT, AN_GRAPH

```

<Analysis: types>+≡

```

type :: analysis_object_t
private

```

```

    type(string_t) :: id
    integer :: type = AN_UNDEFINED
    type(observable_t), pointer :: obs => null ()
    type(histogram_t), pointer :: h => null ()
    type(plot_t), pointer :: p => null ()
    type(graph_t), pointer :: g => null ()
    type(analysis_object_t), pointer :: next => null ()
end type analysis_object_t

```

Initializer/finalizer

Allocate with the correct type but do not fill initial values.

(Analysis: procedures)+≡

```

subroutine analysis_object_init (obj, id, type)
    type(analysis_object_t), intent(out) :: obj
    type(string_t), intent(in) :: id
    integer, intent(in) :: type
    obj%id = id
    obj%type = type
    select case (obj%type)
    case (AN_OBSERVABLE); allocate (obj%obs)
    case (AN_HISTOGRAM); allocate (obj%h)
    case (AN_PLOT); allocate (obj%p)
    case (AN_GRAPH); allocate (obj%g)
    end select
end subroutine analysis_object_init

```

(Analysis: procedures)+≡

```

subroutine analysis_object_final (obj)
    type(analysis_object_t), intent(inout) :: obj
    select case (obj%type)
    case (AN_OBSERVABLE)
        deallocate (obj%obs)
    case (AN_HISTOGRAM)
        deallocate (obj%h)
    case (AN_PLOT)
        call plot_final (obj%p)
        deallocate (obj%p)
    case (AN_GRAPH)
        call graph_final (obj%g)
        deallocate (obj%g)
    end select
    obj%type = AN_UNDEFINED
end subroutine analysis_object_final

```

Clear the analysis object, i.e., reset it to its initial state. Not applicable to graphs, which are always combinations of other existing objects.

(Analysis: procedures)+≡

```

subroutine analysis_object_clear (obj)
    type(analysis_object_t), intent(inout) :: obj
    select case (obj%type)

```

```

case (AN_OBSERVABLE)
  call observable_clear (obj%obs)
case (AN_HISTOGRAM)
  call histogram_clear (obj%h)
case (AN_PLOT)
  call plot_clear (obj%p)
end select
end subroutine analysis_object_clear

```

Fill with data

Record data. The effect depends on the type of analysis object.

<Analysis: procedures>+≡

```

subroutine analysis_object_record_data (obj, &
  x, y, yerr, xerr, weight, excess, success)
  type(analysis_object_t), intent(inout) :: obj
  real(default), intent(in) :: x
  real(default), intent(in), optional :: y, yerr, xerr, weight, excess
  logical, intent(out), optional :: success
  select case (obj%type)
  case (AN_OBSERVABLE)
    if (present (weight)) then
      call observable_record_value_weighted (obj%obs, x, weight, success)
    else
      call observable_record_value_unweighted (obj%obs, x, success)
    end if
  case (AN_HISTOGRAM)
    if (present (weight)) then
      call histogram_record_value_weighted (obj%h, x, weight, success)
    else
      call histogram_record_value_unweighted (obj%h, x, excess, success)
    end if
  case (AN_PLOT)
    if (present (y)) then
      call plot_record_value (obj%p, x, y, yerr, xerr, success)
    else
      if (present (success)) success = .false.
    end if
  case default
    if (present (success)) success = .false.
  end select
end subroutine analysis_object_record_data

```

Explicitly set the pointer to the next object in the list.

<Analysis: procedures>+≡

```

subroutine analysis_object_set_next_ptr (obj, next)
  type(analysis_object_t), intent(inout) :: obj
  type(analysis_object_t), pointer :: next
  obj%next => next
end subroutine analysis_object_set_next_ptr

```

Access contents

Return a pointer to the next object in the list.

```
<Analysis: procedures>+≡
function analysis_object_get_next_ptr (obj) result (next)
    type(analysis_object_t), pointer :: next
    type(analysis_object_t), intent(in) :: obj
    next => obj%next
end function analysis_object_get_next_ptr
```

Return data as appropriate for the object type.

```
<Analysis: procedures>+≡
function analysis_object_get_n_elements (obj) result (n)
    integer :: n
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_HISTOGRAM)
        n = 1
    case (AN_PLOT)
        n = 1
    case (AN_GRAPH)
        n = graph_get_n_elements (obj%g)
    case default
        n = 0
    end select
end function analysis_object_get_n_elements

function analysis_object_get_n_entries (obj, within_bounds) result (n)
    integer :: n
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb
    select case (obj%type)
    case (AN_OBSERVABLE)
        n = observable_get_n_entries (obj%obs)
    case (AN_HISTOGRAM)
        wb = .false.; if (present (within_bounds)) wb = within_bounds
        if (wb) then
            n = histogram_get_n_entries_within_bounds (obj%h)
        else
            n = histogram_get_n_entries (obj%h)
        end if
    case (AN_PLOT)
        n = plot_get_n_entries (obj%p)
    case default
        n = 0
    end select
end function analysis_object_get_n_entries

function analysis_object_get_average (obj, within_bounds) result (avg)
    real(default) :: avg
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb
```



```

select case (obj%type)
case (AN_OBSERVABLE)
    avg = observable_get_average (obj%obs)
case (AN_HISTOGRAM)
    wb = .false.; if (present (within_bounds)) wb = within_bounds
    if (wb) then
        avg = histogram_get_average_within_bounds (obj%h)
    else
        avg = histogram_get_average (obj%h)
    end if
case default
    avg = 0
end select
end function analysis_object_get_average

function analysis_object_get_error (obj, within_bounds) result (err)
    real(default) :: err
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb
    select case (obj%type)
    case (AN_OBSERVABLE)
        err = observable_get_error (obj%obs)
    case (AN_HISTOGRAM)
        wb = .false.; if (present (within_bounds)) wb = within_bounds
        if (wb) then
            err = histogram_get_error_within_bounds (obj%h)
        else
            err = histogram_get_error (obj%h)
        end if
    case default
        err = 0
    end select
end function analysis_object_get_error

```

Return pointers to the actual contents:

(Analysis: procedures)+≡

```

function analysis_object_get_observable_ptr (obj) result (obs)
    type(observable_t), pointer :: obs
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_OBSERVABLE); obs => obj%obs
    case default;         obs => null ()
    end select
end function analysis_object_get_observable_ptr

function analysis_object_get_histogram_ptr (obj) result (h)
    type(histogram_t), pointer :: h
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_HISTOGRAM); h => obj%h
    case default;       h => null ()
    end select
end function analysis_object_get_histogram_ptr

```

```

function analysis_object_get_plot_ptr (obj) result (plot)
  type(plot_t), pointer :: plot
  type(analysis_object_t), intent(in) :: obj
  select case (obj%type)
    case (AN_PLOT); plot => obj%p
    case default; plot => null ()
  end select
end function analysis_object_get_plot_ptr

function analysis_object_get_graph_ptr (obj) result (g)
  type(graph_t), pointer :: g
  type(analysis_object_t), intent(in) :: obj
  select case (obj%type)
    case (AN_GRAPH); g => obj%g
    case default; g => null ()
  end select
end function analysis_object_get_graph_ptr

```

Return true if the object has a graphical representation:

<Analysis: procedures>+≡

```

function analysis_object_has_plot (obj) result (flag)
  logical :: flag
  type(analysis_object_t), intent(in) :: obj
  select case (obj%type)
    case (AN_HISTOGRAM); flag = .true.
    case (AN_PLOT); flag = .true.
    case (AN_GRAPH); flag = .true.
    case default; flag = .false.
  end select
end function analysis_object_has_plot

```

Output

<Analysis: procedures>+≡

```

subroutine analysis_object_write (obj, unit, verbose)
  type(analysis_object_t), intent(in) :: obj
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  logical :: verb
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  verb = .false.; if (present (verbose)) verb = verbose
  write (u, "(A)") repeat ("#", 79)
  select case (obj%type)
    case (AN_OBSERVABLE)
      write (u, "(A)", advance="no") "# Observable:"
    case (AN_HISTOGRAM)
      write (u, "(A)", advance="no") "# Histogram: "
    case (AN_PLOT)
      write (u, "(A)", advance="no") "# Plot: "
    case (AN_GRAPH)

```

```

        write (u, "(A)", advance="no")    "# Graph: "
    case default
        write (u, "(A)")    "# [undefined analysis object]"
        return
    end select
    write (u, "(1x,A)")    char (obj%id)
    select case (obj%type)
    case (AN_OBSERVABLE)
        call observable_write (obj%obs, unit)
    case (AN_HISTOGRAM)
        if (verb) then
            call obj%h%graph_options%write (unit)
            write (u, *)
            call obj%h%drawing_options%write (unit)
            write (u, *)
        end if
        call histogram_write (obj%h, unit)
    case (AN_PLOT)
        if (verb) then
            call obj%p%graph_options%write (unit)
            write (u, *)
            call obj%p%drawing_options%write (unit)
            write (u, *)
        end if
        call plot_write (obj%p, unit)
    case (AN_GRAPH)
        call graph_write (obj%g, unit)
    end select
end subroutine analysis_object_write

```

Write the object part of the L^AT_EX driver file.

```

<Analysis: procedures>+≡
subroutine analysis_object_write_driver (obj, filename, unit)
    type(analysis_object_t), intent(in) :: obj
    type(string_t), intent(in) :: filename
    integer, intent(in), optional :: unit
    select case (obj%type)
    case (AN_OBSERVABLE)
        call observable_write_driver (obj%obs, unit)
    case (AN_HISTOGRAM)
        call histogram_write_gml_driver (obj%h, filename, unit)
    case (AN_PLOT)
        call plot_write_gml_driver (obj%p, filename, unit)
    case (AN_GRAPH)
        call graph_write_gml_driver (obj%g, filename, unit)
    end select
end subroutine analysis_object_write_driver

```

Return a data header for external formats, in ifile form.

```

<Analysis: procedures>+≡
subroutine analysis_object_get_header (obj, header, comment)
    type(analysis_object_t), intent(in) :: obj
    type(ifile_t), intent(inout) :: header

```

```

type(string_t), intent(in), optional :: comment
select case (obj%type)
case (AN_HISTOGRAM)
    call histogram_get_header (obj%h, header, comment)
case (AN_PLOT)
    call plot_get_header (obj%p, header, comment)
end select
end subroutine analysis_object_get_header

```

13.5.10 Analysis object iterator

Analysis objects are containers which have iterable data structures: histograms/bins and plots/points. If they are to be treated on a common basis, it is useful to have an iterator which hides the implementation details.

The iterator is used only for elementary analysis objects that contain plot data: histograms or plots. It is invalid for meta-objects (graphs) and non-graphical objects (observables).

```

<Analysis: types>+≡
type :: analysis_iterator_t
private
integer :: type = AN_UNDEFINED
type(analysis_object_t), pointer :: object => null ()
integer :: index = 1
type(point_t), pointer :: point => null ()
end type

```

The initializer places the iterator at the beginning of the analysis object.

```

<Analysis: procedures>+≡
subroutine analysis_iterator_init (iterator, object)
type(analysis_iterator_t), intent(out) :: iterator
type(analysis_object_t), intent(in), target :: object
iterator%object => object
if (associated (iterator%object)) then
    iterator%type = iterator%object%type
    select case (iterator%type)
    case (AN_PLOT)
        iterator%point => iterator%object%p%first
    end select
end if
end subroutine analysis_iterator_init

```

The iterator is valid as long as it points to an existing entry. An iterator for a data object without array data (observable) is always invalid.

```

<Analysis: procedures>+≡
function analysis_iterator_is_valid (iterator) result (valid)
logical :: valid
type(analysis_iterator_t), intent(in) :: iterator
if (associated (iterator%object)) then
    select case (iterator%type)
    case (AN_HISTOGRAM)
        valid = iterator%index <= histogram_get_n_bins (iterator%object%h)
    end select
end if
end function analysis_iterator_is_valid

```

```

        case (AN_PLOT)
            valid = associated (iterator%point)
        case default
            valid = .false.
        end select
    else
        valid = .false.
    end if
end function analysis_iterator_is_valid

```

Advance the iterator.

```

<Analysis: procedures>+≡
subroutine analysis_iterator_advance (iterator)
    type(analysis_iterator_t), intent(inout) :: iterator
    if (associated (iterator%object)) then
        select case (iterator%type)
            case (AN_PLOT)
                iterator%point => iterator%point%next
            end select
        iterator%index = iterator%index + 1
    end if
end subroutine analysis_iterator_advance

```

Retrieve the object type:

```

<Analysis: procedures>+≡
function analysis_iterator_get_type (iterator) result (type)
    integer :: type
    type(analysis_iterator_t), intent(in) :: iterator
    type = iterator%type
end function analysis_iterator_get_type

```

Use the iterator to retrieve data. We implement a common routine which takes the data descriptors as optional arguments. Data which do not occur in the selected type trigger to an error condition.

The iterator must point to a valid entry.

```

<Analysis: procedures>+≡
subroutine analysis_iterator_get_data (iterator, &
    x, y, yerr, xerr, width, excess, index, n_total)
    type(analysis_iterator_t), intent(in) :: iterator
    real(default), intent(out), optional :: x, y, yerr, xerr, width, excess
    integer, intent(out), optional :: index, n_total
    select case (iterator%type)
        case (AN_HISTOGRAM)
            if (present (x)) &
                x = bin_get_midpoint (iterator%object%h%bin(iterator%index))
            if (present (y)) &
                y = bin_get_sum (iterator%object%h%bin(iterator%index))
            if (present (yerr)) &
                yerr = bin_get_error (iterator%object%h%bin(iterator%index))
            if (present (xerr)) &
                call invalid ("histogram", "xerr")
            if (present (width)) &

```

```

        width = bin_get_width (iterator%object%h%bin(iterator%index))
    if (present (excess)) &
        excess = bin_get_excess (iterator%object%h%bin(iterator%index))
    if (present (index)) &
        index = iterator%index
    if (present (n_total)) &
        n_total = histogram_get_n_bins (iterator%object%h)
case (AN_PLOT)
    if (present (x)) &
        x = point_get_x (iterator%point)
    if (present (y)) &
        y = point_get_y (iterator%point)
    if (present (yerr)) &
        yerr = point_get_yerr (iterator%point)
    if (present (xerr)) &
        xerr = point_get_xerr (iterator%point)
    if (present (width)) &
        call invalid ("plot", "width")
    if (present (excess)) &
        call invalid ("plot", "excess")
    if (present (index)) &
        index = iterator%index
    if (present (n_total)) &
        n_total = plot_get_n_entries (iterator%object%p)
case default
    call msg_bug ("analysis_iterator_get_data: called " &
        // "for unsupported analysis object type")
end select
contains
subroutine invalid (typestr, objstr)
    character(*), intent(in) :: typestr, objstr
    call msg_bug ("analysis_iterator_get_data: attempt to get '" &
        // objstr // "' for type '" // typestr // "'")
end subroutine invalid
end subroutine analysis_iterator_get_data

```

13.5.11 Analysis store

This data structure holds all observables, histograms and such that are currently active. We have one global store; individual items are identified by their ID strings and types.

```

<Analysis: variables>≡
    type(analysis_store_t), save :: analysis_store

<Analysis: types>+≡
    type :: analysis_store_t
    private
    type(analysis_object_t), pointer :: first => null ()
    type(analysis_object_t), pointer :: last => null ()
end type analysis_store_t

```

Delete the analysis store

```
<Analysis: public>+≡
    public :: analysis_final

<Analysis: sub interfaces>+≡
    module subroutine analysis_final ()
    end subroutine analysis_final

<Analysis: procedures>+≡
    module subroutine analysis_final ()
        type(analysis_object_t), pointer :: current
        do while (associated (analysis_store%first))
            current => analysis_store%first
            analysis_store%first => current%next
            call analysis_object_final (current)
        end do
        analysis_store%last => null ()
    end subroutine analysis_final
```

Append a new analysis object

```
<Analysis: procedures>+≡
    subroutine analysis_store_append_object (id, type)
        type(string_t), intent(in) :: id
        integer, intent(in) :: type
        type(analysis_object_t), pointer :: obj
        allocate (obj)
        call analysis_object_init (obj, id, type)
        if (associated (analysis_store%last)) then
            analysis_store%last%next => obj
        else
            analysis_store%first => obj
        end if
        analysis_store%last => obj
    end subroutine analysis_store_append_object
```

Return a pointer to the analysis object with given ID.

```
<Analysis: procedures>+≡
    function analysis_store_get_object_ptr (id) result (obj)
        type(string_t), intent(in) :: id
        type(analysis_object_t), pointer :: obj
        obj => analysis_store%first
        do while (associated (obj))
            if (obj%id == id) return
            obj => obj%next
        end do
    end function analysis_store_get_object_ptr
```

Initialize an analysis object: either reset it if present, or append a new entry.

```
<Analysis: procedures>+≡
    subroutine analysis_store_init_object (id, type, obj)
        type(string_t), intent(in) :: id
        integer, intent(in) :: type
        type(analysis_object_t), pointer :: obj, next
```

```

obj => analysis_store_get_object_ptr (id)
if (associated (obj)) then
    next => analysis_object_get_next_ptr (obj)
    call analysis_object_final (obj)
    call analysis_object_init (obj, id, type)
    call analysis_object_set_next_ptr (obj, next)
else
    call analysis_store_append_object (id, type)
    obj => analysis_store%last
end if
end subroutine analysis_store_init_object

```

Get the type of a analysis object

```

<Analysis: public>+≡
public :: analysis_store_get_object_type

<Analysis: sub interfaces>+≡
module function analysis_store_get_object_type (id) result (type)
    type(string_t), intent(in) :: id
    integer :: type
end function analysis_store_get_object_type

<Analysis: procedures>+≡
module function analysis_store_get_object_type (id) result (type)
    type(string_t), intent(in) :: id
    integer :: type
    type(analysis_object_t), pointer :: object
    object => analysis_store_get_object_ptr (id)
    if (associated (object)) then
        type = object%type
    else
        type = AN_UNDEFINED
    end if
end function analysis_store_get_object_type

```

Return the number of objects in the store.

```

<Analysis: procedures>+≡
function analysis_store_get_n_objects () result (n)
    integer :: n
    type(analysis_object_t), pointer :: current
    n = 0
    current => analysis_store%first
    do while (associated (current))
        n = n + 1
        current => current%next
    end do
end function analysis_store_get_n_objects

```

Allocate an array and fill it with all existing IDs.

```

<Analysis: public>+≡
public :: analysis_store_get_ids

```



```

<Analysis: sub interfaces>+≡
    module subroutine analysis_store_get_ids (id)
        type(string_t), dimension(:), allocatable, intent(out) :: id
    end subroutine analysis_store_get_ids

<Analysis: procedures>+≡
    module subroutine analysis_store_get_ids (id)
        type(string_t), dimension(:), allocatable, intent(out) :: id
        type(analysis_object_t), pointer :: current
        integer :: i
        allocate (id (analysis_store_get_n_objects()))
        i = 0
        current => analysis_store%first
        do while (associated (current))
            i = i + 1
            id(i) = current%id
            current => current%next
        end do
    end subroutine analysis_store_get_ids

```

13.5.12 L^AT_EX driver file

Write a driver file for all objects in the store.

```

<Analysis: procedures>+≡
    subroutine analysis_store_write_driver_all (filename_data, unit)
        type(string_t), intent(in) :: filename_data
        integer, intent(in), optional :: unit
        type(analysis_object_t), pointer :: obj
        call analysis_store_write_driver_header (unit)
        obj => analysis_store%first
        do while (associated (obj))
            call analysis_object_write_driver (obj, filename_data, unit)
            obj => obj%next
        end do
        call analysis_store_write_driver_footer (unit)
    end subroutine analysis_store_write_driver_all

```

Write a driver file for an array of objects.

```

<Analysis: procedures>+≡
    subroutine analysis_store_write_driver_obj (filename_data, id, unit)
        type(string_t), intent(in) :: filename_data
        type(string_t), dimension(:), intent(in) :: id
        integer, intent(in), optional :: unit
        type(analysis_object_t), pointer :: obj
        integer :: i
        call analysis_store_write_driver_header (unit)
        do i = 1, size (id)
            obj => analysis_store_get_object_ptr (id(i))
            if (associated (obj)) &
                call analysis_object_write_driver (obj, filename_data, unit)
        end do
        call analysis_store_write_driver_footer (unit)
    end subroutine analysis_store_write_driver_obj

```

```
end subroutine analysis_store_write_driver_obj
```

The beginning of the driver file.

<Analysis: procedures>+≡

```
subroutine analysis_store_write_driver_header (unit)
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, '(A)') "\documentclass[12pt]{article}"
  write (u, *)
  write (u, '(A)') "\usepackage{gamelan}"
  write (u, '(A)') "\usepackage{amsmath}"
  write (u, '(A)') "\usepackage{ifpdf}"
  write (u, '(A)') "\ifpdf"
  write (u, '(A)') "  \DeclareGraphicsRule{*}{mps}{*}{"
  write (u, '(A)') "\else"
  write (u, '(A)') "  \DeclareGraphicsRule{*}{eps}{*}{"
  write (u, '(A)') "\fi"
  write (u, *)
  write (u, '(A)') "\begin{document}"
  write (u, '(A)') "\begin{gmlfile}"
  write (u, *)
  write (u, '(A)') "\begin{gmlcode}"
  write (u, '(A)') "  color col.default, col.excess;"
  write (u, '(A)') "  col.default = 0.9white;"
  write (u, '(A)') "  col.excess = red;"
  write (u, '(A)') "  boolean show_excess;"
  !!! Future excess options for plots
  ! if (mcs(1)%plot_excess .and. mcs(1)%unweighted) then
  !   write (u, '(A)') "  show_excess = true;"
  ! else
  write (u, '(A)') "  show_excess = false;"
  ! end if
  write (u, '(A)') "\end{gmlcode}"
  write (u, *)
end subroutine analysis_store_write_driver_header
```

The end of the driver file.

<Analysis: procedures>+≡

```
subroutine analysis_store_write_driver_footer (unit)
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write(u, *)
  write(u, '(A)') "\end{gmlfile}"
  write(u, '(A)') "\end{document}"
end subroutine analysis_store_write_driver_footer
```

13.5.13 API

Creating new objects

The specific versions below:

```
<Analysis: public>+≡
    public :: analysis_init_observable

<Analysis: sub interfaces>+≡
    module subroutine analysis_init_observable (id, obs_label, obs_unit, graph_options)
        type(string_t), intent(in) :: id
        type(string_t), intent(in), optional :: obs_label, obs_unit
        type(graph_options_t), intent(in), optional :: graph_options
    end subroutine analysis_init_observable

<Analysis: procedures>+≡
    module subroutine analysis_init_observable (id, obs_label, obs_unit, graph_options)
        type(string_t), intent(in) :: id
        type(string_t), intent(in), optional :: obs_label, obs_unit
        type(graph_options_t), intent(in), optional :: graph_options
        type(analysis_object_t), pointer :: obj
        type(observable_t), pointer :: obs
        call analysis_store_init_object (id, AN_OBSERVABLE, obj)
        obs => analysis_object_get_observable_ptr (obj)
        call observable_init (obs, obs_label, obs_unit, graph_options)
    end subroutine analysis_init_observable

<Analysis: public>+≡
    public :: analysis_init_histogram

<Analysis: interfaces>+≡
    interface analysis_init_histogram
        module procedure analysis_init_histogram_n_bins
        module procedure analysis_init_histogram_bin_width
    end interface

<Analysis: sub interfaces>+≡
    module subroutine analysis_init_histogram_n_bins &
        (id, lower_bound, upper_bound, n_bins, normalize_bins, &
         obs_label, obs_unit, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: lower_bound, upper_bound
        integer, intent(in) :: n_bins
        logical, intent(in) :: normalize_bins
        type(string_t), intent(in), optional :: obs_label, obs_unit
        type(graph_options_t), intent(in), optional :: graph_options
        type(drawing_options_t), intent(in), optional :: drawing_options
    end subroutine analysis_init_histogram_n_bins
    module subroutine analysis_init_histogram_bin_width &
        (id, lower_bound, upper_bound, bin_width, normalize_bins, &
         obs_label, obs_unit, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: lower_bound, upper_bound, bin_width
        logical, intent(in) :: normalize_bins
        type(string_t), intent(in), optional :: obs_label, obs_unit
```

```

        type(graph_options_t), intent(in), optional :: graph_options
        type(drawing_options_t), intent(in), optional :: drawing_options
    end subroutine analysis_init_histogram_bin_width

<Analysis: procedures>+≡
    module subroutine analysis_init_histogram_n_bins &
        (id, lower_bound, upper_bound, n_bins, normalize_bins, &
         obs_label, obs_unit, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: lower_bound, upper_bound
        integer, intent(in) :: n_bins
        logical, intent(in) :: normalize_bins
        type(string_t), intent(in), optional :: obs_label, obs_unit
        type(graph_options_t), intent(in), optional :: graph_options
        type(drawing_options_t), intent(in), optional :: drawing_options
        type(analysis_object_t), pointer :: obj
        type(histogram_t), pointer :: h
        call analysis_store_init_object (id, AN_HISTOGRAM, obj)
        h => analysis_object_get_histogram_ptr (obj)
        call histogram_init (h, id, &
            lower_bound, upper_bound, n_bins, normalize_bins, &
            obs_label, obs_unit, graph_options, drawing_options)
    end subroutine analysis_init_histogram_n_bins

    module subroutine analysis_init_histogram_bin_width &
        (id, lower_bound, upper_bound, bin_width, normalize_bins, &
         obs_label, obs_unit, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: lower_bound, upper_bound, bin_width
        logical, intent(in) :: normalize_bins
        type(string_t), intent(in), optional :: obs_label, obs_unit
        type(graph_options_t), intent(in), optional :: graph_options
        type(drawing_options_t), intent(in), optional :: drawing_options
        type(analysis_object_t), pointer :: obj
        type(histogram_t), pointer :: h
        call analysis_store_init_object (id, AN_HISTOGRAM, obj)
        h => analysis_object_get_histogram_ptr (obj)
        call histogram_init (h, id, &
            lower_bound, upper_bound, bin_width, normalize_bins, &
            obs_label, obs_unit, graph_options, drawing_options)
    end subroutine analysis_init_histogram_bin_width

<Analysis: public>+≡
    public :: analysis_init_plot

<Analysis: sub interfaces>+≡
    module subroutine analysis_init_plot (id, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        type(graph_options_t), intent(in), optional :: graph_options
        type(drawing_options_t), intent(in), optional :: drawing_options
    end subroutine analysis_init_plot

<Analysis: procedures>+≡
    module subroutine analysis_init_plot (id, graph_options, drawing_options)
        type(string_t), intent(in) :: id
        type(graph_options_t), intent(in), optional :: graph_options

```

```

    type(drawing_options_t), intent(in), optional :: drawing_options
    type(analysis_object_t), pointer :: obj
    type(plot_t), pointer :: plot
    call analysis_store_init_object (id, AN_PLOT, obj)
    plot => analysis_object_get_plot_ptr (obj)
    call plot_init (plot, id, graph_options, drawing_options)
end subroutine analysis_init_plot

```

```

<Analysis: public>+≡
    public :: analysis_init_graph

```

```

<Analysis: sub interfaces>+≡
    module subroutine analysis_init_graph (id, n_elements, graph_options)
        type(string_t), intent(in) :: id
        integer, intent(in) :: n_elements
        type(graph_options_t), intent(in), optional :: graph_options
    end subroutine analysis_init_graph

```

```

<Analysis: procedures>+≡
    module subroutine analysis_init_graph (id, n_elements, graph_options)
        type(string_t), intent(in) :: id
        integer, intent(in) :: n_elements
        type(graph_options_t), intent(in), optional :: graph_options
        type(analysis_object_t), pointer :: obj
        type(graph_t), pointer :: graph
        call analysis_store_init_object (id, AN_GRAPH, obj)
        graph => analysis_object_get_graph_ptr (obj)
        call graph_init (graph, id, n_elements, graph_options)
    end subroutine analysis_init_graph

```

Recording data

This procedure resets an object or the whole store to its initial state.

```

<Analysis: public>+≡
    public :: analysis_clear

```

```

<Analysis: interfaces>+≡
    interface analysis_clear
        module procedure analysis_store_clear_obj
        module procedure analysis_store_clear_all
    end interface

```

```

<Analysis: sub interfaces>+≡
    module subroutine analysis_store_clear_obj (id)
        type(string_t), intent(in) :: id
    end subroutine analysis_store_clear_obj
    module subroutine analysis_store_clear_all ()
    end subroutine analysis_store_clear_all

```

```

<Analysis: procedures>+≡
    module subroutine analysis_store_clear_obj (id)
        type(string_t), intent(in) :: id
        type(analysis_object_t), pointer :: obj
        obj => analysis_store_get_object_ptr (id)
    end subroutine analysis_store_clear_obj

```

```

        if (associated (obj)) then
            call analysis_object_clear (obj)
        end if
    end subroutine analysis_store_clear_obj

    module subroutine analysis_store_clear_all ()
        type(analysis_object_t), pointer :: obj
        obj => analysis_store%first
        do while (associated (obj))
            call analysis_object_clear (obj)
            obj => obj%next
        end do
    end subroutine analysis_store_clear_all

```

There is one generic recording function whose behavior depends on the type of analysis object.

```

<Analysis: public>+≡
    public :: analysis_record_data

<Analysis: sub interfaces>+≡
    module subroutine analysis_record_data (id, x, y, yerr, xerr, &
        weight, excess, success, exist)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: x
        real(default), intent(in), optional :: y, yerr, xerr, weight, excess
        logical, intent(out), optional :: success, exist
    end subroutine analysis_record_data

<Analysis: procedures>+≡
    module subroutine analysis_record_data (id, x, y, yerr, xerr, &
        weight, excess, success, exist)
        type(string_t), intent(in) :: id
        real(default), intent(in) :: x
        real(default), intent(in), optional :: y, yerr, xerr, weight, excess
        logical, intent(out), optional :: success, exist
        type(analysis_object_t), pointer :: obj
        obj => analysis_store_get_object_ptr (id)
        if (associated (obj)) then
            call analysis_object_record_data (obj, x, y, yerr, xerr, &
                weight, excess, success)
            if (present (exist)) exist = .true.
        else
            if (present (success)) success = .false.
            if (present (exist)) exist = .false.
        end if
    end subroutine analysis_record_data

```

Build a graph

This routine sets up the array of graph elements by copying the graph elements given as input. The object must exist and already be initialized as a graph.

```

<Analysis: public>+≡
    public :: analysis_fill_graph

```

```

<Analysis: sub interfaces>+≡
    module subroutine analysis_fill_graph (id, i, id_in, drawing_options)
        type(string_t), intent(in) :: id
        integer, intent(in) :: i
        type(string_t), intent(in) :: id_in
        type(drawing_options_t), intent(in), optional :: drawing_options
    end subroutine analysis_fill_graph

<Analysis: procedures>+≡
    module subroutine analysis_fill_graph (id, i, id_in, drawing_options)
        type(string_t), intent(in) :: id
        integer, intent(in) :: i
        type(string_t), intent(in) :: id_in
        type(drawing_options_t), intent(in), optional :: drawing_options
        type(analysis_object_t), pointer :: obj
        type(graph_t), pointer :: g
        type(histogram_t), pointer :: h
        type(plot_t), pointer :: p
        obj => analysis_store_get_object_ptr (id)
        g => analysis_object_get_graph_ptr (obj)
        obj => analysis_store_get_object_ptr (id_in)
        if (associated (obj)) then
            select case (obj%type)
            case (AN_HISTOGRAM)
                h => analysis_object_get_histogram_ptr (obj)
                call graph_insert_histogram (g, i, h, drawing_options)
            case (AN_PLOT)
                p => analysis_object_get_plot_ptr (obj)
                call graph_insert_plot (g, i, p, drawing_options)
            case default
                call msg_error ("Graph '" // char (id) // "': Element '" &
                    // char (id_in) // "' is neither histogram nor plot.")
            end select
        else
            call msg_error ("Graph '" // char (id) // "': Element '" &
                // char (id_in) // "' is undefined.")
        end if
    end subroutine analysis_fill_graph

```

Retrieve generic results

Check if a named object exists.

```

<Analysis: public>+≡
    public :: analysis_exists

<Analysis: sub interfaces>+≡
    module function analysis_exists (id) result (flag)
        type(string_t), intent(in) :: id
        logical :: flag
    end function analysis_exists

<Analysis: procedures>+≡
    module function analysis_exists (id) result (flag)
        type(string_t), intent(in) :: id

```

```

logical :: flag
type(analysis_object_t), pointer :: obj
flag = .true.
obj => analysis_store%first
do while (associated (obj))
    if (obj%id == id) return
    obj => obj%next
end do
flag = .false.
end function analysis_exists

```

The following functions should work for all kinds of analysis object:

<Analysis: public>+≡

```

public :: analysis_get_n_elements
public :: analysis_get_n_entries
public :: analysis_get_average
public :: analysis_get_error

```

<Analysis: sub interfaces>+≡

```

module function analysis_get_n_elements (id) result (n)
    integer :: n
    type(string_t), intent(in) :: id
end function analysis_get_n_elements
module function analysis_get_n_entries (id, within_bounds) result (n)
    integer :: n
    type(string_t), intent(in) :: id
    logical, intent(in), optional :: within_bounds
end function analysis_get_n_entries
module function analysis_get_average (id, within_bounds) result (avg)
    real(default) :: avg
    type(string_t), intent(in) :: id
    logical, intent(in), optional :: within_bounds
end function analysis_get_average
module function analysis_get_error (id, within_bounds) result (err)
    real(default) :: err
    type(string_t), intent(in) :: id
    logical, intent(in), optional :: within_bounds
end function analysis_get_error

```

<Analysis: procedures>+≡

```

module function analysis_get_n_elements (id) result (n)
    integer :: n
    type(string_t), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        n = analysis_object_get_n_elements (obj)
    else
        n = 0
    end if
end function analysis_get_n_elements

module function analysis_get_n_entries (id, within_bounds) result (n)
    integer :: n

```



```

    type(string_t), intent(in) :: id
    logical, intent(in), optional :: within_bounds
    type(analysis_object_t), pointer :: obj
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        n = analysis_object_get_n_entries (obj, within_bounds)
    else
        n = 0
    end if
end function analysis_get_n_entries

module function analysis_get_average (id, within_bounds) result (avg)
    real(default) :: avg
    type(string_t), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    logical, intent(in), optional :: within_bounds
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        avg = analysis_object_get_average (obj, within_bounds)
    else
        avg = 0
    end if
end function analysis_get_average

module function analysis_get_error (id, within_bounds) result (err)
    real(default) :: err
    type(string_t), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    logical, intent(in), optional :: within_bounds
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        err = analysis_object_get_error (obj, within_bounds)
    else
        err = 0
    end if
end function analysis_get_error

```

Return true if any analysis object is graphical

<Analysis: public>+≡

```
public :: analysis_has_plots
```

<Analysis: interfaces>+≡

```
interface analysis_has_plots
    module procedure analysis_has_plots_any
    module procedure analysis_has_plots_obj
end interface

```

<Analysis: sub interfaces>+≡

```

module function analysis_has_plots_any () result (flag)
    logical :: flag
end function analysis_has_plots_any
module function analysis_has_plots_obj (id) result (flag)
    logical :: flag
    type(string_t), dimension(:), intent(in) :: id

```

```

        end function analysis_has_plots_obj
<Analysis: procedures>+≡
module function analysis_has_plots_any () result (flag)
    logical :: flag
    type(analysis_object_t), pointer :: obj
    flag = .false.
    obj => analysis_store%first
    do while (associated (obj))
        flag = analysis_object_has_plot (obj)
        if (flag) return
    end do
end function analysis_has_plots_any

module function analysis_has_plots_obj (id) result (flag)
    logical :: flag
    type(string_t), dimension(:), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    integer :: i
    flag = .false.
    do i = 1, size (id)
        obj => analysis_store_get_object_ptr (id(i))
        if (associated (obj)) then
            flag = analysis_object_has_plot (obj)
            if (flag) return
        end if
    end do
end function analysis_has_plots_obj

```

Iterators

Initialize an iterator for the given object. If the object does not exist or has wrong type, the iterator will be invalid.

```

<Analysis: procedures>+≡
subroutine analysis_init_iterator (id, iterator)
    type(string_t), intent(in) :: id
    type(analysis_iterator_t), intent(out) :: iterator
    type(analysis_object_t), pointer :: obj
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) call analysis_iterator_init (iterator, obj)
end subroutine analysis_init_iterator

```

Output

```

<Analysis: public>+≡
public :: analysis_write
<Analysis: interfaces>+≡
interface analysis_write
    module procedure analysis_write_object
    module procedure analysis_write_all
end interface

```

<Analysis: sub interfaces>+≡

```

module subroutine analysis_write_object (id, unit, verbose)
  type(string_t), intent(in) :: id
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
end subroutine analysis_write_object
module subroutine analysis_write_all (unit, verbose)
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
end subroutine analysis_write_all

```

<Analysis: procedures>+≡

```

module subroutine analysis_write_object (id, unit, verbose)
  type(string_t), intent(in) :: id
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  type(analysis_object_t), pointer :: obj
  obj => analysis_store_get_object_ptr (id)
  if (associated (obj)) then
    call analysis_object_write (obj, unit, verbose)
  else
    call msg_error ("Analysis object '" // char (id) // "' not found")
  end if
end subroutine analysis_write_object

module subroutine analysis_write_all (unit, verbose)
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  type(analysis_object_t), pointer :: obj
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  obj => analysis_store%first
  do while (associated (obj))
    call analysis_object_write (obj, unit, verbose)
    obj => obj%next
  end do
end subroutine analysis_write_all

```

<Analysis: public>+≡

```

public :: analysis_write_driver

```

<Analysis: sub interfaces>+≡

```

module subroutine analysis_write_driver (filename_data, id, unit)
  type(string_t), intent(in) :: filename_data
  type(string_t), dimension(:), intent(in), optional :: id
  integer, intent(in), optional :: unit
end subroutine analysis_write_driver

```

<Analysis: procedures>+≡

```

module subroutine analysis_write_driver (filename_data, id, unit)
  type(string_t), intent(in) :: filename_data
  type(string_t), dimension(:), intent(in), optional :: id
  integer, intent(in), optional :: unit
  if (present (id)) then
    call analysis_store_write_driver_obj (filename_data, id, unit)
  else

```

```

        call analysis_store_write_driver_all (filename_data, unit)
    end if
end subroutine analysis_write_driver

```

<Analysis: public>+≡

```

public :: analysis_compile_tex

```

<Analysis: sub interfaces>+≡

```

module subroutine analysis_compile_tex (file, has_gmlcode, os_data)
    type(string_t), intent(in) :: file
    logical, intent(in) :: has_gmlcode
    type(os_data_t), intent(in) :: os_data
end subroutine analysis_compile_tex

```

<Analysis: procedures>+≡

```

module subroutine analysis_compile_tex (file, has_gmlcode, os_data)
    type(string_t), intent(in) :: file
    logical, intent(in) :: has_gmlcode
    type(os_data_t), intent(in) :: os_data
    integer :: status
    if (os_data%event_analysis_ps) then
        call os_system_call ("make compile " // os_data%makeflags // " -f " // &
            char (file) // "_ana.makefile", status)
        if (status /= 0) then
            call msg_error ("Unable to compile analysis output file")
        end if
    else
        call msg_warning ("Skipping results display because " &
            // "latex/mpost/dvips is not available")
    end if
end subroutine analysis_compile_tex

```

Write header for generic data output to an ifile.

<Analysis: procedures>+≡

```

subroutine analysis_get_header (id, header, comment)
    type(string_t), intent(in) :: id
    type(ifile_t), intent(inout) :: header
    type(string_t), intent(in), optional :: comment
    type(analysis_object_t), pointer :: object
    object => analysis_store_get_object_ptr (id)
    if (associated (object)) then
        call analysis_object_get_header (object, header, comment)
    end if
end subroutine analysis_get_header

```

Write a makefile in order to do the compile steps.

<Analysis: public>+≡

```

public :: analysis_write_makefile

```

<Analysis: sub interfaces>+≡

```

module subroutine analysis_write_makefile (filename, unit, has_gmlcode, os_data)
    type(string_t), intent(in) :: filename
    integer, intent(in) :: unit
    logical, intent(in) :: has_gmlcode

```

```

        type(os_data_t), intent(in) :: os_data
    end subroutine analysis_write_makefile

<Analysis: procedures>+≡
    module subroutine analysis_write_makefile (filename, unit, has_gmlcode, os_data)
        type(string_t), intent(in) :: filename
        integer, intent(in) :: unit
        logical, intent(in) :: has_gmlcode
        type(os_data_t), intent(in) :: os_data
        write (unit, "(3A)")  "# WHIZARD: Makefile for analysis '", &
            char (filename), "'"
        write (unit, "(A)")  "# Automatically generated file, do not edit"
        write (unit, "(A)")  ""
        write (unit, "(A)")  "# LaTeX setup"
        write (unit, "(A)")  "LATEX = " // char (os_data%latex)
        write (unit, "(A)")  "MPOST = " // char (os_data%mpost)
        write (unit, "(A)")  "GML = " // char (os_data%gml)
        write (unit, "(A)")  "DVIPS = " // char (os_data%dvips)
        write (unit, "(A)")  "PS2PDF = " // char (os_data%ps2pdf)
        write (unit, "(A)")  'TEX_FLAGS = "$TEXINPUTS:' // &
            char(os_data%whizard_texpath) // ', "'
        write (unit, "(A)")  'MP_FLAGS = "$MPINPUTS:' // &
            char(os_data%whizard_texpath) // ', "'
        write (unit, "(A)")  ""
        write (unit, "(5A)")  "TEX_SOURCES = ", char (filename), ".tex"
        if (os_data%event_analysis_pdf) then
            write (unit, "(5A)")  "TEX_OBJECTS = ", char (filename), ".pdf"
        else
            write (unit, "(5A)")  "TEX_OBJECTS = ", char (filename), ".ps"
        end if
        if (os_data%event_analysis_ps) then
            if (os_data%event_analysis_pdf) then
                write (unit, "(5A)")  char (filename), ".pdf: ", &
                    char (filename), ".tex"
            else
                write (unit, "(5A)")  char (filename), ".ps: ", &
                    char (filename), ".tex"
            end if
        write (unit, "(5A)")  TAB, "-TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
            char (filename) // ".tex"
        if (has_gmlcode) then
            write (unit, "(5A)")  TAB, "$(GML) " // char (filename)
            write (unit, "(5A)")  TAB, "TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
                char (filename) // ".tex"
        end if
        write (unit, "(5A)")  TAB, "$(DVIPS) -o " // char (filename) // ".ps " // &
            char (filename) // ".dvi"
        if (os_data%event_analysis_pdf) then
            write (unit, "(5A)")  TAB, "$(PS2PDF) " // char (filename) // ".ps"
        end if
    end if
    write (unit, "(A)")
    write (unit, "(A)")  "compile: $(TEX_OBJECTS)"
    write (unit, "(A)")  ".PHONY: compile"
    write (unit, "(A)")

```

```

write (unit, "(5A)") "CLEAN_OBJECTS = ", char (filename), ".aux"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".log"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".dvi"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".out"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9][0-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9][0-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".ltp"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".mp"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".mpx"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".dvi"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".ps"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".pdf"
write (unit, "(A)")
write (unit, "(A)") "# Generic cleanup targets"
write (unit, "(A)") "clean-objects:"
write (unit, "(A)") TAB // "rm -f $(CLEAN_OBJECTS)"
write (unit, "(A)") ""
write (unit, "(A)") "clean: clean-objects"
write (unit, "(A)") ".PHONY: clean"
end subroutine analysis_write_makefile

```

13.5.14 Unit tests

Test module, followed by the corresponding implementation module.

<analysis_ut.f90>≡

<File header>

```

module analysis_ut
  use unit_tests
  use analysis_uti

```

<Standard module head>

<Analysis: public test>

contains

<Analysis: test driver>

```

end module analysis_ut

```

<analysis_uti.f90>≡

<File header>

```

module analysis_uti

```

<Use kinds>

<Use strings>

```

  use format_defs, only: FMT_19

```

```

    use analysis

    <Standard module head>

    <Analysis: test declarations>

contains

    <Analysis: tests>

end module analysis_util

API: driver for the unit tests below.
<Analysis: public test>≡
    public :: analysis_test

<Analysis: test driver>≡
    subroutine analysis_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Analysis: execute tests>
    end subroutine analysis_test

<Analysis: execute tests>≡
    call test (analysis_1, "analysis_1", &
        "check elementary analysis building blocks", &
        u, results)

<Analysis: test declarations>≡
    public :: analysis_1

<Analysis: tests>≡
    subroutine analysis_1 (u)
        integer, intent(in) :: u
        type(string_t) :: id1, id2, id3, id4
        integer :: i
        id1 = "foo"
        id2 = "bar"
        id3 = "hist"
        id4 = "plot"

        write (u, "(A)")  "* Test output: Analysis"
        write (u, "(A)")  "* Purpose: test the analysis routines"
        write (u, "(A)")

        call analysis_init_observable (id1)
        call analysis_init_observable (id2)
        call analysis_init_histogram &
            (id3, 0.5_default, 5.5_default, 1._default, normalize_bins=.false.)
        call analysis_init_plot (id4)
        do i = 1, 3
            write (u, "(A,1x," // FMT_19 // ")") "data = ", real(i,default)
            call analysis_record_data (id1, real(i,default))
            call analysis_record_data (id2, real(i,default), &
                weight=real(i,default))

```

```

        call analysis_record_data (id3, real(i,default))
        call analysis_record_data (id4, real(i,default), real(i,default)**2)
    end do
write (u, "(A,10(1x,I5))") "n_entries = ", &
    analysis_get_n_entries (id1), &
    analysis_get_n_entries (id2), &
    analysis_get_n_entries (id3), &
    analysis_get_n_entries (id3, within_bounds = .true.), &
    analysis_get_n_entries (id4), &
    analysis_get_n_entries (id4, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "average = ", &
    analysis_get_average (id1), &
    analysis_get_average (id2), &
    analysis_get_average (id3), &
    analysis_get_average (id3, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "error = ", &
    analysis_get_error (id1), &
    analysis_get_error (id2), &
    analysis_get_error (id3), &
    analysis_get_error (id3, within_bounds = .true.)

write (u, "(A)")
write (u, "(A)") "* Clear analysis #2"
write (u, "(A)")

call analysis_clear (id2)
do i = 4, 6
    print *, "data = ", real(i,default)
    call analysis_record_data (id1, real(i,default))
    call analysis_record_data (id2, real(i,default), &
        weight=real(i,default))
    call analysis_record_data (id3, real(i,default))
    call analysis_record_data (id4, real(i,default), real(i,default)**2)
end do
write (u, "(A,10(1x,I5))") "n_entries = ", &
    analysis_get_n_entries (id1), &
    analysis_get_n_entries (id2), &
    analysis_get_n_entries (id3), &
    analysis_get_n_entries (id3, within_bounds = .true.), &
    analysis_get_n_entries (id4), &
    analysis_get_n_entries (id4, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "average = ", &
    analysis_get_average (id1), &
    analysis_get_average (id2), &
    analysis_get_average (id3), &
    analysis_get_average (id3, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "error = ", &
    analysis_get_error (id1), &
    analysis_get_error (id2), &
    analysis_get_error (id3), &
    analysis_get_error (id3, within_bounds = .true.)
write (u, "(A)")
call analysis_write (u)

```



```
write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call analysis_clear ()
call analysis_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: analysis_1"
end subroutine analysis_1
```

Chapter 14

Matrix Element Handling

In this chapter, we support internal and external matrix elements: initialization, automatic generation where necessary, and numerical evaluation. We provide the interface for code generation and linking. Matrix-element code is organized in processes and process libraries.

process_constants A record of static process properties, for easy transfer between various WHIZARD modules.

prclib_interfaces This module deals with matrix-element code which is accessible via external libraries (Fortran libraries or generic C-compatible libraries) and must either be generated by the program or provided by the user explicitly.

The module defines and uses an abstract type `prc_writer_t` and two abstract extensions, one for a Fortran module and one for a C-compatible library. The implementation provides the specific methods for writing the appropriate parts in external matrix element code.

prc_core_def This module defines the abstract types `prc_core_def_t` and `prc_driver_t`. The implementation of the former provides the configuration for processes of a certain class, while the latter accesses the corresponding matrix element, in particular those generated by the appropriate `prc_writer_t` object.

process_libraries This module combines the functionality of the previous module with the means for holding processes definitions (the internal counterpart of appropriate declarations in the user interface), for handling matrix elements which do not need external code, and for accessing the matrix elements by the procedures for matrix-element evaluation, integration and event generation.

prclib_stacks Collect process libraries.

test_me This module provides a test implementation for the abstract types in the `prc_core_def` module. The implementation is intended for self-tests of several later modules. The implementation is internal, i.e., no external code has is generated.

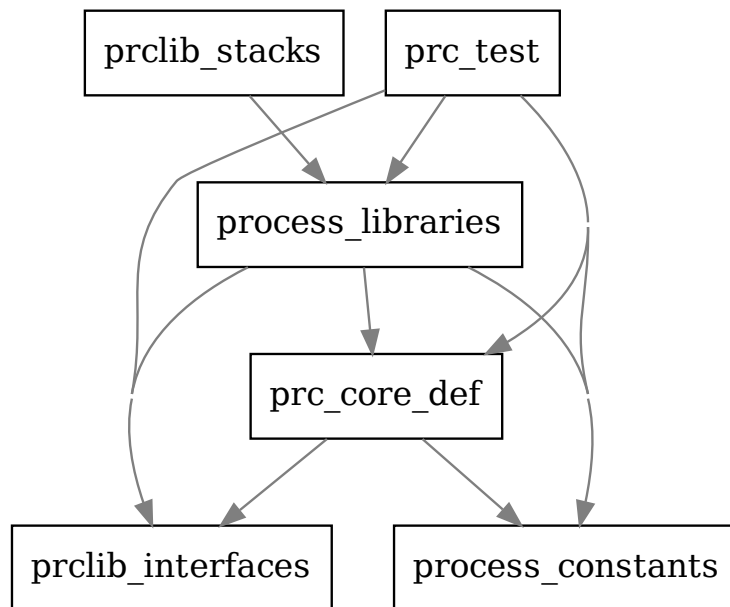


Figure 14.1: Module dependencies in `src/matrix_elements`.

All data structures which are specific for a particular way of generating code or evaluating matrix element are kept abstract and thus generic. Later modules such as `prc_omega` provide implementations, in the form of type extensions for the various abstract types.

14.1 Process data block

We define a simple transparent type that contains universal constant process data. We will reference objects of this type for the phase-space setup, for interfacing with process libraries, for implementing matrix-element generation, and in the master process-handling module.

```
<process_constants.f90>≡
  <File header>

  module process_constants

    <Use kinds>
    <Use strings>
    use pdg_arrays

    <Standard module head>

    <Process constants: public>

    <Process constants: types>

    interface
    <Process constants: sub interfaces>
    end interface

  end module process_constants

<process_constants_sub.f90>≡
  <File header>

  submodule (process_constants) process_constants_s

    use io_units, only: given_output_unit, free_unit
    use format_utils, only: write_integer_array
    use md5, only: md5sum

    implicit none

  contains

    <Process constants: procedures>

  end submodule process_constants_s
```

The data type is just a block of public objects, only elementary types, no type-bound procedures.

```
<Process constants: public>≡
  public :: process_constants_t

<Process constants: types>≡
  type :: process_constants_t
    type(string_t) :: id
    type(string_t) :: model_name
    character(32) :: md5sum = ""
```

```

logical :: openmp_supported = .false.
integer :: n_in = 0
integer :: n_out = 0
integer :: n_flv = 0
integer :: n_hel = 0
integer :: n_col = 0
integer :: n_cin = 0
integer :: n_cf = 0
integer, dimension(:,:), allocatable :: flv_state
integer, dimension(:,:), allocatable :: hel_state
integer, dimension(:,:), allocatable :: col_state
logical, dimension(:,:), allocatable :: ghost_flag
complex(default), dimension(:), allocatable :: color_factors
integer, dimension(:,:), allocatable :: cf_index
integer, dimension(:), allocatable :: eqv_flv_index
integer, dimension(:), allocatable :: eqv_hel_index
contains
<Process constants: process constants: TBP>
end type process_constants_t

<Process constants: process constants: TBP>≡
procedure :: get_n_tot => process_constants_get_n_tot

<Process constants: sub interfaces>≡
elemental module function process_constants_get_n_tot (prc_const) result (n_tot)
integer :: n_tot
class(process_constants_t), intent(in) :: prc_const
end function process_constants_get_n_tot

<Process constants: procedures>≡
elemental module function process_constants_get_n_tot (prc_const) result (n_tot)
integer :: n_tot
class(process_constants_t), intent(in) :: prc_const
n_tot = prc_const%n_in + prc_const%n_out
end function process_constants_get_n_tot

<Process constants: process constants: TBP>+≡
procedure :: get_flv_state => process_constants_get_flv_state

<Process constants: sub interfaces>+≡
module subroutine process_constants_get_flv_state (prc_const, flv_state)
class(process_constants_t), intent(in) :: prc_const
integer, dimension(:,:), allocatable, intent(out) :: flv_state
end subroutine process_constants_get_flv_state

<Process constants: procedures>+≡
module subroutine process_constants_get_flv_state (prc_const, flv_state)
class(process_constants_t), intent(in) :: prc_const
integer, dimension(:,:), allocatable, intent(out) :: flv_state
allocate (flv_state (size (prc_const%flv_state, 1), &
size (prc_const%flv_state, 2)))
flv_state = prc_const%flv_state
end subroutine process_constants_get_flv_state

```

```

<Process constants: process constants: TBP>+≡
    procedure :: get_n_flv => process_constants_get_n_flv
<Process constants: sub interfaces>+≡
    module function process_constants_get_n_flv (data) result (n_flv)
        integer :: n_flv
        class(process_constants_t), intent(in) :: data
    end function process_constants_get_n_flv
<Process constants: procedures>+≡
    module function process_constants_get_n_flv (data) result (n_flv)
        integer :: n_flv
        class(process_constants_t), intent(in) :: data
        n_flv = data%n_flv
    end function process_constants_get_n_flv

<Process constants: process constants: TBP>+≡
    procedure :: get_n_hel => process_constants_get_n_hel
<Process constants: sub interfaces>+≡
    module function process_constants_get_n_hel (data) result (n_hel)
        integer :: n_hel
        class(process_constants_t), intent(in) :: data
    end function process_constants_get_n_hel
<Process constants: procedures>+≡
    module function process_constants_get_n_hel (data) result (n_hel)
        integer :: n_hel
        class(process_constants_t), intent(in) :: data
        n_hel = data%n_hel
    end function process_constants_get_n_hel

<Process constants: process constants: TBP>+≡
    procedure :: get_hel_state => process_constants_get_hel_state
<Process constants: sub interfaces>+≡
    module subroutine process_constants_get_hel_state (prc_const, hel_state)
        class(process_constants_t), intent(in) :: prc_const
        integer, dimension(:,:), allocatable, intent(out) :: hel_state
    end subroutine process_constants_get_hel_state
<Process constants: procedures>+≡
    module subroutine process_constants_get_hel_state (prc_const, hel_state)
        class(process_constants_t), intent(in) :: prc_const
        integer, dimension(:,:), allocatable, intent(out) :: hel_state
        allocate (hel_state (size (prc_const%hel_state, 1), &
            size (prc_const%hel_state, 2)))
        hel_state = prc_const%hel_state
    end subroutine process_constants_get_hel_state

<Process constants: process constants: TBP>+≡
    procedure :: get_col_state => process_constants_get_col_state
<Process constants: sub interfaces>+≡
    module subroutine process_constants_get_col_state (prc_const, col_state)
        class(process_constants_t), intent(in) :: prc_const
        integer, dimension(:,:), allocatable, intent(out) :: col_state
    end subroutine process_constants_get_col_state

```

```

<Process constants: procedures>+≡
  module subroutine process_constants_get_col_state (prc_const, col_state)
    class(process_constants_t), intent(in) :: prc_const
    integer, dimension(:,:,:), allocatable, intent(out) :: col_state
    allocate (col_state (size (prc_const%col_state, 1), &
      size (prc_const%col_state, 2), size (prc_const%col_state, 3)))
    col_state = prc_const%col_state
  end subroutine process_constants_get_col_state

<Process constants: process constants: TBP>+≡
  procedure :: get_ghost_flag => process_constants_get_ghost_flag

<Process constants: sub interfaces>+≡
  module subroutine process_constants_get_ghost_flag (prc_const, ghost_flag)
    class(process_constants_t), intent(in) :: prc_const
    logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
  end subroutine process_constants_get_ghost_flag

<Process constants: procedures>+≡
  module subroutine process_constants_get_ghost_flag (prc_const, ghost_flag)
    class(process_constants_t), intent(in) :: prc_const
    logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
    allocate (ghost_flag (size (prc_const%ghost_flag, 1), &
      size (prc_const%ghost_flag, 2)))
    ghost_flag = prc_const%ghost_flag
  end subroutine process_constants_get_ghost_flag

<Process constants: process constants: TBP>+≡
  procedure :: get_color_factors => process_constants_get_color_factors

<Process constants: sub interfaces>+≡
  module subroutine process_constants_get_color_factors (prc_const, col_facts)
    class(process_constants_t), intent(in) :: prc_const
    complex(default), dimension(:), allocatable, intent(out) :: col_facts
  end subroutine process_constants_get_color_factors

<Process constants: procedures>+≡
  module subroutine process_constants_get_color_factors (prc_const, col_facts)
    class(process_constants_t), intent(in) :: prc_const
    complex(default), dimension(:), allocatable, intent(out) :: col_facts
    allocate (col_facts (size (prc_const%color_factors)))
    col_facts = prc_const%color_factors
  end subroutine process_constants_get_color_factors

<Process constants: process constants: TBP>+≡
  procedure :: get_cf_index => process_constants_get_cf_index

<Process constants: sub interfaces>+≡
  module subroutine process_constants_get_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(in) :: prc_const
    integer, intent(out), dimension(:,:), allocatable :: cf_index
  end subroutine process_constants_get_cf_index

```



```

<Process constants: procedures>+≡
  module subroutine process_constants_get_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(in) :: prc_const
    integer, intent(out), dimension(:,:), allocatable :: cf_index
    allocate (cf_index (size (prc_const%cf_index, 1), &
      size (prc_const%cf_index, 2)))
    cf_index = prc_const%cf_index
  end subroutine process_constants_get_cf_index

<Process constants: process constants: TBP>+≡
  procedure :: set_flv_state => process_constants_set_flv_state

<Process constants: sub interfaces>+≡
  module subroutine process_constants_set_flv_state (prc_const, flv_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:), allocatable :: flv_state
  end subroutine process_constants_set_flv_state

<Process constants: procedures>+≡
  module subroutine process_constants_set_flv_state (prc_const, flv_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:), allocatable :: flv_state
    if (allocated (prc_const%flv_state)) deallocate (prc_const%flv_state)
    allocate (prc_const%flv_state (size (flv_state, 1), &
      size (flv_state, 2)))
    prc_const%flv_state = flv_state
    prc_const%n_flv = size (flv_state, 2)
  end subroutine process_constants_set_flv_state

<Process constants: process constants: TBP>+≡
  procedure :: set_col_state => process_constants_set_col_state

<Process constants: sub interfaces>+≡
  module subroutine process_constants_set_col_state (prc_const, col_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:,:), allocatable :: col_state
  end subroutine process_constants_set_col_state

<Process constants: procedures>+≡
  module subroutine process_constants_set_col_state (prc_const, col_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:,:), allocatable :: col_state
    allocate (prc_const%col_state (size (col_state, 1), &
      size (col_state, 2), size (col_state, 3)))
    prc_const%col_state = col_state
  end subroutine process_constants_set_col_state

<Process constants: process constants: TBP>+≡
  procedure :: set_cf_index => process_constants_set_cf_index

<Process constants: sub interfaces>+≡
  module subroutine process_constants_set_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(inout) :: prc_const
    integer, dimension(:,:), intent(in), allocatable :: cf_index
  end subroutine process_constants_set_cf_index

```

```

<Process constants: procedures>+≡
  module subroutine process_constants_set_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(inout) :: prc_const
    integer, dimension(:,:), intent(in), allocatable :: cf_index
    allocate (prc_const%cf_index (size (cf_index, 1), &
      size (cf_index, 2)))
    prc_const%cf_index = cf_index
  end subroutine process_constants_set_cf_index

<Process constants: process constants: TBP>+≡
  procedure :: set_color_factors => process_constants_set_color_factors

<Process constants: sub interfaces>+≡
  module subroutine process_constants_set_color_factors (prc_const, color_factors)
    class(process_constants_t), intent(inout) :: prc_const
    complex(default), dimension(:), intent(in), allocatable :: color_factors
  end subroutine process_constants_set_color_factors

<Process constants: procedures>+≡
  module subroutine process_constants_set_color_factors (prc_const, color_factors)
    class(process_constants_t), intent(inout) :: prc_const
    complex(default), dimension(:), intent(in), allocatable :: color_factors
    allocate (prc_const%color_factors (size (color_factors)))
    prc_const%color_factors = color_factors
  end subroutine process_constants_set_color_factors

<Process constants: process constants: TBP>+≡
  procedure :: set_ghost_flag => process_constants_set_ghost_flag

<Process constants: sub interfaces>+≡
  module subroutine process_constants_set_ghost_flag (prc_const, ghost_flag)
    class(process_constants_t), intent(inout) :: prc_const
    logical, dimension(:,:), allocatable, intent(in) :: ghost_flag
  end subroutine process_constants_set_ghost_flag

<Process constants: procedures>+≡
  module subroutine process_constants_set_ghost_flag (prc_const, ghost_flag)
    class(process_constants_t), intent(inout) :: prc_const
    logical, dimension(:,:), allocatable, intent(in) :: ghost_flag
    allocate (prc_const%ghost_flag (size (ghost_flag, 1), &
      size (ghost_flag, 2)))
    prc_const%ghost_flag = ghost_flag
  end subroutine process_constants_set_ghost_flag

<Process constants: process constants: TBP>+≡
  procedure :: get_pdg_in => process_constants_get_pdg_in

<Process constants: sub interfaces>+≡
  module function process_constants_get_pdg_in (prc_const) result (pdg_in)
    type(pdg_array_t), dimension(:), allocatable :: pdg_in
    class(process_constants_t), intent(in) :: prc_const
  end function process_constants_get_pdg_in

<Process constants: procedures>+≡
  module function process_constants_get_pdg_in (prc_const) result (pdg_in)
    type(pdg_array_t), dimension(:), allocatable :: pdg_in
    class(process_constants_t), intent(in) :: prc_const

```

```

type(pdg_array_t) :: pdg_tmp
integer :: i
allocate (pdg_in (prc_const%n_in))
do i = 1, prc_const%n_in
    pdg_tmp = prc_const%flv_state(i,:)
    pdg_in(i) = sort_abs (pdg_tmp, unique = .true.)
end do
end function process_constants_get_pdg_in

```

<Process constants: process constants: TBP>+≡

```

procedure :: compute_md5sum => process_constants_compute_md5sum

```

<Process constants: sub interfaces>+≡

```

module subroutine process_constants_compute_md5sum (prc_const, include_id)
    class(process_constants_t), intent(inout) :: prc_const
    logical, intent(in) :: include_id
end subroutine process_constants_compute_md5sum

```

<Process constants: procedures>+≡

```

module subroutine process_constants_compute_md5sum (prc_const, include_id)
    class(process_constants_t), intent(inout) :: prc_const
    logical, intent(in) :: include_id
    integer :: unit
    unit = prc_const%fill_unit_for_md5sum (include_id)
    rewind (unit)
    prc_const%md5sum = md5sum (unit)
    close (unit)
end subroutine process_constants_compute_md5sum

```

<Process constants: process constants: TBP>+≡

```

procedure :: fill_unit_for_md5sum => process_constants_fill_unit_for_md5sum

```

<Process constants: sub interfaces>+≡

```

module function process_constants_fill_unit_for_md5sum &
    (prc_const, include_id) result (unit)
    integer :: unit
    class(process_constants_t), intent(in) :: prc_const
    logical, intent(in) :: include_id
end function process_constants_fill_unit_for_md5sum

```

<Process constants: procedures>+≡

```

module function process_constants_fill_unit_for_md5sum &
    (prc_const, include_id) result (unit)
    integer :: unit
    class(process_constants_t), intent(in) :: prc_const
    logical, intent(in) :: include_id
    integer :: i, j, k
    unit = free_unit ()
    open (unit, status="scratch", action="readwrite")
    if (include_id) write (unit, '(A)') char (prc_const%id)
    write (unit, '(A)') char (prc_const%model_name)
    write (unit, '(L1)') prc_const%openmp_supported
    write (unit, '(IO)') prc_const%n_in
    write (unit, '(IO)') prc_const%n_out
    write (unit, '(IO)') prc_const%n_flv

```

```

write (unit, '(I0)') prc_const%n_hel
write (unit, '(I0)') prc_const%n_col
write (unit, '(I0)') prc_const%n_cin
write (unit, '(I0)') prc_const%n_cf
do i = 1, size (prc_const%flv_state, dim=1)
  do j = 1, size (prc_const%flv_state, dim=2)
    write (unit, '(I0)') prc_const%flv_state (i, j)
  end do
end do
do i = 1, size (prc_const%hel_state, dim=1)
  do j = 1, size (prc_const%hel_state, dim=2)
    write (unit, '(I0)') prc_const%hel_state (i, j)
  end do
end do
do i = 1, size (prc_const%col_state, dim=1)
  do j = 1, size (prc_const%col_state, dim=2)
    do k = 1, size (prc_const%col_state, dim=3)
      write (unit, '(I0)') prc_const%col_state (i, j, k)
    end do
  end do
end do
do i = 1, size (prc_const%ghost_flag, dim=1)
  do j = 1, size (prc_const%ghost_flag, dim=2)
    write (unit, '(L1)') prc_const%ghost_flag (i, j)
  end do
end do
do i = 1, size (prc_const%color_factors)
  write (unit, '(F0.0,F0.0)') real (prc_const%color_factors(i)), &
    aimag (prc_const%color_factors(i))
end do
do i = 1, size (prc_const%cf_index, dim=1)
  do j = 1, size (prc_const%cf_index, dim=2)
    write (unit, '(I0)') prc_const%cf_index(i, j)
  end do
end do
end function process_constants_fill_unit_for_md5sum

```

<Process constants: process constants: TBP>+≡

```
procedure :: write => process_constants_write
```

<Process constants: sub interfaces>+≡

```

module subroutine process_constants_write (prc_const, unit)
  class(process_constants_t), intent(in) :: prc_const
  integer, intent(in), optional :: unit
end subroutine process_constants_write

```

<Process constants: procedures>+≡

```

module subroutine process_constants_write (prc_const, unit)
  class(process_constants_t), intent(in) :: prc_const
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A,A)") "Process data of id: ", char (prc_const%id)
  write (u, "(1x,A,A)") "Associated model: ", char (prc_const%model_name)
  write (u, "(1x,A,I0)") "n_in: ", prc_const%n_in

```

```

write (u, "(1x,A,I0)") "n_out: ", prc_const%n_out
write (u, "(1x,A,I0)") "n_flv: ", prc_const%n_flv
write (u, "(1x,A,I0)") "n_hel: ", prc_const%n_hel
write (u, "(1x,A,I0)") "n_col: ", prc_const%n_col
write (u, "(1x,A,I0)") "n_cin: ", prc_const%n_cin
write (u, "(1x,A,I0)") "n_cf: ", prc_const%n_cf
write (u, "(1x,A)") "Flavors: "
do i = 1, prc_const%n_flv
  write (u, "(1x,A,I0)") "i_flv: ", i
  call write_integer_array (prc_const%flv_state (:,i))
end do
end subroutine process_constants_write

```

14.2 Process library interface

The module `prclib_interfaces` handles external matrix-element code.

14.2.1 Overview

The top-level data structure is the `prclib_driver_t` data type. The associated type-bound procedures deal with the generation of external code, compilation and linking, and accessing the active external library.

An object of type `prclib_driver_t` consists of the following parts:

1. Metadata that identify name and status of the library driver, etc.
2. An array of process records (`prclib_driver_record_t`), one for each external matrix element.
3. A record of type `dlaccess_t` which handles the operating-system part of linking a dynamically loadable library.
4. A collection of procedure pointers which have a counterpart in the external library interface. Given the unique identifier of a matrix element, the procedures retrieve generic matrix-element information such as the particle content and helicity combination tables. There is also a procedure which returns pointers to the more specific procedures that a matrix element provides, called *features*.

The process records of type `prclib_driver_record_t` handle the individual matrix elements. Each record identifies a process by name (`id`), names the physics model to be loaded for this process, lists the features that the associated matrix-element code provides, and holds a `writer` object which handles all operations that depend on the process type. The numbering of process records is identical to the numbering of matrix-element codes in the external library.

The writer object is of abstract type `prc_writer_t`. The module defines two basic, also abstract, extensions: `prc_writer_f_module_t` and `prc_writer_c_lib_t`. The first version is for matrix-element code that is available in form of Fortran modules. The writer contains type-bound procedures which create appropriate `use` directives and C-compatible wrapper functions for the given set of Fortran modules and their features. The second version is for matrix-element code that

is available in form of a C-compatible library (this includes Fortran libraries with proper C bindings). The writer needs not write wrapper function, but explicit interface blocks for the matrix-element features.

Each matrix-element variant is encoded in an appropriate extension of `prc_writer_t`. For instance, O’MEGA matrix elements provide an implementation `omega_writer_t` which extends `prc_writer_f_module_t`.

14.2.2 Workflow

We expect that the functionality provided by this module is called in the following order:

1. The caller initializes the `prclib_driver_t` object and fills the array of `prclib_record_t` entries with the appropriate process data and process-specific writer objects.
2. It calls the `generate_makefile` method to set up an appropriate makefile in the current directory. The makefile will handle source generation, compilation and linking both for the individual matrix elements (unless this has to be done manually) and for the common external driver code which interfaces those matrix element.
3. The `generate_driver_code` writes the common driver as source code to file.
4. The methods `make_source`, `make_compile`, and `make_link` individually perform the corresponding steps in building the library. Wherever possible, they simply use the generated makefile. By calling `make`, we make sure that we can avoid unnecessary recompilation. For the compilation and linking steps, the makefile will employ `libtool`.
5. The `load` method loads the library procedures into the corresponding procedure pointers, using the `dlopen` mechanism via the `dlaccess` subobject.

14.2.3 The module

```

<prclib_interfaces.f90>≡
  <File header>

  module prclib_interfaces

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use os_interface

    <Standard module head>

    <Prclib interfaces: public>

    <Prclib interfaces: types>

```

```

    <Prclib interfaces: interfaces>

    interface
    <Prclib interfaces: sub interfaces>
    end interface

    contains

    <Prclib interfaces: main procedures>

    end module prclib_interfaces

<prclib_interfaces_sub.f90>≡
<File header>

submodule (prclib_interfaces) prclib_interfaces_s

    use io_units
    use system_defs, only: TAB
    use string_utils, only: lower_case
    use diagnostics

    implicit none

    contains

    <Prclib interfaces: procedures>

    end submodule prclib_interfaces_s

```

14.2.4 Writers

External matrix element code provides externally visible procedures, which we denote as *features*. The features consist of informational subroutines and functions which are mandatory (universal features) and matrix-element specific subroutines and functions (specific features). The driver interfaces the generic features directly, while it returns the specific features in form of `bind(C)` procedure pointers to the caller. For instance, function `n_in` is generic, while the matrix matrix-element value itself is specific.

To implement these tasks, the driver needs `use` directives for Fortran module procedures, interface blocks for other external stuff, wrapper code, and Makefile snippets.

Generic writer

In the `prc_writer_t` data type, we collect the procedures which implement the writing tasks. The type is abstract. The concrete implementations are defined by an extension which is specific for the process type.

The MD5 sum stored here should be the MD5 checksum of the current process component, which can be calculated once the process is configured completely. It can be used by implementations which work with external files, such

```

as O'MEGA.
<Prclib interfaces: public>≡
  public :: prc_writer_t
<Prclib interfaces: types>≡
  type, abstract :: prc_writer_t
    character(32) :: md5sum = ""
    contains
    <Prclib interfaces: prc writer: TBP>
  end type prc_writer_t

```

In any case, it is useful to have a string representation of the writer type. This must be implemented by all extensions.

```

<Prclib interfaces: prc writer: TBP>≡
  procedure(get_const_string), nopass, deferred :: type_name
<Prclib interfaces: interfaces>≡
  abstract interface
    function get_const_string () result (string)
      import
      type(string_t) :: string
    end function get_const_string
  end interface

```

Return the name of a procedure that implements a given feature, as it is provided by the external matrix-element code. For a reasonable default, we take the feature name unchanged. Due to a bug of bind(C) features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure, nopass :: get_procname => prc_writer_get_procname
<Prclib interfaces: main procedures>≡
  function prc_writer_get_procname (feature) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: feature
    name = feature
  end function prc_writer_get_procname

```

Return the name of a procedure that implements a given feature with the bind(C) property, so it can be accessed via a C procedure pointer and handled by dlopen. We need this for all special features of a matrix element, since the interface has to return a C function pointer for it. For a default implementation, we prefix the external procedure name by the process ID. Due to a bug of bind(C) features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure :: get_c_procname => prc_writer_get_c_procname
<Prclib interfaces: main procedures>+≡
  function prc_writer_get_c_procname (writer, id, feature) result (name)
    class(prc_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id, feature

```



```

    type(string_t) :: name
    name = id // "_" // feature
end function prc_writer_get_c_procname

```

Common signature of code-writing procedures. The procedure may use the process ID, and the feature name. (Not necessarily all of them.)

(Prclib interfaces: interfaces)+≡

```

abstract interface
    subroutine write_code_file (writer, id)
    import
    class(prc_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    end subroutine write_code_file
end interface

abstract interface
    subroutine write_code (writer, unit, id)
    import
    class(prc_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    end subroutine write_code
end interface

abstract interface
    subroutine write_code_os &
        (writer, unit, id, os_data, verbose, testflag)
    import
    class(prc_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    end subroutine write_code_os
end interface

abstract interface
    subroutine write_feature_code (writer, unit, id, feature)
    import
    class(prc_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    end subroutine write_feature_code
end interface

```

There must be a procedure which writes an interface block for a given feature. If the external matrix element is implemented as a Fortran module, this is required only for the specific features which are returned as procedure pointers.

(Prclib interfaces: prc writer: TBP)+≡

```

    procedure(write_feature_code), deferred :: write_interface

```

There must also be a procedure which writes Makefile code which is specific for

the current process, but not the feature.

```
<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_os), deferred :: write_makefile_code
```

This procedure writes code process-specific source-code file (which need not be Fortran). It is called before `make source` is called. It may be a no-op, if the source code is generated by Make instead.

```
<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_file), deferred :: write_source_code
```

This procedure is executed, once for each process, before (after) `make compile` is called, respectively.

```
<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_file), deferred :: before_compile
  procedure(write_code_file), deferred :: after_compile
```

Writer for Fortran-module matrix elements

If the matrix element is available as a Fortran module, we have specific requirements: (i) the features are imported via `use` directives, (ii) the specific features require `bind(C)` wrappers.

The type is still abstract, all methods must be implemented explicitly for a specific matrix-element variant.

```
<Prclib interfaces: public>+≡
  public :: prc_writer_f_module_t

<Prclib interfaces: types>+≡
  type, extends (prc_writer_t), abstract :: prc_writer_f_module_t
  contains
    <Prclib interfaces: prc writer f module: TBP>
  end type prc_writer_f_module_t
```

Return the name of the Fortran module. As a default implementation, we take the process ID unchanged. Due to a bug of `bind(C)` features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```
<Prclib interfaces: prc writer f module: TBP>≡
  procedure, nopass :: get_module_name => prc_writer_get_module_name

<Prclib interfaces: main procedures>+≡
  function prc_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = id
  end function prc_writer_get_module_name
```

Write a `use` directive that associates the driver reference with the procedure in the matrix element code. By default, we use the C name for this.

```
<Prclib interfaces: prc writer f module: TBP>+≡
  procedure :: write_use_line => prc_writer_write_use_line
```

```

<Prclib interfaces: sub interfaces>≡
    module subroutine prc_writer_write_use_line (writer, unit, id, feature)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t) :: id, feature
    end subroutine prc_writer_write_use_line
<Prclib interfaces: procedures>≡
    module subroutine prc_writer_write_use_line (writer, unit, id, feature)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t) :: id, feature
        write (unit, "(2x,9A)") "use ", char (writer%get_module_name (id)), &
            ", only: ", char (writer%get_c_procname (id, feature)), &
            " => ", char (writer%get_procname (feature))
    end subroutine prc_writer_write_use_line

```

Write a wrapper routine for a feature. This also associates a C name the module procedure. The details depend on the writer variant.

```

<Prclib interfaces: prc writer f module: TBP>+≡
    procedure(prc_write_wrapper), deferred :: write_wrapper
<Prclib interfaces: interfaces>+≡
    abstract interface
        subroutine prc_write_wrapper (writer, unit, id, feature)
            import
            class(prc_writer_f_module_t), intent(in) :: writer
            integer, intent(in) :: unit
            type(string_t), intent(in) :: id, feature
        end subroutine prc_write_wrapper
    end interface

```

This is used for testing only: initialize the writer with a specific MD5 sum string.

```

<Prclib interfaces: prc writer: TBP>+≡
    procedure :: init_test => prc_writer_init_test
<Prclib interfaces: sub interfaces>+≡
    module subroutine prc_writer_init_test (writer)
        class(prc_writer_t), intent(out) :: writer
    end subroutine prc_writer_init_test
<Prclib interfaces: procedures>+≡
    module subroutine prc_writer_init_test (writer)
        class(prc_writer_t), intent(out) :: writer
        writer%md5sum = "1234567890abcdef1234567890abcdef"
    end subroutine prc_writer_init_test

```

Writer for C-library matrix elements

This applies if the matrix element is available as a C library or a Fortran library with bind(C) compatible interface. We can use the basic version.

The type is still abstract, all methods must be implemented explicitly for a specific matrix-element variant.

```

<Prclib interfaces: public>+≡

```

```

    public :: prc_writer_c_lib_t
  <Prclib interfaces: types>+≡
    type, extends (prc_writer_t), abstract :: prc_writer_c_lib_t
    contains
    <Prclib interfaces: prc writer c lib: TBP>
  end type prc_writer_c_lib_t

```

14.2.5 Process records in the library driver

A process record holds the process (component) ID, the physics `model_name`, and the array of `features` that are implemented by the corresponding matrix element code.

The `writer` component holds procedures. The procedures write source code for the current record, either for the driver or for the Makefile.

```

  <Prclib interfaces: types>+≡
    type :: prclib_driver_record_t
    type(string_t) :: id
    type(string_t) :: model_name
    type(string_t), dimension(:), allocatable :: feature
    class(prc_writer_t), pointer :: writer => null ()
    contains
    <Prclib interfaces: prclib driver record: TBP>
  end type prclib_driver_record_t

```

Output routine. We indent the output, so it smoothly integrates into the output routine for the whole driver.

Note: the pointer `writer` is introduced as a workaround for a NAG compiler bug.

```

  <Prclib interfaces: prclib driver record: TBP>≡
    procedure :: write => prclib_driver_record_write

  <Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_record_write (object, unit)
      class(prclib_driver_record_t), intent(in) :: object
      integer, intent(in) :: unit
    end subroutine prclib_driver_record_write

  <Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_record_write (object, unit)
      class(prclib_driver_record_t), intent(in) :: object
      integer, intent(in) :: unit
      integer :: j
      class(prc_writer_t), pointer :: writer
      write (unit, "(3x,A,2x,['',A,']')") &
        char (object%id), char (object%model_name)
      if (allocated (object%feature)) then
        writer => object%writer
        write (unit, "(5x,A,A)", advance="no") &
          char (writer%type_name ()), ":"
        do j = 1, size (object%feature)
          write (unit, "(1x,A)", advance="no") &
            char (object%feature(j))

```

```

        end do
        write (unit, *)
    end if
end subroutine prclib_driver_record_write

```

Get the C procedure name for a feature. Due to a bug of bind(C) features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: get_c_procname => prclib_driver_record_get_c_procname

<Prclib interfaces: main procedures>+≡
    function prclib_driver_record_get_c_procname (record, feature) result (name)
        type(string_t) :: name
        class(prclib_driver_record_t), intent(in) :: record
        type(string_t), intent(in) :: feature
        name = record%writer%get_c_procname (record%id, feature)
    end function prclib_driver_record_get_c_procname

```

Write a USE directive for a given feature. Applies only if the record corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_use_line => prclib_driver_record_write_use_line

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_record_write_use_line (record, unit, feature)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(string_t), intent(in) :: feature
    end subroutine prclib_driver_record_write_use_line

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_record_write_use_line (record, unit, feature)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(string_t), intent(in) :: feature
        select type (writer => record%writer)
            class is (prc_writer_f_module_t)
                call writer%write_use_line (unit, record%id, feature)
            end select
    end subroutine prclib_driver_record_write_use_line

```

The alternative: write an interface block for a given feature, unless the record corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_interface => prclib_driver_record_write_interface

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_record_write_interface (record, unit, feature)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(string_t), intent(in) :: feature
    end subroutine prclib_driver_record_write_interface

```

```

<Prclib interfaces: procedures>+≡
module subroutine prclib_driver_record_write_interface (record, unit, feature)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  type(string_t), intent(in) :: feature
  select type (writer => record%writer)
  class is (prc_writer_f_module_t)
  class default
    call writer%write_interface (unit, record%id, feature)
  end select
end subroutine prclib_driver_record_write_interface

```

Write all special feature interfaces for the current record. Do this for all process variants.

```

<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: write_interfaces => prclib_driver_record_write_interfaces

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_record_write_interfaces (record, unit)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit
  end subroutine prclib_driver_record_write_interfaces

<Prclib interfaces: procedures>+≡
module subroutine prclib_driver_record_write_interfaces (record, unit)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  integer :: i
  do i = 1, size (record%feature)
    call record%writer%write_interface (unit, record%id, record%feature(i))
  end do
end subroutine prclib_driver_record_write_interfaces

```

Write the wrapper routines for this record, if it corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: write_wrappers => prclib_driver_record_write_wrappers

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_record_write_wrappers (record, unit)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit
  end subroutine prclib_driver_record_write_wrappers

<Prclib interfaces: procedures>+≡
module subroutine prclib_driver_record_write_wrappers (record, unit)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  integer :: i
  select type (writer => record%writer)
  class is (prc_writer_f_module_t)
    do i = 1, size (record%feature)
      call writer%write_wrapper (unit, record%id, record%feature(i))
    end do
  end select
end subroutine prclib_driver_record_write_wrappers

```

Write the Makefile code for this record.

```

<Prclib interfaces: prclib driver record: TBP>+=
    procedure :: write_makefile_code => prclib_driver_record_write_makefile_code

<Prclib interfaces: sub interfaces>+=
    module subroutine prclib_driver_record_write_makefile_code &
        (record, unit, os_data, verbose, testflag)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
    end subroutine prclib_driver_record_write_makefile_code

<Prclib interfaces: procedures>+=
    module subroutine prclib_driver_record_write_makefile_code &
        (record, unit, os_data, verbose, testflag)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        call record%writer%write_makefile_code &
            (unit, record%id, os_data, verbose, testflag)
    end subroutine prclib_driver_record_write_makefile_code

```

Write source-code files for this record. This can be used as an alternative to handling source code via Makefile. In fact, this procedure is executed before `make source` is called. Usually, does nothing.

```

<Prclib interfaces: prclib driver record: TBP>+=
    procedure :: write_source_code => prclib_driver_record_write_source_code

<Prclib interfaces: sub interfaces>+=
    module subroutine prclib_driver_record_write_source_code (record)
        class(prclib_driver_record_t), intent(in) :: record
    end subroutine prclib_driver_record_write_source_code

<Prclib interfaces: procedures>+=
    module subroutine prclib_driver_record_write_source_code (record)
        class(prclib_driver_record_t), intent(in) :: record
        call record%writer%write_source_code (record%id)
    end subroutine prclib_driver_record_write_source_code

```

Execute commands for this record that depend on the sources, so they cannot be included in the previous procedure. This procedure is executed before (after) `make compile` is called, respectively. Usually, does nothing.

```

<Prclib interfaces: prclib driver record: TBP>+=
    procedure :: before_compile => prclib_driver_record_before_compile
    procedure :: after_compile => prclib_driver_record_after_compile

<Prclib interfaces: sub interfaces>+=
    module subroutine prclib_driver_record_before_compile (record)
        class(prclib_driver_record_t), intent(in) :: record
    end subroutine prclib_driver_record_before_compile
    module subroutine prclib_driver_record_after_compile (record)

```

```

        class(prclib_driver_record_t), intent(in) :: record
    end subroutine prclib_driver_record_after_compile

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_record_before_compile (record)
        class(prclib_driver_record_t), intent(in) :: record
        call record%writer%before_compile (record%id)
    end subroutine prclib_driver_record_before_compile

    module subroutine prclib_driver_record_after_compile (record)
        class(prclib_driver_record_t), intent(in) :: record
        call record%writer%after_compile (record%id)
    end subroutine prclib_driver_record_after_compile

```

14.2.6 The process library driver object

A `prclib_driver_t` object provides the interface to external matrix element code. The code is provided by an external library which is either statically or dynamically linked.

The dynamic and static versions of the library are two different implementations of the abstract base type.

The `basename` identifies the library, both by file names and by Fortran variable names.

The `loaded` flag becomes true once all procedure pointers to the matrix element have been assigned.

For a dynamical external library, the communication proceeds via a `dlaccess` object.

`n_processes` is the number of external process code components that are referenced by this library. The code is addressed by index (`i_lib` in the process library entry above). This number should be equal to the number returned by `get_n_prc`.

For each external process, there is a separate `record` which holds the data that are needed for the driver parts which are specific for a given process component. The actual pointers for the loaded library will be assigned elsewhere.

The remainder is a collection of procedure pointers, which can be assigned once all external code has been compiled and linked. The procedure pointers all take a process component code index as an argument. Most return information about the process component that should match the process definition. The `get_fptr` procedures return a function pointer, which is the actual means to compute matrix elements or retrieve associated data.

Finally, the `unload_hook` and `reload_hook` pointers allow for the insertion of additional code when a library is loaded.

```

<Prclib interfaces: public>+≡
    public :: prclib_driver_t

<Prclib interfaces: types>+≡
    type, abstract :: prclib_driver_t
        type(string_t) :: basename
        character(32) :: md5sum = ""
        logical :: loaded = .false.
        type(string_t) :: libname

```



```

type(string_t) :: modellibs_ldflags
integer :: n_processes = 0
type(prclib_driver_record_t), dimension(:), allocatable :: record
procedure(prc_get_n_processes), nopass, pointer :: &
    get_n_processes => null ()
procedure(prc_get_stringptr), nopass, pointer :: &
    get_process_id_ptr => null ()
procedure(prc_get_stringptr), nopass, pointer :: &
    get_model_name_ptr => null ()
procedure(prc_get_stringptr), nopass, pointer :: &
    get_md5sum_ptr => null ()
procedure(prc_get_log), nopass, pointer :: &
    get_omp_status => null ()
procedure(prc_get_int), nopass, pointer :: get_n_in => null ()
procedure(prc_get_int), nopass, pointer :: get_n_out => null ()
procedure(prc_get_int), nopass, pointer :: get_n_flv => null ()
procedure(prc_get_int), nopass, pointer :: get_n_hel => null ()
procedure(prc_get_int), nopass, pointer :: get_n_col => null ()
procedure(prc_get_int), nopass, pointer :: get_n_cin => null ()
procedure(prc_get_int), nopass, pointer :: get_n_cf => null ()
procedure(prc_set_int_tab1), nopass, pointer :: &
    set_flv_state_ptr => null ()
procedure(prc_set_int_tab1), nopass, pointer :: &
    set_hel_state_ptr => null ()
procedure(prc_set_col_state), nopass, pointer :: &
    set_col_state_ptr => null ()
procedure(prc_set_color_factors), nopass, pointer :: &
    set_color_factors_ptr => null ()
procedure(prc_get_fptr), nopass, pointer :: get_fptr => null ()
contains
    <Prclib interfaces: prclib driver: TBP>
end type prclib_driver_t

```

This is the dynamic version. It contains a dlaccess object for communicating with the OS.

```

<Prclib interfaces: public>+≡
    public :: prclib_driver_dynamic_t
<Prclib interfaces: types>+≡
    type, extends (prclib_driver_t) :: prclib_driver_dynamic_t
        type(dlaccess_t) :: dlaccess
    contains
        <Prclib interfaces: prclib driver dynamic: TBP>
    end type prclib_driver_dynamic_t

```

Print just the metadata. Procedure pointers cannot be printed.

```

<Prclib interfaces: prclib driver: TBP>≡
    procedure :: write => prclib_driver_write
<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_write (object, unit, libpath)
        class(prclib_driver_t), intent(in) :: object
        integer, intent(in) :: unit
        logical, intent(in), optional :: libpath
    end subroutine prclib_driver_write

```

```

end subroutine prclib_driver_write
<Prclib interfaces: procedures>+=
module subroutine prclib_driver_write (object, unit, libpath)
  class(prclib_driver_t), intent(in) :: object
  integer, intent(in) :: unit
  logical, intent(in), optional :: libpath
  logical :: write_lib
  integer :: i
  write_lib = .true.
  if (present (libpath)) write_lib = libpath
  write (unit, "(1x,A,A)") &
    "External matrix-element code library: ", char (object%basename)
  select type (object)
  type is (prclib_driver_dynamic_t)
    write (unit, "(3x,A,L1)") "static      = F"
  class default
    write (unit, "(3x,A,L1)") "static      = T"
  end select
  write (unit, "(3x,A,L1)") "loaded      = ", object%loaded
  write (unit, "(3x,A,A,A)") "MD5 sum    = '", object%md5sum, "'"
  if (write_lib) then
    write (unit, "(3x,A,A,A)") "Mdl flags = '", &
      char (object%modellibs_ldflags), "'"
  end if
  select type (object)
  type is (prclib_driver_dynamic_t)
    write (unit, *)
    call object%dlaccess%write (unit)
  end select
  write (unit, *)
  if (allocated (object%record)) then
    write (unit, "(1x,A)") "Matrix-element code entries:"
    do i = 1, object%n_processes
      call object%record(i)%write (unit)
    end do
  else
    write (unit, "(1x,A)") "Matrix-element code entries: [undefined]"
  end if
end subroutine prclib_driver_write

```

Allocate a library as either static or dynamic. For static libraries, the procedure defers control to an external procedure which knows about the available static libraries. By default, this procedure is empty, but when we build a stand-alone executable, we replace the dummy by an actual dispatcher for the available static libraries. If the static dispatcher was not successful, we allocate a dynamic library.

The default version of `dispatch_prclib_static` resides in the `prebuilt` section of the `WHIZARD` tree, in a separate library. It does nothing, but can be replaced by a different procedure that allocates a static library driver if requested by name. Due to a bug of `bind(C)` features with submodules in `gfortran 7/8/9` (and maybe together with `MPI`) this needs to be in the module, not the submodule.

```

<Prclib interfaces: public>+≡
    public :: dispatch_prclib_driver

<Prclib interfaces: main procedures>+≡
    subroutine dispatch_prclib_driver &
        (driver, basename, modellibs_ldflags)
        class(prclib_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        type(string_t), intent(in), optional :: modellibs_ldflags
        procedure(dispatch_prclib_driver) :: dispatch_prclib_static
        if (allocated (driver)) deallocate (driver)
        call dispatch_prclib_static (driver, basename)
        if (.not. allocated (driver)) then
            allocate (prclib_driver_dynamic_t :: driver)
        end if
        driver%basename = basename
        driver%modellibs_ldflags = modellibs_ldflags
    end subroutine dispatch_prclib_driver

```

Initialize the ID array and set `n_processes` accordingly.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: init => prclib_driver_init

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_init (driver, n_processes)
        class(prclib_driver_t), intent(inout) :: driver
        integer, intent(in) :: n_processes
    end subroutine prclib_driver_init

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_init (driver, n_processes)
        class(prclib_driver_t), intent(inout) :: driver
        integer, intent(in) :: n_processes
        driver%n_processes = n_processes
        allocate (driver%record (n_processes))
    end subroutine prclib_driver_init

```

Set the MD5 sum. This is separate because the MD5 sum may be known only after initialization.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: set_md5sum => prclib_driver_set_md5sum

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_set_md5sum (driver, md5sum)
        class(prclib_driver_t), intent(inout) :: driver
        character(32), intent(in) :: md5sum
    end subroutine prclib_driver_set_md5sum

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_set_md5sum (driver, md5sum)
        class(prclib_driver_t), intent(inout) :: driver
        character(32), intent(in) :: md5sum
        driver%md5sum = md5sum
    end subroutine prclib_driver_set_md5sum

```

Set the process record for a specific library entry. If the index is zero, we do nothing.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: set_record => prclib_driver_set_record

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_set_record (driver, i, &
    id, model_name, features, writer)
    class(prclib_driver_t), intent(inout) :: driver
    integer, intent(in) :: i
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: features
    class(prc_writer_t), intent(in), pointer :: writer
  end subroutine prclib_driver_set_record

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_set_record (driver, i, &
    id, model_name, features, writer)
    class(prclib_driver_t), intent(inout) :: driver
    integer, intent(in) :: i
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: features
    class(prc_writer_t), intent(in), pointer :: writer
    if (i > 0) then
      associate (record => driver%record(i))
        record%id = id
        record%model_name = model_name
        allocate (record%feature (size (features)))
        record%feature = features
        record%writer => writer
      end associate
    end if
  end subroutine prclib_driver_set_record

```

Write all USE directives for a given feature, scanning the array of processes. Only Fortran-module processes count. Then, write interface blocks for the remaining processes.

The implicit none statement must go in-between.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_interfaces => prclib_driver_write_interfaces

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_write_interfaces (driver, unit, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: feature
  end subroutine prclib_driver_write_interfaces

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_write_interfaces (driver, unit, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: feature

```

```

integer :: i
do i = 1, driver%n_processes
    call driver%record(i)%write_use_line (unit, feature)
end do
write (unit, "(2x,9A)") "implicit none"
do i = 1, driver%n_processes
    call driver%record(i)%write_interface (unit, feature)
end do
end subroutine prclib_driver_write_interfaces

```

14.2.7 Write makefile

The makefile contains constant parts, parts that depend on the library name, and parts that depend on the specific processes and their types.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: generate_makefile => prclib_driver_generate_makefile

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_generate_makefile (driver, unit, os_data, verbose, testflag)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
    end subroutine prclib_driver_generate_makefile

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_generate_makefile (driver, unit, os_data, verbose, testflag)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        integer :: i
        write (unit, "(A)") "# WHIZARD: Makefile for process library '" &
            // char (driver%basename) // "'"
        write (unit, "(A)") "# Automatically generated file, do not edit"
        write (unit, "(A)") ""
        write (unit, "(A)") "# Integrity check (don't modify the following line!)"
        write (unit, "(A)") "MD5SUM = '" // driver%md5sum // "'"
        write (unit, "(A)") ""
        write (unit, "(A)") "# Library name"
        write (unit, "(A)") "BASE = " // char (driver%basename)
        write (unit, "(A)") ""
        write (unit, "(A)") "# Compiler"
        write (unit, "(A)") "FC = " // char (os_data%fc)
        write (unit, "(A)") "CC = " // char (os_data%cc)
        write (unit, "(A)") ""
        write (unit, "(A)") "# Included libraries"
        write (unit, "(A)") "FCINCL = " // char (os_data%whizard_includes)
        write (unit, "(A)") ""
        write (unit, "(A)") "# Compiler flags"
        write (unit, "(A)") "FCFLAGS = " // char (os_data%fcflags)
    end subroutine prclib_driver_generate_makefile

```

```

write (unit, "(A)") "FCFLAGS_PIC = " // char (os_data%fcflags_pic)
write (unit, "(A)") "CFLAGS = " // char (os_data%cflags)
write (unit, "(A)") "CFLAGS_PIC = " // char (os_data%cflags_pic)
write (unit, "(A)") "LDFLAGS = " // char (os_data%whizard_ldflags) &
// " " // char (os_data%ldflags) // " " // &
char (driver%modellibs_ldflags)
write (unit, "(A)") ""
write (unit, "(A)") "# LaTeX setup"
write (unit, "(A)") "LATEX = " // char (os_data%latex)
write (unit, "(A)") "MPOST = " // char (os_data%mpost)
write (unit, "(A)") "DVIPS = " // char (os_data%dvips)
write (unit, "(A)") "PS2PDF = " // char (os_data%ps2pdf)
write (unit, "(A)") 'TEX_FLAGS = "$TEXINPUTS:" // &
char(os_data%whizard_texpath) // ''
write (unit, "(A)") 'MP_FLAGS = "$MPINPUTS:" // &
char(os_data%whizard_texpath) // ''
write (unit, "(A)") ""
write (unit, "(A)") "# Libtool"
write (unit, "(A)") "LIBTOOL = " // char (os_data%whizard_libtool)
if (verbose) then
write (unit, "(A)") "FCOMPILE = $(LIBTOOL) -tag=FC -mode=compile"
write (unit, "(A)") "CCOMPILE = $(LIBTOOL) -tag=CC -mode=compile"
write (unit, "(A)") "LINK = $(LIBTOOL) -tag=FC -mode=link"
else
write (unit, "(A)") "FCOMPILE = @$(LIBTOOL) -silent -tag=FC -mode=compile"
write (unit, "(A)") "CCOMPILE = @$(LIBTOOL) -silent -tag=CC -mode=compile"
write (unit, "(A)") "LINK = @$(LIBTOOL) -silent -tag=FC -mode=link"
end if
write (unit, "(A)") ""
write (unit, "(A)") "# Compile commands (default)"
write (unit, "(A)") "LTF_COMPILE = $(FCOMPILE) $(FC) -c &
&$(FCINCL) $(FCFLAGS) $(FCFLAGS_PIC)"
write (unit, "(A)") "LTCC_COMPILE = $(CCOMPILE) $(CC) -c &
&$(CFLAGS) $(CFLAGS_PIC)"
write (unit, "(A)") ""
write (unit, "(A)") "# Default target"
write (unit, "(A)") "all: link diags"
write (unit, "(A)") ""
write (unit, "(A)") "# Matrix-element code files"
do i = 1, size (driver%record)
call driver%record(i)%write_makefile_code (unit, os_data, verbose, testflag)
end do
write (unit, "(A)") ""
write (unit, "(A)") "# Library driver"
write (unit, "(A)") "$(BASE).lo: $(BASE).f90 $(OBJECTS)"
write (unit, "(A)") TAB // "$(LTF_COMPILE) $<"
if (.not. verbose) then
write (unit, "(A)") TAB // '@echo " FC " $@'
end if
write (unit, "(A)") ""
write (unit, "(A)") "# Library"
write (unit, "(A)") "$(BASE).la: $(BASE).lo $(OBJECTS)"
if (.not. verbose) then
write (unit, "(A)") TAB // '@echo " FCLD " $@'

```

```

end if
write (unit, "(A)") TAB // "$(LINK) $(FC) -module -rpath /dev/null &
    &$(FCFLAGS) $(LDFLAGS) -o $(BASE).la $"
write (unit, "(A)") ""
write (unit, "(A)") "# Main targets"
write (unit, "(A)") "link: compile $(BASE).la"
write (unit, "(A)") "compile: source $(OBJECTS) $(TEX_OBJECTS) $(BASE).lo"
write (unit, "(A)") "compile_tex: $(TEX_OBJECTS)"
write (unit, "(A)") "source: $(SOURCES) $(BASE).f90 $(TEX_SOURCES)"
write (unit, "(A)") ".PHONY: link diags compile compile_tex source"
write (unit, "(A)") ""
write (unit, "(A)") "# Specific cleanup targets"
do i = 1, size (driver%record)
    write (unit, "(A)") "clean-" // char (driver%record(i)%id) // ":"
    write (unit, "(A)") ".PHONY: clean-" // char (driver%record(i)%id)
end do
write (unit, "(A)") ""
write (unit, "(A)") "# Generic cleanup targets"
write (unit, "(A)") "clean-library:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(BASE).la"
else
    write (unit, "(A)") TAB // '@echo " RM          $(BASE).la"'
    write (unit, "(A)") TAB // "@rm -f $(BASE).la"
end if
write (unit, "(A)") "clean-objects:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(BASE).lo $(BASE)_driver.mod &
        &$(CLEAN_OBJECTS)"
else
    write (unit, "(A)") TAB // '@echo " RM          $(BASE).lo &
        &$(BASE)_driver.mod $(CLEAN_OBJECTS)"'
    write (unit, "(A)") TAB // "@rm -f $(BASE).lo $(BASE)_driver.mod &
        &$(CLEAN_OBJECTS)"
end if
write (unit, "(A)") "clean-source:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(CLEAN_SOURCES)"
else
    write (unit, "(A)") TAB // '@echo " RM          $(CLEAN_SOURCES)"'
    write (unit, "(A)") TAB // "@rm -f $(CLEAN_SOURCES)"
end if
write (unit, "(A)") "clean-driver:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(BASE).f90"
else
    write (unit, "(A)") TAB // '@echo " RM          $(BASE).f90"'
    write (unit, "(A)") TAB // "@rm -f $(BASE).f90"
end if
write (unit, "(A)") "clean-makefile:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(BASE).makefile"
else
    write (unit, "(A)") TAB // '@echo " RM          $(BASE).makefile"'

```

```

        write (unit, "(A)") TAB // "@rm -f $(BASE).makefile"
    end if
    write (unit, "(A)") ".PHONY: clean-library clean-objects &
        &clean-source clean-driver clean-makefile"
    write (unit, "(A)") ""
    write (unit, "(A)") "clean: clean-library clean-objects clean-source"
    write (unit, "(A)") "distclean: clean clean-driver clean-makefile"
    write (unit, "(A)") ".PHONY: clean distclean"
end subroutine prclib_driver_generate_makefile

```

14.2.8 Write driver file

This procedure writes the process library driver source code to the specified output unit. The individual routines for writing source-code procedures are given below.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: generate_driver_code => prclib_driver_generate_code

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_generate_code (driver, unit)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
    end subroutine prclib_driver_generate_code

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_generate_code (driver, unit)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t) :: prefix
        integer :: i

        prefix = driver%basename // "_"

        write (unit, "(A)") "! WHIZARD matrix-element code interface"
        write (unit, "(A)") "!"
        write (unit, "(A)") "! Automatically generated file, do not edit"
        call driver%write_module (unit, prefix)
        call driver%write_lib_md5sum_fun (unit, prefix)
        call driver%write_get_n_processes_fun (unit, prefix)
        call driver%write_get_process_id_fun (unit, prefix)
        call driver%write_get_model_name_fun (unit, prefix)
        call driver%write_get_md5sum_fun (unit, prefix)
        call driver%write_string_to_array_fun (unit, prefix)
        call driver%write_get_openmp_status_fun (unit, prefix)
        call driver%write_get_int_fun (unit, prefix, var_str ("n_in"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_out"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_flv"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_hel"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_col"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_cin"))
        call driver%write_get_int_fun (unit, prefix, var_str ("n_cf"))
        call driver%write_set_int_sub (unit, prefix, var_str ("flv_state"))
        call driver%write_set_int_sub (unit, prefix, var_str ("hel_state"))

```



```

call driver%write_set_col_state_sub (unit, prefix)
call driver%write_set_color_factors_sub (unit, prefix)
call driver%write_get_fptr_sub (unit, prefix)
do i = 1, driver%n_processes
    call driver%record(i)%write_wrappers (unit)
end do
end subroutine prclib_driver_generate_code

```

The driver module is used and required *only* if we intend to link the library statically. Then, it provides the (static) driver type as a concrete implementation of the abstract library driver. This type contains the internal dispatcher for assigning the library procedures to their appropriate procedure pointers. In the dynamical case, the assignment is done via the base-type dispatcher which invokes the DL mechanism.

However, compiling this together with the rest in any case should not do any harm.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure, nopass :: write_module => prclib_driver_write_module

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_write_module (unit, prefix)
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
    end subroutine prclib_driver_write_module

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_write_module (unit, prefix)
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
        write (unit, "(A)") ""
        write (unit, "(A)") "! Module: define library driver as an extension &
            &of the abstract driver type."
        write (unit, "(A)") "! This is used _only_ by the library dispatcher &
            &of a static executable."
        write (unit, "(A)") "! For a dynamical library, the stand-alone proce&
            &dures are linked via libdl."
        write (unit, "(A)") ""
        write (unit, "(A)") "module " &
            // char (prefix) // "driver"
        write (unit, "(A)") "    use iso_c_binding"
        write (unit, "(A)") "    use iso_varying_string, string_t => varying_string"
        write (unit, "(A)") "    use diagnostics"
        write (unit, "(A)") "    use prclib_interfaces"
        write (unit, "(A)") ""
        write (unit, "(A)") "    implicit none"
        write (unit, "(A)") ""
        write (unit, "(A)") "    type, extends (prclib_driver_t) :: " &
            // char (prefix) // "driver_t"
        write (unit, "(A)") "        contains"
        write (unit, "(A)") "        procedure :: get_c_funptr => " &
            // char (prefix) // "driver_get_c_funptr"
        write (unit, "(A)") "    end type " &
            // char (prefix) // "driver_t"
        write (unit, "(A)") ""

```

```

write (unit, "(A)") "contains"
write (unit, "(A)") ""
write (unit, "(A)") " function " &
    // char (prefix) // "driver_get_c_funptr (driver, feature) result &
    &(c_funptr)"
write (unit, "(A)") " class(" &
    // char (prefix) // "driver_t), intent(inout) :: driver"
write (unit, "(A)") " type(string_t), intent(in) :: feature"
write (unit, "(A)") " type(c_funptr) :: c_funptr"
call write_decl ("get_n_processes", "get_n_processes")
call write_decl ("get_stringptr", "get_process_id_ptr")
call write_decl ("get_stringptr", "get_model_name_ptr")
call write_decl ("get_stringptr", "get_md5sum_ptr")
call write_decl ("get_log", "get_openmp_status")
call write_decl ("get_int", "get_n_in")
call write_decl ("get_int", "get_n_out")
call write_decl ("get_int", "get_n_flv")
call write_decl ("get_int", "get_n_hel")
call write_decl ("get_int", "get_n_col")
call write_decl ("get_int", "get_n_cin")
call write_decl ("get_int", "get_n_cf")
call write_decl ("set_int_tab1", "set_flv_state_ptr")
call write_decl ("set_int_tab1", "set_hel_state_ptr")
call write_decl ("set_col_state", "set_col_state_ptr")
call write_decl ("set_color_factors", "set_color_factors_ptr")
call write_decl ("get_fptr", "get_fptr")
write (unit, "(A)") " select case (char (feature))"
call write_case ("get_n_processes")
call write_case ("get_process_id_ptr")
call write_case ("get_model_name_ptr")
call write_case ("get_md5sum_ptr")
call write_case ("get_openmp_status")
call write_case ("get_n_in")
call write_case ("get_n_out")
call write_case ("get_n_flv")
call write_case ("get_n_hel")
call write_case ("get_n_col")
call write_case ("get_n_cin")
call write_case ("get_n_cf")
call write_case ("set_flv_state_ptr")
call write_case ("set_hel_state_ptr")
call write_case ("set_col_state_ptr")
call write_case ("set_color_factors_ptr")
call write_case ("get_fptr")
write (unit, "(A)") " case default"
write (unit, "(A)") " call msg_bug ('prclib2 driver setup: unknown &
    &function name')"
write (unit, "(A)") " end select"
write (unit, "(A)") " end function " &
    // char (prefix) // "driver_get_c_funptr"
write (unit, "(A)") ""
write (unit, "(A)") "end module " &
    // char (prefix) // "driver"
write (unit, "(A)") ""

```

```

        write (unit, "(A)")  "! Stand-alone external procedures: used for both &
                               &static and dynamic linkage"
contains
  subroutine write_decl (template, feature)
    character(*), intent(in) :: template, feature
    write (unit, "(A)")  "    procedure(prc_" // template // ") &"
    write (unit, "(A)")  "        :: " &
        // char (prefix) // feature
  end subroutine write_decl
  subroutine write_case (feature)
    character(*), intent(in) :: feature
    write (unit, "(A)")  "    case ('" // feature // "')"
    write (unit, "(A)")  "        c_fptr = c_funloc (" &
        // char (prefix) // feature // ")"
  end subroutine write_case
end subroutine prclib_driver_write_module

```

This function provides the overall library MD5sum. The function is for internal use (therefore not bind(C)), the external interface is via the `get_md5sum_ptr` procedure with index 0.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_lib_md5sum_fun => prclib_driver_write_lib_md5sum_fun

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_write_lib_md5sum_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
  end subroutine prclib_driver_write_lib_md5sum_fun

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_write_lib_md5sum_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    write (unit, "(A)")  ""
    write (unit, "(A)")  "! The MD5 sum of the library"
    write (unit, "(A)")  "function " // char (prefix) &
        // "md5sum () result (md5sum)"
    write (unit, "(A)")  "  implicit none"
    write (unit, "(A)")  "  character(32) :: md5sum"
    write (unit, "(A)")  "  md5sum = ' " // driver%md5sum // "'
    write (unit, "(A)")  "end function " // char (prefix) // "md5sum"
  end subroutine prclib_driver_write_lib_md5sum_fun

```

14.2.9 Interface bodies for informational functions

These interfaces implement the communication between WHIZARD (the main program) and the process-library driver. The procedures are all BIND(C), so they can safely be exposed by the library and handled by the `dlopen` mechanism, which apparently understands only C calling conventions.

In the sections below, for each procedure, we provide both the interface itself and a procedure that writes the corresponding procedure as source code to the process library driver.

Process count

Return the number of processes contained in the library.

```
<Prclib interfaces: public>+≡
  public :: prc_get_n_processes

<Prclib interfaces: interfaces>+≡
  abstract interface
    function prc_get_n_processes () result (n) bind(C)
    import
    integer(c_int) :: n
    end function prc_get_n_processes
  end interface
```

Here is the code.

```
<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_n_processes_fun

<Prclib interfaces: sub interfaces>+≡
  module subroutine write_get_n_processes_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    end subroutine write_get_n_processes_fun

<Prclib interfaces: procedures>+≡
  module subroutine write_get_n_processes_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    write (unit, "(A)") ""
    write (unit, "(A)") "! Return the number of processes in this library"
    write (unit, "(A)") "function " // char (prefix) &
      // "get_n_processes () result (n) bind(C)"
    write (unit, "(A)") " use iso_c_binding"
    write (unit, "(A)") " implicit none"
    write (unit, "(A)") " integer(c_int) :: n"
    write (unit, "(A,I0)") " n = ", driver%n_processes
    write (unit, "(A)") "end function " // char (prefix) &
      // "get_n_processes"
    end subroutine write_get_n_processes_fun
```

Informational string functions

These functions return constant information about the matrix-element code.

The following procedures have to return strings. With the BIND(C) constraint, we choose to return the C pointer to a string, and its length, so the procedures implement this interface. They are actually subroutines.

```
<Prclib interfaces: public>+≡
  public :: prc_get_stringptr
```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_get_stringptr (i, cptr, len) bind(C)
      import
      integer(c_int), intent(in) :: i
      type(c_ptr), intent(out) :: cptr
      integer(c_int), intent(out) :: len
    end subroutine prc_get_stringptr
  end interface

```

To hide this complication, we introduce a subroutine that converts the returned C pointer to a `string_t` object. As a side effect, we deallocate the original after conversion – otherwise, we might have a memory leak.

For the conversion, we first pointer-convert the C pointer to a Fortran character array pointer, length 1 and size `len`. Using argument association and an internal subroutine, we convert this to a character array with length `len` and size 1. Using ordinary assignment, we finally convert this to `string_t`.

The function takes the pointer-returning function as an argument. The index `i` identifies the process in the library.

```

<Prclib interfaces: procedures>+≡
  subroutine get_string_via_cptr (string, i, get_stringptr)
    type(string_t), intent(out) :: string
    integer, intent(in) :: i
    procedure(prc_get_stringptr) :: get_stringptr
    type(c_ptr) :: cptr
    integer(c_int) :: pid, len
    character(kind=c_char), dimension(:), pointer :: c_array
    pid = i
    call get_stringptr (pid, cptr, len)
    if (c_associated (cptr)) then
      call c_f_pointer (cptr, c_array, shape = [len])
      call set_string (c_array)
      call get_stringptr (0_c_int, cptr, len)
    else
      string = ""
    end if
  contains
    subroutine set_string (buffer)
      character(len, kind=c_char), dimension(1), intent(in) :: buffer
      string = buffer(1)
    end subroutine set_string
  end subroutine get_string_via_cptr

```

Since the module procedures return Fortran strings, we have to convert them. This is the necessary auxiliary routine. The routine is not `BIND(C)`, it is not accessed from outside.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure, nopass :: write_string_to_array_fun

<Prclib interfaces: sub interfaces>+≡
  module subroutine write_string_to_array_fun (unit, prefix)
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
  end subroutine write_string_to_array_fun

```

<Prclib interfaces: procedures>+≡

```

module subroutine write_string_to_array_fun (unit, prefix)
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  write (unit, "(A)") ""
  write (unit, "(A)") "! Auxiliary: convert character string &
    &to array pointer"
  write (unit, "(A)") "subroutine " // char (prefix) &
    // "string_to_array (string, a)"
  write (unit, "(A)") " use iso_c_binding"
  write (unit, "(A)") " implicit none"
  write (unit, "(A)") " character(*), intent(in) :: string"
  write (unit, "(A)") " character(kind=c_char), dimension(:), &
    &allocatable, intent(out) :: a"
  write (unit, "(A)") " integer :: i"
  write (unit, "(A)") " allocate (a (len (string)))"
  write (unit, "(A)") " do i = 1, size (a)"
  write (unit, "(A)") "   a(i) = string(i:i)"
  write (unit, "(A)") " end do"
  write (unit, "(A)") "end subroutine " // char (prefix) &
    // "string_to_array"
end subroutine write_string_to_array_fun

```

The above routine is called by other functions. It is not in a module, so they need its interface explicitly.

<Prclib interfaces: procedures>+≡

```

subroutine write_string_to_array_interface (unit, prefix)
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  write (unit, "(2x,A)") "interface"
  write (unit, "(2x,A)") " subroutine " // char (prefix) &
    // "string_to_array (string, a)"
  write (unit, "(2x,A)") " use iso_c_binding"
  write (unit, "(2x,A)") " implicit none"
  write (unit, "(2x,A)") " character(*), intent(in) :: string"
  write (unit, "(2x,A)") " character(kind=c_char), dimension(:), &
    &allocatable, intent(out) :: a"
  write (unit, "(2x,A)") " end subroutine " // char (prefix) &
    // "string_to_array"
  write (unit, "(2x,A)") "end interface"
end subroutine write_string_to_array_interface

```

Here are the info functions which return strings, implementing the interface `prc_get_stringptr`.

Return the process ID for each process.

<Prclib interfaces: prclib driver: TBP>+≡

```

procedure :: write_get_process_id_fun

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine write_get_process_id_fun (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix

```

```

end subroutine write_get_process_id_fun

<Prclib interfaces: procedures>+≡
module subroutine write_get_process_id_fun (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  integer :: i
  write (unit, "(A)") ""
  write (unit, "(A)") "! Return the process ID of process #i &
    &(as a C pointer to a character array)"
  write (unit, "(A)") "subroutine " // char (prefix) &
    // "get_process_id_ptr (i, cptr, len) bind(C)"
  write (unit, "(A)") " use iso_c_binding"
  write (unit, "(A)") " implicit none"
  write (unit, "(A)") " integer(c_int), intent(in) :: i"
  write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
  write (unit, "(A)") " integer(c_int), intent(out) :: len"
  write (unit, "(A)") " character(kind=c_char), dimension(:), &
    &allocatable, target, save :: a"
  call write_string_to_array_interface (unit, prefix)
  write (unit, "(A)") " select case (i)"
  write (unit, "(A)") " case (0); if (allocated (a)) deallocate (a)"
  do i = 1, driver%n_processes
    write (unit, "(A,I0,9A)") " case (" , i, "); ", &
      "call ", char (prefix), "string_to_array ('", &
      char (driver%record(i)%id), "'", a)"
  end do
  write (unit, "(A)") " end select"
  write (unit, "(A)") " if (allocated (a)) then"
  write (unit, "(A)") " cptr = c_loc (a)"
  write (unit, "(A)") " len = size (a)"
  write (unit, "(A)") " else"
  write (unit, "(A)") " cptr = c_null_ptr"
  write (unit, "(A)") " len = 0"
  write (unit, "(A)") " end if"
  write (unit, "(A)") "end subroutine " // char (prefix) &
    // "get_process_id_ptr"
end subroutine write_get_process_id_fun

```

Return the model name, given explicitly.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_model_name_fun

<Prclib interfaces: sub interfaces>+≡
  module subroutine write_get_model_name_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
  end subroutine write_get_model_name_fun

<Prclib interfaces: procedures>+≡
  module subroutine write_get_model_name_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit

```

```

type(string_t), intent(in) :: prefix
integer :: i
write (unit, "(A)") ""
write (unit, "(A)") " ! Return the model name for process #i &
    &(as a C pointer to a character array)"
write (unit, "(A)") " subroutine " // char (prefix) &
    // "get_model_name_ptr (i, cptr, len) bind(C)"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " implicit none"
write (unit, "(A)") " integer(c_int), intent(in) :: i"
write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
write (unit, "(A)") " integer(c_int), intent(out) :: len"
write (unit, "(A)") " character(kind=c_char), dimension(:), &
    &allocatable, target, save :: a"
call write_string_to_array_interface (unit, prefix)
write (unit, "(A)") " select case (i)"
write (unit, "(A)") " case (0); if (allocated (a)) deallocate (a)"
do i = 1, driver%n_processes
    write (unit, "(A,I0,9A)") " case (" , i, "); " , &
        "call " , char (prefix), "string_to_array ('" , &
        char (driver%record(i)%model_name), &
        "' , a)"
end do
write (unit, "(A)") " end select"
write (unit, "(A)") " if (allocated (a)) then"
write (unit, "(A)") " cptr = c_loc (a)"
write (unit, "(A)") " len = size (a)"
write (unit, "(A)") " else"
write (unit, "(A)") " cptr = c_null_ptr"
write (unit, "(A)") " len = 0"
write (unit, "(A)") " end if"
write (unit, "(A)") "end subroutine " // char (prefix) &
    // "get_model_name_ptr"
end subroutine write_get_model_name_fun

```

Call the MD5 sum function for the process. The function calls the corresponding function of the matrix-element code, and it returns the C address of a character array with length 32.

<Prclib interfaces: prclib driver: TBP>+≡

```

procedure :: write_get_md5sum_fun

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine write_get_md5sum_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
end subroutine write_get_md5sum_fun

```

<Prclib interfaces: procedures>+≡

```

module subroutine write_get_md5sum_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    integer :: i

```



```

write (unit, "(A)") ""
write (unit, "(A)") "! Return the MD5 sum for the process configuration &
&(as a C pointer to a character array)"
write (unit, "(A)") "subroutine " // char (prefix) &
// "get_md5sum_ptr (i, cptr, len) bind(C)"
write (unit, "(A)") " use iso_c_binding"
call driver%write_interfaces (unit, var_str ("md5sum"))
write (unit, "(A)") " interface"
write (unit, "(A)") " function " // char (prefix) &
// "md5sum () result (md5sum)"
write (unit, "(A)") " character(32) :: md5sum"
write (unit, "(A)") " end function " // char (prefix) // "md5sum"
write (unit, "(A)") " end interface"
write (unit, "(A)") " integer(c_int), intent(in) :: i"
write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
write (unit, "(A)") " integer(c_int), intent(out) :: len"
write (unit, "(A)") " character(kind=c_char), dimension(32), &
&target, save :: md5sum"
write (unit, "(A)") " select case (i)"
write (unit, "(A)") " case (0)"
write (unit, "(A)") " call copy (" // char (prefix) // "md5sum ()"
write (unit, "(A)") " cptr = c_loc (md5sum)"
do i = 1, driver%n_processes
write (unit, "(A,I0,A)") " case (" , i, ")"
call driver%record(i)%write_md5sum_call (unit)
end do
write (unit, "(A)") " case default"
write (unit, "(A)") " cptr = c_null_ptr"
write (unit, "(A)") " end select"
write (unit, "(A)") " len = 32"
write (unit, "(A)") "contains"
write (unit, "(A)") " subroutine copy (md5sum_tmp)"
write (unit, "(A)") " character, dimension(32), intent(in) :: &
&md5sum_tmp"
write (unit, "(A)") " md5sum = md5sum_tmp"
write (unit, "(A)") " end subroutine copy"
write (unit, "(A)") "end subroutine " // char (prefix) &
// "get_md5sum_ptr"
end subroutine write_get_md5sum_fun

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib_driver_record: TBP>+≡
procedure :: write_md5sum_call => prclib_driver_record_write_md5sum_call

<Prclib interfaces: sub interfaces>+≡
module subroutine prclib_driver_record_write_md5sum_call (record, unit)
class(prclib_driver_record_t), intent(in) :: record
integer, intent(in) :: unit
end subroutine prclib_driver_record_write_md5sum_call

<Prclib interfaces: procedures>+≡
module subroutine prclib_driver_record_write_md5sum_call (record, unit)
class(prclib_driver_record_t), intent(in) :: record
integer, intent(in) :: unit
call record%writer%write_md5sum_call (unit, record%id)

```

```
end subroutine prclib_driver_record_write_md5sum_call
```

The interface goes into the writer base type:

```
<Prclib interfaces: prc writer: TBP>+≡
```

```
procedure(write_code), deferred :: write_md5sum_call
```

In the Fortran module case, we take a detour. The string returned by the Fortran function is copied into a fixed-size array. The copy routine is an internal subroutine of `get_md5sum_ptr`. We return the C address of the target array.

```
<Prclib interfaces: prc writer f module: TBP>+≡
```

```
procedure :: write_md5sum_call => prc_writer_f_module_write_md5sum_call
```

```
<Prclib interfaces: sub interfaces>+≡
```

```
module subroutine prc_writer_f_module_write_md5sum_call (writer, unit, id)
  class(prc_writer_f_module_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
end subroutine prc_writer_f_module_write_md5sum_call
```

```
<Prclib interfaces: procedures>+≡
```

```
module subroutine prc_writer_f_module_write_md5sum_call (writer, unit, id)
  class(prc_writer_f_module_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)") "call copy (" , &
    char (writer%get_c_procname (id, var_str ("md5sum"))), " ()"
  write (unit, "(5x,9A)") "cptr = c_loc (md5sum)"
end subroutine prc_writer_f_module_write_md5sum_call
```

In the C library case, the library function returns a C pointer, which we can just copy.

```
<Prclib interfaces: prc writer c lib: TBP>≡
```

```
procedure :: write_md5sum_call => prc_writer_c_lib_write_md5sum_call
```

```
<Prclib interfaces: sub interfaces>+≡
```

```
module subroutine prc_writer_c_lib_write_md5sum_call (writer, unit, id)
  class(prc_writer_c_lib_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
end subroutine prc_writer_c_lib_write_md5sum_call
```

```
<Prclib interfaces: procedures>+≡
```

```
module subroutine prc_writer_c_lib_write_md5sum_call (writer, unit, id)
  class(prc_writer_c_lib_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)") &
    "cptr = ", &
    char (writer%get_c_procname (id, var_str ("get_md5sum"))), " ()"
end subroutine prc_writer_c_lib_write_md5sum_call
```

Actual references to the info functions

The string-valued info functions return C character arrays. For the API of the library driver, we provide convenience functions which (re)convert those arrays into `string_t` objects.

```
(Prclib interfaces: prclib driver: TBP)+≡
  procedure :: get_process_id => prclib_driver_get_process_id
  procedure :: get_model_name => prclib_driver_get_model_name
  procedure :: get_md5sum => prclib_driver_get_md5sum

(Prclib interfaces: sub interfaces)+≡
  module function prclib_driver_get_process_id (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
  end function prclib_driver_get_process_id
  module function prclib_driver_get_model_name (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
  end function prclib_driver_get_model_name
  module function prclib_driver_get_md5sum (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
  end function prclib_driver_get_md5sum

(Prclib interfaces: procedures)+≡
  module function prclib_driver_get_process_id (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    call get_string_via_cptr (string, i, driver%get_process_id_ptr)
  end function prclib_driver_get_process_id

  module function prclib_driver_get_model_name (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    call get_string_via_cptr (string, i, driver%get_model_name_ptr)
  end function prclib_driver_get_model_name

  module function prclib_driver_get_md5sum (driver, i) result (string)
    type(string_t) :: string
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    call get_string_via_cptr (string, i, driver%get_md5sum_ptr)
  end function prclib_driver_get_md5sum
```

Informational logical functions

When returning a logical value, we use the C boolean type, which may differ from Fortran.

```
(Prclib interfaces: public)+≡
```

```

    public :: prc_get_log
<Prclib interfaces: interfaces>+≡
    abstract interface
        function prc_get_log (pid) result (l) bind(C)
            import
            integer(c_int), intent(in) :: pid
            logical(c_bool) :: l
        end function prc_get_log
    end interface

Return a logical flag which tells whether OpenMP is supported for a specific
process code.

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: write_get_openmp_status_fun

<Prclib interfaces: sub interfaces>+≡
    module subroutine write_get_openmp_status_fun (driver, unit, prefix)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
    end subroutine write_get_openmp_status_fun

<Prclib interfaces: procedures>+≡
    module subroutine write_get_openmp_status_fun (driver, unit, prefix)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
        integer :: i
        write (unit, "(A)") ""
        write (unit, "(A)") "! Return the OpenMP support status"
        write (unit, "(A)") "function " // char (prefix) &
            // "get_openmp_status (i) result (openmp_status) bind(C)"
        write (unit, "(A)") " use iso_c_binding"
        call driver%write_interfaces (unit, var_str ("openmp_supported"))
        write (unit, "(A)") " integer(c_int), intent(in) :: i"
        write (unit, "(A)") " logical(c_bool) :: openmp_status"
        write (unit, "(A)") " select case (i)"
        do i = 1, driver%n_processes
            write (unit, "(A,I0,9A)") " case (" , i, "); ", &
                "openmp_status = ", &
                char (driver%record(i)%get_c_procname &
                    (var_str ("openmp_supported"))), " ()"
        end do
        write (unit, "(A)") " end select"
        write (unit, "(A)") "end function " // char (prefix) &
            // "get_openmp_status"
    end subroutine write_get_openmp_status_fun

```

Informational integer functions

Various process metadata are integer values. We can use a single interface for all of them.

```

<Prclib interfaces: public>+≡
    public :: prc_get_int

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    function prc_get_int (pid) result (n) bind(C)
      import
        integer(c_int), intent(in) :: pid
        integer(c_int) :: n
      end function prc_get_int
  end interface

```

This function returns any data of type integer, for each process.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_int_fun

```

```

<Prclib interfaces: sub interfaces>+≡
  module subroutine write_get_int_fun (driver, unit, prefix, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    type(string_t), intent(in) :: feature
  end subroutine write_get_int_fun

```

```

<Prclib interfaces: procedures>+≡
  module subroutine write_get_int_fun (driver, unit, prefix, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    type(string_t), intent(in) :: feature
    integer :: i
    write (unit, "(A)") ""
    write (unit, "(9A)") "! Return the value of ", char (feature)
    write (unit, "(9A)") "function ", char (prefix), &
      "get_", char (feature), " (pid)", &
      " result (" , char (feature), ") bind(C)"
    write (unit, "(9A)") " use iso_c_binding"
    call driver%write_interfaces (unit, feature)
    write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
    write (unit, "(9A)") " integer(c_int) :: ", char (feature)
    write (unit, "(9A)") " select case (pid)"
    do i = 1, driver%n_processes
      write (unit, "(2x,A,I0,9A)" "case (" , i, "); ", &
        char (feature), " = ", &
        char (driver%record(i)%get_c_procname (feature)), &
        " ()"
    end do
    write (unit, "(9A)") " end select"
    write (unit, "(9A)") "end function ", char (prefix), &
      "get_", char (feature)
  end subroutine write_get_int_fun

```

Write a **case** line that assigns the value of the external function to the current return value.

```

<Prclib interfaces: procedures>+≡
  subroutine write_case_int_fun (record, unit, i, feature)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit

```

```

integer, intent(in) :: i
type(string_t), intent(in) :: feature
write (unit, "(5x,A,I0,9A)") "case (" , i, ")"; " , &
      char (feature), " = " , char (record%get_c_procname (feature))
end subroutine write_case_int_fun

```

Flavor and helicity tables

Transferring tables is more complicated. First, a two-dimensional array.

```

<Prclib interfaces: public>+≡
public :: prc_set_int_tab1

<Prclib interfaces: interfaces>+≡
abstract interface
  subroutine prc_set_int_tab1 (pid, tab, shape) bind(C)
    import
    integer(c_int), intent(in) :: pid
    integer(c_int), dimension(*), intent(out) :: tab
    integer(c_int), dimension(2), intent(in) :: shape
  end subroutine prc_set_int_tab1
end interface

```

This subroutine returns a table of integers.

```

<Prclib interfaces: prclib driver: TBP>+≡
procedure :: write_set_int_sub

<Prclib interfaces: sub interfaces>+≡
module subroutine write_set_int_sub (driver, unit, prefix, feature)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  type(string_t), intent(in) :: feature
end subroutine write_set_int_sub

<Prclib interfaces: procedures>+≡
module subroutine write_set_int_sub (driver, unit, prefix, feature)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  type(string_t), intent(in) :: feature
  integer :: i
  write (unit, "(A)") ""
  write (unit, "(9A)") "! Set table: " , char (feature)
  write (unit, "(9A)") "subroutine " , char (prefix), &
    "set-" , char (feature), "_ptr (pid, " , char (feature), &
    " , shape) bind(C)"
  write (unit, "(9A)") " use iso_c_binding"
  call driver%write_interfaces (unit, feature)
  write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
  write (unit, "(9A)") " integer(c_int), dimension(*), intent(out) :: " , &
    char (feature)
  write (unit, "(9A)") " integer(c_int), dimension(2), intent(in) :: shape"
  write (unit, "(9A)") " integer, dimension(:,:) , allocatable :: " , &
    char (feature), "_tmp"
  write (unit, "(9A)") " integer :: i, j"

```

```

write (unit, "(9A)") " select case (pid)"
do i = 1, driver%n_processes
  write (unit, "(2x,A,I0,A)") "case (", i, ")"
  call driver%record(i)%write_int_sub_call (unit, feature)
end do
write (unit, "(9A)") " end select"
write (unit, "(9A)") "end subroutine ", char (prefix), &
  "set_", char (feature), "_ptr"
end subroutine write_set_int_sub

```

The actual call depends on the type of matrix element.

<Prclib interfaces: prclib driver record: TBP>+≡

```

procedure :: write_int_sub_call => prclib_driver_record_write_int_sub_call

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine prclib_driver_record_write_int_sub_call (record, unit, feature)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  type(string_t), intent(in) :: feature
end subroutine prclib_driver_record_write_int_sub_call

```

<Prclib interfaces: procedures>+≡

```

module subroutine prclib_driver_record_write_int_sub_call (record, unit, feature)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  type(string_t), intent(in) :: feature
  call record%writer%write_int_sub_call (unit, record%id, feature)
end subroutine prclib_driver_record_write_int_sub_call

```

The interface goes into the writer base type:

<Prclib interfaces: prc writer: TBP>+≡

```

procedure(write_feature_code), deferred :: write_int_sub_call

```

In the Fortran module case, we need an extra copy in the (academical) situation where default integer and `c_int` differ. Otherwise, we just associate a Fortran array with the C pointer and let the matrix-element subroutine fill the array.

<Prclib interfaces: prc writer f module: TBP>+≡

```

procedure :: write_int_sub_call => prc_writer_f_module_write_int_sub_call

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine prc_writer_f_module_write_int_sub_call (writer, unit, id, feature)
  class(prc_writer_f_module_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
end subroutine prc_writer_f_module_write_int_sub_call

```

<Prclib interfaces: procedures>+≡

```

module subroutine prc_writer_f_module_write_int_sub_call (writer, unit, id, feature)
  class(prc_writer_f_module_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(5x,9A)") "allocate (", char (feature), "_tmp ", &
    "(shape(1), shape(2)))"
  write (unit, "(5x,9A)") "call ", &
    char (writer%get_c_procname (id, feature)), &

```

```

        "(", char(feature), "_tmp)"
    write(unit, "(5x,9A)" forall (i=1:shape(1), j=1:shape(2)) "
    write(unit, "(8x,9A)" char(feature), "(i + shape(1)*(j-1)) = ", &
        char(feature), "_tmp", "(i,j)"
    write(unit, "(5x,9A)" "end forall"
end subroutine prc_writer_f_module_write_int_sub_call

```

In the C library case, we just transfer the C pointer to the library function.

```

<Prclib interfaces: prc_writer_c_lib: TBP>+≡
    procedure :: write_int_sub_call => prc_writer_c_lib_write_int_sub_call

<Prclib interfaces: sub interfaces>+≡
    module subroutine prc_writer_c_lib_write_int_sub_call (writer, unit, id, feature)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
    end subroutine prc_writer_c_lib_write_int_sub_call

<Prclib interfaces: procedures>+≡
    module subroutine prc_writer_c_lib_write_int_sub_call (writer, unit, id, feature)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
        write(unit, "(5x,9A)" "call ", &
            char(writer%get_c_procname(id, feature)), "(", char(feature), ")")
    end subroutine prc_writer_c_lib_write_int_sub_call

```

Color state table

The color-state specification needs a table of integers (one array per color flow) and a corresponding array of color-ghost flags.

```

<Prclib interfaces: public>+≡
    public :: prc_set_col_state

<Prclib interfaces: interfaces>+≡
    abstract interface
        subroutine prc_set_col_state (pid, col_state, ghost_flag, shape) bind(C)
            import
            integer(c_int), intent(in) :: pid
            integer(c_int), dimension(*), intent(out) :: col_state
            logical(c_bool), dimension(*), intent(out) :: ghost_flag
            integer(c_int), dimension(3), intent(in) :: shape
        end subroutine prc_set_col_state
    end interface

<Prclib interfaces: prclib_driver: TBP>+≡
    procedure :: write_set_col_state_sub

<Prclib interfaces: sub interfaces>+≡
    module subroutine write_set_col_state_sub (driver, unit, prefix)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
    end subroutine write_set_col_state_sub

```


<Prclib interfaces: procedures>+≡

```

module subroutine write_set_col_state_sub (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  integer :: i
  type(string_t) :: feature
  feature = "col_state"
  write (unit, "(A)") ""
  write (unit, "(9A)") "! Set tables: col_state, ghost_flag"
  write (unit, "(9A)") "subroutine ", char (prefix), &
    "set_col_state_ptr (pid, col_state, ghost_flag, shape) bind(C)"
  write (unit, "(9A)") " use iso_c_binding"
  call driver%write_interfaces (unit, feature)
  write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
  write (unit, "(9A)") &
    " integer(c_int), dimension(*), intent(out) :: col_state"
  write (unit, "(9A)") &
    " logical(c_bool), dimension(*), intent(out) :: ghost_flag"
  write (unit, "(9A)") &
    " integer(c_int), dimension(3), intent(in) :: shape"
  write (unit, "(9A)") &
    " integer, dimension(:, :, :), allocatable :: col_state_tmp"
  write (unit, "(9A)") &
    " logical, dimension(:, :, :), allocatable :: ghost_flag_tmp"
  write (unit, "(9A)") " integer :: i, j, k"
  write (unit, "(A)") " select case (pid)"
  do i = 1, driver%n_processes
    write (unit, "(A,I0,A)") " case (" , i, ")"
    call driver%record(i)%write_col_state_call (unit)
  end do
  write (unit, "(A)") " end select"
  write (unit, "(9A)") "end subroutine ", char (prefix), &
    "set_col_state_ptr"
end subroutine write_set_col_state_sub

```

The actual call depends on the type of matrix element.

<Prclib interfaces: prclib driver record: TBP>+≡

```

procedure :: write_col_state_call => prclib_driver_record_write_col_state_call

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine prclib_driver_record_write_col_state_call (record, unit)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
end subroutine prclib_driver_record_write_col_state_call

```

<Prclib interfaces: procedures>+≡

```

module subroutine prclib_driver_record_write_col_state_call (record, unit)
  class(prclib_driver_record_t), intent(in) :: record
  integer, intent(in) :: unit
  call record%writer%write_col_state_call (unit, record%id)
end subroutine prclib_driver_record_write_col_state_call

```

The interface goes into the writer base type:

```
<Prclib interfaces: prc writer: TBP>+≡
```

```
    procedure(write_code), deferred :: write_col_state_call
```

In the Fortran module case, we need an extra copy in the (academical) situation where default integer and `c_int` differ. Otherwise, we just associate a Fortran array with the C pointer and let the matrix-element subroutine fill the array.

```
<Prclib interfaces: prc writer f module: TBP>+≡
```

```
    procedure :: write_col_state_call => prc_writer_f_module_write_col_state_call
```

```
<Prclib interfaces: sub interfaces>+≡
```

```
    module subroutine prc_writer_f_module_write_col_state_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
    end subroutine prc_writer_f_module_write_col_state_call
```

```
<Prclib interfaces: procedures>+≡
```

```
    module subroutine prc_writer_f_module_write_col_state_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        write (unit, "(9A)") " allocate (col_state_tmp ", &
            "(shape(1), shape(2), shape(3)))"
        write (unit, "(5x,9A)") "allocate (ghost_flag_tmp ", &
            "(shape(2), shape(3)))"
        write (unit, "(5x,9A)") "call ", &
            char (writer%get_c_procname (id, var_str ("col_state"))), &
            " (col_state_tmp, ghost_flag_tmp)"
        write (unit, "(5x,9A)") "forall (i = 1:shape(2), j = 1:shape(3))"
        write (unit, "(8x,9A)") "forall (k = 1:shape(1))"
        write (unit, "(11x,9A)") &
            "col_state(k + shape(1) * (i + shape(2)*(j-1) - 1)) ", &
            "= col_state_tmp(k,i,j)"
        write (unit, "(8x,9A)") "end forall"
        write (unit, "(8x,9A)") &
            "ghost_flag(i + shape(2)*(j-1)) = ghost_flag_tmp(i,j)"
        write (unit, "(5x,9A)") "end forall"
    end subroutine prc_writer_f_module_write_col_state_call
```

In the C library case, we just transfer the C pointer to the library function.

```
<Prclib interfaces: prc writer c lib: TBP>+≡
```

```
    procedure :: write_col_state_call => prc_writer_c_lib_write_col_state_call
```

```
<Prclib interfaces: sub interfaces>+≡
```

```
    module subroutine prc_writer_c_lib_write_col_state_call (writer, unit, id)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
    end subroutine prc_writer_c_lib_write_col_state_call
```

```
<Prclib interfaces: procedures>+≡
```

```
    module subroutine prc_writer_c_lib_write_col_state_call (writer, unit, id)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
```

```

write (unit, "(5x,9A)") "call ", &
char (writer%get_c_procname (id, var_str ("col_state"))), &
" (col_state, ghost_flag)"
end subroutine prc_writer_c_lib_write_col_state_call

```

Color factors

For the color-factor information, we return two integer arrays and a complex array.

```

<Prclib interfaces: public>+≡
public :: prc_set_color_factors

<Prclib interfaces: interfaces>+≡
abstract interface
  subroutine prc_set_color_factors &
    (pid, cf_index1, cf_index2, color_factors, shape) bind(C)
  import
  integer(c_int), intent(in) :: pid
  integer(c_int), dimension(*), intent(out) :: cf_index1, cf_index2
  complex(c_default_complex), dimension(*), intent(out) :: color_factors
  integer(c_int), dimension(1), intent(in) :: shape
end subroutine prc_set_color_factors
end interface

```

This subroutine returns the color-flavor factor table.

```

<Prclib interfaces: prclib driver: TBP>+≡
procedure :: write_set_color_factors_sub

<Prclib interfaces: sub interfaces>+≡
module subroutine write_set_color_factors_sub (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
end subroutine write_set_color_factors_sub

<Prclib interfaces: procedures>+≡
module subroutine write_set_color_factors_sub (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  integer :: i
  type(string_t) :: feature
  feature = "color_factors"
  write (unit, "(A)") ""
  write (unit, "(A)") "!! Set tables: color factors"
  write (unit, "(9A)") "subroutine ", char (prefix), &
    "set_color_factors_ptr (pid, cf_index1, cf_index2, color_factors, ", &
    "shape) bind(C)"
  write (unit, "(A)") " use iso_c_binding"
  write (unit, "(A)") " use kinds"
  write (unit, "(A)") " use omega_color"
  call driver%write_interfaces (unit, feature)
  write (unit, "(A)") " integer(c_int), intent(in) :: pid"

```

```

write (unit, "(A)") " integer(c_int), dimension(1), intent(in) :: shape"
write (unit, "(A)") " integer(c_int), dimension(*), intent(out) :: &
    &cf_index1, cf_index2"
write (unit, "(A)") " complex(c_default_complex), dimension(*), &
    &intent(out) :: color_factors"
write (unit, "(A)") " type(omega_color_factor), dimension(:), &
    &allocatable :: cf"
write (unit, "(A)") " select case (pid)"
do i = 1, driver%n_processes
    write (unit, "(2x,A,I0,A)") "case (", i, ")"
    call driver%record(i)%write_color_factors_call (unit)
end do
write (unit, "(A)") " end select"
write (unit, "(A)") "end subroutine " // char (prefix) &
    // "set_color_factors_ptr"
end subroutine write_set_color_factors_sub

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_color_factors_call => prclib_driver_record_write_color_factors_call

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_record_write_color_factors_call (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
    end subroutine prclib_driver_record_write_color_factors_call

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_record_write_color_factors_call (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        call record%writer%write_color_factors_call (unit, record%id)
    end subroutine prclib_driver_record_write_color_factors_call

```

The interface goes into the writer base type:

```

<Prclib interfaces: prc writer: TBP>+≡
    procedure(write_code), deferred :: write_color_factors_call

In the Fortran module case, the matrix-element procedure fills an array of
omega_color_factor elements. We distribute this array among two integer
arrays and one complex-valued array, for which we have the C pointers.

<Prclib interfaces: prc writer f module: TBP>+≡
    procedure :: write_color_factors_call => prc_writer_f_module_write_color_factors_call

<Prclib interfaces: sub interfaces>+≡
    module subroutine prc_writer_f_module_write_color_factors_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
    end subroutine prc_writer_f_module_write_color_factors_call

<Prclib interfaces: procedures>+≡
    module subroutine prc_writer_f_module_write_color_factors_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit

```

```

type(string_t), intent(in) :: id
write (unit, "(5x,A)") "allocate (cf (shape(1)))"
write (unit, "(5x,9A)") "call ", &
    char (writer%get_c_procname (id, var_str ("color_factors"))), " (cf)"
write (unit, "(5x,9A)") "cf_index1(1:shape(1)) = cf%i1"
write (unit, "(5x,9A)") "cf_index2(1:shape(1)) = cf%i2"
write (unit, "(5x,9A)") "color_factors(1:shape(1)) = cf%factor"
end subroutine prc_writer_f_module_write_color_factors_call

```

In the C library case, we just transfer the C pointers to the library function. There are three arrays.

```

<Prclib interfaces: prc writer c lib: TBP>+=
    procedure :: write_color_factors_call => &
        prc_writer_c_lib_write_color_factors_call

<Prclib interfaces: sub interfaces>+=
    module subroutine prc_writer_c_lib_write_color_factors_call (writer, unit, id)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
    end subroutine prc_writer_c_lib_write_color_factors_call

<Prclib interfaces: procedures>+=
    module subroutine prc_writer_c_lib_write_color_factors_call (writer, unit, id)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        write (unit, "(5x,9A)") "call ", &
            char (writer%get_c_procname (id, var_str ("color_factors"))), &
            " (cf_index1, cf_index2, color_factors)"
    end subroutine prc_writer_c_lib_write_color_factors_call

```

14.2.10 Interfaces for C-library matrix element

If the matrix element code is not provided as a Fortran module but as a C or bind(C) Fortran library, we need explicit interfaces for the library functions. They are not identical to the Fortran module versions. They transfer pointers directly.

The implementation is part of the `prc_writer_c_lib` type, which serves as base type for all C-library writers. It writes specific interfaces depending on the feature.

We bind this as the method `write_standard_interface` instead of `write_interface`, because we have to override the latter. Otherwise we could not call the method because the writer type is abstract.

```

<Prclib interfaces: prc writer c lib: TBP>+=
    procedure :: write_standard_interface => prc_writer_c_lib_write_interface

<Prclib interfaces: sub interfaces>+=
    module subroutine prc_writer_c_lib_write_interface (writer, unit, id, feature)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
    end subroutine prc_writer_c_lib_write_interface

```

<Prclib interfaces: procedures>+≡

```

module subroutine prc_writer_c_lib_write_interface (writer, unit, id, feature)
  class(prc_writer_c_lib_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  select case (char (feature))
  case ("md5sum")
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "function ", &
      char (writer%get_c_procname (id, var_str ("get_md5sum"))), &
      " () result (c_ptr) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "implicit none"
    write (unit, "(7x,9A)") "type(c_ptr) :: c_ptr"
    write (unit, "(5x,9A)") "end function ", &
      char (writer%get_c_procname (id, var_str ("get_md5sum")))
    write (unit, "(2x,9A)") "end interface"
  case ("openmp_supported")
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "function ", &
      char (writer%get_c_procname (id, feature)), &
      " () result (status) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "implicit none"
    write (unit, "(7x,9A)") "logical(c_bool) :: status"
    write (unit, "(5x,9A)") "end function ", &
      char (writer%get_c_procname (id, feature))
    write (unit, "(2x,9A)") "end interface"
  case ("n_in", "n_out", "n_flv", "n_hel", "n_col", "n_cin", "n_cf")
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "function ", &
      char (writer%get_c_procname (id, feature)), &
      " () result (n) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "implicit none"
    write (unit, "(7x,9A)") "integer(c_int) :: n"
    write (unit, "(5x,9A)") "end function ", &
      char (writer%get_c_procname (id, feature))
    write (unit, "(2x,9A)") "end interface"
  case ("flv_state", "hel_state")
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "subroutine ", &
      char (writer%get_c_procname (id, feature)), &
      " (", char (feature), ") bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "implicit none"
    write (unit, "(7x,9A)") "integer(c_int), dimension(*), intent(out) ", &
      ":", char (feature)
    write (unit, "(5x,9A)") "end subroutine ", &
      char (writer%get_c_procname (id, feature))
    write (unit, "(2x,9A)") "end interface"
  case ("col_state")
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "subroutine ", &

```

```

        char (writer%get_c_procname (id, feature)), &
        " (col_state, ghost_flag) bind(C)"
write (unit, "(7x,9A)") "import"
write (unit, "(7x,9A)") "implicit none"
write (unit, "(7x,9A)") "integer(c_int), dimension(*), intent(out) ", &
    ":: col_state"
write (unit, "(7x,9A)") "logical(c_bool), dimension(*), intent(out) ", &
    ":: ghost_flag"
write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
write (unit, "(2x,9A)") "end interface"
case ("color_factors")
write (unit, "(2x,9A)") "interface"
write (unit, "(5x,9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (cf_index1, cf_index2, color_factors) bind(C)"
write (unit, "(7x,9A)") "import"
write (unit, "(7x,9A)") "implicit none"
write (unit, "(7x,9A)") "integer(c_int), dimension(*), &
    &intent(out) :: cf_index1"
write (unit, "(7x,9A)") "integer(c_int), dimension(*), &
    &intent(out) :: cf_index2"
write (unit, "(7x,9A)") "complex(c_default_complex), dimension(*), &
    &intent(out) :: color_factors"
write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
write (unit, "(2x,9A)") "end interface"
end select
end subroutine prc_writer_c_lib_write_interface

```

14.2.11 Retrieving the tables

In the previous section we had the writer routines for procedures that return tables, actually C pointers to tables. Here, we write convenience routines that unpack them and move the contents to suitable Fortran arrays.

The flavor and helicity tables are two-dimensional integer arrays. We use intermediate storage for correctly transforming C to Fortran data types.

<Prclib interfaces: prclib driver: TBP>+≡

```

procedure :: set_flv_state => prclib_driver_set_flv_state
procedure :: set_hel_state => prclib_driver_set_hel_state

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine prclib_driver_set_flv_state (driver, i, flv_state)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    integer, dimension(:,:), allocatable, intent(out) :: flv_state
end subroutine prclib_driver_set_flv_state
module subroutine prclib_driver_set_hel_state (driver, i, hel_state)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    integer, dimension(:,:), allocatable, intent(out) :: hel_state
end subroutine prclib_driver_set_hel_state

```

<Prclib interfaces: procedures>+≡

```

module subroutine prclib_driver_set_flv_state (driver, i, flv_state)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  integer, dimension(:,:), allocatable, intent(out) :: flv_state
  integer :: n_tot, n_flv
  integer(c_int) :: pid
  integer(c_int), dimension(:,:), allocatable :: c_flv_state
  pid = i
  n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
  n_flv = driver%get_n_flv (pid)
  allocate (flv_state (n_tot, n_flv))
  allocate (c_flv_state (n_tot, n_flv))
  call driver%set_flv_state_ptr &
    (pid, c_flv_state, int ([n_tot, n_flv], kind=c_int))
  flv_state = c_flv_state
end subroutine prclib_driver_set_flv_state

```

```

module subroutine prclib_driver_set_hel_state (driver, i, hel_state)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  integer, dimension(:,:), allocatable, intent(out) :: hel_state
  integer :: n_tot, n_hel
  integer(c_int) :: pid
  integer(c_int), dimension(:,:), allocatable, target :: c_hel_state
  pid = i
  n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
  n_hel = driver%get_n_hel (pid)
  allocate (hel_state (n_tot, n_hel))
  allocate (c_hel_state (n_tot, n_hel))
  call driver%set_hel_state_ptr &
    (pid, c_hel_state, int ([n_tot, n_hel], kind=c_int))
  hel_state = c_hel_state
end subroutine prclib_driver_set_hel_state

```

The color-flow table is three-dimensional, otherwise similar. We simultaneously set the ghost-flag table, which consists of logical entries.

<Prclib interfaces: prclib driver: TBP>+≡

```

procedure :: set_col_state => prclib_driver_set_col_state

```

<Prclib interfaces: sub interfaces>+≡

```

module subroutine prclib_driver_set_col_state (driver, i, col_state, ghost_flag)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  integer, dimension(:,:), allocatable, intent(out) :: col_state
  logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
end subroutine prclib_driver_set_col_state

```

<Prclib interfaces: procedures>+≡

```

module subroutine prclib_driver_set_col_state (driver, i, col_state, ghost_flag)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  integer, dimension(:,:), allocatable, intent(out) :: col_state
  logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
  integer :: n_cin, n_tot, n_col

```



```

integer(c_int) :: pid
integer(c_int), dimension(:,:), allocatable :: c_col_state
logical(c_bool), dimension(:,:), allocatable :: c_ghost_flag
pid = i
n_cin = driver%get_n_cin (pid)
n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
n_col = driver%get_n_col (pid)
allocate (col_state (n_cin, n_tot, n_col))
allocate (c_col_state (n_cin, n_tot, n_col))
allocate (ghost_flag (n_tot, n_col))
allocate (c_ghost_flag (n_tot, n_col))
call driver%set_col_state_ptr (pid, &
    c_col_state, c_ghost_flag, int ([n_cin, n_tot, n_col], kind=c_int))
col_state = c_col_state
ghost_flag = c_ghost_flag
end subroutine prclib_driver_set_col_state

```

The color-factor table is a sparse matrix: a two-column array of indices and one array which contains the corresponding factors.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: set_color_factors => prclib_driver_set_color_factors

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_set_color_factors (driver, i, color_factors, cf_index)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        complex(default), dimension(:), allocatable, intent(out) :: color_factors
        integer, dimension(:,:), allocatable, intent(out) :: cf_index
    end subroutine prclib_driver_set_color_factors

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_set_color_factors (driver, i, color_factors, cf_index)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        complex(default), dimension(:), allocatable, intent(out) :: color_factors
        integer, dimension(:,:), allocatable, intent(out) :: cf_index
        integer :: n_cf
        integer(c_int) :: pid
        complex(c_default_complex), dimension(:), allocatable, target :: c_color_factors
        integer(c_int), dimension(:), allocatable, target :: c_cf_index1
        integer(c_int), dimension(:), allocatable, target :: c_cf_index2
        pid = i
        n_cf = driver%get_n_cf (pid)
        allocate (color_factors (n_cf))
        allocate (c_color_factors (n_cf))
        allocate (c_cf_index1 (n_cf))
        allocate (c_cf_index2 (n_cf))
        call driver%set_color_factors_ptr (pid, &
            c_cf_index1, c_cf_index2, &
            c_color_factors, int ([n_cf], kind=c_int))
        color_factors = c_color_factors
        allocate (cf_index (2, n_cf))
        cf_index(1,:) = c_cf_index1
        cf_index(2,:) = c_cf_index2
    end subroutine prclib_driver_set_color_factors

```

14.2.12 Returning a procedure pointer

The functions that directly access the matrix element, event by event, are assigned to a process-specific driver object as procedure pointers. For the `dlopen` interface, we use C function pointers. This subroutine returns such a pointer:

```

<Prclib interfaces: public>+≡
  public :: prc_get_fptr

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_get_fptr (pid, fid, fptr) bind(C)
      import
      integer(c_int), intent(in) :: pid
      integer(c_int), intent(in) :: fid
      type(c_funptr), intent(out) :: fptr
    end subroutine prc_get_fptr
  end interface

```

This procedure writes the source code for the procedure pointer returning subroutine.

All C functions that are provided by the matrix element code of a specific process are handled here. The selection consists of a double layered `select case` construct.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_fptr_sub

<Prclib interfaces: sub interfaces>+≡
  module subroutine write_get_fptr_sub (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
  end subroutine write_get_fptr_sub

<Prclib interfaces: procedures>+≡
  module subroutine write_get_fptr_sub (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    integer :: i, j
    write (unit, "(A)") ""
    write (unit, "(A)") "! Return C pointer to a procedure:"
    write (unit, "(A)") "! pid = process index; fid = function index"
    write (unit, "(4A)") "subroutine ", char (prefix), "get_fptr ", &
      "(pid, fid, fptr) bind(C)"
    write (unit, "(A)") " use iso_c_binding"
    write (unit, "(A)") " use kinds"
    write (unit, "(A)") " implicit none"
    write (unit, "(A)") " integer(c_int), intent(in) :: pid"
    write (unit, "(A)") " integer(c_int), intent(in) :: fid"
    write (unit, "(A)") " type(c_funptr), intent(out) :: fptr"
    do i = 1, driver%n_processes
      call driver%record(i)%write_interfaces (unit)
    end do
  end module

```

```

end do
write (unit, "(A)") " select case (pid)"
do i = 1, driver%n_processes
  write (unit, "(2x,A,I0,A)") "case (" , i, ")"
  write (unit, "(5x,A)") "select case (fid)"
  associate (record => driver%record(i))
    do j = 1, size (record%feature)
      write (unit, "(5x,A,I0,9A)") "case (" , j, "); " , &
        "fptr = c_funloc (" , &
          char (record%get_c_procname (record%feature(j))), &
          ")"
    end do
  end associate
  write (unit, "(5x,A)") "end select"
end do
write (unit, "(A)") " end select"
write (unit, "(3A)") "end subroutine " , char (prefix), "get_fptr"
end subroutine write_get_fptr_sub

```

The procedures for which we want to return a pointer (the 'features' of the matrix element code) are actually Fortran module procedures. If we want to have a C signature, we must write wrapper functions for all of them. The procedures, their signatures, and the appropriate writer routines are specific for the process type.

To keep this generic, we do not provide the writer routines here, but just the interface for a writer routine. The actual routines are stored in the process record.

The `prefix` indicates the library, the `id` indicates the process, and `procname` is the bare name of the procedure to be written.

```

<Prclib interfaces: public>+≡
  public :: write_driver_code

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine write_driver_code (unit, prefix, id, procname)
      import
      integer, intent(in) :: unit
      type(string_t), intent(in) :: prefix
      type(string_t), intent(in) :: id
      type(string_t), intent(in) :: procname
    end subroutine write_driver_code
  end interface

```

14.2.13 Hooks

Interface for additional library unload / reload hooks (currently unused!)

```

<Prclib interfaces: public>+≡
  public :: prclib_unload_hook
  public :: prclib_reload_hook

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prclib_unload_hook (libname)
      import
      type(string_t), intent(in) :: libname
    end subroutine prclib_unload_hook

    subroutine prclib_reload_hook (libname)
      import
      type(string_t), intent(in) :: libname
    end subroutine prclib_reload_hook
  end interface

```

14.2.14 Make source, compile, link

Since we should have written a Makefile, these tasks amount to simple `make` calls. Note that the Makefile targets depend on each other, so calling `link` executes also the `source` and `compile` steps, when necessary.

Optionally, we can use a subdirectory. We construct a prefix for the subdirectory, and generate a shell `cd` call that moves us into the workspace.

The `prefix` version is intended to be prepended to a filename, and can be empty. The `path` version is intended to be prepended with a following slash, so the default is `..`.

```

<Prclib interfaces: public>+≡
  public :: workspace_prefix
  public :: workspace_path

<Prclib interfaces: sub interfaces>+≡
  module function workspace_prefix (workspace) result (prefix)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: prefix
  end function workspace_prefix
  module function workspace_path (workspace) result (path)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: path
  end function workspace_path
  module function workspace_cmd (workspace) result (cmd)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: cmd
  end function workspace_cmd

<Prclib interfaces: procedures>+≡
  module function workspace_prefix (workspace) result (prefix)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: prefix
    if (present (workspace)) then
      if (workspace /= "") then
        prefix = workspace // "/"
      else
        prefix = ""
      end if
    else
      prefix = ""
    end if
  end function

```

```

end function workspace_prefix

module function workspace_path (workspace) result (path)
  type(string_t), intent(in), optional :: workspace
  type(string_t) :: path
  if (present (workspace)) then
    if (workspace /= "") then
      path = workspace
    else
      path = "."
    end if
  else
    path = "."
  end if
end function workspace_path

module function workspace_cmd (workspace) result (cmd)
  type(string_t), intent(in), optional :: workspace
  type(string_t) :: cmd
  if (present (workspace)) then
    if (workspace /= "") then
      cmd = "cd " // workspace // " && "
    else
      cmd = ""
    end if
  else
    cmd = ""
  end if
end function workspace_cmd

```

The first routine writes source-code files for the individual processes. First it calls the writer routines directly for each process, then it calls `make source`. The make command may either post-process the files, or it may do the complete work, e.g., calling an external program that generates the files.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: make_source => prclib_driver_make_source

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_make_source (driver, os_data, workspace)
    class(prclib_driver_t), intent(in) :: driver
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in), optional :: workspace
  end subroutine prclib_driver_make_source

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_make_source (driver, os_data, workspace)
    class(prclib_driver_t), intent(in) :: driver
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in), optional :: workspace
    integer :: i
    do i = 1, driver%n_processes
      call driver%record(i)%write_source_code ()
    end do
    call os_system_call ( &

```

```

        workspace_cmd (workspace) &
        // "make source " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
    end subroutine prclib_driver_make_source

```

Compile matrix element source code and the driver source code. As above, we first iterate through all processes and call `before_compile`. This is usually empty, but can execute code that depends on `make_source` already completed. Similarly, `after_compile` scans all processes again.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: make_compile => prclib_driver_make_compile

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_make_compile (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_make_compile

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_make_compile (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
        integer :: i
        do i = 1, driver%n_processes
            call driver%record(i)%before_compile ()
        end do
        call os_system_call ( &
            workspace_cmd (workspace) &
            // "make compile " // os_data%makeflags &
            // " -f " // driver%basename // ".makefile")
        do i = 1, driver%n_processes
            call driver%record(i)%after_compile ()
        end do
    end subroutine prclib_driver_make_compile

```

Combine all matrix-element code together with the driver in a process library on disk.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: make_link => prclib_driver_make_link

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_make_link (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_make_link

<Prclib interfaces: procedures>+≡
    module subroutine prclib_driver_make_link (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
        integer :: i

```

```

call os_system_call ( &
    workspace_cmd (workspace) &
    // "make link " // os_data%makeflags &
    // " -f " // driver%basename // ".makefile")
end subroutine prclib_driver_make_link

```

14.2.15 Clean up generated files

The task of cleaning any generated files should also be deferred to Makefile targets. Apart from removing everything, removing specific files may be useful for partial rebuilds. (Note that removing the makefile itself can only be done once, for obvious reasons.)

If there is no makefile, do nothing.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: clean_library => prclib_driver_clean_library
    procedure :: clean_objects => prclib_driver_clean_objects
    procedure :: clean_source => prclib_driver_clean_source
    procedure :: clean_driver => prclib_driver_clean_driver
    procedure :: clean_makefile => prclib_driver_clean_makefile
    procedure :: clean => prclib_driver_clean
    procedure :: distclean => prclib_driver_distclean

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_clean_library (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean_library
    module subroutine prclib_driver_clean_objects (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean_objects
    module subroutine prclib_driver_clean_source (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean_source
    module subroutine prclib_driver_clean_driver (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean_driver
    module subroutine prclib_driver_clean_makefile (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean_makefile
    module subroutine prclib_driver_clean (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_clean

```

```

end subroutine prclib_driver_clean
module subroutine prclib_driver_distclean (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
end subroutine prclib_driver_distclean

(Prclib interfaces: procedures)+=≡
module subroutine prclib_driver_clean_library (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean-library " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean_library

module subroutine prclib_driver_clean_objects (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean-objects " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean_objects

module subroutine prclib_driver_clean_source (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean-source " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean_source

module subroutine prclib_driver_clean_driver (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean-driver " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean_driver

```



```

module subroutine prclib_driver_clean_makefile (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean-makefile " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean_makefile

module subroutine prclib_driver_clean (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make clean " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_clean

module subroutine prclib_driver_distclean (driver, os_data, workspace)
  class(prclib_driver_t), intent(in) :: driver
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  if (driver%makefile_exists ()) then
    call os_system_call ( &
      workspace_cmd (workspace) &
      // "make distclean " // os_data%makeflags &
      // " -f " // driver%basename // ".makefile")
  end if
end subroutine prclib_driver_distclean

```

This Make target should remove all files that apply to a specific process. We execute this when we want to force remaking source code. Note that source targets need not have prerequisites, so just calling `make_source` would not do anything if the files exist.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: clean_proc => prclib_driver_clean_proc

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_clean_proc (driver, i, os_data, workspace)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in), optional :: workspace
  end subroutine prclib_driver_clean_proc

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_clean_proc (driver, i, os_data, workspace)

```

```

class(prclib_driver_t), intent(in) :: driver
integer, intent(in) :: i
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
type(string_t) :: id
if (driver%makefile_exists ()) then
    id = driver%record(i)%id
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-" // driver%record(i)%id // " " &
        // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
end if
end subroutine prclib_driver_clean_proc

```

14.2.16 Further Tools

Check for the appropriate makefile.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: makefile_exists => prclib_driver_makefile_exists

<Prclib interfaces: sub interfaces>+≡
    module function prclib_driver_makefile_exists (driver, workspace) result (flag)
        class(prclib_driver_t), intent(in) :: driver
        type(string_t), intent(in), optional :: workspace
        logical :: flag
    end function prclib_driver_makefile_exists

<Prclib interfaces: procedures>+≡
    module function prclib_driver_makefile_exists (driver, workspace) result (flag)
        class(prclib_driver_t), intent(in) :: driver
        type(string_t), intent(in), optional :: workspace
        logical :: flag
        inquire (file = char (workspace_prefix (workspace) &
            & // driver%basename) // ".makefile", &
            exist = flag)
    end function prclib_driver_makefile_exists

```

14.2.17 Load the library

Once the library has been linked, we can dlopen it and assign all procedure pointers to their proper places in the library driver object. The loaded flag is set only if all required pointers have become assigned.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: load => prclib_driver_load

<Prclib interfaces: sub interfaces>+≡
    module subroutine prclib_driver_load (driver, os_data, noerror, workspace)
        class(prclib_driver_t), intent(inout) :: driver
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: noerror
        type(string_t), intent(in), optional :: workspace
    end subroutine prclib_driver_load

```

<Prclib interfaces: procedures>+≡

```

module subroutine prclib_driver_load (driver, os_data, noerror, workspace)
  class(prclib_driver_t), intent(inout) :: driver
  type(os_data_t), intent(in) :: os_data
  logical, intent(in), optional :: noerror
  type(string_t), intent(in), optional :: workspace
  type(c_funptr) :: c_fptr
  logical :: ignore

  ignore = .false.; if (present (noerror)) ignore = noerror

  driver%libname = os_get_dlname ( &
    workspace_prefix (workspace) // driver%basename, &
    os_data, noerror, noerror)
  if (driver%libname == "") return
  select type (driver)
  type is (prclib_driver_dynamic_t)
    if (.not. dlaccess_is_open (driver%dlaccess)) then
      call dlaccess_init &
        (driver%dlaccess, workspace_path (workspace), &
        driver%libname, os_data)
      if (.not. ignore) call driver%check_dlerror ()
    end if
    driver%loaded = dlaccess_is_open (driver%dlaccess)
  class default
    driver%loaded = .true.
  end select
  if (.not. driver%loaded) return

  c_fptr = driver%get_c_funptr (var_str ("get_n_processes"))
  call c_f_procpointer (c_fptr, driver%get_n_processes)
  driver%loaded = driver%loaded .and. associated (driver%get_n_processes)

  c_fptr = driver%get_c_funptr (var_str ("get_process_id_ptr"))
  call c_f_procpointer (c_fptr, driver%get_process_id_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_process_id_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_model_name_ptr"))
  call c_f_procpointer (c_fptr, driver%get_model_name_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_model_name_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_md5sum_ptr"))
  call c_f_procpointer (c_fptr, driver%get_md5sum_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_md5sum_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_openmp_status"))
  call c_f_procpointer (c_fptr, driver%get_openmp_status)
  driver%loaded = driver%loaded .and. associated (driver%get_openmp_status)

  c_fptr = driver%get_c_funptr (var_str ("get_n_in"))
  call c_f_procpointer (c_fptr, driver%get_n_in)
  driver%loaded = driver%loaded .and. associated (driver%get_n_in)

  c_fptr = driver%get_c_funptr (var_str ("get_n_out"))

```

```

call c_f_procpointer (c_fptr, driver%get_n_out)
driver%loaded = driver%loaded .and. associated (driver%get_n_out)

c_fptr = driver%get_c_funptr (var_str ("get_n_flv"))
call c_f_procpointer (c_fptr, driver%get_n_flv)
driver%loaded = driver%loaded .and. associated (driver%get_n_flv)

c_fptr = driver%get_c_funptr (var_str ("get_n_hel"))
call c_f_procpointer (c_fptr, driver%get_n_hel)
driver%loaded = driver%loaded .and. associated (driver%get_n_hel)

c_fptr = driver%get_c_funptr (var_str ("get_n_col"))
call c_f_procpointer (c_fptr, driver%get_n_col)
driver%loaded = driver%loaded .and. associated (driver%get_n_col)

c_fptr = driver%get_c_funptr (var_str ("get_n_cin"))
call c_f_procpointer (c_fptr, driver%get_n_cin)
driver%loaded = driver%loaded .and. associated (driver%get_n_cin)

c_fptr = driver%get_c_funptr (var_str ("get_n_cf"))
call c_f_procpointer (c_fptr, driver%get_n_cf)
driver%loaded = driver%loaded .and. associated (driver%get_n_cf)

c_fptr = driver%get_c_funptr (var_str ("set_flv_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_flv_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_flv_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_hel_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_hel_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_hel_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_col_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_col_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_col_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_color_factors_ptr"))
call c_f_procpointer (c_fptr, driver%set_color_factors_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_color_factors_ptr)

c_fptr = driver%get_c_funptr (var_str ("get_fptr"))
call c_f_procpointer (c_fptr, driver%get_fptr)
driver%loaded = driver%loaded .and. associated (driver%get_fptr)

end subroutine prclib_driver_load

```

Unload. To be sure, nullify the procedure pointers.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: unload => prclib_driver_unload

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_unload (driver)
    class(prclib_driver_t), intent(inout) :: driver
  end subroutine prclib_driver_unload

<Prclib interfaces: procedures>+≡

```

```

module subroutine prclib_driver_unload (driver)
  class(prclib_driver_t), intent(inout) :: driver
  select type (driver)
  type is (prclib_driver_dynamic_t)
    if (dlaccess_is_open (driver%dlaccess)) then
      call dlaccess_final (driver%dlaccess)
      call driver%check_dlerror ()
    end if
  end select
  driver%loaded = .false.
  nullify (driver%get_n_processes)
  nullify (driver%get_process_id_ptr)
  nullify (driver%get_model_name_ptr)
  nullify (driver%get_md5sum_ptr)
  nullify (driver%get_openmp_status)
  nullify (driver%get_n_in)
  nullify (driver%get_n_out)
  nullify (driver%get_n_flv)
  nullify (driver%get_n_hel)
  nullify (driver%get_n_col)
  nullify (driver%get_n_cin)
  nullify (driver%get_n_cf)
  nullify (driver%set_flv_state_ptr)
  nullify (driver%set_hel_state_ptr)
  nullify (driver%set_col_state_ptr)
  nullify (driver%set_color_factors_ptr)
  nullify (driver%get_fptr)
end subroutine prclib_driver_unload

```

This subroutine checks the `dlerror` content and issues a fatal error if it finds an error there.

```

<Prclib interfaces: prclib driver dynamic: TBP>≡
  procedure :: check_dlerror => prclib_driver_check_dlerror

<Prclib interfaces: sub interfaces>+≡
  module subroutine prclib_driver_check_dlerror (driver)
    class(prclib_driver_dynamic_t), intent(in) :: driver
  end subroutine prclib_driver_check_dlerror

<Prclib interfaces: procedures>+≡
  module subroutine prclib_driver_check_dlerror (driver)
    class(prclib_driver_dynamic_t), intent(in) :: driver
    if (dlaccess_has_error (driver%dlaccess)) then
      call msg_fatal (char (dlaccess_get_error (driver%dlaccess)))
    end if
  end subroutine prclib_driver_check_dlerror

```

Get the handle (C function pointer) for a given “feature” of the matrix element code, so it can be assigned to the appropriate procedure pointer slot. In the static case, this is a trivial pointer assignment, hard-coded into the driver type implementation.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure (prclib_driver_get_c_funptr), deferred :: get_c_funptr

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    function prclib_driver_get_c_funptr (driver, feature) result (c_fptr)
      import
      class(prclib_driver_t), intent(inout) :: driver
      type(string_t), intent(in) :: feature
      type(c_funptr) :: c_fptr
    end function prclib_driver_get_c_funptr
  end interface

```

In the dynamic-library case, we call the DL interface to retrieve the C pointer to a named procedure.

```

<Prclib interfaces: prclib driver dynamic: TBP>+≡
  procedure :: get_c_funptr => prclib_driver_dynamic_get_c_funptr

<Prclib interfaces: sub interfaces>+≡
  module function prclib_driver_dynamic_get_c_funptr &
    (driver, feature) result (c_fptr)
    class(prclib_driver_dynamic_t), intent(inout) :: driver
    type(string_t), intent(in) :: feature
    type(c_funptr) :: c_fptr
  end function prclib_driver_dynamic_get_c_funptr

<Prclib interfaces: procedures>+≡
  module function prclib_driver_dynamic_get_c_funptr &
    (driver, feature) result (c_fptr)
    class(prclib_driver_dynamic_t), intent(inout) :: driver
    type(string_t), intent(in) :: feature
    type(c_funptr) :: c_fptr
    type(string_t) :: prefix, full_name
    prefix = lower_case (driver%basename) // "_"
    full_name = prefix // feature
    c_fptr = dlaccess_get_c_funptr (driver%dlaccess, full_name)
    call driver%check_dlerror ()
  end function prclib_driver_dynamic_get_c_funptr

```

14.2.18 MD5 sums

Recall the MD5 sum written in the Makefile

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: get_md5sum_makefile => prclib_driver_get_md5sum_makefile

<Prclib interfaces: sub interfaces>+≡
  module function prclib_driver_get_md5sum_makefile &
    (driver, workspace) result (md5sum)
    class(prclib_driver_t), intent(in) :: driver
    type(string_t), intent(in), optional :: workspace
    character(32) :: md5sum
  end function prclib_driver_get_md5sum_makefile

<Prclib interfaces: procedures>+≡
  module function prclib_driver_get_md5sum_makefile &
    (driver, workspace) result (md5sum)
    class(prclib_driver_t), intent(in) :: driver

```

```

type(string_t), intent(in), optional :: workspace
character(32) :: md5sum
type(string_t) :: filename
character(80) :: buffer
logical :: exist
integer :: u, iostat
md5sum = ""
filename = workspace_prefix (workspace) // driver%basename // ".makefile"
inquire (file = char (filename), exist = exist)
if (exist) then
    u = free_unit ()
    open (u, file = char (filename), action = "read", status = "old")
    iostat = 0
    do
        read (u, "(A)", iostat = iostat) buffer
        if (iostat /= 0) exit
        buffer = adjustl (buffer)
        select case (buffer(1:9))
        case ("MD5SUM = ")
            read (buffer(11:), "(A32)") md5sum
            exit
        end select
    end do
    close (u)
end if
end function prclib_driver_get_md5sum_makefile

```

Recall the MD5 sum written in the driver source code.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: get_md5sum_driver => prclib_driver_get_md5sum_driver

<Prclib interfaces: sub interfaces>+≡
    module function prclib_driver_get_md5sum_driver (driver, workspace) result (md5sum)
        class(prclib_driver_t), intent(in) :: driver
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum
    end function prclib_driver_get_md5sum_driver

<Prclib interfaces: procedures>+≡
    module function prclib_driver_get_md5sum_driver (driver, workspace) result (md5sum)
        class(prclib_driver_t), intent(in) :: driver
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum
        type(string_t) :: filename
        character(80) :: buffer
        logical :: exist
        integer :: u, iostat
        md5sum = ""
        filename = workspace_prefix (workspace) // driver%basename // ".f90"
        inquire (file = char (filename), exist = exist)
        if (exist) then
            u = free_unit ()
            open (u, file = char (filename), action = "read", status = "old")
            iostat = 0
            do

```

```

        read (u, "(A)", iostat = iostat)  buffer
        if (iostat /= 0)  exit
        buffer = adjustl (buffer)
        select case (buffer(1:9))
        case ("md5sum = ")
            read (buffer(11:), "(A32)")  md5sum
            exit
        end select
    end do
    close (u)
end if
end function prclib_driver_get_md5sum_driver

```

Recall the MD5 sum written in the matrix element source code.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: get_md5sum_source => prclib_driver_get_md5sum_source

<Prclib interfaces: sub interfaces>+≡
    module function prclib_driver_get_md5sum_source &
        (driver, i, workspace) result (md5sum)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum
    end function prclib_driver_get_md5sum_source

<Prclib interfaces: procedures>+≡
    module function prclib_driver_get_md5sum_source &
        (driver, i, workspace) result (md5sum)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum
        type(string_t) :: filename
        character(80) :: buffer
        logical :: exist
        integer :: u, iostat
        md5sum = ""

        filename = workspace_prefix (workspace) // driver%record(i)%id // ".f90"
        inquire (file = char (filename), exist = exist)
        if (exist) then
            u = free_unit ()
            open (u, file = char (filename), action = "read", status = "old")
            iostat = 0
            do
                read (u, "(A)", iostat = iostat)  buffer
                if (iostat /= 0)  exit
                buffer = adjustl (buffer)
                select case (buffer(1:9))
                case ("md5sum = ")
                    read (buffer(11:), "(A32)")  md5sum
                    exit
                end select
            end do
        end if
    end function prclib_driver_get_md5sum_source

```



```

        close (u)
    end if
end function prclib_driver_get_md5sum_source

```

14.2.19 Unit Test

Test module, followed by the corresponding implementation module.

```

<prclib_interfaces_ut.f90>≡
  <File header>

  module prclib_interfaces_ut
    use kinds
    use system_dependencies, only: CC_IS_GNU, CC_HAS_QUADMATH
    use unit_tests
    use prclib_interfaces_uti

    <Standard module head>

    <Prclib interfaces: public test>

    <Prclib interfaces: public test auxiliary>

    contains

    <Prclib interfaces: test driver>

  end module prclib_interfaces_ut
<prclib_interfaces_uti.f90>≡
  <File header>

  module prclib_interfaces_uti

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    use system_dependencies, only: CC_HAS_QUADMATH, DEFAULT_FC_PRECISION
  <Use strings>
    use io_units
    use system_defs, only: TAB
    use os_interface

    use prclib_interfaces

    <Standard module head>

    <Prclib interfaces: public test auxiliary>

    <Prclib interfaces: test declarations>

    <Prclib interfaces: test types>

    contains

```

<Prclib interfaces: tests>

<Prclib interfaces: test auxiliary>

end module prclib_interfaces_uti

API: driver for the unit tests below.

<Prclib interfaces: public test>≡

public :: prclib_interfaces_test

<Prclib interfaces: test driver>≡

subroutine prclib_interfaces_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Prclib interfaces: execute tests>

end subroutine prclib_interfaces_test

Empty process list

Test 1: Create a driver object and display its contents. One of the feature lists references a writer procedure; this is just a dummy that does nothing useful.

<Prclib interfaces: execute tests>≡

call test (prclib_interfaces_1, "prclib_interfaces_1", &
"create driver object", &
u, results)

<Prclib interfaces: test declarations>≡

public :: prclib_interfaces_1

<Prclib interfaces: tests>≡

subroutine prclib_interfaces_1 (u)

integer, intent(in) :: u

class(prclib_driver_t), allocatable :: driver

character(32), parameter :: md5sum = "prclib_interfaces_1_md5sum "

class(prc_writer_t), pointer :: test_writer_1

write (u, "(A)") "* Test output: prclib_interfaces_1"

write (u, "(A)") "* Purpose: display the driver object contents"

write (u, *)

write (u, "(A)") "* Create a prclib driver object"

write (u, "(A)")

call dispatch_prclib_driver (driver, var_str ("prclib"), var_str (""))

call driver%init (3)

call driver%set_md5sum (md5sum)

allocate (test_writer_1_t :: test_writer_1)

call driver%set_record (1, var_str ("test1"), var_str ("test_model"), &
[var_str ("init")], test_writer_1)

call driver%set_record (2, var_str ("test2"), var_str ("foo_model"), &

```

[var_str ("another_proc")], test_writer_1)

call driver%set_record (3, var_str ("test3"), var_str ("test_model"), &
[var_str ("init"), var_str ("some_proc")], test_writer_1)

call driver%write (u)

deallocate (test_writer_1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_1"
end subroutine prclib_interfaces_1

```

The writer: the procedures write just comment lines. We can fix an instance of this as a parameter (since it has no mutable content) and just reference the fixed parameter.

NOTE: temporarily made public.

```

<Prclib interfaces: test types>≡
type, extends (prc_writer_t) :: test_writer_1_t
contains
  procedure, nopass :: type_name => test_writer_1_type_name
  procedure :: write_makefile_code => test_writer_1_mk
  procedure :: write_source_code => test_writer_1_src
  procedure :: write_interface => test_writer_1_if
  procedure :: write_md5sum_call => test_writer_1_md5sum
  procedure :: write_int_sub_call => test_writer_1_int_sub
  procedure :: write_col_state_call => test_writer_1_col_state
  procedure :: write_color_factors_call => test_writer_1_col_factors
  procedure :: before_compile => test_writer_1_before_compile
  procedure :: after_compile => test_writer_1_after_compile
end type test_writer_1_t

```

```

<Prclib interfaces: test auxiliary>≡
function test_writer_1_type_name () result (string)
  type(string_t) :: string
  string = "test_1"
end function test_writer_1_type_name

subroutine test_writer_1_mk &
  (writer, unit, id, os_data, verbose, testflag)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
  write (unit, "(5A)")  "# Makefile code for process ", char (id), &
    " goes here."
end subroutine test_writer_1_mk

subroutine test_writer_1_src (writer, id)
  class(test_writer_1_t), intent(in) :: writer
  type(string_t), intent(in) :: id

```

```

end subroutine test_writer_1_src

subroutine test_writer_1_if (writer, unit, id, feature)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(2x,9A)")  "! Interface code for ", &
    char (id), "_", char (writer%get_procname (feature)), &
    " goes here."
end subroutine test_writer_1_if

subroutine test_writer_1_md5sum (writer, unit, id)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)")  "! MD5sum call for ", char (id), " goes here."
end subroutine test_writer_1_md5sum

subroutine test_writer_1_int_sub (writer, unit, id, feature)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(5x,9A)")  "! ", char (feature), " call for ", &
    char (id), " goes here."
end subroutine test_writer_1_int_sub

subroutine test_writer_1_col_state (writer, unit, id)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)")  "! col_state call for ", &
    char (id), " goes here."
end subroutine test_writer_1_col_state

subroutine test_writer_1_col_factors (writer, unit, id)
  class(test_writer_1_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)")  "! color_factors call for ", &
    char (id), " goes here."
end subroutine test_writer_1_col_factors

subroutine test_writer_1_before_compile (writer, id)
  class(test_writer_1_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_1_before_compile

subroutine test_writer_1_after_compile (writer, id)
  class(test_writer_1_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_1_after_compile

```

Process library driver file

Test 2: Write the driver file for a test case with two processes. The first process needs no wrapper (C library), the second one needs wrappers (Fortran module library).

```
<Prclib interfaces: execute tests>+≡
    call test (prclib_interfaces_2, "prclib_interfaces_2", &
               "write driver file", &
               u, results)

<Prclib interfaces: test declarations>+≡
    public :: prclib_interfaces_2

<Prclib interfaces: tests>+≡
    subroutine prclib_interfaces_2 (u)
        integer, intent(in) :: u
        class(prclib_driver_t), allocatable :: driver
        character(32), parameter :: md5sum = "prclib_interfaces_2_md5sum"
        class(prc_writer_t), pointer :: test_writer_1, test_writer_2

        write (u, "(A)")  "* Test output: prclib_interfaces_2"
        write (u, "(A)")  "* Purpose: check the generated driver source code"
        write (u, "(A)")
        write (u, "(A)")  "* Create a prclib driver object (2 processes)"
        write (u, "(A)")

        call dispatch_prclib_driver (driver, var_str ("prclib2"), var_str (""))
        call driver%init (2)
        call driver%set_md5sum (md5sum)

        allocate (test_writer_1_t :: test_writer_1)
        allocate (test_writer_2_t :: test_writer_2)

        call driver%set_record (1, var_str ("test1"), var_str ("Test_model"), &
                                [var_str ("proc1")], test_writer_1)

        call driver%set_record (2, var_str ("test2"), var_str ("Test_model"), &
                                [var_str ("proc1"), var_str ("proc2")], test_writer_2)

        call driver%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Write the driver file"
        write (u, "(A)")  "* File contents:"
        write (u, "(A)")

        call driver%generate_driver_code (u)

        deallocate (test_writer_1)
        deallocate (test_writer_2)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: prclib_interfaces_2"
    end subroutine prclib_interfaces_2
```

A writer with wrapper code: the procedures again write just comment lines. Since all procedures are NOPASS, we can reuse two of the TBP.

```

<Prclib interfaces: test types>+≡
type, extends (prc_writer_f_module_t) :: test_writer_2_t
contains
  procedure, nopass :: type_name => test_writer_2_type_name
  procedure :: write_makefile_code => test_writer_2_mk
  procedure :: write_source_code => test_writer_2_src
  procedure :: write_interface => test_writer_2_if
  procedure :: write_wrapper => test_writer_2_wr
  procedure :: before_compile => test_writer_2_before_compile
  procedure :: after_compile => test_writer_2_after_compile
end type test_writer_2_t

<Prclib interfaces: test auxiliary>+≡
function test_writer_2_type_name () result (string)
  type(string_t) :: string
  string = "test_2"
end function test_writer_2_type_name

subroutine test_writer_2_mk &
  (writer, unit, id, os_data, verbose, testflag)
  class(test_writer_2_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
  write (unit, "(5A)")  "# Makefile code for process ", char (id), &
    " goes here."
end subroutine test_writer_2_mk

subroutine test_writer_2_src (writer, id)
  class(test_writer_2_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_2_src

subroutine test_writer_2_if (writer, unit, id, feature)
  class(test_writer_2_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(2x,9A)")  "! Interface code for ", &
    char (writer%get_module_name (id)), "_", &
    char (writer%get_procname (feature)), " goes here."
end subroutine test_writer_2_if

subroutine test_writer_2_wr (writer, unit, id, feature)
  class(test_writer_2_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, *)
  write (unit, "(9A)")  "! Wrapper code for ", &
    char (writer%get_c_procname (id, feature)), " goes here."

```

```

end subroutine test_writer_2_wr

subroutine test_writer_2_before_compile (writer, id)
  class(test_writer_2_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_2_before_compile

subroutine test_writer_2_after_compile (writer, id)
  class(test_writer_2_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_2_after_compile

```

Process library makefile

Test 3: Write the makefile for compiling and linking the process library (processes and driver code). There are two processes, one with one method, one with two methods.

To have predictable output, we reset the system-dependent initial components of `os_data` to known values.

```

<Prclib interfaces: execute tests>+≡
  call test (prclib_interfaces_3, "prclib_interfaces_3", &
    "write makefile", &
    u, results)

<Prclib interfaces: test declarations>+≡
  public :: prclib_interfaces_3

<Prclib interfaces: tests>+≡
  subroutine prclib_interfaces_3 (u)
    integer, intent(in) :: u
    class(prclib_driver_t), allocatable :: driver
    type(os_data_t) :: os_data
    character(32), parameter :: md5sum = "prclib_interfaces_3_md5sum"
    class(prc_writer_t), pointer :: test_writer_1, test_writer_2

    call os_data%init ()
    os_data%fc = "fortran-compiler"
    os_data%whizard_includes = "-I module-dir"
    os_data%fcflags = "-C=all"
    os_data%fcflags_pic = "-PIC"
    os_data%cc = "c-compiler"
    os_data%cflags = "-I include-dir"
    os_data%cflags_pic = "-PIC"
    os_data%whizard_ldflags = ""
    os_data%ldflags = ""
    os_data%whizard_libtool = "my-libtool"
    os_data%latex = "latex -halt-on-error"
    os_data%mpost = "mpost -math=scaled -halt-on-error"
    os_data%dvips = "dvips"
    os_data%ps2pdf = "ps2pdf14"
    os_data%whizard_texpath = ""

    write (u, "(A)")  "*" Test output: prclib_interfaces_3"

```

```

write (u, "(A)")  "*" Purpose: check the generated Makefile"
write (u, *)
write (u, "(A)")  "*" Create a prclib driver object (2 processes)"
write (u, "(A)")

call dispatch_prclib_driver (driver, var_str ("prclib3"), var_str (""))
call driver%init (2)
call driver%set_md5sum (md5sum)

allocate (test_writer_1_t :: test_writer_1)
allocate (test_writer_2_t :: test_writer_2)

call driver%set_record (1, var_str ("test1"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_1)

call driver%set_record (2, var_str ("test2"), var_str ("Test_model"), &
    [var_str ("proc1"), var_str ("proc2")], test_writer_2)

call driver%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Write Makefile"
write (u, "(A)")  "*" File contents:"
write (u, "(A)")

call driver%generate_makefile (u, os_data, verbose = .true.)

deallocate (test_writer_1)
deallocate (test_writer_2)

write (u, "(A)")
write (u, "(A)")  "*" Test output end: prclib_interfaces_3"
end subroutine prclib_interfaces_3

```

Compile test with Fortran module

Test 4: Write driver and makefile and try to compile and link the library driver.

There is a single test process with a single feature. The process code is provided as a Fortran module, therefore we need a wrapper for the featured procedure.

```

<Prclib interfaces: execute tests>+≡
    call test (prclib_interfaces_4, "prclib_interfaces_4", &
        "compile and link (Fortran module)", &
        u, results)

<Prclib interfaces: test declarations>+≡
    public :: prclib_interfaces_4

<Prclib interfaces: tests>+≡
    subroutine prclib_interfaces_4 (u)
        integer, intent(in) :: u
        class(prclib_driver_t), allocatable :: driver
        class(prc_writer_t), pointer :: test_writer_4

```



```

type(os_data_t) :: os_data
integer :: u_file

integer, dimension(:,:), allocatable :: flv_state
integer, dimension(:,:), allocatable :: hel_state
integer, dimension(:,:,:), allocatable :: col_state
logical, dimension(:,:), allocatable :: ghost_flag
integer, dimension(:,:), allocatable :: cf_index
complex(default), dimension(:), allocatable :: color_factors
character(32), parameter :: md5sum = "prclib_interfaces_4_md5sum      "
character(32) :: md5sum_file

type(c_funptr) :: proc1_ptr
interface
    subroutine proc1_t (n) bind(C)
        import
        integer(c_int), intent(out) :: n
    end subroutine proc1_t
end interface
procedure(proc1_t), pointer :: proc1
integer(c_int) :: n

write (u, "(A)")  "* Test output: prclib_interfaces_4"
write (u, "(A)")  "* Purpose: compile, link, and load process library"
write (u, "(A)")  "*           with (fake) matrix-element code &
    &as a Fortran module"
write (u, *)
write (u, "(A)")  "* Create a prclib driver object (1 process)"
write (u, "(A)")

call os_data%init ()

allocate (test_writer_4_t :: test_writer_4)
call test_writer_4%init_test ()

call dispatch_prclib_driver (driver, var_str ("prclib4"), var_str (""))
call driver%init (1)
call driver%set_md5sum (md5sum)

call driver%set_record (1, var_str ("test4"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_4)

call driver%write (u)

write (u, *)
write (u, "(A)")  "* Write Makefile"
u_file = free_unit ()
open (u_file, file="prclib4.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from Makefile"
write (u, "(A)")

```

```

md5sum_file = driver%get_md5sum_makefile ()
write (u, "(1x,A,A,A)") "MD5 sum = ', md5sum_file, "'

write (u, "(A)")
write (u, "(A)")  "* Write driver source code"

u_file = free_unit ()
open (u_file, file="prclib4.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from driver source"
write (u, "(A)")

md5sum_file = driver%get_md5sum_driver ()
write (u, "(1x,A,A,A)") "MD5 sum = ', md5sum_file, "'

write (u, "(A)")
write (u, "(A)")  "* Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from matrix-element source"
write (u, "(A)")

md5sum_file = driver%get_md5sum_source (1)
write (u, "(1x,A,A,A)") "MD5 sum = ', md5sum_file, "'

write (u, "(A)")
write (u, "(A)")  "* Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "* Link library"
call driver%make_link (os_data)

write (u, "(A)")  "* Load library"
call driver%load (os_data)

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
  write (u, "(A)")  "* Call library functions:"
  write (u, *)
  write (u, "(1x,A,I0)") "n_processes   = ", driver%get_n_processes ()
  write (u, "(1x,A,A,A)") "process_id   = ', &
    char (driver%get_process_id (1)), "'
  write (u, "(1x,A,A,A)") "model_name   = ', &
    char (driver%get_model_name (1)), "'
  write (u, "(1x,A,A,A)") "md5sum (lib) = ', &
    char (driver%get_md5sum (0)), "'

```

```

write (u, "(1x,A,A,A)") "md5sum (proc) = ', &
      char (driver%get_md5sum (1)), "'
write (u, "(1x,A,L1)") "openmp_status = ", driver%get_openmp_status (1)
write (u, "(1x,A,I0)") "n_in = ", driver%get_n_in (1)
write (u, "(1x,A,I0)") "n_out = ", driver%get_n_out (1)
write (u, "(1x,A,I0)") "n_flv = ", driver%get_n_flv (1)
write (u, "(1x,A,I0)") "n_hel = ", driver%get_n_hel (1)
write (u, "(1x,A,I0)") "n_col = ", driver%get_n_col (1)
write (u, "(1x,A,I0)") "n_cin = ", driver%get_n_cin (1)
write (u, "(1x,A,I0)") "n_cf = ", driver%get_n_cf (1)

call driver%set_flv_state (1, flv_state)
write (u, "(1x,A,10(1x,I0))") "flv_state =", flv_state

call driver%set_hel_state (1, hel_state)
write (u, "(1x,A,10(1x,I0))") "hel_state =", hel_state

call driver%set_col_state (1, col_state, ghost_flag)
write (u, "(1x,A,10(1x,I0))") "col_state =", col_state
write (u, "(1x,A,10(1x,L1))") "ghost_flag =", ghost_flag

call driver%set_color_factors (1, color_factors, cf_index)
write (u, "(1x,A,10(1x,F5.3))") "color_factors =", color_factors
write (u, "(1x,A,10(1x,I0))") "cf_index =", cf_index

call driver%get_fptr (1, 1, proc1_ptr)
call c_f_procpointer (proc1_ptr, proc1)
if (associated (proc1)) then
  write (u, *)
  call proc1 (n)
  write (u, "(1x,A,I0)") "proc1(1) = ", n
end if

end if

deallocate (test_writer_4)

write (u, "(A)")
write (u, "(A)") "* Test output end: prclib_interfaces_4"
end subroutine prclib_interfaces_4

```

This version of test-code writer actually writes an interface and wrapper code.

The wrapped function is a no-parameter function with integer result.

The stored MD5 sum may be modified.

We will reuse this later, therefore public.

```

<Prclib interfaces: public test auxiliary>≡
  public :: test_writer_4_t

<Prclib interfaces: test types>+≡
  type, extends (prc_writer_f_module_t) :: test_writer_4_t
  contains
    procedure, nopass :: type_name => test_writer_4_type_name
    procedure, nopass :: get_module_name => &
      test_writer_4_get_module_name

```

```

    procedure :: write_makefile_code => test_writer_4_mk
    procedure :: write_source_code => test_writer_4_src
    procedure :: write_interface => test_writer_4_if
    procedure :: write_wrapper => test_writer_4_wr
    procedure :: before_compile => test_writer_4_before_compile
    procedure :: after_compile => test_writer_4_after_compile
end type test_writer_4_t

```

(Prclib interfaces: test auxiliary)+≡

```

function test_writer_4_type_name () result (string)
    type(string_t) :: string
    string = "test_4"
end function test_writer_4_type_name

```

```

function test_writer_4_get_module_name (id) result (name)
    type(string_t), intent(in) :: id
    type(string_t) :: name
    name = "tpr_" // id
end function test_writer_4_get_module_name

```

```

subroutine test_writer_4_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_4_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
    write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
    write (unit, "(5A)") "CLEAN_OBJECTS += tpr_", char (id), ".mod"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " FC      " $@"
    end if
    write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
end subroutine test_writer_4_mk

```

```

subroutine test_writer_4_src (writer, id)
    class(test_writer_4_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    call write_test_module_file (id, var_str ("proc1"), writer%md5sum)
end subroutine test_writer_4_src

```

```

subroutine test_writer_4_if (writer, unit, id, feature)
    class(test_writer_4_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    write (unit, "(2x,9A)") "interface"
    write (unit, "(5x,9A)") "subroutine ", &
        char (writer%get_c_procname (id, feature)), &
        " (n) bind(C)"

```

```

write (unit, "(7x,9A)") "import"
write (unit, "(7x,9A)") "implicit none"
write (unit, "(7x,9A)") "integer(c_int), intent(out) :: n"
write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
write (unit, "(2x,9A)") "end interface"
end subroutine test_writer_4_if

subroutine test_writer_4_wr (writer, unit, id, feature)
class(test_writer_4_t), intent(in) :: writer
integer, intent(in) :: unit
type(string_t), intent(in) :: id, feature
write (unit, *)
write (unit, "(9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (n) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use tpr_", char (id), ", only: ", &
    char (writer%get_c_procname (feature))
write (unit, "(2x,9A)") "implicit none"
write (unit, "(2x,9A)") "integer(c_int), intent(out) :: n"
write (unit, "(2x,9A)") "call ", char (feature), " (n)"
write (unit, "(9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
end subroutine test_writer_4_wr

subroutine test_writer_4_before_compile (writer, id)
class(test_writer_4_t), intent(in) :: writer
type(string_t), intent(in) :: id
end subroutine test_writer_4_before_compile

subroutine test_writer_4_after_compile (writer, id)
class(test_writer_4_t), intent(in) :: writer
type(string_t), intent(in) :: id
end subroutine test_writer_4_after_compile

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature), the name given as an argument.

(Prelib interfaces: test auxiliary)+≡

```

subroutine write_test_module_file (basename, feature, md5sum)
type(string_t), intent(in) :: basename
type(string_t), intent(in) :: feature
character(32), intent(in) :: md5sum
integer :: u
u = free_unit ()
open (u, file = char (basename) // ".f90", &
    status = "replace", action = "write")
write (u, "(A)") "!(Pseudo) matrix element code file &
    &for WHIZARD self-test"
write (u, *)
write (u, "(A)") "module tpr_" // char (basename)

```

```

write (u, *)
write (u, "(2x,A)") "use kinds"
write (u, "(2x,A)") "use omega_color, OCF => omega_color_factor"
write (u, *)
write (u, "(2x,A)") "implicit none"
write (u, "(2x,A)") "private"
write (u, *)
call write_test_me_code_1 (u)
write (u, *)
write (u, "(2x,A)") "public :: " // char (feature)
write (u, *)
write (u, "(A)") "contains"
write (u, *)
call write_test_me_code_2 (u, md5sum)
write (u, *)
write (u, "(2x,A)") "subroutine " // char (feature) // " (n)"
write (u, "(2x,A)") " integer, intent(out) :: n"
write (u, "(2x,A)") " n = 42"
write (u, "(2x,A)") "end subroutine " // char (feature)
write (u, *)
write (u, "(A)") "end module tpr_" // char (basename)
close (u)
end subroutine write_test_module_file

```

The following two subroutines provide building blocks for a matrix-element source code file, useful only for testing the workflow. The first routine writes the header part, the other routine the implementation of the procedures listed in the header.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_me_code_1 (u)
integer, intent(in) :: u
write (u, "(2x,A)") "public :: md5sum"
write (u, "(2x,A)") "public :: openmp_supported"
write (u, *)
write (u, "(2x,A)") "public :: n_in"
write (u, "(2x,A)") "public :: n_out"
write (u, "(2x,A)") "public :: n_flv"
write (u, "(2x,A)") "public :: n_hel"
write (u, "(2x,A)") "public :: n_cin"
write (u, "(2x,A)") "public :: n_col"
write (u, "(2x,A)") "public :: n_cf"
write (u, *)
write (u, "(2x,A)") "public :: flv_state"
write (u, "(2x,A)") "public :: hel_state"
write (u, "(2x,A)") "public :: col_state"
write (u, "(2x,A)") "public :: color_factors"
end subroutine write_test_me_code_1

subroutine write_test_me_code_2 (u, md5sum)
integer, intent(in) :: u
character(32), intent(in) :: md5sum
write (u, "(2x,A)") "pure function md5sum ()"
write (u, "(2x,A)") " character(len=32) :: md5sum"

```

```

write (u, "(2x,A)") " md5sum = ' " // md5sum // "'
write (u, "(2x,A)") "end function md5sum"
write (u, *)
write (u, "(2x,A)") "pure function openmp_supported () result (status)"
write (u, "(2x,A)") " logical :: status"
write (u, "(2x,A)") " status = .false."
write (u, "(2x,A)") "end function openmp_supported"
write (u, *)
write (u, "(2x,A)") "pure function n_in () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 1"
write (u, "(2x,A)") "end function n_in"
write (u, *)
write (u, "(2x,A)") "pure function n_out () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 2"
write (u, "(2x,A)") "end function n_out"
write (u, *)
write (u, "(2x,A)") "pure function n_flv () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 1"
write (u, "(2x,A)") "end function n_flv"
write (u, *)
write (u, "(2x,A)") "pure function n_hel () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 1"
write (u, "(2x,A)") "end function n_hel"
write (u, *)
write (u, "(2x,A)") "pure function n_cin () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 2"
write (u, "(2x,A)") "end function n_cin"
write (u, *)
write (u, "(2x,A)") "pure function n_col () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 1"
write (u, "(2x,A)") "end function n_col"
write (u, *)
write (u, "(2x,A)") "pure function n_cf () result (n)"
write (u, "(2x,A)") " integer :: n"
write (u, "(2x,A)") " n = 1"
write (u, "(2x,A)") "end function n_cf"
write (u, *)
write (u, "(2x,A)") "pure subroutine flv_state (a)"
write (u, "(2x,A)") " integer, dimension(:,:), intent(out) :: a"
write (u, "(2x,A)") " a = reshape ([1,2,3], [3,1])"
write (u, "(2x,A)") "end subroutine flv_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine hel_state (a)"
write (u, "(2x,A)") " integer, dimension(:,:), intent(out) :: a"
write (u, "(2x,A)") " a = reshape ([0,0,0], [3,1])"
write (u, "(2x,A)") "end subroutine hel_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine col_state (a, g)"

```

```

write (u, "(2x,A)") " integer, dimension(:,:,:), intent(out) :: a"
write (u, "(2x,A)") " logical, dimension(:,:), intent(out) :: g"
write (u, "(2x,A)") " a = reshape ([0,0, 0,0, 0,0], [2,3,1])"
write (u, "(2x,A)") " g = reshape ([.false., .false., .false.], [3,1])"
write (u, "(2x,A)") "end subroutine col_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine color_factors (cf)"
write (u, "(2x,A)") " type(OCF), dimension(:), intent(out) :: cf"
write (u, "(2x,A)") " cf = [ OCF(1,1,+1._default) ]"
write (u, "(2x,A)") "end subroutine color_factors"
end subroutine write_test_me_code_2

```

Compile test with Fortran bind(C) library

Test 5: Write driver and makefile and try to compile and link the library driver.

There is a single test process with a single feature. The process code is provided as a Fortran library of independent procedures. These procedures are bind(C).

```

<Prclib interfaces: execute tests>+≡
call test (prclib_interfaces_5, "prclib_interfaces_5", &
"compile and link (Fortran library)", &
u, results)

<Prclib interfaces: test declarations>+≡
public :: prclib_interfaces_5

<Prclib interfaces: tests>+≡
subroutine prclib_interfaces_5 (u)
integer, intent(in) :: u
class(prclib_driver_t), allocatable :: driver
class(prc_writer_t), pointer :: test_writer_5
type(os_data_t) :: os_data
integer :: u_file

integer, dimension(:,:), allocatable :: flv_state
integer, dimension(:,:), allocatable :: hel_state
integer, dimension(:,:,:), allocatable :: col_state
logical, dimension(:,:), allocatable :: ghost_flag
integer, dimension(:,:), allocatable :: cf_index
complex(default), dimension(:), allocatable :: color_factors
character(32), parameter :: md5sum = "prclib_interfaces_5_md5sum"

type(c_funptr) :: proc1_ptr
interface
subroutine proc1_t (n) bind(C)
import
integer(c_int), intent(out) :: n
end subroutine proc1_t
end interface
procedure(proc1_t), pointer :: proc1
integer(c_int) :: n

write (u, "(A)") "* Test output: prclib_interfaces_5"

```



```

write (u, "(A)")  "*" Purpose: compile, link, and load process library"
write (u, "(A)")  "*"           with (fake) matrix-element code &
                        &as a Fortran bind(C) library"
write (u, *)
write (u, "(A)")  "*" Create a prclib driver object (1 process)"
write (u, "(A)")

call os_data%init ()
allocate (test_writer_5_t :: test_writer_5)

call dispatch_prclib_driver (driver, var_str ("prclib5"), var_str (""))
call driver%init (1)
call driver%set_md5sum (md5sum)

call driver%set_record (1, var_str ("test5"), var_str ("Test_model"), &
                        [var_str ("proc1")], test_writer_5)

call driver%write (u)

write (u, *)
write (u, "(A)")  "*" Write makefile"
u_file = free_unit ()
open (u_file, file="prclib5.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")  "*" Write driver source code"
u_file = free_unit ()
open (u_file, file="prclib5.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")  "*" Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")  "*" Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "*" Link library"
call driver%make_link (os_data)

write (u, "(A)")  "*" Load library"
call driver%load (os_data)

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
    write (u, "(A)")  "*" Call library functions:"
    write (u, *)
    write (u, "(1x,A,I0)")  "n_processes   = ", driver%get_n_processes ()
    write (u, "(1x,A,A)")  "process_id    = ", &
        char (driver%get_process_id (1))

```

```

write (u, "(1x,A,A)") "model_name      = ", &
char (driver%get_model_name (1))
write (u, "(1x,A,A)") "md5sum         = ", &
char (driver%get_md5sum (1))
write (u, "(1x,A,L1)") "openmp_status = ", driver%get_openmp_status (1)
write (u, "(1x,A,I0)") "n_in      = ", driver%get_n_in (1)
write (u, "(1x,A,I0)") "n_out     = ", driver%get_n_out (1)
write (u, "(1x,A,I0)") "n_flv     = ", driver%get_n_flv (1)
write (u, "(1x,A,I0)") "n_hel     = ", driver%get_n_hel (1)
write (u, "(1x,A,I0)") "n_col     = ", driver%get_n_col (1)
write (u, "(1x,A,I0)") "n_cin     = ", driver%get_n_cin (1)
write (u, "(1x,A,I0)") "n_cf      = ", driver%get_n_cf (1)

call driver%set_flv_state (1, flv_state)
write (u, "(1x,A,10(1x,I0))") "flv_state =", flv_state

call driver%set_hel_state (1, hel_state)
write (u, "(1x,A,10(1x,I0))") "hel_state =", hel_state

call driver%set_col_state (1, col_state, ghost_flag)
write (u, "(1x,A,10(1x,I0))") "col_state =", col_state
write (u, "(1x,A,10(1x,L1))") "ghost_flag =", ghost_flag

call driver%set_color_factors (1, color_factors, cf_index)
write (u, "(1x,A,10(1x,F5.3))") "color_factors =", color_factors
write (u, "(1x,A,10(1x,I0))") "cf_index =", cf_index

call driver%get_fptr (1, 1, proc1_ptr)
call c_f_procpointer (proc1_ptr, proc1)
if (associated (proc1)) then
  write (u, *)
  call proc1 (n)
  write (u, "(1x,A,I0)") "proc1(1) = ", n
end if

end if

deallocate (test_writer_5)

write (u, "(A)")
write (u, "(A)") "* Test output end: prclib_interfaces_5"
end subroutine prclib_interfaces_5

```

This version of test-code writer writes interfaces for all standard features plus one specific feature. The interfaces are all bind(C), so no wrapper is needed.

<Prclib interfaces: test types>+≡

```

type, extends (prc_writer_c_lib_t) :: test_writer_5_t
contains
  procedure, nopass :: type_name => test_writer_5_type_name
  procedure :: write_makefile_code => test_writer_5_mk
  procedure :: write_source_code => test_writer_5_src
  procedure :: write_interface => test_writer_5_if
  procedure :: before_compile => test_writer_5_before_compile

```

```

    procedure :: after_compile => test_writer_5_after_compile
end type test_writer_5_t

```

The

(Prclib interfaces: test auxiliary)+≡

```

function test_writer_5_type_name () result (string)
    type(string_t) :: string
    string = "test_5"
end function test_writer_5_type_name

subroutine test_writer_5_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_5_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
    write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " FC " $@"
    end if
    write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
end subroutine test_writer_5_mk

subroutine test_writer_5_src (writer, id)
    class(test_writer_5_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    call write_test_f_lib_file (id, var_str ("proc1"))
end subroutine test_writer_5_src

subroutine test_writer_5_if (writer, unit, id, feature)
    class(test_writer_5_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    select case (char (feature))
    case ("proc1")
        write (unit, "(2x,9A)") "interface"
        write (unit, "(5x,9A)") "subroutine ", &
            char (writer%get_c_procname (id, feature)), &
            " (n) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "implicit none"
        write (unit, "(7x,9A)") "integer(c_int), intent(out) :: n"
        write (unit, "(5x,9A)") "end subroutine ", &
            char (writer%get_c_procname (id, feature))
        write (unit, "(2x,9A)") "end interface"
    case default
        call writer%write_standard_interface (unit, id, feature)
    end select
end subroutine test_writer_5_if

```

```

subroutine test_writer_5_before_compile (writer, id)
  class(test_writer_5_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_5_before_compile

subroutine test_writer_5_after_compile (writer, id)
  class(test_writer_5_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_5_after_compile

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature), the name given as an argument.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_f_lib_file (basename, feature)
  type(string_t), intent(in) :: basename
  type(string_t), intent(in) :: feature
  integer :: u
  u = free_unit ()
  open (u, file = char (basename) // ".f90", &
        status = "replace", action = "write")
  write (u, "(A)") "!(Pseudo) matrix element code file &
    &for WHIZARD self-test"
  call write_test_me_code_3 (u, char (basename))
  write (u, *)
  write (u, "(A)") "subroutine " // char (basename) // "_" &
    // char (feature) // " (n) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " integer(c_int), intent(out) :: n"
  write (u, "(A)") " n = 42"
  write (u, "(A)") "end subroutine " // char (basename) // "_" &
    // char (feature)
  close (u)
end subroutine write_test_f_lib_file

```

The following matrix-element source code is identical to the previous one, but modified such as to provide independent procedures without a module envelope.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_me_code_3 (u, id)
  integer, intent(in) :: u
  character(*), intent(in) :: id
  write (u, "(A)") "function " // id // "_get_md5sum () &
    &result (cptr) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " type(c_ptr) :: cptr"
  write (u, "(A)") " character(c_char), dimension(32), &
    &target, save :: md5sum"
  write (u, "(A)") " md5sum = copy (c_char_&
    &'1234567890abcdef1234567890abcdef')"
  write (u, "(A)") " cptr = c_loc (md5sum)"

```

```

write (u, "(A)") "contains"
write (u, "(A)") "  function copy (md5sum)"
write (u, "(A)") "    character(c_char), dimension(32) :: copy"
write (u, "(A)") "    character(c_char), dimension(32), intent(in) :: &
&md5sum"
write (u, "(A)") "      copy = md5sum"
write (u, "(A)") "    end function copy"
write (u, "(A)") "end function " // id // "_get_md5sum"
write (u, *)
write (u, "(A)") "function " // id // "_openmp_supported () &
&result (status) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  logical(c_bool) :: status"
write (u, "(A)") "  status = .false."
write (u, "(A)") "end function " // id // "_openmp_supported"
write (u, *)
write (u, "(A)") "function " // id // "_n_in () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  integer(c_int) :: n"
write (u, "(A)") "  n = 1"
write (u, "(A)") "end function " // id // "_n_in"
write (u, *)
write (u, "(A)") "function " // id // "_n_out () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  integer(c_int) :: n"
write (u, "(A)") "  n = 2"
write (u, "(A)") "end function " // id // "_n_out"
write (u, *)
write (u, "(A)") "function " // id // "_n_flv () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  integer(c_int) :: n"
write (u, "(A)") "  n = 1"
write (u, "(A)") "end function " // id // "_n_flv"
write (u, *)
write (u, "(A)") "function " // id // "_n_hel () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  integer(c_int) :: n"
write (u, "(A)") "  n = 1"
write (u, "(A)") "end function " // id // "_n_hel"
write (u, *)
write (u, "(A)") "function " // id // "_n_cin () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"
write (u, "(A)") "  implicit none"
write (u, "(A)") "  integer(c_int) :: n"
write (u, "(A)") "  n = 2"
write (u, "(A)") "end function " // id // "_n_cin"
write (u, *)
write (u, "(A)") "function " // id // "_n_col () result (n) bind(C)"
write (u, "(A)") "  use iso_c_binding"

```

```

write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 1"
write (u, "(A)") "end function " // id // "_n_col"
write (u, *)
write (u, "(A)") "function " // id // "_n_cf () result (n) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 1"
write (u, "(A)") "end function " // id // "_n_cf"
write (u, *)
write (u, "(A)") "subroutine " // id // "_flv_state (flv_state) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: flv_state"
write (u, "(A)") " flv_state(1:3) = [1,2,3]"
write (u, "(A)") "end subroutine " // id // "_flv_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_hel_state (hel_state) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: hel_state"
write (u, "(A)") " hel_state(1:3) = [0,0,0]"
write (u, "(A)") "end subroutine " // id // "_hel_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_col_state &
&(col_state, ghost_flag) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) &
&:: col_state"
write (u, "(A)") " logical(c_bool), dimension(*), intent(out) &
&:: ghost_flag"
write (u, "(A)") " col_state(1:6) = [0,0, 0,0, 0,0]"
write (u, "(A)") " ghost_flag(1:3) = [.false., .false., .false.]"
write (u, "(A)") "end subroutine " // id // "_col_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_color_factors &
&(cf_index1, cf_index2, color_factors) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " use kinds"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: cf_index1"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: cf_index2"
write (u, "(A)") " complex(c_default_complex), dimension(*), &
&intent(out) :: color_factors"
write (u, "(A)") " cf_index1(1:1) = [1]"
write (u, "(A)") " cf_index2(1:1) = [1]"
write (u, "(A)") " color_factors(1:1) = [1]"
write (u, "(A)") "end subroutine " // id // "_color_factors"
end subroutine write_test_me_code_3

```

Compile test with genuine C library

Test 6: Write driver and makefile and try to compile and link the library driver.

There is a single test process with a single feature. The process code is provided as a C library of independent procedures. These procedures should match the Fortran bind(C) interface.

```
<Prclib interfaces: execute tests>+≡
  if (default == double .or. (CC_IS_GNU .and. CC_HAS_QUADMATH)) then
    call test (prclib_interfaces_6, "prclib_interfaces_6", &
      "compile and link (C library)", &
      u, results)
  end if

<Prclib interfaces: test declarations>+≡
  public :: prclib_interfaces_6

<Prclib interfaces: tests>+≡
  subroutine prclib_interfaces_6 (u)
    integer, intent(in) :: u
    class(prclib_driver_t), allocatable :: driver
    class(prc_writer_t), pointer :: test_writer_6
    type(os_data_t) :: os_data
    integer :: u_file

    integer, dimension(:,:), allocatable :: flv_state
    integer, dimension(:,:), allocatable :: hel_state
    integer, dimension(:,:,:), allocatable :: col_state
    logical, dimension(:,:), allocatable :: ghost_flag
    integer, dimension(:,:), allocatable :: cf_index
    complex(default), dimension(:), allocatable :: color_factors
    character(32), parameter :: md5sum = "prclib_interfaces_6_md5sum"

    type(c_funptr) :: proc1_ptr
    interface
      subroutine proc1_t (n) bind(C)
        import
        integer(c_int), intent(out) :: n
      end subroutine proc1_t
    end interface
    procedure(proc1_t), pointer :: proc1
    integer(c_int) :: n

    write (u, "(A)")  "* Test output: prclib_interfaces_6"
    write (u, "(A)")  "* Purpose: compile, link, and load process library"
    write (u, "(A)")  "*           with (fake) matrix-element code &
      &as a C library"
    write (u, *)
    write (u, "(A)")  "* Create a prclib driver object (1 process)"
    write (u, "(A)")

    call os_data%init ()
    allocate (test_writer_6_t :: test_writer_6)

    call dispatch_prclib_driver (driver, var_str ("prclib6"), var_str (""))
    call driver%init (1)
```

```

call driver%set_md5sum (md5sum)

call driver%set_record (1, var_str ("test6"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_6)

call driver%write (u)

write (u, *)
write (u, "(A)")  "* Write makefile"
u_file = free_unit ()
open (u_file, file="prclib6.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")  "* Write driver source code"
u_file = free_unit ()
open (u_file, file="prclib6.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")  "* Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")  "* Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "* Link library"
call driver%make_link (os_data)

write (u, "(A)")  "* Load library"
call driver%load (os_data)

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
    write (u, "(A)")  "* Call library functions:"
    write (u, *)
    write (u, "(1x,A,I0)")  "n_processes   = ", driver%get_n_processes ()
    write (u, "(1x,A,A)")  "process_id   = ", &
        char (driver%get_process_id (1))
    write (u, "(1x,A,A)")  "model_name   = ", &
        char (driver%get_model_name (1))
    write (u, "(1x,A,A)")  "md5sum       = ", &
        char (driver%get_md5sum (1))
    write (u, "(1x,A,L1)")  "openmp_status = ", driver%get_openmp_status (1)
    write (u, "(1x,A,I0)")  "n_in        = ", driver%get_n_in (1)
    write (u, "(1x,A,I0)")  "n_out       = ", driver%get_n_out (1)
    write (u, "(1x,A,I0)")  "n_flv       = ", driver%get_n_flv (1)
    write (u, "(1x,A,I0)")  "n_hel       = ", driver%get_n_hel (1)
    write (u, "(1x,A,I0)")  "n_col       = ", driver%get_n_col (1)
    write (u, "(1x,A,I0)")  "n_cin       = ", driver%get_n_cin (1)
    write (u, "(1x,A,I0)")  "n_cf        = ", driver%get_n_cf (1)

```



```

call driver%set_flv_state (1, flv_state)
write (u, "(1x,A,10(1x,I0))") "flv_state =", flv_state

call driver%set_hel_state (1, hel_state)
write (u, "(1x,A,10(1x,I0))") "hel_state =", hel_state

call driver%set_col_state (1, col_state, ghost_flag)
write (u, "(1x,A,10(1x,I0))") "col_state =", col_state
write (u, "(1x,A,10(1x,L1))") "ghost_flag =", ghost_flag

call driver%set_color_factors (1, color_factors, cf_index)
write (u, "(1x,A,10(1x,F5.3))") "color_factors =", color_factors
write (u, "(1x,A,10(1x,I0))") "cf_index =", cf_index

call driver%get_fptr (1, 1, proc1_ptr)
call c_f_procpointer (proc1_ptr, proc1)
if (associated (proc1)) then
  write (u, *)
  call proc1 (n)
  write (u, "(1x,A,I0)") "proc1(1) = ", n
end if

end if

deallocate (test_writer_6)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_6"
end subroutine prclib_interfaces_6

```

This version of test-code writer writes interfaces for all standard features plus one specific feature. The interfaces are all `bind(C)`, so no wrapper is needed.

The driver part is identical to the Fortran case, so we simply extend the previous `test_writer_5` type. We only have to override the Makefile writer.

```

<Prclib interfaces: test types>+≡
type, extends (test_writer_5_t) :: test_writer_6_t
contains
  procedure, nopass :: type_name => test_writer_6_type_name
  procedure :: write_makefile_code => test_writer_6_mk
  procedure :: write_source_code => test_writer_6_src
end type test_writer_6_t

<Prclib interfaces: test auxiliary>+≡
function test_writer_6_type_name () result (string)
  type(string_t) :: string
  string = "test_6"
end function test_writer_6_type_name

subroutine test_writer_6_mk &
  (writer, unit, id, os_data, verbose, testflag)
  class(test_writer_6_t), intent(in) :: writer
  integer, intent(in) :: unit

```

```

type(string_t), intent(in) :: id
type(os_data_t), intent(in) :: os_data
logical, intent(in) :: verbose
logical, intent(in), optional :: testflag
write (unit, "(5A)") "SOURCES += ", char (id), ".c"
write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
write (unit, "(5A)") char (id), ".lo: ", char (id), ".c"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " FC          "$@'
end if
write (unit, "(5A)") TAB, "$(LTCCOMPILE) $<"
end subroutine test_writer_6_mk

subroutine test_writer_6_src (writer, id)
class(test_writer_6_t), intent(in) :: writer
type(string_t), intent(in) :: id
call write_test_c_lib_file (id, var_str ("proc1"))
end subroutine test_writer_6_src

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature), the name given as an argument.

```

<Prclib interfaces: test auxiliary>+≡
subroutine write_test_c_lib_file (basename, feature)
type(string_t), intent(in) :: basename
type(string_t), intent(in) :: feature
integer :: u
u = free_unit ()
open (u, file = char (basename) // ".c", &
      status = "replace", action = "write")
write (u, "(A)") "/* (Pseudo) matrix element code file &
&for WHIZARD self-test */"
write (u, "(A)") "#include <stdbool.h>"
if (CC_HAS_QUADMATH) then
    write (u, "(A)") "#include <quadmath.h>"
end if
write (u, *)
call write_test_me_code_4 (u, char (basename))
write (u, *)
write (u, "(A)") "void " // char (basename) // "_" &
// char (feature) // "(int* n) {"
write (u, "(A)") "    *n = 42;"
write (u, "(A)") "}"
close (u)
end subroutine write_test_c_lib_file

```

The following matrix-element source code is equivalent to the code in the previous example, but coded in C.

```

<Prclib interfaces: test auxiliary>+≡
subroutine write_test_me_code_4 (u, id)
integer, intent(in) :: u
character(*), intent(in) :: id

```

```

write (u, "(A)") "char* " // id // "_get_md5sum() {"
write (u, "(A)") " return ""1234567890abcdef1234567890abcdef"";"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "bool " // id // "_openmp_supported() {"
write (u, "(A)") " return false;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_in() {"
write (u, "(A)") " return 1;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_out() {"
write (u, "(A)") " return 2;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_flv() {"
write (u, "(A)") " return 1;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_hel() {"
write (u, "(A)") " return 1;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_cin() {"
write (u, "(A)") " return 2;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_col() {"
write (u, "(A)") " return 1;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "int " // id // "_n_cf() {"
write (u, "(A)") " return 1;"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "void " // id // "_flv_state( int (*a)[] ) {"
write (u, "(A)") " static int flv_state[1][3] = { { 1, 2, 3 } };"
write (u, "(A)") " int j;"
write (u, "(A)") " for (j = 0; j < 3; j++) { (*a)[j] &
    &= flv_state[0][j]; }"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "void " // id // "_hel_state( int (*a)[] ) {"
write (u, "(A)") " static int hel_state[1][3] = { { 0, 0, 0 } };"
write (u, "(A)") " int j;"
write (u, "(A)") " for (j = 0; j < 3; j++) { (*a)[j] &
    &= hel_state[0][j]; }"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "void " // id // "_col_state&
    &( int (*a)[], bool (*g)[] ) {"
write (u, "(A)") " static int col_state[1][3][2] = &
    &{ { {0, 0}, {0, 0}, {0, 0} } };"

```

```

write (u, "(A)") " static bool ghost_flag[1][3] = &
&{ { false, false, false } };"
write (u, "(A)") " int j,k;"
write (u, "(A)") " for (j = 0; j < 3; j++) {"
write (u, "(A)") " for (k = 0; k < 2; k++) {"
write (u, "(A)") " (*a)[j*2+k] = col_state[0][j][k];"
write (u, "(A)") " }"
write (u, "(A)") " (*g)[j] = ghost_flag[0][j];"
write (u, "(A)") " }"
write (u, "(A)") "}"
write (u, *)
select case (DEFAULT_FC_PRECISION)
case ("quadruple")
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&__complex128 (*color_factors)[] ) {"
case ("extended")
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&long double _Complex (*color_factors)[] ) {"
case default
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&double _Complex (*color_factors)[] ) {"
end select
write (u, "(A)") " (*color_factors)[0] = 1;"
write (u, "(A)") " (*cf_index1)[0] = 1;"
write (u, "(A)") " (*cf_index2)[0] = 1;"
write (u, "(A)") "}"
end subroutine write_test_me_code_4

```

Test cleanup targets

Test 7: Repeat test 4 (create, compile, link Fortran module and driver) and properly clean up all generated files.

<Prclib interfaces: execute tests>+≡

```

call test (prclib_interfaces_7, "prclib_interfaces_7", &
"cleanup", &
u, results)

```

<Prclib interfaces: test declarations>+≡

```

public :: prclib_interfaces_7

```

<Prclib interfaces: tests>+≡

```

subroutine prclib_interfaces_7 (u)
integer, intent(in) :: u
class(prclib_driver_t), allocatable :: driver
class(prc_writer_t), pointer :: test_writer_4
type(os_data_t) :: os_data
integer :: u_file
character(32), parameter :: md5sum = "1234567890abcdef1234567890abcdef"

write (u, "(A)") "* Test output: prclib_interfaces_7"
write (u, "(A)") "* Purpose: compile and link process library"

```

```

write (u, "(A)")  "*"           with (fake) matrix-element code &
                        &as a Fortran module"
write (u, "(A)")  "*"           then clean up generated files"
write (u, *)
write (u, "(A)")  "** Create a prclib driver object (1 process)"

allocate (test_writer_4_t :: test_writer_4)

call os_data%init ()
call dispatch_prclib_driver (driver, var_str ("prclib7"), var_str (""))
call driver%init (1)
call driver%set_md5sum (md5sum)
call driver%set_record (1, var_str ("test7"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_4)

write (u, "(A)")  "** Write makefile"
u_file = free_unit ()
open (u_file, file="prclib7.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")  "** Write driver source code"
u_file = free_unit ()
open (u_file, file="prclib7.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")  "** Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")  "** Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "** Link library"
call driver%make_link (os_data)

write (u, "(A)")  "** File check"
write (u, *)
call check_file (u, "test7.f90")
call check_file (u, "tpr_test7.mod")
call check_file (u, "test7.lo")
call check_file (u, "prclib7.makefile")
call check_file (u, "prclib7.f90")
call check_file (u, "prclib7.lo")
call check_file (u, "prclib7.la")

write (u, *)
write (u, "(A)")  "** Delete library"
write (u, *)
call driver%clean_library (os_data)
call check_file (u, "prclib7.la")

write (u, *)

```

```

write (u, "(A)")  "* Delete object code"
write (u, *)
call driver%clean_objects (os_data)
call check_file (u, "test7.lo")
call check_file (u, "tpr_test7.mod")
call check_file (u, "prclib7.lo")

write (u, *)
write (u, "(A)")  "* Delete source code"
write (u, *)
call driver%clean_source (os_data)
call check_file (u, "test7.f90")

write (u, *)
write (u, "(A)")  "* Delete driver source code"
write (u, *)
call driver%clean_driver (os_data)
call check_file (u, "prclib7.f90")

write (u, *)
write (u, "(A)")  "* Delete makefile"
write (u, *)
call driver%clean_makefile (os_data)
call check_file (u, "prclib7.makefile")

deallocate (test_writer_4)

write (u, *)
write (u, "(A)")  "* Test output end: prclib_interfaces_7"
end subroutine prclib_interfaces_7

```

Auxiliary routine: check and report existence of a file

```

<Prclib interfaces: test auxiliary>+≡
subroutine check_file (u, file)
integer, intent(in) :: u
character(*), intent(in) :: file
logical :: exist
inquire (file=file, exist=exist)
write (u, "(2x,A,A,L1)") file, " = ", exist
end subroutine check_file

```

14.3 Abstract process core configuration

In this module, we define abstract data types that handle the method-specific part of defining a process (including all of its options) and accessing an external matrix element.

There are no unit tests, these are deferred to the `process_libraries` module below.

```

<prc_core_def.f90>≡
<File header>

```

```

module prc_core_def

  <Use strings>
    use process_constants
    use prclib_interfaces

  <Standard module head>

  <Prc core def: public>

  <Prc core def: types>

  <Prc core def: interfaces>

    interface
  <Prc core def: sub interfaces>
    end interface

end module prc_core_def
<prc_core_def_sub.f90>≡
  <File header>

  submodule (prc_core_def) prc_core_def_s

    use io_units
    use diagnostics

    implicit none

  contains

  <Prc core def: procedures>

end submodule prc_core_def_s

```

14.3.1 Process core definition type

For storing configuration data that depend on the specific process variant, we introduce a polymorphic type. At this point, we just declare an abstract base type. This allows us to defer the implementation to later modules.

There should be no components that need explicit finalization, otherwise we would have to call a finalizer from the `process_component_def_t` wrapper. Translate a `prc_core_def_t` to above named integers

```

<Prc core def: public>≡
  public :: prc_core_def_t

<Prc core def: types>≡
  type, abstract :: prc_core_def_t
    class(prc_writer_t), allocatable :: writer
  contains
  <Prc core def: process core def: TBP>

```

```
end type prc_core_def_t
```

Interfaces for the deferred methods.

This returns a string. No passed argument; the string is constant and depends just on the type.

```
<Prc core def: process core def: TBP>≡
  procedure (prc_core_def_get_string), nopass, deferred :: type_string

<Prc core def: interfaces>≡
  abstract interface
    function prc_core_def_get_string () result (string)
      import
        type(string_t) :: string
    end function prc_core_def_get_string
  end interface
```

The `write` method should display the content completely.

```
<Prc core def: process core def: TBP>+≡
  procedure (prc_core_def_write), deferred :: write

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_write (object, unit)
      import
        class(prc_core_def_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine prc_core_def_write
  end interface
```

The `read` method should fill the content completely.

```
<Prc core def: process core def: TBP>+≡
  procedure (prc_core_def_read), deferred :: read

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_read (object, unit)
      import
        class(prc_core_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine prc_core_def_read
  end interface
```

This communicates a MD5 checksum to the writer inside the `core_def` object, if there is any. Usually, this checksum is not yet known at the time when the writer is initialized.

```
<Prc core def: process core def: TBP>+≡
  procedure :: set_md5sum => prc_core_def_set_md5sum

<Prc core def: sub interfaces>≡
  module subroutine prc_core_def_set_md5sum (core_def, md5sum)
    class(prc_core_def_t), intent(inout) :: core_def
    character(32) :: md5sum
  end subroutine prc_core_def_set_md5sum
```



```

<Prc core def: procedures>≡
  module subroutine prc_core_def_set_md5sum (core_def, md5sum)
    class(prc_core_def_t), intent(inout) :: core_def
    character(32) :: md5sum
    if (allocated (core_def%writer)) core_def%writer%md5sum = md5sum
  end subroutine prc_core_def_set_md5sum

```

Allocate an appropriate driver object which corresponds to the chosen process core definition.

For internal matrix element (i.e., those which do not need external code), the driver should have access to all matrix element information from the beginning. In short, it is the matrix-element code.

For external matrix elements, the driver will get access to the external matrix element code.

```

<Prc core def: process core def: TBP>+≡
  procedure(prc_core_def_allocate_driver), deferred :: allocate_driver

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_allocate_driver (object, driver, basename)
      import
      class(prc_core_def_t), intent(in) :: object
      class(prc_core_driver_t), intent(out), allocatable :: driver
      type(string_t), intent(in) :: basename
    end subroutine prc_core_def_allocate_driver
  end interface

```

This flag tells whether the particular variant needs external code. We implement a default function which returns false. The flag depends only on the type, therefore we implement it as `nopass`.

```

<Prc core def: process core def: TBP>+≡
  procedure, nopass :: needs_code => prc_core_def_needs_code

<Prc core def: sub interfaces>+≡
  module function prc_core_def_needs_code () result (flag)
    logical :: flag
  end function prc_core_def_needs_code

<Prc core def: procedures>+≡
  module function prc_core_def_needs_code () result (flag)
    logical :: flag
    flag = .false.
  end function prc_core_def_needs_code

```

This subroutine allocates an array which holds the name of all features that this process core implements. This feature applies to matrix element code that is not coded as a Fortran module but communicates via independent library functions, which follow the C calling conventions. The addresses of those functions are returned as C function pointers, which can be converted into Fortran procedure pointers. The conversion is done in code specific for the process variant; here we just retrieve the C function pointer.

The array returned here serves the purpose of writing specific driver code. The driver interfaces only those C functions which are supported for the given process core.

If the process core does not require external code, this array is meaningless.

```

<Prc core def: process core def: TBP>+≡
    procedure(prc_core_def_get_features), nopass, deferred &
        :: get_features

<Prc core def: interfaces>+≡
    abstract interface
        subroutine prc_core_def_get_features (features)
            import
            type(string_t), dimension(:), allocatable, intent(out) :: features
        end subroutine prc_core_def_get_features
    end interface

```

Assign pointers to the process-specific procedures to the driver, if the process is external.

```

<Prc core def: process core def: TBP>+≡
    procedure(prc_core_def_connect), deferred :: connect

<Prc core def: interfaces>+≡
    abstract interface
        subroutine prc_core_def_connect (def, lib_driver, i, proc_driver)
            import
            class(prc_core_def_t), intent(in) :: def
            class(prclib_driver_t), intent(in) :: lib_driver
            integer, intent(in) :: i
            class(prc_core_driver_t), intent(inout) :: proc_driver
        end subroutine prc_core_def_connect
    end interface

```

14.3.2 Process core template

We must be able to automatically allocate a process core definition object with the appropriate type, given only the type name.

To this end, we introduce a `prc_template_t` type which is simply a wrapper for an empty `prc_core_def_t` object. Choosing one of the templates from an array, we can allocate the target object.

```

<Prc core def: public>+≡
    public :: prc_template_t

<Prc core def: types>+≡
    type :: prc_template_t
        class(prc_core_def_t), allocatable :: core_def
    end type prc_template_t

```

The allocation routine. We use the `source` option of the `allocate` statement. The `mold` option would probably more appropriate, but is a F2008 feature.

```

<Prc core def: public>+≡
    public :: allocate_core_def

```

```

<Prc core def: sub interfaces>+≡
    module subroutine allocate_core_def (template, name, core_def)
        type(prc_template_t), dimension(:), intent(in) :: template
        type(string_t), intent(in) :: name
        class(prc_core_def_t), allocatable :: core_def
    end subroutine allocate_core_def

<Prc core def: procedures>+≡
    module subroutine allocate_core_def (template, name, core_def)
        type(prc_template_t), dimension(:), intent(in) :: template
        type(string_t), intent(in) :: name
        class(prc_core_def_t), allocatable :: core_def
        integer :: i
        do i = 1, size (template)
            if (template(i)%core_def%type_string () == name) then
                allocate (core_def, source = template(i)%core_def)
                return
            end if
        end do
    end subroutine allocate_core_def

```

14.3.3 Process driver

For each process component, we implement a driver object which holds the calls to the matrix element and various auxiliary routines as procedure pointers. Any actual calculation will use this object to communicate with the process.

Depending on the type of process (as described by a corresponding `prc_core_def` object), the procedure pointers may refer to external or internal code, and there may be additional procedures for certain types. The base type defined here is abstract.

```

<Prc core def: public>+≡
    public :: prc_core_driver_t

<Prc core def: types>+≡
    type, abstract :: prc_core_driver_t
    contains
    <Prc core def: process driver: TBP>
    end type prc_core_driver_t

```

This returns the process type. No reference to contents.

```

<Prc core def: process driver: TBP>≡
    procedure(prc_core_driver_type_name), nopass, deferred :: type_name

<Prc core def: interfaces>+≡
    abstract interface
        function prc_core_driver_type_name () result (type)
            import
            type(string_t) :: type
        end function prc_core_driver_type_name
    end interface

```

14.3.4 Process driver for intrinsic process

This is an abstract extension for the driver type. It has one additional method, namely a subroutine that fills the record of constant process data. For an external process, this task is performed by the external library driver instead.

```
<Prc core def: public>+≡
    public :: process_driver_internal_t

<Prc core def: types>+≡
    type, extends (prc_core_driver_t), abstract :: process_driver_internal_t
    contains
    <Prc core def: process driver internal: TBP>
    end type process_driver_internal_t

<Prc core def: process driver internal: TBP>≡
    procedure(process_driver_fill_constants), deferred :: fill_constants

<Prc core def: interfaces>+≡
    abstract interface
        subroutine process_driver_fill_constants (driver, data)
            import
            class(process_driver_internal_t), intent(in) :: driver
            type(process_constants_t), intent(out) :: data
        end subroutine process_driver_fill_constants
    end interface
```

14.4 Process library access

Processes (the code and data that are necessary for evaluating matrix elements of a particular process or process component) are organized in process libraries. In full form, process libraries contain generated and dynamically compiled and linked code, so they are actual libraries on the OS level. Alternatively, there may be simple processes that can be generated without referring to external libraries, and external libraries that are just linked in.

This module interfaces the OS to create, build, and use process libraries.

We work with two related data structures. There is the list of process configurations that stores the user input and data derived from it. A given process configuration list is scanned for creating a process library, which consists of both data and code. The creation step involves calling external programs and incorporating external code.

For the subsequent integration and event generation steps, we read the process library. We also support partial (re)creation of the process library. To this end, we should be able to reconstruct the configuration data records from the process library.

```
<process_libraries.f90>≡
    <File header>

    module process_libraries

        use, intrinsic :: iso_c_binding !NODEP!
```

```

    <Use strings>
    use physics_defs
    use os_interface
    use model_data
    use particle_specifiers
    use process_constants
    use prclib_interfaces
    use prc_core_def

    <Standard module head>

    <Process libraries: public>

    <Process libraries: parameters>

    <Process libraries: types>

    interface
    <Process libraries: sub interfaces>
    end interface

end module process_libraries

<process_libraries_sub.f90>≡
    <File header>

    submodule (process_libraries) process_libraries_s

        use io_units
        use diagnostics
        use md5

        implicit none

    contains

    <Process libraries: procedures>

end submodule process_libraries_s

```

14.4.1 Auxiliary stuff

Here is a small subroutine that strips the left-hand side and the equals sign off an equation.

```

    <Process libraries: public>≡
        public :: strip_equation_lhs

    <Process libraries: sub interfaces>≡
        module subroutine strip_equation_lhs (buffer)
            character(*), intent(inout) :: buffer
            end subroutine strip_equation_lhs

```

```

<Process libraries: procedures>≡
module subroutine strip_equation_lhs (buffer)
  character(*), intent(inout) :: buffer
  type(string_t) :: string, prefix
  string = buffer
  call split (string, prefix, "=")
  buffer = string
end subroutine strip_equation_lhs

```

14.4.2 Process definition objects

We collect process configuration data in a derived type, `process_def_t`. A process can be a collection of several components which are treated as a single entity for the purpose of observables and event generation. Multiple process components may initially be defined by the user. The system may add additional components, e.g., subtraction terms. The common data type is `process_component_def_t`. Within each component, there are several universal data items, and a part which depend on the particular process variant. The latter is covered by an abstract type `prc_core_def_t` and its extensions.

Wrapper for components

We define a wrapper type for the configuration of individual components.

The string `basename` is used for building file, module, and function names for the current process component. Initially, it will be built from the corresponding process basename by appending an alphanumeric suffix.

The logical `initial` tells whether this is a user-defined (true) or system-generated (false) configuration.

The numbers `n_in`, `n_out`, and `n_tot` denote the incoming, outgoing and total number of particles (partons) participating in the process component, respectively. These are the nominal particles, as input by the user (recombination may change the particle content, for the output events).

The string arrays `prt_in` and `prt_out` hold the particle specifications as provided by the user. For a system-generated process component, they remain deallocated.

The `method` string is used to determine the type of process matrix element and how it is obtained.

The `description` string collects the information about particle content and method in a single human-readable string.

The pointer object `core_def` is allocated according to the actual process variant, which depends on the method. The subobject holds any additional configuration data that is relevant for the process component.

We assume that no finalizer is needed.

```

<Process libraries: public>+≡
  public :: process_component_def_t

<Process libraries: types>≡
  type :: process_component_def_t
  private
  type(string_t) :: basename

```

```

logical :: initial = .false.
integer :: n_in = 0
integer :: n_out = 0
integer :: n_tot = 0
type(prt_spec_t), dimension(:), allocatable :: prt_in
type(prt_spec_t), dimension(:), allocatable :: prt_out
type(string_t) :: method
type(string_t) :: description
class(prc_core_def_t), allocatable :: core_def
character(32) :: md5sum = ""
integer :: nlo_type = BORN
integer, dimension(N_ASSOCIATED_COMPONENTS) :: associated_components = 0
logical :: active
integer :: fixed_emitter = -1
integer :: alpha_power = 0
integer :: alphas_power = 0
contains
  <Process libraries: process component def: TBP>
end type process_component_def_t

```

Display the complete content.

```

<Process libraries: process component def: TBP>≡
  procedure :: write => process_component_def_write

<Process libraries: sub interfaces>+≡
  module subroutine process_component_def_write (object, unit)
    class(process_component_def_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine process_component_def_write

<Process libraries: procedures>+≡
  module subroutine process_component_def_write (object, unit)
    class(process_component_def_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,A)") "Component ID          = ", char (object%basename)
    write (u, "(3x,A,L1)") "Initial component    = ", object%initial
    write (u, "(3x,A,I0,1x,I0,1x,I0)") "N (in, out, tot)    = ", &
      object%n_in, object%n_out, object%n_tot
    write (u, "(3x,A)", advance="no") "Particle content    = "
    if (allocated (object%prt_in)) then
      call prt_spec_write (object%prt_in, u, advance="no")
    else
      write (u, "(A)", advance="no") "[undefined]"
    end if
    write (u, "(A)", advance="no") " => "
    if (allocated (object%prt_out)) then
      call prt_spec_write (object%prt_out, u, advance="no")
    else
      write (u, "(A)", advance="no") "[undefined]"
    end if
    write (u, "(A)")
    if (object%method /= "") then
      write (u, "(3x,A,A)") "Method              = ", &

```

```

        char (object%method)
    else
        write (u, "(3x,A)") "Method" = [undefined]"
    end if
    if (allocated (object%core_def)) then
        write (u, "(3x,A,A)") "Process variant" = ", &
        char (object%core_def%type_string ())
        call object%core_def%write (u)
    else
        write (u, "(3x,A)") "Process variant" = [undefined]"
    end if
    write (u, "(3x,A,A,A)") "MD5 sum (def)" = "'", object%md5sum, "'"
end subroutine process_component_def_write

```

Read the process component definition. Allocate the process variant definition with appropriate type, matching the type name on file with the provided templates.

(Process libraries: process component def: TBP)+≡

```

procedure :: read => process_component_def_read

```

(Process libraries: sub interfaces)+≡

```

module subroutine process_component_def_read (component, unit, core_def_templates)
    class(process_component_def_t), intent(out) :: component
    integer, intent(in) :: unit
    type(prc_template_t), dimension(:), intent(in) :: core_def_templates
end subroutine process_component_def_read

```

(Process libraries: procedures)+≡

```

module subroutine process_component_def_read (component, unit, core_def_templates)
    class(process_component_def_t), intent(out) :: component
    integer, intent(in) :: unit
    type(prc_template_t), dimension(:), intent(in) :: core_def_templates
    character(80) :: buffer
    type(string_t) :: var_buffer, prefix, in_state, out_state
    type(string_t) :: variant_type

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    component%basename = trim (adjustl (buffer))

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) component%initial

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) component%n_in, component%n_out, component%n_tot

    call get (unit, var_buffer)
    call split (var_buffer, prefix, "=") ! keeps 'in => out'
    call split (var_buffer, prefix, "=") ! actually: separator is '=>'

    in_state = prefix
    if (component%n_in > 0) then

```



```

        call prt_spec_read (component%prt_in, in_state)
    end if

    out_state = extract (var_buffer, 2)
    if (component%n_out > 0) then
        call prt_spec_read (component%prt_out, out_state)
    end if

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    component%method = trim (adjustl (buffer))
    if (component%method == "[undefined]") &
        component%method = ""

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    variant_type = trim (adjustl (buffer))
    call allocate_core_def &
        (core_def_templates, variant_type, component%core_def)
    if (allocated (component%core_def)) then
        call component%core_def%read (unit)
    end if

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer(3:34), "(A32)") component%md5sum

end subroutine process_component_def_read

```

Short account.

```

<Process libraries: process component def: TBP>+≡
    procedure :: show => process_component_def_show

<Process libraries: sub interfaces>+≡
    module subroutine process_component_def_show (object, unit)
        class(process_component_def_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_component_def_show

<Process libraries: procedures>+≡
    module subroutine process_component_def_show (object, unit)
        class(process_component_def_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(6x,A)", advance="no") char (object%basename)
        if (.not. object%initial) &
            write (u, "('*')", advance="no")
        write (u, "(:',1x)", advance="no")
        if (allocated (object%prt_in)) then
            call prt_spec_write (object%prt_in, u, advance="no")
        else
            write (u, "(A)", advance="no") "[undefined]"
        end if
        write (u, "(A)", advance="no") " => "
    end subroutine process_component_def_show

```

```

    if (allocated (object%prt_out)) then
        call prt_spec_write (object%prt_out, u, advance="no")
    else
        write (u, "(A)", advance="no") "[undefined]"
    end if
    if (object%method /= "") then
        write (u, "(2x,['',A,']')") char (object%method)
    else
        write (u, *)
    end if
end subroutine process_component_def_show

```

Compute the MD5 sum of a process component. We reset the stored MD5 sum to the empty string (so a previous value is not included in the calculation), then write a temporary file and calculate the MD5 sum of that file.

This implies that all data that are displayed by the `write` method become part of the MD5 sum calculation.

The `model` is not part of the object, but must be included in the MD5 sum. Otherwise, modifying the model and nothing else would not trigger remaking the process-component source. Note that the model parameters may change later and therefore are not incorporated.

After the MD5 sum of the component has been computed, we communicate it to the `writer` subobject of the specific `core_def` component. Although these types are abstract, the MD5-related features are valid for the abstract types.

(Process libraries: process component def: TBP)+≡

```

    procedure :: compute_md5sum => process_component_def_compute_md5sum

```

(Process libraries: sub interfaces)+≡

```

    module subroutine process_component_def_compute_md5sum (component, model)
        class(process_component_def_t), intent(inout) :: component
        class(model_data_t), intent(in), optional, target :: model
    end subroutine process_component_def_compute_md5sum

```

(Process libraries: procedures)+≡

```

    module subroutine process_component_def_compute_md5sum (component, model)
        class(process_component_def_t), intent(inout) :: component
        class(model_data_t), intent(in), optional, target :: model
        integer :: u
        component%md5sum = ""
        u = free_unit ()
        open (u, status = "scratch", action = "readwrite")
        if (present (model)) write (u, "(A32)") model%get_md5sum ()
        call component%write (u)
        rewind (u)
        component%md5sum = md5sum (u)
        close (u)
        if (allocated (component%core_def)) then
            call component%core_def%set_md5sum (component%md5sum)
        end if
    end subroutine process_component_def_compute_md5sum

```

(Process libraries: process component def: TBP)+≡

```

    procedure :: get_def_type_string => process_component_def_get_def_type_string

```

```

<Process libraries: sub interfaces>+≡
    module function process_component_def_get_def_type_string (component) result (type_string)
        type(string_t) :: type_string
        class(process_component_def_t), intent(in) :: component
    end function process_component_def_get_def_type_string

```

```

<Process libraries: procedures>+≡
    module function process_component_def_get_def_type_string (component) result (type_string)
        type(string_t) :: type_string
        class(process_component_def_t), intent(in) :: component
        type_string = component%core_def%type_string ()
    end function process_component_def_get_def_type_string

```

Allocate the process driver (with a suitable type) for a process component. For internal processes, we may set all data already at this stage.

```

<Process libraries: process component def: TBP>+≡
    procedure :: allocate_driver => process_component_def_allocate_driver

<Process libraries: sub interfaces>+≡
    module subroutine process_component_def_allocate_driver (component, driver)
        class(process_component_def_t), intent(in) :: component
        class(prc_core_driver_t), intent(out), allocatable :: driver
    end subroutine process_component_def_allocate_driver

<Process libraries: procedures>+≡
    module subroutine process_component_def_allocate_driver (component, driver)
        class(process_component_def_t), intent(in) :: component
        class(prc_core_driver_t), intent(out), allocatable :: driver
        if (allocated (component%core_def)) then
            call component%core_def%allocate_driver (driver, component%basename)
        end if
    end subroutine process_component_def_allocate_driver

```

Tell whether the process core needs external code.

```

<Process libraries: process component def: TBP>+≡
    procedure :: needs_code => process_component_def_needs_code

<Process libraries: sub interfaces>+≡
    module function process_component_def_needs_code (component) result (flag)
        class(process_component_def_t), intent(in) :: component
        logical :: flag
    end function process_component_def_needs_code

<Process libraries: procedures>+≡
    module function process_component_def_needs_code (component) result (flag)
        class(process_component_def_t), intent(in) :: component
        logical :: flag
        flag = component%core_def%needs_code ()
    end function process_component_def_needs_code

```

If there is external code, the `core_def` subobject should provide a writer object. This method returns a pointer to the writer.

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_writer_ptr => process_component_def_get_writer_ptr

```

```

(Process libraries: sub interfaces)+≡
    module function process_component_def_get_writer_ptr (component) result (writer)
        class(process_component_def_t), intent(in), target :: component
        class(prc_writer_t), pointer :: writer
    end function process_component_def_get_writer_ptr

```

```

(Process libraries: procedures)+≡
    module function process_component_def_get_writer_ptr (component) result (writer)
        class(process_component_def_t), intent(in), target :: component
        class(prc_writer_t), pointer :: writer
        writer => component%core_def%writer
    end function process_component_def_get_writer_ptr

```

Return an array which holds the names of all C functions that this process component implements.

```

(Process libraries: process component def: TBP)+≡
    procedure :: get_features => process_component_def_get_features

(Process libraries: sub interfaces)+≡
    module function process_component_def_get_features (component) result (features)
        class(process_component_def_t), intent(in) :: component
        type(string_t), dimension(:), allocatable :: features
    end function process_component_def_get_features

(Process libraries: procedures)+≡
    module function process_component_def_get_features (component) result (features)
        class(process_component_def_t), intent(in) :: component
        type(string_t), dimension(:), allocatable :: features
        call component%core_def%get_features (features)
    end function process_component_def_get_features

```

Assign procedure pointers in the driver component (external processes). For internal processes, this is meaningless.

```

(Process libraries: process component def: TBP)+≡
    procedure :: connect => process_component_def_connect

(Process libraries: sub interfaces)+≡
    module subroutine process_component_def_connect &
        (component, lib_driver, i, proc_driver)
        class(process_component_def_t), intent(in) :: component
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
    end subroutine process_component_def_connect

(Process libraries: procedures)+≡
    module subroutine process_component_def_connect &
        (component, lib_driver, i, proc_driver)
        class(process_component_def_t), intent(in) :: component
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
        select type (proc_driver)
        class is (process_driver_internal_t)
            !!! Nothing to do

```

```

class default
  call component%core_def%connect (lib_driver, i, proc_driver)
end select
end subroutine process_component_def_connect

```

Return a pointer to the process core definition, which is of abstract type.

```

(Process libraries: process component def: TBP)+≡
  procedure :: get_core_def_ptr => process_component_get_core_def_ptr

(Process libraries: sub interfaces)+≡
  module function process_component_get_core_def_ptr (component) result (ptr)
    class(process_component_def_t), intent(in), target :: component
    class(prc_core_def_t), pointer :: ptr
  end function process_component_get_core_def_ptr

(Process libraries: procedures)+≡
  module function process_component_get_core_def_ptr (component) result (ptr)
    class(process_component_def_t), intent(in), target :: component
    class(prc_core_def_t), pointer :: ptr
    ptr => component%core_def
  end function process_component_get_core_def_ptr

```

Return nominal particle counts, as input by the user.

```

(Process libraries: process component def: TBP)+≡
  procedure :: get_n_in  => process_component_def_get_n_in
  procedure :: get_n_out => process_component_def_get_n_out
  procedure :: get_n_tot => process_component_def_get_n_tot

(Process libraries: sub interfaces)+≡
  module function process_component_def_get_n_in (component) result (n_in)
    class(process_component_def_t), intent(in) :: component
    integer :: n_in
  end function process_component_def_get_n_in
  module function process_component_def_get_n_out (component) result (n_out)
    class(process_component_def_t), intent(in) :: component
    integer :: n_out
  end function process_component_def_get_n_out
  module function process_component_def_get_n_tot (component) result (n_tot)
    class(process_component_def_t), intent(in) :: component
    integer :: n_tot
  end function process_component_def_get_n_tot

(Process libraries: procedures)+≡
  module function process_component_def_get_n_in (component) result (n_in)
    class(process_component_def_t), intent(in) :: component
    integer :: n_in
    n_in = component%n_in
  end function process_component_def_get_n_in

  module function process_component_def_get_n_out (component) result (n_out)
    class(process_component_def_t), intent(in) :: component
    integer :: n_out
    n_out = component%n_out
  end function process_component_def_get_n_out

```

```

module function process_component_def_get_n_tot (component) result (n_tot)
  class(process_component_def_t), intent(in) :: component
  integer :: n_tot
  n_tot = component%n_tot
end function process_component_def_get_n_tot

```

Allocate and return string arrays for the incoming and outgoing particles.

(Process libraries: process component def: TBP)+≡

```

procedure :: get_prt_in => process_component_def_get_prt_in
procedure :: get_prt_out => process_component_def_get_prt_out

```

(Process libraries: sub interfaces)+≡

```

module subroutine process_component_def_get_prt_in (component, prt)
  class(process_component_def_t), intent(in) :: component
  type(string_t), dimension(:), intent(out), allocatable :: prt
end subroutine process_component_def_get_prt_in
module subroutine process_component_def_get_prt_out (component, prt)
  class(process_component_def_t), intent(in) :: component
  type(string_t), dimension(:), intent(out), allocatable :: prt
end subroutine process_component_def_get_prt_out

```

(Process libraries: procedures)+≡

```

module subroutine process_component_def_get_prt_in (component, prt)
  class(process_component_def_t), intent(in) :: component
  type(string_t), dimension(:), intent(out), allocatable :: prt
  integer :: i
  allocate (prt (component%n_in))
  do i = 1, component%n_in
    prt(i) = component%prt_in(i)%to_string ()
  end do
end subroutine process_component_def_get_prt_in

```

```

module subroutine process_component_def_get_prt_out (component, prt)
  class(process_component_def_t), intent(in) :: component
  type(string_t), dimension(:), intent(out), allocatable :: prt
  integer :: i
  allocate (prt (component%n_out))
  do i = 1, component%n_out
    prt(i) = component%prt_out(i)%to_string ()
  end do
end subroutine process_component_def_get_prt_out

```

Return the incoming and outgoing particle specifiers as-is.

(Process libraries: process component def: TBP)+≡

```

procedure :: get_prt_spec_in => process_component_def_get_prt_spec_in
procedure :: get_prt_spec_out => process_component_def_get_prt_spec_out

```

(Process libraries: sub interfaces)+≡

```

module function process_component_def_get_prt_spec_in (component) result (prt)
  class(process_component_def_t), intent(in) :: component
  type(prt_spec_t), dimension(:), allocatable :: prt
end function process_component_def_get_prt_spec_in
module function process_component_def_get_prt_spec_out (component) result (prt)
  class(process_component_def_t), intent(in) :: component

```

```

        type(prt_spec_t), dimension(:), allocatable :: prt
    end function process_component_def_get_prt_spec_out

<Process libraries: procedures>+≡
    module function process_component_def_get_prt_spec_in (component) result (prt)
        class(process_component_def_t), intent(in) :: component
        type(prt_spec_t), dimension(:), allocatable :: prt
        allocate (prt (component%n_in))
        prt(:) = component%prt_in(:)
    end function process_component_def_get_prt_spec_in

    module function process_component_def_get_prt_spec_out (component) result (prt)
        class(process_component_def_t), intent(in) :: component
        type(prt_spec_t), dimension(:), allocatable :: prt
        allocate (prt (component%n_out))
        prt(:) = component%prt_out(:)
    end function process_component_def_get_prt_spec_out

```

Return the combination of incoming particles as a PDG code

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_pdg_in => process_component_def_get_pdg_in

<Process libraries: sub interfaces>+≡
    module subroutine process_component_def_get_pdg_in (component, model, pdg)
        class(process_component_def_t), intent(in) :: component
        class(model_data_t), intent(in), target :: model
        integer, intent(out), dimension(:) :: pdg
    end subroutine process_component_def_get_pdg_in

<Process libraries: procedures>+≡
    module subroutine process_component_def_get_pdg_in (component, model, pdg)
        class(process_component_def_t), intent(in) :: component
        class(model_data_t), intent(in), target :: model
        integer, intent(out), dimension(:) :: pdg
        integer :: i
        do i = 1, size (pdg)
            pdg(i) = model%get_pdg (component%prt_in(i)%to_string ())
        end do
    end subroutine process_component_def_get_pdg_in

```

Return the MD5 sum.

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_md5sum => process_component_def_get_md5sum

<Process libraries: sub interfaces>+≡
    pure module function process_component_def_get_md5sum (component) result (md5sum)
        class(process_component_def_t), intent(in) :: component
        character(32) :: md5sum
    end function process_component_def_get_md5sum

<Process libraries: procedures>+≡
    pure module function process_component_def_get_md5sum (component) result (md5sum)
        class(process_component_def_t), intent(in) :: component
        character(32) :: md5sum
        md5sum = component%md5sum
    end function process_component_def_get_md5sum

```

Get NLO data

```

(Process libraries: process component def: TBP)+≡
  procedure :: get_nlo_type => process_component_def_get_nlo_type
  procedure :: get_associated_born &
    => process_component_def_get_associated_born
  procedure :: get_associated_real_fin &
    => process_component_def_get_associated_real_fin
  procedure :: get_associated_real_sing &
    => process_component_def_get_associated_real_sing
  procedure :: get_associated_subtraction &
    => process_component_def_get_associated_subtraction
  procedure :: get_association_list &
    => process_component_def_get_association_list
  procedure :: can_be_integrated &
    => process_component_def_can_be_integrated
  procedure :: get_associated_real => process_component_def_get_associated_real

(Process libraries: sub interfaces)+≡
  elemental module function process_component_def_get_nlo_type &
    (component) result (nlo_type)
    integer :: nlo_type
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_get_nlo_type
  elemental module function process_component_def_get_associated_born &
    (component) result (i_born)
    integer :: i_born
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_get_associated_born
  elemental module function process_component_def_get_associated_real_fin &
    (component) result (i_rfin)
    integer :: i_rfin
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_get_associated_real_fin
  elemental module function process_component_def_get_associated_real_sing &
    (component) result (i_rsing)
    integer :: i_rsing
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_get_associated_real_sing
  elemental module function process_component_def_get_associated_subtraction &
    (component) result (i_sub)
    integer :: i_sub
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_get_associated_subtraction
  elemental module function process_component_def_can_be_integrated &
    (component) result (active)
    logical :: active
    class(process_component_def_t), intent(in) :: component
  end function process_component_def_can_be_integrated
  module function process_component_def_get_association_list &
    (component, i_skip_in) result (list)
    integer, dimension(:), allocatable :: list
    class(process_component_def_t), intent(in) :: component
    integer, intent(in), optional :: i_skip_in
  end function process_component_def_get_association_list
  module function process_component_def_get_associated_real &

```



```

        (component) result (i_real)
        integer :: i_real
        class(process_component_def_t), intent(in) :: component
    end function process_component_def_get_associated_real

    <Process libraries: procedures>+≡
    elemental module function process_component_def_get_nlo_type &
        (component) result (nlo_type)
        integer :: nlo_type
        class(process_component_def_t), intent(in) :: component
        nlo_type = component%nlo_type
    end function process_component_def_get_nlo_type

    elemental module function process_component_def_get_associated_born &
        (component) result (i_born)
        integer :: i_born
        class(process_component_def_t), intent(in) :: component
        i_born = component%associated_components(ASSOCIATED_BORN)
    end function process_component_def_get_associated_born

    elemental module function process_component_def_get_associated_real_fin &
        (component) result (i_rfin)
        integer :: i_rfin
        class(process_component_def_t), intent(in) :: component
        i_rfin = component%associated_components(ASSOCIATED_REAL_FIN)
    end function process_component_def_get_associated_real_fin

    elemental module function process_component_def_get_associated_real_sing &
        (component) result (i_rsing)
        integer :: i_rsing
        class(process_component_def_t), intent(in) :: component
        i_rsing = component%associated_components(ASSOCIATED_REAL_SING)
    end function process_component_def_get_associated_real_sing

    elemental module function process_component_def_get_associated_subtraction &
        (component) result (i_sub)
        integer :: i_sub
        class(process_component_def_t), intent(in) :: component
        i_sub = component%associated_components(ASSOCIATED_SUB)
    end function process_component_def_get_associated_subtraction

    elemental module function process_component_def_can_be_integrated &
        (component) result (active)
        logical :: active
        class(process_component_def_t), intent(in) :: component
        active = component%active
    end function process_component_def_can_be_integrated

    module function process_component_def_get_association_list &
        (component, i_skip_in) result (list)
        integer, dimension(:), allocatable :: list
        class(process_component_def_t), intent(in) :: component
        integer, intent(in), optional :: i_skip_in
        integer :: i, j, n, i_skip
        logical :: valid

```

```

i_skip = 0; if (present (i_skip_in)) i_skip = i_skip_in
n = count (component%associated_components /= 0) - 1
if (i_skip > 0) then
    if (component%associated_components(i_skip) > 0) n = n - 1
end if
allocate (list (n))
j = 1
do i = 1, size(component%associated_components)
    valid = component%associated_components(i) /= 0 &
        .and. i /= ASSOCIATED_SUB .and. i /= i_skip
    if (valid) then
        list(j) = component%associated_components(i)
        j = j + 1
    end if
end do
end function process_component_def_get_association_list

module function process_component_def_get_associated_real &
    (component) result (i_real)
    integer :: i_real
    class(process_component_def_t), intent(in) :: component
    i_real = component%associated_components(ASSOCIATED_REAL)
end function process_component_def_get_associated_real

```

(Process libraries: process component def: TBP)+≡

```
procedure :: get_me_method => process_component_def_get_me_method
```

(Process libraries: sub interfaces)+≡

```

elemental module function process_component_def_get_me_method (component) result (method)
    type(string_t) :: method
    class(process_component_def_t), intent(in) :: component
end function process_component_def_get_me_method

```

(Process libraries: procedures)+≡

```

elemental module function process_component_def_get_me_method (component) result (method)
    type(string_t) :: method
    class(process_component_def_t), intent(in) :: component
    method = component%method
end function process_component_def_get_me_method

```

(Process libraries: process component def: TBP)+≡

```
procedure :: get_fixed_emitter => process_component_def_get_fixed_emitter
```

(Process libraries: sub interfaces)+≡

```

module function process_component_def_get_fixed_emitter (component) result (emitter)
    integer :: emitter
    class(process_component_def_t), intent(in) :: component
end function process_component_def_get_fixed_emitter

```

(Process libraries: procedures)+≡

```

module function process_component_def_get_fixed_emitter (component) result (emitter)
    integer :: emitter
    class(process_component_def_t), intent(in) :: component
    emitter = component%fixed_emitter
end function process_component_def_get_fixed_emitter

```

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_coupling_powers => process_component_def_get_coupling_powers

<Process libraries: sub interfaces>+≡
    pure module subroutine process_component_def_get_coupling_powers &
        (component, alpha_power, alphas_power)
        class(process_component_def_t), intent(in) :: component
        integer, intent(out) :: alpha_power, alphas_power
    end subroutine process_component_def_get_coupling_powers

<Process libraries: procedures>+≡
    pure module subroutine process_component_def_get_coupling_powers &
        (component, alpha_power, alphas_power)
        class(process_component_def_t), intent(in) :: component
        integer, intent(out) :: alpha_power, alphas_power
        alpha_power = component%alpha_power
        alphas_power = component%alphas_power
    end subroutine process_component_def_get_coupling_powers

```

Process definition

The process component definitions are collected in a common process definition object.

The `id` is the ID string that the user has provided for identifying this process. It must be a string that is allowed as part of a Fortran variable name, since it may be used for generating code.

The number `n_in` is 1 or 2 for a decay or scattering process, respectively. This must be identical to `n_in` for all components.

The initial and extra component definitions (see above) are allocated as the `initial` and `extra` arrays, respectively. The latter are determined from the former.

The `md5sum` is used to verify the integrity of the configuration.

```

<Process libraries: public>+≡
    public :: process_def_t

<Process libraries: types>+≡
    type :: process_def_t
    private
    type(string_t) :: id
    integer :: num_id = 0
    class(model_data_t), pointer :: model => null ()
    type(string_t) :: model_name
    integer :: n_in = 0
    integer :: n_initial = 0
    integer :: n_extra = 0
    type(process_component_def_t), dimension(:), allocatable :: initial
    type(process_component_def_t), dimension(:), allocatable :: extra
    character(32) :: md5sum = ""
    logical :: nlo_process = .false.
    logical :: negative_sf = .false.
    logical :: requires_resonances = .false.
contains
    <Process libraries: process def: TBP>

```

```
end type process_def_t
```

Write the process definition including components:

(Process libraries: process def: TBP)≡

```
procedure :: write => process_def_write
```

(Process libraries: sub interfaces)+≡

```
module subroutine process_def_write (object, unit)
  class(process_def_t), intent(in) :: object
  integer, intent(in) :: unit
end subroutine process_def_write
```

(Process libraries: procedures)+≡

```
module subroutine process_def_write (object, unit)
  class(process_def_t), intent(in) :: object
  integer, intent(in) :: unit
  integer :: i
  write (unit, "(1x,A,A,A)") "ID = ", char (object%id), ""
  if (object%num_id /= 0) &
    write (unit, "(1x,A,IO)") "ID(num) = ", object%num_id
  select case (object%n_in)
  case (1); write (unit, "(1x,A)") "Decay"
  case (2); write (unit, "(1x,A)") "Scattering"
  case default
    write (unit, "(1x,A)") "[Undefined process]"
    return
  end select
  if (object%model_name /= "") then
    write (unit, "(1x,A,A)") "Model = ", char (object%model_name)
  else
    write (unit, "(1x,A)") "Model = [undefined]"
  end if
  write (unit, "(1x,A,IO)") "Initially defined component(s) = ", &
    object%n_initial
  write (unit, "(1x,A,IO)") "Extra generated component(s) = ", &
    object%n_extra
  if (object%requires_resonances) then
    ! This line has to matched with the reader below!
    write (unit, "(1x,A,IO)") "Resonant subprocesses required"
  end if
  write (unit, "(1x,A,A,A)") "MD5 sum = ", object%md5sum, ""
  if (allocated (object%initial)) then
    do i = 1, size (object%initial)
      write (unit, "(1x,A,IO)") "Component #", i
      call object%initial(i)%write (unit)
    end do
  end if
  if (allocated (object%extra)) then
    do i = 1, size (object%extra)
      write (unit, "(1x,A,IO)") "Component #", object%n_initial + i
      call object%extra(i)%write (unit)
    end do
  end if
end subroutine process_def_write
```

Read the process definition including components.

```

(Process libraries: process def: TBP)+≡
  procedure :: read => process_def_read

(Process libraries: sub interfaces)+≡
  module subroutine process_def_read (object, unit, core_def_templates)
    class(process_def_t), intent(out) :: object
    integer, intent(in) :: unit
    type(prc_template_t), dimension(:), intent(in) :: core_def_templates
  end subroutine process_def_read

(Process libraries: procedures)+≡
  module subroutine process_def_read (object, unit, core_def_templates)
    class(process_def_t), intent(out) :: object
    integer, intent(in) :: unit
    type(prc_template_t), dimension(:), intent(in) :: core_def_templates
    integer :: i, i1, i2
    character(80) :: buffer, ref
    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    i1 = scan (buffer, "'")
    i2 = scan (buffer, "'", back=.true.)
    if (i2 > i1) then
      object%id = buffer(i1+1:i2-1)
    else
      object%id = ""
    end if

    read (unit, "(A)") buffer
    select case (buffer(2:11))
    case ("Decay      "); object%n_in = 1
    case ("Scattering"); object%n_in = 2
    case default
      return
    end select

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    object%model_name = trim (adjustl (buffer))
    if (object%model_name == "[undefined]") object%model_name = ""

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%n_initial

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%n_extra

    read (unit, "(A)") buffer
    if (buffer(1:9) == " Resonant") then
      object%requires_resonances = .true.
      read (unit, "(A)") buffer
    else
      object%requires_resonances = .false.
    end if
  end module

```

```

end if

call strip_equation_lhs (buffer)
read (buffer(3:34), "(A32)") object%md5sum

if (object%n_initial > 0) then
  allocate (object%initial (object%n_initial))
  do i = 1, object%n_initial
    read (unit, "(A)") buffer
    write (ref, "(1x,A,I0)") "Component #", i
    if (buffer /= ref) return ! Wrong component header
    call object%initial(i)%read (unit, core_def_templates)
  end do
end if

end subroutine process_def_read

```

Short account.

```

<Process libraries: process def: TBP>+≡
  procedure :: show => process_def_show

<Process libraries: sub interfaces>+≡
  module subroutine process_def_show (object, unit)
    class(process_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine process_def_show

<Process libraries: procedures>+≡
  module subroutine process_def_show (object, unit)
    class(process_def_t), intent(in) :: object
    integer, intent(in) :: unit
    integer :: i
    write (unit, "(4x,A)", advance="no") char (object%id)
    if (object%num_id /= 0) &
      write (unit, "(1x,'( ',I0,' )'", advance="no") object%num_id
    if (object%model_name /= "") &
      write (unit, "(1x,'[ ',A,' ]'", advance="no") char (object%model_name)
    if (object%requires_resonances) then
      write (unit, "(1x,A)", advance="no") "[+ resonant subprocesses]"
    end if
    write (unit, *)
    if (allocated (object%initial)) then
      do i = 1, size (object%initial)
        call object%initial(i)%show (unit)
      end do
    end if
    if (allocated (object%extra)) then
      do i = 1, size (object%extra)
        call object%extra(i)%show (unit)
      end do
    end if
  end subroutine process_def_show

```

Initialize an entry (initialize the process definition inside). We allocate the 'initial' set of components. Extra components remain unallocated.

The model should be present as a pointer. This allows us to retrieve the model's MD5 sum. However, for various tests it is sufficient to have the name.

We create the basenames for the process components by appending a suffix which we increment for each component.

```

(Process libraries: process def: TBP)+≡
  procedure :: init => process_def_init

(Process libraries: sub interfaces)+≡
  module subroutine process_def_init (def, id, &
    model, model_name, n_in, n_components, num_id, &
    nlo_process, negative_sf, requires_resonances)
    class(process_def_t), intent(out) :: def
    type(string_t), intent(in), optional :: id
    class(model_data_t), intent(in), optional, target :: model
    type(string_t), intent(in), optional :: model_name
    integer, intent(in), optional :: n_in
    integer, intent(in), optional :: n_components
    integer, intent(in), optional :: num_id
    logical, intent(in), optional :: nlo_process
    logical, intent(in), optional :: negative_sf
    logical, intent(in), optional :: requires_resonances
  end subroutine process_def_init

(Process libraries: procedures)+≡
  module subroutine process_def_init (def, id, &
    model, model_name, n_in, n_components, num_id, &
    nlo_process, negative_sf, requires_resonances)
    class(process_def_t), intent(out) :: def
    type(string_t), intent(in), optional :: id
    class(model_data_t), intent(in), optional, target :: model
    type(string_t), intent(in), optional :: model_name
    integer, intent(in), optional :: n_in
    integer, intent(in), optional :: n_components
    integer, intent(in), optional :: num_id
    logical, intent(in), optional :: nlo_process
    logical, intent(in), optional :: negative_sf
    logical, intent(in), optional :: requires_resonances
    character(16) :: suffix
    integer :: i
    if (present (id)) then
      def%id = id
    else
      def%id = ""
    end if
    if (present (num_id)) then
      def%num_id = num_id
    end if
    if (present (model)) then
      def%model => model
      def%model_name = model%get_name ()
    else
      def%model => null ()
      if (present (model_name)) then

```

```

        def%model_name = model_name
    else
        def%model_name = ""
    end if
end if
if (present (n_in)) def%n_in = n_in
if (present (n_components)) then
    def%n_initial = n_components
    allocate (def%initial (n_components))
end if
if (present (nlo_process)) then
    def%nlo_process = nlo_process
end if
if (present (negative_sf)) then
    def%negative_sf = negative_sf
end if
if (present (requires_resonances)) then
    def%requires_resonances = requires_resonances
end if
def%initial%initial = .true.
def%initial%method = ""
do i = 1, def%n_initial
    write (suffix, "(A,I0)") "_i", i
    def%initial(i)%basename = def%id // trim (suffix)
end do
def%initial%description = ""
end subroutine process_def_init

```

Explicitly set the model name (for unit test).

```

<Process libraries: process def: TBP>+≡
    procedure :: set_model_name => process_def_set_model_name

<Process libraries: sub interfaces>+≡
    module subroutine process_def_set_model_name (def, model_name)
        class(process_def_t), intent(inout) :: def
        type(string_t), intent(in) :: model_name
    end subroutine process_def_set_model_name

<Process libraries: procedures>+≡
    module subroutine process_def_set_model_name (def, model_name)
        class(process_def_t), intent(inout) :: def
        type(string_t), intent(in) :: model_name
        def%model_name = model_name
    end subroutine process_def_set_model_name

```

Initialize an initial component. The particle content must be specified. The process core block is not (yet) allocated.

We assume that the particle arrays match the `n_in` and `n_out` values in size. The model is referred to by name; it is identified as an existing model later. The index `i` must refer to an existing element of the component array.

Data specific for the process core of a component are imported as the `core_def` argument. We should allocate an object of class `prc_core_def_t` with the appropriate specific type, fill it, and transfer it to the process compo-

nent definition here. The allocation is moved, so the original allocated object is returned empty.

<Process libraries: process def: TBP>+≡

```
procedure :: import_component => process_def_import_component
```

<Process libraries: sub interfaces>+≡

```
module subroutine process_def_import_component (def, &
    i, n_out, prt_in, prt_out, method, variant, &
    nlo_type, can_be_integrated)
class(process_def_t), intent(inout) :: def
integer, intent(in) :: i
integer, intent(in), optional :: n_out
type(prt_spec_t), dimension(:), intent(in), optional :: prt_in
type(prt_spec_t), dimension(:), intent(in), optional :: prt_out
type(string_t), intent(in), optional :: method
integer, intent(in), optional :: nlo_type
logical, intent(in), optional :: can_be_integrated
class(prc_core_def_t), &
    intent(inout), allocatable, optional :: variant
end subroutine process_def_import_component
```

<Process libraries: procedures>+≡

```
module subroutine process_def_import_component (def, &
    i, n_out, prt_in, prt_out, method, variant, &
    nlo_type, can_be_integrated)
class(process_def_t), intent(inout) :: def
integer, intent(in) :: i
integer, intent(in), optional :: n_out
type(prt_spec_t), dimension(:), intent(in), optional :: prt_in
type(prt_spec_t), dimension(:), intent(in), optional :: prt_out
type(string_t), intent(in), optional :: method
integer, intent(in), optional :: nlo_type
logical, intent(in), optional :: can_be_integrated
type(string_t) :: nlo_type_string
class(prc_core_def_t), &
    intent(inout), allocatable, optional :: variant
integer :: p
associate (comp => def%initial(i))
    if (present (n_out)) then
        comp%n_in = def%n_in
        comp%n_out = n_out
        comp%n_tot = def%n_in + n_out
    end if
    if (present (prt_in)) then
        allocate (comp%prt_in (size (prt_in)))
        comp%prt_in = prt_in
    end if
    if (present (prt_out)) then
        allocate (comp%prt_out (size (prt_out)))
        comp%prt_out = prt_out
    end if
    if (present (method)) comp%method = method
    if (present (variant)) then
        call move_alloc (variant, comp%core_def)
    end if
end if
```

```

    if (present (nlo_type)) then
        comp%nlo_type = nlo_type
    end if
    if (present (can_be_integrated)) then
        comp%active = can_be_integrated
    else
        comp%active = .true.
    end if
    if (allocated (comp%prt_in) .and. allocated (comp%prt_out)) then
        associate (d => comp%description)
            d = ""
            do p = 1, size (prt_in)
                if (p > 1) d = d // ", "
                d = d // comp%prt_in(p)%to_string ()
            end do
            d = d // " => "
            do p = 1, size (prt_out)
                if (p > 1) d = d // ", "
                d = d // comp%prt_out(p)%to_string ()
            end do
            if (comp%method /= "") then
                if ((def%nlo_process .and. .not. comp%active) .or. &
                    comp%nlo_type == NLO_SUBTRACTION) then
                    d = d // " [inactive]"
                else
                    d = d // " [" // comp%method // "]"
                end if
            end if
            nlo_type_string = component_status (comp%nlo_type)
            if (nlo_type_string /= "born") then
                d = d // ", [" // nlo_type_string // "]"
            end if
        end associate
    end if
end associate
end subroutine process_def_import_component

```

```

<Process libraries: process def: TBP>+≡
    procedure :: get_n_components => process_def_get_n_components

<Process libraries: sub interfaces>+≡
    module function process_def_get_n_components (def) result (n)
        class(process_def_t), intent(in) :: def
        integer :: n
    end function process_def_get_n_components

<Process libraries: procedures>+≡
    module function process_def_get_n_components (def) result (n)
        class(process_def_t), intent(in) :: def
        integer :: n
        n = size (def%initial)
    end function process_def_get_n_components

```

```

<Process libraries: process def: TBP>+≡
    procedure :: set_fixed_emitter => process_def_set_fixed_emitter

```

```

(Process libraries: sub interfaces)+≡
    module subroutine process_def_set_fixed_emitter (def, i, emitter)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: i, emitter
    end subroutine process_def_set_fixed_emitter

(Process libraries: procedures)+≡
    module subroutine process_def_set_fixed_emitter (def, i, emitter)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: i, emitter
        def%initial(i)%fixed_emitter = emitter
    end subroutine process_def_set_fixed_emitter

(Process libraries: process def: TBP)+≡
    procedure :: set_coupling_powers => process_def_set_coupling_powers

(Process libraries: sub interfaces)+≡
    module subroutine process_def_set_coupling_powers (def, alpha_power, alphas_power)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: alpha_power, alphas_power
    end subroutine process_def_set_coupling_powers

(Process libraries: procedures)+≡
    module subroutine process_def_set_coupling_powers (def, alpha_power, alphas_power)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: alpha_power, alphas_power
        def%initial(1)%alpha_power = alpha_power
        def%initial(1)%alphas_power = alphas_power
    end subroutine process_def_set_coupling_powers

(Process libraries: process def: TBP)+≡
    procedure :: set_associated_components => &
        process_def_set_associated_components

(Process libraries: sub interfaces)+≡
    module subroutine process_def_set_associated_components (def, i, &
        i_list, remnant, real_finite, mismatch)
        class(process_def_t), intent(inout) :: def
        logical, intent(in) :: remnant, real_finite, mismatch
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: i_list
    end subroutine process_def_set_associated_components

(Process libraries: procedures)+≡
    module subroutine process_def_set_associated_components (def, i, &
        i_list, remnant, real_finite, mismatch)
        class(process_def_t), intent(inout) :: def
        logical, intent(in) :: remnant, real_finite, mismatch
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: i_list
        integer :: add_index
        add_index = 0
        associate (comp => def%initial(i)%associated_components)
            comp(ASSOCIATED_BORN) = i_list(1)
            comp(ASSOCIATED_REAL) = i_list(2)
            comp(ASSOCIATED_VIRT) = i_list(3)
        end associate
    end subroutine process_def_set_associated_components

```

```

    comp(ASSOCIATED_SUB) = i_list(4)
    if (remnant) then
        comp(ASSOCIATED_PDF) = i_list(5)
        add_index = add_index + 1
    end if
    if (real_finite) then
        comp(ASSOCIATED_REAL_FIN) = i_list(5+add_index)
        add_index = add_index + 1
    end if
    if (mismatch) then
        !!! incomplete
    end if
end associate
end subroutine process_def_set_associated_components

```

Compute the MD5 sum for this process definition. We compute the MD5 sums for all components individually, then concatenate a string of those and compute the MD5 sum of this string. We also include the model name. All other data part of the component definitions.

```

<Process libraries: process def: TBP>+≡
    procedure :: compute_md5sum => process_def_compute_md5sum

<Process libraries: sub interfaces>+≡
    module subroutine process_def_compute_md5sum (def, model)
        class(process_def_t), intent(inout) :: def
        class(model_data_t), intent(in), optional, target :: model
    end subroutine process_def_compute_md5sum

<Process libraries: procedures>+≡
    module subroutine process_def_compute_md5sum (def, model)
        class(process_def_t), intent(inout) :: def
        class(model_data_t), intent(in), optional, target :: model
        integer :: i
        type(string_t) :: buffer
        buffer = def%model_name
        do i = 1, def%n_initial
            call def%initial(i)%compute_md5sum (model)
            buffer = buffer // def%initial(i)%md5sum
        end do
        do i = 1, def%n_extra
            call def%extra(i)%compute_md5sum (model)
            buffer = buffer // def%initial(i)%md5sum
        end do
        def%md5sum = md5sum (char (buffer))
    end subroutine process_def_compute_md5sum

```

Return the MD5 sum of the process or of a process component.

```

<Process libraries: process def: TBP>+≡
    procedure :: get_md5sum => process_def_get_md5sum

<Process libraries: sub interfaces>+≡
    module function process_def_get_md5sum (def, i_component) result (md5sum)
        class(process_def_t), intent(in) :: def
        integer, intent(in), optional :: i_component
    end function process_def_get_md5sum

```

```

        character(32) :: md5sum
    end function process_def_get_md5sum

<Process libraries: procedures>+≡
    module function process_def_get_md5sum (def, i_component) result (md5sum)
        class(process_def_t), intent(in) :: def
        integer, intent(in), optional :: i_component
        character(32) :: md5sum
        if (present (i_component)) then
            md5sum = def%initial(i_component)%md5sum
        else
            md5sum = def%md5sum
        end if
    end function process_def_get_md5sum

```

Return a pointer to the definition of a particular component (for test purposes).

```

<Process libraries: process def: TBP>+≡
    procedure :: get_core_def_ptr => process_def_get_core_def_ptr

<Process libraries: sub interfaces>+≡
    module function process_def_get_core_def_ptr (def, i_component) result (ptr)
        class(process_def_t), intent(in), target :: def
        integer, intent(in) :: i_component
        class(prc_core_def_t), pointer :: ptr
    end function process_def_get_core_def_ptr

<Process libraries: procedures>+≡
    module function process_def_get_core_def_ptr (def, i_component) result (ptr)
        class(process_def_t), intent(in), target :: def
        integer, intent(in) :: i_component
        class(prc_core_def_t), pointer :: ptr
        ptr => def%initial(i_component)%get_core_def_ptr ()
    end function process_def_get_core_def_ptr

```

This query tells whether a specific process component relies on external code. This includes all traditional WHIZARD matrix elements which rely on O'MEGA for code generation. Other process components (trivial decays, subtraction terms) do not require external code.

NOTE: Implemented only for initial component.

The query is passed to the process component.

```

<Process libraries: process def: TBP>+≡
    procedure :: needs_code => process_def_needs_code

<Process libraries: sub interfaces>+≡
    module function process_def_needs_code (def, i_component) result (flag)
        class(process_def_t), intent(in) :: def
        integer, intent(in) :: i_component
        logical :: flag
    end function process_def_needs_code

<Process libraries: procedures>+≡
    module function process_def_needs_code (def, i_component) result (flag)
        class(process_def_t), intent(in) :: def
        integer, intent(in) :: i_component
        logical :: flag
    end function process_def_needs_code

```

```

        flag = def%initial(i_component)%needs_code ()
    end function process_def_needs_code

```

Return the first entry for the incoming particle(s), PDG code, of this process.

<Process libraries: process def: TBP>+≡

```

    procedure :: get_pdg_in_1 => process_def_get_pdg_in_1

```

<Process libraries: sub interfaces>+≡

```

    module subroutine process_def_get_pdg_in_1 (def, pdg)
        class(process_def_t), intent(in), target :: def
        integer, dimension(:), intent(out) :: pdg
    end subroutine process_def_get_pdg_in_1

```

<Process libraries: procedures>+≡

```

    module subroutine process_def_get_pdg_in_1 (def, pdg)
        class(process_def_t), intent(in), target :: def
        integer, dimension(:), intent(out) :: pdg
        call def%initial(1)%get_pdg_in (def%model, pdg)
    end subroutine process_def_get_pdg_in_1

```

<Process libraries: process def: TBP>+≡

```

    procedure :: is_nlo => process_def_is_nlo

```

<Process libraries: sub interfaces>+≡

```

    elemental module function process_def_is_nlo (def) result (flag)
        logical :: flag
        class(process_def_t), intent(in) :: def
    end function process_def_is_nlo

```

<Process libraries: procedures>+≡

```

    elemental module function process_def_is_nlo (def) result (flag)
        logical :: flag
        class(process_def_t), intent(in) :: def
        flag = def%nlo_process
    end function process_def_is_nlo

```

<Process libraries: process def: TBP>+≡

```

    procedure :: get_nlo_type => process_def_get_nlo_type

```

<Process libraries: sub interfaces>+≡

```

    elemental module function process_def_get_nlo_type (def, i_component) result (nlo_type)
        integer :: nlo_type
        class(process_def_t), intent(in) :: def
        integer, intent(in) :: i_component
    end function process_def_get_nlo_type

```

<Process libraries: procedures>+≡

```

    elemental module function process_def_get_nlo_type (def, i_component) result (nlo_type)
        integer :: nlo_type
        class(process_def_t), intent(in) :: def
        integer, intent(in) :: i_component
        nlo_type = def%initial(i_component)%nlo_type
    end function process_def_get_nlo_type

```

```

<Process libraries: process def: TBP>+≡
    procedure :: get_negative_sf => process_def_get_negative_sf

<Process libraries: sub interfaces>+≡
    elemental module function process_def_get_negative_sf (def) result (neg_sf)
        logical :: neg_sf
        class(process_def_t), intent(in) :: def
    end function process_def_get_negative_sf

<Process libraries: procedures>+≡
    elemental module function process_def_get_negative_sf (def) result (neg_sf)
        logical :: neg_sf
        class(process_def_t), intent(in) :: def
        neg_sf = def%negative_sf
    end function process_def_get_negative_sf

```

Number of incoming particles, common to all components.

```

<Process libraries: process def: TBP>+≡
    procedure :: get_n_in => process_def_get_n_in

<Process libraries: sub interfaces>+≡
    module function process_def_get_n_in (def) result (n_in)
        class(process_def_t), intent(in) :: def
        integer :: n_in
    end function process_def_get_n_in

<Process libraries: procedures>+≡
    module function process_def_get_n_in (def) result (n_in)
        class(process_def_t), intent(in) :: def
        integer :: n_in
        n_in = def%n_in
    end function process_def_get_n_in

```

Pointer to a particular component definition record.

```

<Process libraries: process def: TBP>+≡
    procedure :: get_component_def_ptr => process_def_get_component_def_ptr

<Process libraries: sub interfaces>+≡
    module function process_def_get_component_def_ptr (def, i) result (component)
        type(process_component_def_t), pointer :: component
        class(process_def_t), intent(in), target :: def
        integer, intent(in) :: i
    end function process_def_get_component_def_ptr

<Process libraries: procedures>+≡
    module function process_def_get_component_def_ptr (def, i) result (component)
        type(process_component_def_t), pointer :: component
        class(process_def_t), intent(in), target :: def
        integer, intent(in) :: i
        if (i <= def%n_initial) then
            component => def%initial(i)
        else
            component => null ()
        end if
    end function process_def_get_component_def_ptr

```

Process definition list

A list of process definitions is the starting point for creating a process library. The list is built when reading the user input. When reading an existing process library, the list is used for cross-checking and updating the configuration.

We need a type for the list entry. The simplest way is to extend the process definition type, so all methods apply to the process definition directly.

```
<Process libraries: public>+≡
    public :: process_def_entry_t

<Process libraries: types>+≡
    type, extends (process_def_t) :: process_def_entry_t
    private
        type(process_def_entry_t), pointer :: next => null ()
    end type process_def_entry_t
```

This is the type for the list itself.

```
<Process libraries: public>+≡
    public :: process_def_list_t

<Process libraries: types>+≡
    type :: process_def_list_t
    private
        type(process_def_entry_t), pointer :: first => null ()
        type(process_def_entry_t), pointer :: last => null ()
    contains
        <Process libraries: process def list: TBP>
    end type process_def_list_t
```

The deallocates the list iteratively. We assume that the list entries do not need finalization themselves.

```
<Process libraries: process def list: TBP>≡
    procedure :: final => process_def_list_final

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_final (list)
        class(process_def_list_t), intent(inout) :: list
    end subroutine process_def_list_final

<Process libraries: procedures>+≡
    module subroutine process_def_list_final (list)
        class(process_def_list_t), intent(inout) :: list
        type(process_def_entry_t), pointer :: current
        nullify (list%last)
        do while (associated (list%first))
            current => list%first
            list%first => current%next
            deallocate (current)
        end do
    end subroutine process_def_list_final
```

Write the complete list.

```
<Process libraries: process def list: TBP>+≡
    procedure :: write => process_def_list_write
```



```

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_write (object, unit, libpath)
        class(process_def_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
    end subroutine process_def_list_write

<Process libraries: procedures>+≡
    module subroutine process_def_list_write (object, unit, libpath)
        class(process_def_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
        type(process_def_entry_t), pointer :: entry
        integer :: i, u
        u = given_output_unit (unit)
        if (associated (object%first)) then
            i = 1
            entry => object%first
            do while (associated (entry))
                write (u, "(1x,A,I0,A)") "Process #", i, ":"
                call entry%write (u)
                i = i + 1
                entry => entry%next
                if (associated (entry)) write (u, *)
            end do
        else
            write (u, "(1x,A)") "Process definition list: [empty]"
        end if
    end subroutine process_def_list_write

```

Short account.

```

<Process libraries: process def list: TBP>+≡
    procedure :: show => process_def_list_show

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_show (object, unit)
        class(process_def_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_def_list_show

<Process libraries: procedures>+≡
    module subroutine process_def_list_show (object, unit)
        class(process_def_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        type(process_def_entry_t), pointer :: entry
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%first)) then
            write (u, "(2x,A)") "Processes:"
            entry => object%first
            do while (associated (entry))
                call entry%show (u)
                entry => entry%next
            end do
        else

```

```

        write (u, "(2x,A)") "Processes: [empty]"
    end if
end subroutine process_def_list_show

```

Read the complete list. We need an array of templates for the component sub-objects of abstract `prc_core_t` type, to allocate them with the correct specific type.

NOTE: Error handling is missing. Reading will just be aborted on error, or an I/O error occurs.

```

<Process libraries: process def list: TBP>+≡
    procedure :: read => process_def_list_read

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_read (object, unit, core_def_templates)
        class(process_def_list_t), intent(out) :: object
        integer, intent(in) :: unit
        type(prc_template_t), dimension(:), intent(in) :: core_def_templates
    end subroutine process_def_list_read

<Process libraries: procedures>+≡
    module subroutine process_def_list_read (object, unit, core_def_templates)
        class(process_def_list_t), intent(out) :: object
        integer, intent(in) :: unit
        type(prc_template_t), dimension(:), intent(in) :: core_def_templates
        type(process_def_entry_t), pointer :: entry
        character(80) :: buffer, ref
        integer :: i
        read (unit, "(A)") buffer
        write (ref, "(1x,A)") "Process definition list: [empty]"
        if (buffer == ref) return ! OK: empty library
        backspace (unit)
        READ_ENTRIES: do i = 1, huge(0)-1
            if (i > 1) read (unit, *, end=1)
            read (unit, "(A)") buffer

            write (ref, "(1x,A,I0,A)") "Process #", i, ":"
            if (buffer /= ref) return ! Wrong process header: done.
            allocate (entry)
            call entry%read (unit, core_def_templates)
            call object%append (entry)
        end do READ_ENTRIES
1    continue ! EOF: done
    end subroutine process_def_list_read

```

Append an entry to the list. The entry should be allocated as a pointer, and the pointer allocation is transferred. The original pointer is returned null.

```

<Process libraries: process def list: TBP>+≡
    procedure :: append => process_def_list_append

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_append (list, entry)
        class(process_def_list_t), intent(inout) :: list
        type(process_def_entry_t), intent(inout), pointer :: entry
    end subroutine process_def_list_append

```

```

<Process libraries: procedures>+≡
module subroutine process_def_list_append (list, entry)
  class(process_def_list_t), intent(inout) :: list
  type(process_def_entry_t), intent(inout), pointer :: entry
  if (list%contains (entry%id)) then
    call msg_fatal ("Recording process: '" // char (entry%id) &
      // "' has already been defined")
  end if
  if (associated (list%first)) then
    list%last%next => entry
  else
    list%first => entry
  end if
  list%last => entry
  entry => null ()
end subroutine process_def_list_append

```

Probe the process definition list

Return the number of processes supported by the library.

```

<Process libraries: process def list: TBP>+≡
  procedure :: get_n_processes => process_def_list_get_n_processes

<Process libraries: sub interfaces>+≡
  module function process_def_list_get_n_processes (list) result (n)
    integer :: n
    class(process_def_list_t), intent(in) :: list
    end function process_def_list_get_n_processes

<Process libraries: procedures>+≡
module function process_def_list_get_n_processes (list) result (n)
  integer :: n
  class(process_def_list_t), intent(in) :: list
  type(process_def_entry_t), pointer :: current
  n = 0
  current => list%first
  do while (associated (current))
    n = n + 1
    current => current%next
  end do
end function process_def_list_get_n_processes

```

Allocate an array with the process IDs supported by the library.

```

<Process libraries: process def list: TBP>+≡
  procedure :: get_process_id_list => process_def_list_get_process_id_list

<Process libraries: sub interfaces>+≡
  module subroutine process_def_list_get_process_id_list (list, id)
    class(process_def_list_t), intent(in) :: list
    type(string_t), dimension(:), allocatable, intent(out) :: id
  end subroutine process_def_list_get_process_id_list

```

(Process libraries: procedures)+≡

```

module subroutine process_def_list_get_process_id_list (list, id)
  class(process_def_list_t), intent(in) :: list
  type(string_t), dimension(:), allocatable, intent(out) :: id
  type(process_def_entry_t), pointer :: current
  integer :: i
  allocate (id (list%get_n_processes ()))
  i = 0
  current => list%first
  do while (associated (current))
    i = i + 1
    id(i) = current%id
    current => current%next
  end do
end subroutine process_def_list_get_process_id_list

```

Return just the processes which require resonant subprocesses.

(Process libraries: process def list: TBP)+≡

```

procedure :: get_process_id_req_resonant => &
  process_def_list_get_process_id_req_resonant

```

(Process libraries: sub interfaces)+≡

```

module subroutine process_def_list_get_process_id_req_resonant (list, id)
  class(process_def_list_t), intent(in) :: list
  type(string_t), dimension(:), allocatable, intent(out) :: id
end subroutine process_def_list_get_process_id_req_resonant

```

(Process libraries: procedures)+≡

```

module subroutine process_def_list_get_process_id_req_resonant (list, id)
  class(process_def_list_t), intent(in) :: list
  type(string_t), dimension(:), allocatable, intent(out) :: id
  type(process_def_entry_t), pointer :: current
  integer :: i
  allocate (id (list%get_n_processes ()))
  i = 0
  current => list%first
  do while (associated (current))
    if (current%requires_resonances) then
      i = i + 1
      id(i) = current%id
    end if
    current => current%next
  end do
  id = id(1:i)
end subroutine process_def_list_get_process_id_req_resonant

```

Return a pointer to a particular process entry.

(Process libraries: process def list: TBP)+≡

```

procedure :: get_process_def_ptr => process_def_list_get_process_def_ptr

```

(Process libraries: sub interfaces)+≡

```

module function process_def_list_get_process_def_ptr (list, id) result (entry)
  type(process_def_entry_t), pointer :: entry
  class(process_def_list_t), intent(in) :: list

```

```

        type(string_t), intent(in) :: id
    end function process_def_list_get_process_def_ptr

<Process libraries: procedures>+≡
module function process_def_list_get_process_def_ptr (list, id) result (entry)
    type(process_def_entry_t), pointer :: entry
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id
    type(process_def_entry_t), pointer :: current
    current => list%first
    do while (associated (current))
        if (id == current%id) exit
        current => current%next
    end do
    entry => current
end function process_def_list_get_process_def_ptr

```

Return true if a given process is in the library.

```

<Process libraries: process def list: TBP>+≡
    procedure :: contains => process_def_list_contains

<Process libraries: sub interfaces>+≡
    module function process_def_list_contains (list, id) result (flag)
        logical :: flag
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
    end function process_def_list_contains

<Process libraries: procedures>+≡
    module function process_def_list_contains (list, id) result (flag)
        logical :: flag
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        flag = associated (current)
    end function process_def_list_contains

```

Return the index of the entry that corresponds to a given process.

```

<Process libraries: process def list: TBP>+≡
    procedure :: get_entry_index => process_def_list_get_entry_index

<Process libraries: sub interfaces>+≡
    module function process_def_list_get_entry_index (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
    end function process_def_list_get_entry_index

<Process libraries: procedures>+≡
    module function process_def_list_get_entry_index (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current

```

```

n = 0
current => list%first
do while (associated (current))
  n = n + 1
  if (id == current%id) then
    return
  end if
  current => current%next
end do
n = 0
end function process_def_list_get_entry_index

```

Return the numerical ID for a process.

```

(Process libraries: process def list: TBP)+≡
  procedure :: get_num_id => process_def_list_get_num_id

(Process libraries: sub interfaces)+≡
  module function process_def_list_get_num_id (list, id) result (num_id)
    integer :: num_id
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id
  end function process_def_list_get_num_id

(Process libraries: procedures)+≡
  module function process_def_list_get_num_id (list, id) result (num_id)
    integer :: num_id
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id
    type(process_def_entry_t), pointer :: current
    current => list%get_process_def_ptr (id)
    if (associated (current)) then
      num_id = current%num_id
    else
      num_id = 0
    end if
  end function process_def_list_get_num_id

```

Return the model name for a given process in the library.

```

(Process libraries: process def list: TBP)+≡
  procedure :: get_model_name => process_def_list_get_model_name

(Process libraries: sub interfaces)+≡
  module function process_def_list_get_model_name (list, id) result (model_name)
    type(string_t) :: model_name
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id
  end function process_def_list_get_model_name

(Process libraries: procedures)+≡
  module function process_def_list_get_model_name (list, id) result (model_name)
    type(string_t) :: model_name
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id
    type(process_def_entry_t), pointer :: current
    current => list%get_process_def_ptr (id)
  end function process_def_list_get_model_name

```

```

    if (associated (current)) then
        model_name = current%model_name
    else
        model_name = ""
    end if
end function process_def_list_get_model_name

```

Return the number of incoming particles of a given process in the library. This tells us whether the process is a decay or a scattering.

```

<Process libraries: process def list: TBP>+≡
    procedure :: get_n_in => process_def_list_get_n_in

<Process libraries: sub interfaces>+≡
    module function process_def_list_get_n_in (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
    end function process_def_list_get_n_in

<Process libraries: procedures>+≡
    module function process_def_list_get_n_in (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            n = current%n_in
        else
            n = 0
        end if
    end function process_def_list_get_n_in

```

Return the incoming particle pdg codesnumber of incoming particles of a given process in the library. If there is a PDG array, return only the first code for each beam. This serves as a quick way for (re)constructing beam properties.

```

<Process libraries: process def list: TBP>+≡
    procedure :: get_pdg_in_1 => process_def_list_get_pdg_in_1

<Process libraries: sub interfaces>+≡
    module subroutine process_def_list_get_pdg_in_1 (list, id, pdg)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        integer, dimension(:), intent(out) :: pdg
    end subroutine process_def_list_get_pdg_in_1

<Process libraries: procedures>+≡
    module subroutine process_def_list_get_pdg_in_1 (list, id, pdg)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        integer, dimension(:), intent(out) :: pdg
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            call current%get_pdg_in_1 (pdg)
        end if
    end subroutine process_def_list_get_pdg_in_1

```

```

else
    pdg = 0
end if
end subroutine process_def_list_get_pdg_in_1

```

Return the list of component IDs of a given process in the library.

```

(Process libraries: process def list: TBP)+≡
    procedure :: get_component_list => process_def_list_get_component_list

(Process libraries: sub interfaces)+≡
    module subroutine process_def_list_get_component_list (list, id, cid)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(string_t), dimension(:), allocatable, intent(out) :: cid
    end subroutine process_def_list_get_component_list

(Process libraries: procedures)+≡
    module subroutine process_def_list_get_component_list (list, id, cid)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(string_t), dimension(:), allocatable, intent(out) :: cid
        type(process_def_entry_t), pointer :: current
        integer :: i, n
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            allocate (cid (current%n_initial + current%n_extra))
            do i = 1, current%n_initial
                cid(i) = current%initial(i)%basename
            end do
            n = current%n_initial
            do i = 1, current%n_extra
                cid(n + i) = current%extra(i)%basename
            end do
        end if
    end subroutine process_def_list_get_component_list

```

Return the list of component description strings for a given process in the library.

```

(Process libraries: process def list: TBP)+≡
    procedure :: get_component_description_list => &
        process_def_list_get_component_description_list

(Process libraries: sub interfaces)+≡
    module subroutine process_def_list_get_component_description_list &
        (list, id, description)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(string_t), dimension(:), allocatable, intent(out) :: description
    end subroutine process_def_list_get_component_description_list

(Process libraries: procedures)+≡
    module subroutine process_def_list_get_component_description_list &
        (list, id, description)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(string_t), dimension(:), allocatable, intent(out) :: description

```



```

type(process_def_entry_t), pointer :: current
integer :: i, n
current => list%get_process_def_ptr (id)
if (associated (current)) then
    allocate (description (current%n_initial + current%n_extra))
    do i = 1, current%n_initial
        description(i) = current%initial(i)%description
    end do
    n = current%n_initial
    do i = 1, current%n_extra
        description(n + i) = current%extra(i)%description
    end do
end if
end subroutine process_def_list_get_component_description_list

```

Return whether the entry requires construction of a resonant subprocess set.

```

(Process libraries: process def list: TBP)+≡
    procedure :: req_resonant => process_def_list_req_resonant

(Process libraries: sub interfaces)+≡
    module function process_def_list_req_resonant (list, id) result (flag)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        logical :: flag
    end function process_def_list_req_resonant

(Process libraries: procedures)+≡
    module function process_def_list_req_resonant (list, id) result (flag)
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        logical :: flag
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            flag = current%requires_resonances
        else
            flag = .false.
        end if
    end function process_def_list_req_resonant

```

14.4.3 Process library

The process library object is the interface between the process definition data, as provided by the user, generated or linked process code on file, and the process run data that reference the process code.

Process library entry

For each process component that is part of the library, there is a separate library entry (`process_library_entry_t`). The library entry connects a process definition with the specific code (if any) in the compiled driver library.

The **status** indicates how far the process has been processed by the system (definition, code generation, compilation, linking). A process with status **STAT_LOADED** is accessible for computing matrix elements.

The **def** pointer identifies the corresponding process definition. The process component within that definition is identified by the **i_component** index.

The **i_external** index refers to the compiled library driver. If it is zero, there is no associated matrix-element code.

The **driver** component holds the pointers to the matrix-element specific functions, in particular the matrix element function itself.

```

(Process libraries: types)+≡
  type :: process_library_entry_t
  private
    integer :: status = STAT_UNKNOWN
    type(process_def_t), pointer :: def => null ()
    integer :: i_component = 0
    integer :: i_external = 0
    class(prc_core_driver_t), allocatable :: driver
  contains
    (Process libraries: process library entry: TBP)
  end type process_library_entry_t

```

Here are the available status codes. An entry starts with **UNKNOWN** status. Once the association with a valid process definition is established, the status becomes **CONFIGURED**. If matrix element source code is to be generated by the system or provided from elsewhere, **CODE_GENERATED** indicates that this is done. The **COMPILED** status is next, it also applies to processes which are accessed as pre-compiled binaries. Finally, the library is linked and process pointers are set; this is marked as **LOADED**.

For a process library, the initial status is **OPEN**, since process definitions may be added. After configuration, the process content is fixed and the status becomes **CONFIGURED**. The further states are as above, always referring to the lowest status among the process entries.

```

(Process libraries: parameters)≡
  integer, parameter, public :: STAT_UNKNOWN = 0
  integer, parameter, public :: STAT_OPEN = 1
  integer, parameter, public :: STAT_CONFIGURED = 2
  integer, parameter, public :: STAT_SOURCE = 3
  integer, parameter, public :: STAT_COMPILED = 4
  integer, parameter, public :: STAT_LINKED = 5
  integer, parameter, public :: STAT_ACTIVE = 6

  integer, parameter, public :: ASSOCIATED_BORN = 1
  integer, parameter, public :: ASSOCIATED_REAL = 2
  integer, parameter, public :: ASSOCIATED_VIRT = 3
  integer, parameter, public :: ASSOCIATED_SUB = 4
  integer, parameter, public :: ASSOCIATED_PDF = 5
  integer, parameter, public :: ASSOCIATED_REAL_SING = 6
  integer, parameter, public :: ASSOCIATED_REAL_FIN = 7
  integer, parameter, public :: N_ASSOCIATED_COMPONENTS = 7

```

These are the associated code letters, for output:

```

(Process libraries: parameters)+≡
    character, dimension(0:6), parameter :: STATUS_LETTER = &
        ["?", "o", "f", "s", "c", "l", "a"]

```

This produces a condensed account of the library entry. The status is indicated by a letter in brackets, then the ID and component index of the associated process definition, finally the library index, if available.

```

(Process libraries: process library entry: TBP)≡
    procedure :: to_string => process_library_entry_to_string

(Process libraries: sub interfaces)+≡
    module function process_library_entry_to_string (object) result (string)
        type(string_t) :: string
        class(process_library_entry_t), intent(in) :: object
    end function process_library_entry_to_string

(Process libraries: procedures)+≡
    module function process_library_entry_to_string (object) result (string)
        type(string_t) :: string
        class(process_library_entry_t), intent(in) :: object
        character(32) :: buffer
        string = "[" // STATUS_LETTER(object%status) // "]"
        select case (object%status)
        case (STAT_UNKNOWN)
        case default
            if (associated (object%def)) then
                write (buffer, "(IO)") object%i_component
                string = string // " " // object%def%id // "." // trim (buffer)
            end if
            if (object%i_external /= 0) then
                write (buffer, "(IO)") object%i_external
                string = string // " = ext:" // trim (buffer)
            else
                string = string // " = int"
            end if
            if (allocated (object%driver)) then
                string = string // " (" // object%driver%type_name () // ")"
            end if
        end select
    end function process_library_entry_to_string

```

Initialize with data. Used for the unit tests.

```

(Process libraries: process library entry: TBP)+≡
    procedure :: init => process_library_entry_init

(Process libraries: sub interfaces)+≡
    module subroutine process_library_entry_init (object, &
        status, def, i_component, i_external, driver_template)
        class(process_library_entry_t), intent(out) :: object
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &

```

```

        :: driver_template
    end subroutine process_library_entry_init
<Process libraries: procedures>+=
    module subroutine process_library_entry_init (object, &
        status, def, i_component, i_external, driver_template)
        class(process_library_entry_t), intent(out) :: object
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &
            :: driver_template
        object%status = status
        object%def => def
        object%i_component = i_component
        object%i_external = i_external
        if (present (driver_template)) then
            call move_alloc (driver_template, object%driver)
        end if
    end subroutine process_library_entry_init

```

Assign pointers for all process-specific features. We have to combine the method from the `core_def` specification, the assigned pointers within the library driver, the index within that driver, and the process driver which should receive the links.

```

<Process libraries: process library entry: TBP>+=
    procedure :: connect => process_library_entry_connect
<Process libraries: sub interfaces>+=
    module subroutine process_library_entry_connect (entry, lib_driver, i)
        class(process_library_entry_t), intent(inout) :: entry
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
    end subroutine process_library_entry_connect
<Process libraries: procedures>+=
    module subroutine process_library_entry_connect (entry, lib_driver, i)
        class(process_library_entry_t), intent(inout) :: entry
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        call entry%def%initial(entry%i_component)%connect &
            (lib_driver, i, entry%driver)
    end subroutine process_library_entry_connect

```

The process library object

The `process_library_t` type is an extension of the `process_def_list_t` type. Thus, it automatically contains the process definition list.

The `basename` identifies the library generically.

The `external` flag is true if any process within the library needs external code, so the library must correspond to an actual code library (statically or dynamically linked).

The **entry** array contains all process components that can be handled by this library. Each entry refers to the process (component) definition and to the associated external matrix element code, if there is any.

The **driver** object is needed only if **external** is true. This object handles all interactions with external matrix-element code.

The **md5sum** summarizes the complete **process_def_list_t** base object. It can be used to check if the library configuration has changed.

```

(Process libraries: public)+≡
    public :: process_library_t

(Process libraries: types)+≡
    type, extends (process_def_list_t) :: process_library_t
        private
        type(string_t) :: basename
        integer :: n_entries = 0
        logical :: external = .false.
        integer :: status = STAT_UNKNOWN
        logical :: static = .false.
        logical :: driver_exists = .false.
        logical :: makefile_exists = .false.
        integer :: update_counter = 0
        type(process_library_entry_t), dimension(:), allocatable :: entry
        class(prclib_driver_t), allocatable :: driver
        character(32) :: md5sum = ""
        contains
        (Process libraries: process library: TBP)
    end type process_library_t

```

For the output, we write first the metadata and the DL access record, then the library entries in short form, and finally the process definition list which is the base object.

Don't write the MD5 sum since this is used to generate it.

```

(Process libraries: process library: TBP)≡
    procedure :: write => process_library_write

(Process libraries: sub interfaces)+≡
    module subroutine process_library_write (object, unit, libpath)
        class(process_library_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
    end subroutine process_library_write

(Process libraries: procedures)+≡
    module subroutine process_library_write (object, unit, libpath)
        class(process_library_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
        integer :: i, u
        u = given_output_unit (unit)
        write (u, "(1x,A,A)") "Process library: ", char (object%basename)
        write (u, "(3x,A,L1)") "external      = ", object%external
        write (u, "(3x,A,L1)") "makefile exists = ", object%makefile_exists
        write (u, "(3x,A,L1)") "driver exists  = ", object%driver_exists
        write (u, "(3x,A,A1)") "code status    = ", &

```

```

        STATUS_LETTER (object%status)
write (u, *)
if (allocated (object%entry)) then
    write (u, "(1x,A)", advance="no") "Process library entries:"
    write (u, "(1x,I0)") object%n_entries
    do i = 1, size (object%entry)
        write (u, "(1x,A,I0,A,A)") "Entry #", i, ": ", &
            char (object%entry(i)%to_string ())
    end do
    write (u, *)
end if
if (object%external) then
    call object%driver%write (u, libpath)
    write (u, *)
end if
call object%process_def_list_t%write (u)
end subroutine process_library_write

```

Condensed version for screen output.

```

<Process libraries: process library: TBP>+≡
    procedure :: show => process_library_show

<Process libraries: sub interfaces>+≡
    module subroutine process_library_show (object, unit)
        class(process_library_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_library_show

<Process libraries: procedures>+≡
    module subroutine process_library_show (object, unit)
        class(process_library_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A,A)") "Process library: ", char (object%basename)
        write (u, "(2x,A,L1)") "external      = ", object%external
        if (object%static) then
            write (u, "(2x,A,L1)") "static      = ", .true.
        else
            write (u, "(2x,A,L1)") "makefile exists = ", object%makefile_exists
            write (u, "(2x,A,L1)") "driver exists  = ", object%driver_exists
        end if
        write (u, "(2x,A,A1)", advance="no") "code status    = "
        select case (object%status)
        case (STAT_UNKNOWN);    write (u, "(A)") "[unknown]"
        case (STAT_OPEN);       write (u, "(A)") "open"
        case (STAT_CONFIGURED); write (u, "(A)") "configured"
        case (STAT_SOURCE);     write (u, "(A)") "source code exists"
        case (STAT_COMPILED);   write (u, "(A)") "compiled"
        case (STAT_LINKED);     write (u, "(A)") "linked"
        case (STAT_ACTIVE);     write (u, "(A)") "active"
        end select
        call object%process_def_list_t%show (u)
    end subroutine process_library_show

```

The initializer defines just the basename. We may now add process definitions to the library.

```

<Process libraries: process library: TBP>+≡
    procedure :: init => process_library_init

<Process libraries: sub interfaces>+≡
    module subroutine process_library_init (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
    end subroutine process_library_init

<Process libraries: procedures>+≡
    module subroutine process_library_init (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
        lib%basename = basename
        lib%status = STAT_OPEN
        call msg_message ("Process library '" // char (basename) &
            // "': initialized")
    end subroutine process_library_init

```

This alternative initializer declares the library as static. We should now add process definitions to the library, but all external process code exists already. We need the driver object, and we should check the defined processes against the stored ones.

```

<Process libraries: process library: TBP>+≡
    procedure :: init_static => process_library_init_static

<Process libraries: sub interfaces>+≡
    module subroutine process_library_init_static (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
    end subroutine process_library_init_static

<Process libraries: procedures>+≡
    module subroutine process_library_init_static (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
        lib%basename = basename
        lib%status = STAT_OPEN
        lib%static = .true.
        call msg_message ("Static process library '" // char (basename) &
            // "': initialized")
    end subroutine process_library_init_static

```

The `configure` procedure scans the allocated entries in the process definition list. The configuration proceeds in three passes.

In the first pass, we scan the process definition list and count the number of process components and the number of components which need external code. This is used to allocate the `entry` array.

In the second pass, we initialize the `entry` elements which connect process definitions, process driver objects, and external code.

In the third pass, we initialize the library driver object, allocating an entry for each external matrix element.

NOTE: Currently we handle only initial process components; extra components are ignored.

```

(Process libraries: process library: TBP)+≡
    procedure :: configure => process_library_configure

(Process libraries: sub interfaces)+≡
    module subroutine process_library_configure (lib, os_data)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
    end subroutine process_library_configure

(Process libraries: procedures)+≡
    module subroutine process_library_configure (lib, os_data)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        type(process_def_entry_t), pointer :: def_entry
        integer :: n_entries, n_external, i_entry, i_external
        type(string_t) :: model_name
        integer :: i_component

        n_entries = 0
        n_external = 0
        if (allocated (lib%entry)) deallocate (lib%entry)

        def_entry => lib%first
        do while (associated (def_entry))
            do i_component = 1, def_entry%n_initial
                n_entries = n_entries + 1
                if (def_entry%initial(i_component)%needs_code ()) then
                    n_external = n_external + 1
                    lib%external = .true.
                end if
            end do
            def_entry => def_entry%next
        end do

        call lib%allocate_entries (n_entries)

        i_entry = 0
        i_external = 0
        def_entry => lib%first
        do while (associated (def_entry))
            do i_component = 1, def_entry%n_initial
                i_entry = i_entry + 1
                associate (lib_entry => lib%entry(i_entry))
                    lib_entry%status = STAT_CONFIGURED
                    lib_entry%def => def_entry%process_def_t
                    lib_entry%i_component = i_component
                    if (def_entry%initial(i_component)%needs_code ()) then
                        i_external = i_external + 1
                        lib_entry%i_external = i_external
                    end if
                    call def_entry%initial(i_component)%allocate_driver &
                        (lib_entry%driver)
                end associate
            end do
        end do
    end module

```



```

        end do
        def_entry => def_entry%next
    end do

    call dispatch_prclib_driver (lib%driver, &
        lib%basename, lib%get_modellibs_ldflags (os_data))
    call lib%driver%init (n_external)
    do i_entry = 1, n_entries
        associate (lib_entry => lib%entry(i_entry))
            i_component = lib_entry%i_component
            model_name = lib_entry%def%model_name
            associate (def => lib_entry%def%initial(i_component))
                if (def%needs_code ()) then
                    call lib%driver%set_record (lib_entry%i_external, &
                        def%basename, &
                        model_name, &
                        def%get_features (), def%get_writer_ptr ())
                end if
            end associate
        end associate
    end do

    if (lib%static) then
        if (lib%n_entries /= 0) lib%entry%status = STAT_LINKED
        lib%status = STAT_LINKED
    else if (lib%external) then
        where (lib%entry%i_external == 0) lib%entry%status = STAT_LINKED
        lib%status = STAT_CONFIGURED
        lib%makefile_exists = .false.
        lib%driver_exists = .false.
    else
        if (lib%n_entries /= 0) lib%entry%status = STAT_LINKED
        lib%status = STAT_LINKED
    end if
end subroutine process_library_configure

```

Basic setup: allocate the entry array.

(Process libraries: process library: TBP)+≡

```
procedure :: allocate_entries => process_library_allocate_entries
```

(Process libraries: sub interfaces)+≡

```

module subroutine process_library_allocate_entries (lib, n_entries)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: n_entries
end subroutine process_library_allocate_entries

```

(Process libraries: procedures)+≡

```

module subroutine process_library_allocate_entries (lib, n_entries)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: n_entries
    lib%n_entries = n_entries
    allocate (lib%entry (n_entries))
end subroutine process_library_allocate_entries

```

Initialize an entry with data (used by unit tests).

```

(Process libraries: process library: TBP)+≡
    procedure :: init_entry => process_library_init_entry

(Process libraries: sub interfaces)+≡
    module subroutine process_library_init_entry (lib, i, &
        status, def, i_component, i_external, driver_template)
        class(process_library_t), intent(inout) :: lib
        integer, intent(in) :: i
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &
            :: driver_template
    end subroutine process_library_init_entry

(Process libraries: procedures)+≡
    module subroutine process_library_init_entry (lib, i, &
        status, def, i_component, i_external, driver_template)
        class(process_library_t), intent(inout) :: lib
        integer, intent(in) :: i
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &
            :: driver_template
        call lib%entry(i)%init (status, def, i_component, i_external, &
            driver_template)
    end subroutine process_library_init_entry

```

Compute the MD5 sum. We concatenate the individual MD5 sums of all processes (which, in turn, are derived from the MD5 sums of their components) and compute the MD5 sum of that.

This should be executed *after* configuration, where the driver was initialized, since otherwise the MD5 sum stored in the driver would be overwritten.

```

(Process libraries: process library: TBP)+≡
    procedure :: compute_md5sum => process_library_compute_md5sum

(Process libraries: sub interfaces)+≡
    module subroutine process_library_compute_md5sum (lib, model)
        class(process_library_t), intent(inout) :: lib
        class(model_data_t), intent(in), optional, target :: model
    end subroutine process_library_compute_md5sum

(Process libraries: procedures)+≡
    module subroutine process_library_compute_md5sum (lib, model)
        class(process_library_t), intent(inout) :: lib
        class(model_data_t), intent(in), optional, target :: model
        type(process_def_entry_t), pointer :: def_entry
        type(string_t) :: buffer
        buffer = lib%basename
        def_entry => lib%first
        do while (associated (def_entry))

```

```

        call def_entry%compute_md5sum (model)
        buffer = buffer // def_entry%md5sum
        def_entry => def_entry%next
    end do
    lib%md5sum = md5sum (char (buffer))
    call lib%driver%set_md5sum (lib%md5sum)
end subroutine process_library_compute_md5sum

```

Write an appropriate makefile, if there are external processes. Unless `force` is in effect, first check if there is already a makefile with the correct MD5 sum. If yes, do nothing.

The `workspace` optional argument puts any library code in a subdirectory.

```

<Process libraries: process library: TBP>+≡
    procedure :: write_makefile => process_library_write_makefile

<Process libraries: sub interfaces>+≡
    module subroutine process_library_write_makefile &
        (lib, os_data, force, verbose, testflag, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: force, verbose
        logical, intent(in), optional :: testflag
        type(string_t), intent(in), optional :: workspace
    end subroutine process_library_write_makefile

<Process libraries: procedures>+≡
    module subroutine process_library_write_makefile &
        (lib, os_data, force, verbose, testflag, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: force, verbose
        logical, intent(in), optional :: testflag
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum_file
        logical :: generate
        integer :: unit
        if (lib%external .and. .not. lib%static) then
            generate = .true.
            if (.not. force) then
                md5sum_file = lib%driver%get_md5sum_makefile (workspace)
                if (lib%md5sum == md5sum_file) then
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "': keeping makefile")
                    generate = .false.
                end if
            end if
        end if
        if (generate) then
            call msg_message ("Process library '" // char (lib%basename) &
                // "': writing makefile")
            unit = free_unit ()
            open (unit, &
                file = char (workspace_prefix (workspace) &
                    & // lib%driver%basename // ".makefile"), &
                status="replace", action="write")

```

```

        call lib%driver%generate_makefile (unit, os_data, verbose, testflag)
        close (unit)
    end if
    lib%makefile_exists = .true.
end if
end subroutine process_library_write_makefile

```

Write the driver source code for the library to file, if there are external processes.

```

<Process libraries: process library: TBP>+≡
    procedure :: write_driver => process_library_write_driver

<Process libraries: sub interfaces>+≡
    module subroutine process_library_write_driver (lib, force, workspace)
        class(process_library_t), intent(inout) :: lib
        logical, intent(in) :: force
        type(string_t), intent(in), optional :: workspace
    end subroutine process_library_write_driver

<Process libraries: procedures>+≡
    module subroutine process_library_write_driver (lib, force, workspace)
        class(process_library_t), intent(inout) :: lib
        logical, intent(in) :: force
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum_file
        logical :: generate
        integer :: unit
        if (lib%external .and. .not. lib%static) then
            generate = .true.
            if (.not. force) then
                md5sum_file = lib%driver%get_md5sum_driver (workspace)
                if (lib%md5sum == md5sum_file) then
                    call msg_message ("Process library '" // char (lib%basename) &
                                     // "': keeping driver")
                    generate = .false.
                end if
            end if
            if (generate) then
                call msg_message ("Process library '" // char (lib%basename) &
                                 // "': writing driver")
                unit = free_unit ()
                open (unit, &
                     file = char (workspace_prefix (workspace) &
                                 & // lib%driver%basename // ".f90"), &
                     status="replace", action="write")
                call lib%driver%generate_driver_code (unit)
                close (unit)
            end if
            lib%driver_exists = .true.
        end if
    end subroutine process_library_write_driver

```

Update the compilation status of an external library.

Strictly speaking, this is not necessary for a one-time run, since the individual library methods will update the status themselves. However, it allows us to

identify compilation steps that we can skip because the file exists or is already loaded, for the whole library or for particular entries.

Independently, the building process is controlled by a makefile. Thus, previous files are reused if they are not modified by the current compilation.

1. If it is not already loaded, attempt to load the library. If successful, check the overall MD5 sum. If it matches, just keep it loaded and mark as ACTIVE. If not, check the MD5 sum for all linked process components. Where it matches, mark the entry as COMPILED. Then, unload the library and mark as CONFIGURED.

Thus, we can identify compiled files for all matrix elements which are accessible via the previous compiled library, even if it is no longer up to date.

2. If the library is now in CONFIGURED state, look for valid source files. Each entry that is just in CONFIGURED state will advance to SOURCE if the MD5 sum matches. Finally, advance the whole library to SOURCE if all entries are at least in this condition.

```

(Process libraries: process library: TBP)+≡
  procedure :: update_status => process_library_update_status

(Process libraries: sub interfaces)+≡
  module subroutine process_library_update_status (lib, os_data, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in), optional :: workspace
  end subroutine process_library_update_status

(Process libraries: procedures)+≡
  module subroutine process_library_update_status (lib, os_data, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in), optional :: workspace
    character(32) :: md5sum_file
    integer :: i, i_external, i_component
    if (lib%external) then
      select case (lib%status)
      case (STAT_CONFIGURED:STAT_LINKED)
        call lib%driver%load (os_data, noerror=.true., workspace=workspace)
      end select
      if (lib%driver%loaded) then
        md5sum_file = lib%driver%get_md5sum (0)
        if (lib%md5sum == md5sum_file) then
          call lib%load_entries ()
          lib%entry%status = STAT_ACTIVE
          lib%status = STAT_ACTIVE
          call msg_message ("Process library '" // char (lib%basename) &
                           // "': active")
        else
          do i = 1, lib%n_entries
            associate (entry => lib%entry(i))
              i_external = entry%i_external
              i_component = entry%i_component
              if (i_external /= 0) then

```

```

        md5sum_file = lib%driver%get_md5sum (i_external)
        if (entry%def%get_md5sum (i_component) == md5sum_file) then
            entry%status = STAT_COMPILED
        else
            entry%status = STAT_CONFIGURED
        end if
    end if
end associate
end do
call lib%driver%unload ()
lib%status = STAT_CONFIGURED
end if
end if
select case (lib%status)
case (STAT_CONFIGURED)
    do i = 1, lib%n_entries
        associate (entry => lib%entry(i))
            i_external = entry%i_external
            i_component = entry%i_component
            if (i_external /= 0) then
                select case (entry%status)
                case (STAT_CONFIGURED)
                    md5sum_file = lib%driver%get_md5sum_source &
                        (i_external, workspace)
                    if (entry%def%get_md5sum (i_component) == md5sum_file) then
                        entry%status = STAT_SOURCE
                    end if
                end select
            end if
        end associate
    end do
    if (all (lib%entry%status >= STAT_SOURCE)) then
        md5sum_file = lib%driver%get_md5sum_driver (workspace)
        if (lib%md5sum == md5sum_file) then
            lib%status = STAT_SOURCE
        end if
    end if
end select
end if
end subroutine process_library_update_status

```

This procedure triggers code generation for all processes where this is possible.

We generate code only for external processes of status `STAT_CONFIGURED`, which then advance to `STAT_SOURCE`. If, for a particular process, the status is already advanced, we do not remove previous files, so `make` will consider them as up to date if they exist. Otherwise, we remove those files to force a fresh `make`.

Finally, if any source code has been generated, we need a driver file.

```

<Process libraries: process library: TBP>+≡
    procedure :: make_source => process_library_make_source
<Process libraries: sub interfaces>+≡
    module subroutine process_library_make_source &

```

```

        (lib, os_data, keep_old_source, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: keep_old_source
        type(string_t), intent(in), optional :: workspace
    end subroutine process_library_make_source
<Process libraries: procedures>+≡
    module subroutine process_library_make_source &
        (lib, os_data, keep_old_source, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: keep_old_source
        type(string_t), intent(in), optional :: workspace
        logical :: keep_old
        integer :: i, i_external
        keep_old = .false.
        if (present (keep_old_source)) keep_old = keep_old_source
        if (lib%external .and. .not. lib%static) then
            select case (lib%status)
            case (STAT_CONFIGURED)
                if (keep_old) then
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "': keeping source code")
                else
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "': creating source code")
                do i = 1, size (lib%entry)
                    associate (entry => lib%entry(i))
                        i_external = entry%i_external
                        if (i_external /= 0 &
                            .and. lib%entry(i)%status == STAT_CONFIGURED) then
                            call lib%driver%clean_proc &
                                (i_external, os_data, workspace)
                        end if
                    end associate
                    if (signal_is_pending ()) return
                end do
                call lib%driver%make_source (os_data, workspace)
            end if
            lib%status = STAT_SOURCE
            where (lib%entry%i_external /= 0 &
                .and. lib%entry%status == STAT_CONFIGURED)
                lib%entry%status = STAT_SOURCE
            end where
            lib%status = STAT_SOURCE
        end select
    end if
end subroutine process_library_make_source

```

Compile the generated code and update the status codes. Try to make the sources first, just in case. This includes compiling possible L^AT_EX Feynman diagram files.

<Process libraries: process library: TBP>+≡

```

        procedure :: make_compile => process_library_make_compile
    <Process libraries: sub interfaces>+≡
        module subroutine process_library_make_compile &
            (lib, os_data, keep_old_source, workspace)
            class(process_library_t), intent(inout) :: lib
            type(os_data_t), intent(in) :: os_data
            logical, intent(in), optional :: keep_old_source
            type(string_t), intent(in), optional :: workspace
            end subroutine process_library_make_compile
    <Process libraries: procedures>+≡
        module subroutine process_library_make_compile &
            (lib, os_data, keep_old_source, workspace)
            class(process_library_t), intent(inout) :: lib
            type(os_data_t), intent(in) :: os_data
            logical, intent(in), optional :: keep_old_source
            type(string_t), intent(in), optional :: workspace
            if (lib%external .and. .not. lib%static) then
                select case (lib%status)
                case (STAT_CONFIGURED)
                    call lib%make_source (os_data, keep_old_source, workspace)
                end select
                if (signal_is_pending ()) return
                select case (lib%status)
                case (STAT_SOURCE)
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "': compiling sources")
                    call lib%driver%make_compile (os_data, workspace)
                    where (lib%entry%i_external /= 0 &
                        .and. lib%entry%status == STAT_SOURCE)
                        lib%entry%status = STAT_COMPILED
                    end where
                    lib%status = STAT_COMPILED
                end select
            end if
        end subroutine process_library_make_compile

```

Link the process library. Try to compile first, just in case.

```

    <Process libraries: process library: TBP>+≡
        procedure :: make_link => process_library_make_link
    <Process libraries: sub interfaces>+≡
        module subroutine process_library_make_link &
            (lib, os_data, keep_old_source, workspace)
            class(process_library_t), intent(inout) :: lib
            type(os_data_t), intent(in) :: os_data
            logical, intent(in), optional :: keep_old_source
            type(string_t), intent(in), optional :: workspace
            end subroutine process_library_make_link
    <Process libraries: procedures>+≡
        module subroutine process_library_make_link &
            (lib, os_data, keep_old_source, workspace)
            class(process_library_t), intent(inout) :: lib
            type(os_data_t), intent(in) :: os_data

```



```

logical, intent(in), optional :: keep_old_source
type(string_t), intent(in), optional :: workspace
if (lib%external .and. .not. lib%static) then
  select case (lib%status)
  case (STAT_CONFIGURED:STAT_SOURCE)
    call lib%make_compile (os_data, keep_old_source, workspace)
  end select
  if (signal_is_pending ()) return
  select case (lib%status)
  case (STAT_COMPILED)
    call msg_message ("Process library '" // char (lib%basename) &
      // "': linking")
    call lib%driver%make_link (os_data, workspace)
    lib%entry%status = STAT_LINKED
    lib%status = STAT_LINKED
  end select
end if
end subroutine process_library_make_link

```

Load the process library, i.e., assign pointers to the library functions.

(Process libraries: process library: TBP)+≡

```

  procedure :: load => process_library_load

```

(Process libraries: sub interfaces)+≡

```

  module subroutine process_library_load (lib, os_data, keep_old_source, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: keep_old_source
    type(string_t), intent(in), optional :: workspace
  end subroutine process_library_load

```

(Process libraries: procedures)+≡

```

  module subroutine process_library_load (lib, os_data, keep_old_source, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: keep_old_source
    type(string_t), intent(in), optional :: workspace
    select case (lib%status)
    case (STAT_CONFIGURED:STAT_COMPILED)
      call lib%make_link (os_data, keep_old_source, workspace)
    end select
    if (signal_is_pending ()) return
    select case (lib%status)
    case (STAT_LINKED)
      if (lib%external) then
        call msg_message ("Process library '" // char (lib%basename) &
          // "': loading")
        call lib%driver%load (os_data, workspace=workspace)
        call lib%load_entries ()
      end if
      lib%entry%status = STAT_ACTIVE
      lib%status = STAT_ACTIVE
    end select
  end subroutine process_library_load

```

This is the actual loading part for the process methods.

```

(Process libraries: process library: TBP)+≡
    procedure :: load_entries => process_library_load_entries

(Process libraries: sub interfaces)+≡
    module subroutine process_library_load_entries (lib)
        class(process_library_t), intent(inout) :: lib
    end subroutine process_library_load_entries

(Process libraries: procedures)+≡
    module subroutine process_library_load_entries (lib)
        class(process_library_t), intent(inout) :: lib
        integer :: i
        do i = 1, size (lib%entry)
            associate (entry => lib%entry(i))
                if (entry%i_external /= 0) then
                    call entry%connect (lib%driver, entry%i_external)
                end if
            end associate
        end do
    end subroutine process_library_load_entries

```

Unload the library, if possible. This reverts the status to “linked”.

```

(Process libraries: process library: TBP)+≡
    procedure :: unload => process_library_unload

(Process libraries: sub interfaces)+≡
    module subroutine process_library_unload (lib)
        class(process_library_t), intent(inout) :: lib
    end subroutine process_library_unload

(Process libraries: procedures)+≡
    module subroutine process_library_unload (lib)
        class(process_library_t), intent(inout) :: lib
        select case (lib%status)
            case (STAT_ACTIVE)
                if (lib%external) then
                    call msg_message ("Process library '" // char (lib%basename) &
                                     // "': unloading")
                    call lib%driver%unload ()
                end if
                lib%entry%status = STAT_LINKED
                lib%status = STAT_LINKED
            end select
        end subroutine process_library_unload

```

Unload, clean all generated files and revert the library status. If distclean is set, also remove the makefile and the driver source.

```

(Process libraries: process library: TBP)+≡
    procedure :: clean => process_library_clean

(Process libraries: sub interfaces)+≡
    module subroutine process_library_clean (lib, os_data, distclean, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data

```

```

        logical, intent(in) :: distclean
        type(string_t), intent(in), optional :: workspace
    end subroutine process_library_clean

<Process libraries: procedures>+≡
    module subroutine process_library_clean (lib, os_data, distclean, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: distclean
        type(string_t), intent(in), optional :: workspace
        call lib%unload ()
        if (lib%external .and. .not. lib%static) then
            call msg_message ("Process library '" // char (lib%basename) &
                // "': removing old files")
            if (distclean) then
                call lib%driver%distclean (os_data, workspace)
            else
                call lib%driver%clean (os_data, workspace)
            end if
        end if
        where (lib%entry%i_external /= 0)
            lib%entry%status = STAT_CONFIGURED
        elsewhere
            lib%entry%status = STAT_LINKED
        end where
        if (lib%external) then
            lib%status = STAT_CONFIGURED
        else
            lib%status = STAT_LINKED
        end if
    end subroutine process_library_clean

```

Unload and revert the library status to INITIAL. This allows for appending new processes. No files are deleted.

```

<Process libraries: process library: TBP>+≡
    procedure :: open => process_library_open

<Process libraries: sub interfaces>+≡
    module subroutine process_library_open (lib)
        class(process_library_t), intent(inout) :: lib
    end subroutine process_library_open

<Process libraries: procedures>+≡
    module subroutine process_library_open (lib)
        class(process_library_t), intent(inout) :: lib
        select case (lib%status)
        case (STAT_OPEN)
        case default
            call lib%unload ()
            if (.not. lib%static) then
                lib%entry%status = STAT_OPEN
                lib%status = STAT_OPEN
                if (lib%external) lib%update_counter = lib%update_counter + 1
                call msg_message ("Process library '" // char (lib%basename) &
                    // "': open")
            end if
        end select
    end subroutine process_library_open

```

```

        else
            call msg_error ("Static process library '" // char (lib%basename) &
                // "': processes can't be appended")
        end if
    end select
end subroutine process_library_open

```

14.4.4 Use the library

Return the base name of the library

```

<Process libraries: process library: TBP>+≡
    procedure :: get_name => process_library_get_name

<Process libraries: sub interfaces>+≡
    module function process_library_get_name (lib) result (name)
        class(process_library_t), intent(in) :: lib
        type(string_t) :: name
    end function process_library_get_name

<Process libraries: procedures>+≡
    module function process_library_get_name (lib) result (name)
        class(process_library_t), intent(in) :: lib
        type(string_t) :: name
        name = lib%basename
    end function process_library_get_name

```

Once activated, we view the process library object as an interface for accessing the matrix elements.

```

<Process libraries: process library: TBP>+≡
    procedure :: is_active => process_library_is_active

<Process libraries: sub interfaces>+≡
    module function process_library_is_active (lib) result (flag)
        logical :: flag
        class(process_library_t), intent(in) :: lib
    end function process_library_is_active

<Process libraries: procedures>+≡
    module function process_library_is_active (lib) result (flag)
        logical :: flag
        class(process_library_t), intent(in) :: lib
        flag = lib%status == STAT_ACTIVE
    end function process_library_is_active

```

Return the current status code of the library. If an index is provided, return the status of that entry.

```

<Process libraries: process library: TBP>+≡
    procedure :: get_status => process_library_get_status

<Process libraries: sub interfaces>+≡
    module function process_library_get_status (lib, i) result (status)
        class(process_library_t), intent(in) :: lib
        integer, intent(in), optional :: i
        integer :: status
    end function process_library_get_status

```

```

<Process libraries: procedures>+≡
  module function process_library_get_status (lib, i) result (status)
    class(process_library_t), intent(in) :: lib
    integer, intent(in), optional :: i
    integer :: status
    if (present (i)) then
      status = lib%entry(i)%status
    else
      status = lib%status
    end if
  end function process_library_get_status

```

Return the update counter. Since this is incremented each time the library is re-opened, we can use this to check if existing pointers to matrix element code are still valid.

```

<Process libraries: process library: TBP>+≡
  procedure :: get_update_counter => process_library_get_update_counter

<Process libraries: sub interfaces>+≡
  module function process_library_get_update_counter (lib) result (counter)
    class(process_library_t), intent(in) :: lib
    integer :: counter
  end function process_library_get_update_counter

<Process libraries: procedures>+≡
  module function process_library_get_update_counter (lib) result (counter)
    class(process_library_t), intent(in) :: lib
    integer :: counter
    counter = lib%update_counter
  end function process_library_get_update_counter

```

Manually set the current status code of the library. If the optional flag is set, set also the entry status codes. This is used for unit tests.

```

<Process libraries: process library: TBP>+≡
  procedure :: set_status => process_library_set_status

<Process libraries: sub interfaces>+≡
  module subroutine process_library_set_status (lib, status, entries)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: status
    logical, intent(in), optional :: entries
  end subroutine process_library_set_status

<Process libraries: procedures>+≡
  module subroutine process_library_set_status (lib, status, entries)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: status
    logical, intent(in), optional :: entries
    lib%status = status
    if (present (entries)) then
      if (entries) lib%entry%status = status
    end if
  end subroutine process_library_set_status

```

Return the load status of the associated driver.

```

(Process libraries: process library: TBP)+≡
    procedure :: is_loaded => process_library_is_loaded

(Process libraries: sub interfaces)+≡
    module function process_library_is_loaded (lib) result (flag)
        class(process_library_t), intent(in) :: lib
        logical :: flag
    end function process_library_is_loaded

(Process libraries: procedures)+≡
    module function process_library_is_loaded (lib) result (flag)
        class(process_library_t), intent(in) :: lib
        logical :: flag
        flag = lib%driver%loaded
    end function process_library_is_loaded

```

Retrieve constants using the process library driver. We assume that the process code has been loaded, if external.

```

(Process libraries: process library entry: TBP)+≡
    procedure :: fill_constants => process_library_entry_fill_constants

(Process libraries: sub interfaces)+≡
    module subroutine process_library_entry_fill_constants (entry, driver, data)
        class(process_library_entry_t), intent(in) :: entry
        class(prclib_driver_t), intent(in) :: driver
        type(process_constants_t), intent(out) :: data
    end subroutine process_library_entry_fill_constants

(Process libraries: procedures)+≡
    module subroutine process_library_entry_fill_constants (entry, driver, data)
        class(process_library_entry_t), intent(in) :: entry
        class(prclib_driver_t), intent(in) :: driver
        type(process_constants_t), intent(out) :: data
        integer :: i
        if (entry%i_external /= 0) then
            i = entry%i_external
            data%id = driver%get_process_id (i)
            data%model_name = driver%get_model_name (i)
            data%md5sum = driver%get_md5sum (i)
            data%openmp_supported = driver%get_openmp_status (i)
            data%n_in = driver%get_n_in (i)
            data%n_out = driver%get_n_out (i)
            data%n_flv = driver%get_n_flv (i)
            data%n_hel = driver%get_n_hel (i)
            data%n_col = driver%get_n_col (i)
            data%n_cin = driver%get_n_cin (i)
            data%n_cf = driver%get_n_cf (i)
            call driver%set_flv_state (i, data%flv_state)
            call driver%set_hel_state (i, data%hel_state)
            call driver%set_col_state (i, data%col_state, data%ghost_flag)
            call driver%set_color_factors (i, data%color_factors, data%cf_index)
        else
            select type (proc_driver => entry%driver)
            class is (process_driver_internal_t)

```

```

        call proc_driver%fill_constants (data)
    end select
end if
end subroutine process_library_entry_fill_constants

```

Retrieve the constants for a process

```

<Process libraries: process library: TBP>+≡
    procedure :: fill_constants => process_library_fill_constants

<Process libraries: sub interfaces>+≡
    module subroutine process_library_fill_constants (lib, id, i_component, data)
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
    end subroutine process_library_fill_constants

<Process libraries: procedures>+≡
    module subroutine process_library_fill_constants (lib, id, i_component, data)
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
        integer :: i
        do i = 1, size (lib%entry)
            associate (entry => lib%entry(i))
                if (entry%def%id == id .and. entry%i_component == i_component) then
                    call entry%fill_constants (lib%driver, data)
                    return
                end if
            end associate
        end do
    end subroutine process_library_fill_constants

```

Retrieve the constants and a connected driver for a process, identified by a process ID and a subprocess index. We scan the process entries until we have found a match.

```

<Process libraries: process library: TBP>+≡
    procedure :: connect_process => process_library_connect_process

<Process libraries: sub interfaces>+≡
    module subroutine process_library_connect_process &
        (lib, id, i_component, data, proc_driver)
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
        class(prc_core_driver_t), allocatable, intent(out) :: proc_driver
    end subroutine process_library_connect_process

<Process libraries: procedures>+≡
    module subroutine process_library_connect_process &
        (lib, id, i_component, data, proc_driver)
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id

```

```

integer, intent(in) :: i_component
type(process_constants_t), intent(out) :: data
class(prc_core_driver_t), allocatable, intent(out) :: proc_driver
integer :: i
do i = 1, size (lib%entry)
  associate (entry => lib%entry(i))
    if (entry%def%id == id .and. entry%i_component == i_component) then
      call entry%fill_constants (lib%driver, data)
      allocate (proc_driver, source = entry%driver)
      return
    end if
  end associate
end do
call msg_fatal ("Process library '" // char (lib%basename) &
              // "': process '" // char (id) // "' not found")
end subroutine process_library_connect_process

```

Shortcut for use in unit tests: fetch the MD5sum from a specific library entry and inject it into the writer of a specific record.

```

(Process libraries: process library: TBP)+≡
  procedure :: test_transfer_md5sum => process_library_test_transfer_md5sum

(Process libraries: sub interfaces)+≡
  module subroutine process_library_test_transfer_md5sum (lib, r, e, c)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: r, e, c
    end subroutine process_library_test_transfer_md5sum

(Process libraries: procedures)+≡
  module subroutine process_library_test_transfer_md5sum (lib, r, e, c)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: r, e, c
    associate (writer => lib%driver%record(r)%writer)
      writer%md5sum = lib%entry(e)%def%get_md5sum (c)
    end associate
  end subroutine process_library_test_transfer_md5sum

(Process libraries: process library: TBP)+≡
  procedure :: get_nlo_type => process_library_get_nlo_type

(Process libraries: sub interfaces)+≡
  module function process_library_get_nlo_type (lib, id, i_component) result (nlo_type)
    integer :: nlo_type
    class(process_library_t), intent(in) :: lib
    type(string_t), intent(in) :: id
    integer, intent(in) :: i_component
    end function process_library_get_nlo_type

(Process libraries: procedures)+≡
  module function process_library_get_nlo_type (lib, id, i_component) result (nlo_type)
    integer :: nlo_type
    class(process_library_t), intent(in) :: lib
    type(string_t), intent(in) :: id
    integer, intent(in) :: i_component
    integer :: i

```



```

do i = 1, size (lib%entry)
  if (lib%entry(i)%def%id == id .and. lib%entry(i)%i_component == i_component) then
    nlo_type = lib%entry(i)%def%get_nlo_type (i_component)
    exit
  end if
end do
end function process_library_get_nlo_type

```

14.4.5 Collect model-specific libraries

This returns appropriate linker flags for the model parameter libraries that are used by the generated matrix element. At the end, the main libwhizard is appended (again), because functions from that may be required.

Extra models in the local user space need to be treated individually.

```

(Process libraries: process library: TBP)+≡
  procedure :: get_modellibs_ldflags => process_library_get_modellibs_ldflags

(Process libraries: sub interfaces)+≡
  module function process_library_get_modellibs_ldflags (prc_lib, os_data) result (flags)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: flags
  end function process_library_get_modellibs_ldflags

(Process libraries: procedures)+≡
  module function process_library_get_modellibs_ldflags (prc_lib, os_data) result (flags)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: flags
    type(string_t), dimension(:), allocatable :: models
    type(string_t) :: modelname, modllib, modllib_full
    logical :: exist
    integer :: i, j, mi
    flags = "-lomega"
    if ((.not. os_data%use_testfiles) .and. &
        os_dir_exist (os_data%whizard_models_libpath_local)) &
      flags = flags // " -L" // os_data%whizard_models_libpath_local
    flags = flags // " -L" // os_data%whizard_models_libpath
    allocate (models(prc_lib%n_entries + 1))
    models = ""
    mi = 1
    if (allocated (prc_lib%entry)) then
      SCAN: do i = 1, prc_lib%n_entries
        if (associated (prc_lib%entry(i)%def)) then
          if (prc_lib%entry(i)%def%model_name /= "") then
            modelname = prc_lib%entry(i)%def%model_name
          else
            cycle SCAN
          end if
        else
          cycle SCAN
        end if
      end do
    end if
    do j = 1, mi

```

```

        if (models(mi) == modelname) cycle SCAN
    end do
    models(mi) = modelname
    mi = mi + 1
    if (os_data%use_libtool) then
        modellib = "libparameters_" // modelname // ".la"
    else
        modellib = "libparameters_" // modelname // ".a"
    end if
    exist = .false.
    if (.not. os_data%use_testfiles) then
        modellib_full = os_data%whizard_models_libpath_local &
            // "/" // modellib
        inquire (file=char (modellib_full), exist=exist)
    end if
    if (.not. exist) then
        modellib_full = os_data%whizard_models_libpath &
            // "/" // modellib
        inquire (file=char (modellib_full), exist=exist)
    end if
    if (exist) flags = flags // " -lparameters_" // modelname
end do SCAN
end if
deallocate (models)
flags = flags // " -lwhizard"
end function process_library_get_modellibs_ldflags

```

(Process libraries: process library: TBP)+≡

```

procedure :: get_static_modelname => process_library_get_static_modelname

```

(Process libraries: sub interfaces)+≡

```

module function process_library_get_static_modelname (prc_lib, os_data) result (name)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: name
end function process_library_get_static_modelname

```

(Process libraries: procedures)+≡

```

module function process_library_get_static_modelname (prc_lib, os_data) result (name)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: name
    type(string_t), dimension(:), allocatable :: models
    type(string_t) :: modelname, modellib, modellib_full
    logical :: exist
    integer :: i, j, mi
    name = ""
    allocate (models(prc_lib%n_entries + 1))
    models = ""
    mi = 1
    if (allocated (prc_lib%entry)) then
        SCAN: do i = 1, prc_lib%n_entries
            if (associated (prc_lib%entry(i)%def)) then
                if (prc_lib%entry(i)%def%model_name /= "") then
                    modelname = prc_lib%entry(i)%def%model_name

```

```

        else
            cycle SCAN
        end if
    else
        cycle SCAN
    end if
do j = 1, mi
    if (models(mi) == modelname) cycle SCAN
end do
models(mi) = modelname
mi = mi + 1
modellib = "libparameters_" // modelname // ".a"
exist = .false.
if (.not. os_data%use_testfiles) then
    modellib_full = os_data%whizard_models_libpath_local &
        // "/" // modellib
    inquire (file=char (modellib_full), exist=exist)
end if
if (.not. exist) then
    modellib_full = os_data%whizard_models_libpath &
        // "/" // modellib
    inquire (file=char (modellib_full), exist=exist)
end if
if (exist) name = name // " " // modellib_full
end do SCAN
end if
deallocate (models)
end function process_library_get_static_modelname

```

14.4.6 Unit Test

Test module, followed by the corresponding implementation module.

```

<process_libraries_ut.f90>≡
    <File header>

    module process_libraries_ut
        use unit_tests
        use process_libraries_uti

    <Standard module head>

    <Process libraries: public test>

    contains

    <Process libraries: test driver>

    end module process_libraries_ut
<process_libraries_uti.f90>≡
    <File header>

    module process_libraries_uti

```

```

    use, intrinsic :: iso_c_binding !NODEP!

    <Use strings>
    use io_units
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def

    use process_libraries

    use prclib_interfaces_ut, only: test_writer_4_t

    <Standard module head>

    <Process libraries: test declarations>

    <Process libraries: test types>

    contains

    <Process libraries: tests>

    <Process libraries: test auxiliary>

    end module process_libraries_ut
API: driver for the unit tests below.
    <Process libraries: public test>≡
    public :: process_libraries_test
    <Process libraries: test driver>≡
    subroutine process_libraries_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Process libraries: execute tests>
    end subroutine process_libraries_test

```

Empty process list

Test 1: Write an empty process list.

```

    <Process libraries: execute tests>≡
    call test (process_libraries_1, "process_libraries_1", &
        "empty process list", &
        u, results)

    <Process libraries: test declarations>≡
    public :: process_libraries_1

    <Process libraries: tests>≡
    subroutine process_libraries_1 (u)
        integer, intent(in) :: u
        type(process_def_list_t) :: process_def_list

```

```

write (u, "(A)")  "* Test output: process_libraries_1"
write (u, "(A)")  "* Purpose: Display an empty process definition list"
write (u, "(A)")

call process_def_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_1"
end subroutine process_libraries_1

```

Process definition list

Test 2: Process definition list with processes and components. Construct the list, write to file, read it in again, and display. Finalize and delete the list after use.

We define a trivial 'test' type for the process variant. The test type contains just one (meaningless) data item, which is an integer.

```

<Process libraries: test types>≡
type, extends (prc_core_def_t) :: prcdef_2_t
  integer :: data = 0
  logical :: file = .false.
contains
  <Process libraries: prcdef 2: TBP>
end type prcdef_2_t

```

The process variant is named 'test'.

```

<Process libraries: prcdef 2: TBP>≡
  procedure, nopass :: type_string => prcdef_2_type_string

<Process libraries: test auxiliary>≡
  function prcdef_2_type_string () result (string)
    type(string_t) :: string
    string = "test"
  end function prcdef_2_type_string

```

Write the contents (the integer value).

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: write => prcdef_2_write

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_write (object, unit)
    class(prcdef_2_t), intent(in) :: object
    integer, intent(in) :: unit
    write (unit, "(3x,A,I0)") "Test data          = ", object%data
  end subroutine prcdef_2_write

```

Recover the integer value.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: read => prcdef_2_read

```

```

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_read (object, unit)
    class(prcdef_2_t), intent(out) :: object
    integer, intent(in) :: unit
    character(80) :: buffer
    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%data
  end subroutine prcdef_2_read

```

No external procedures.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure, nopass :: get_features => prcdef_2_get_features

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (0))
  end subroutine prcdef_2_get_features

```

No code generated.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: generate_code => prcdef_2_generate_code

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_generate_code (object, &
    basename, model_name, prt_in, prt_out)
    class(prcdef_2_t), intent(in) :: object
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
  end subroutine prcdef_2_generate_code

```

Allocate the driver with the appropriate type.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: allocate_driver => prcdef_2_allocate_driver

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_allocate_driver (object, driver, basename)
    class(prcdef_2_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (prctest_2_t :: driver)
  end subroutine prcdef_2_allocate_driver

```

Nothing to connect.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: connect => prcdef_2_connect

```

```

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_connect (def, lib_driver, i, proc_driver)
    class(prcdef_2_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
  end subroutine prcdef_2_connect

```

The associated driver type.

```

<Process libraries: test types>+≡
  type, extends (process_driver_internal_t) :: prctest_2_t
  contains
    <Process libraries: prctest 2: TBP>
  end type prctest_2_t

```

Return the type name.

```

<Process libraries: prctest 2: TBP>≡
  procedure, nopass :: type_name => prctest_2_type_name

<Process libraries: test auxiliary>+≡
  function prctest_2_type_name () result (type)
    type(string_t) :: type
    type = "test"
  end function prctest_2_type_name

```

This should fill constant process data. We do not check those here, however, therefore nothing done.

```

<Process libraries: prctest 2: TBP>+≡
  procedure :: fill_constants => prctest_2_fill_constants

<Process libraries: test auxiliary>+≡
  subroutine prctest_2_fill_constants (driver, data)
    class(prctest_2_t), intent(in) :: driver
    type(process_constants_t), intent(out) :: data
  end subroutine prctest_2_fill_constants

```

Here is the actual test.

For reading, we need a list of templates, i.e., an array containing allocated objects for all available process variants. This is the purpose of `process_core_templates`. Here, we have only a single template for the 'test' variant.

```

<Process libraries: execute tests>+≡
  call test (process_libraries_2, "process_libraries_2", &
    "process definition list", &
    u, results)

<Process libraries: test declarations>+≡
  public :: process_libraries_2

<Process libraries: tests>+≡
  subroutine process_libraries_2 (u)
    integer, intent(in) :: u
    type(prc_template_t), dimension(:), allocatable :: process_core_templates
    type(process_def_list_t) :: process_def_list

```

```

type(process_def_entry_t), pointer :: entry => null ()
class(prc_core_def_t), allocatable :: test_def
integer :: scratch_unit

write (u, "(A)")  "*" Test output: process_libraries_2"
write (u, "(A)")  "*" Purpose: Construct a process definition list,"
write (u, "(A)")  "*"           write it to file and reread it"
write (u, "(A)")  ""
write (u, "(A)")  "*" Construct a process definition list"
write (u, "(A)")  "*"   First process definition: empty"
write (u, "(A)")  "*"   Second process definition: two components"
write (u, "(A)")  "*"       First component: empty"
write (u, "(A)")  "*"       Second component: test data"
write (u, "(A)")  "*"   Third process definition:"
write (u, "(A)")  "*"       Embedded decays and polarization"
write (u, "(A)")

allocate (process_core_templates (1))
allocate (prcdef_2_t :: process_core_templates(1)%core_def)

allocate (entry)
call entry%init (var_str ("first"), n_in = 0, n_components = 0)
call entry%compute_md5sum ()
call process_def_list%append (entry)

allocate (entry)
call entry%init (var_str ("second"), model_name = var_str ("Test"), &
    n_in = 1, n_components = 2)
allocate (prcdef_2_t :: test_def)
select type (test_def)
type is (prcdef_2_t); test_def%data = 42
end select
call entry%import_component (2, n_out = 2, &
    prt_in  = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method  = var_str ("test"), &
    variant = test_def)
call entry%compute_md5sum ()
call process_def_list%append (entry)

allocate (entry)
call entry%init (var_str ("third"), model_name = var_str ("Test"), &
    n_in = 2, n_components = 1)
allocate (prcdef_2_t :: test_def)
call entry%import_component (1, n_out = 3, &
    prt_in  = &
        new_prt_spec ([var_str ("a"), var_str ("b")]), &
    prt_out = &
        [new_prt_spec (var_str ("c")), &
        new_prt_spec (var_str ("d"), .true.), &
        new_prt_spec (var_str ("e"), [var_str ("e_decay")])], &
    method  = var_str ("test"), &
    variant = test_def)
call entry%compute_md5sum ()

```



```

call process_def_list%append (entry)
call process_def_list%write (u)

write (u, "(A)") ""
write (u, "(A)")  "* Write the process definition list to (scratch) file"

scratch_unit = free_unit ()
open (unit = scratch_unit, status="scratch", action = "readwrite")
call process_def_list%write (scratch_unit)
call process_def_list%final ()

write (u, "(A)")  "* Reread it"
write (u, "(A)") ""

rewind (scratch_unit)
call process_def_list%read (scratch_unit, process_core_templates)
close (scratch_unit)

call process_def_list%write (u)
call process_def_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_2"
end subroutine process_libraries_2

```

Process library object

Test 3: Process library object with several process definitions and library entries. Just construct the object, modify some initial content, and write the result. The modifications are mostly applied directly, so we do not test anything but the contents and the output routine.

```

<Process libraries: execute tests>+≡
  call test (process_libraries_3, "process_libraries_3", &
    "recover process definition list from file", &
    u, results)

<Process libraries: test declarations>+≡
  public :: process_libraries_3

<Process libraries: tests>+≡
  subroutine process_libraries_3 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    type(process_def_entry_t), pointer :: entry
    class(prc_core_driver_t), allocatable :: driver_template

    write (u, "(A)")  "* Test output: process_libraries_3"
    write (u, "(A)")  "* Purpose: Construct a process library object &
      &with entries"
    write (u, "(A)")  ""
    write (u, "(A)")  "* Construct and display a process library object"
    write (u, "(A)")  "*   with 5 entries"
    write (u, "(A)")  "*   associated with 3 matrix element codes"

```

```

write (u, "(A)")  "*"   corresponding to 3 process definitions"
write (u, "(A)")  "*"   with 2, 1, 1 components, respectively"
write (u, "(A)")

call lib%init (var_str ("testlib"))

call lib%set_status (STAT_ACTIVE)
call lib%allocate_entries (5)

allocate (entry)
call entry%init (var_str ("test_a"), n_in = 2, n_components = 2)
allocate (prctest_2_t :: driver_template)
call lib%init_entry (3, STAT_SOURCE, entry%process_def_t, 2, 2, &
    driver_template)
call lib%init_entry (4, STAT_COMPILED, entry%process_def_t, 1, 0)
call lib%append (entry)

allocate (entry)
call entry%init (var_str ("test_b"), n_in = 2, n_components = 1)
call lib%init_entry (2, STAT_CONFIGURED, entry%process_def_t, 1, 1)
call lib%append (entry)

allocate (entry)
call entry%init (var_str ("test_c"), n_in = 2, n_components = 1)
allocate (prctest_2_t :: driver_template)
call lib%init_entry (5, STAT_LINKED, entry%process_def_t, 1, 3, &
    driver_template)
call lib%append (entry)

call lib%write (u)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: process_libraries_3"
end subroutine process_libraries_3

```

Process library for test matrix element (no file)

Test 4: We proceed through the library generation and loading phases with a test matrix element type that needs no code written on file.

```

<Process libraries: execute tests>+≡
    call test (process_libraries_4, "process_libraries_4", &
        "build and load internal process library", &
        u, results)

<Process libraries: test declarations>+≡
    public :: process_libraries_4

<Process libraries: tests>+≡
    subroutine process_libraries_4 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        type(process_def_entry_t), pointer :: entry

```

```

class(prc_core_def_t), allocatable :: core_def
type(os_data_t) :: os_data

write (u, "(A)")  "* Test output: process_libraries_4"
write (u, "(A)")  "* Purpose: build a process library with an &
                    &internal (pseudo) matrix element"
write (u, "(A)")  "*          No Makefile or code should be generated"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry &
                    &(no external code)"
write (u, "(A)")
call os_data%init ()
call lib%init (var_str ("proclibs4"))

allocate (prcdef_2_t :: core_def)

allocate (entry)
call entry%init (var_str ("proclibs4_a"), n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, variant = core_def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Compute MD5 sum"
write (u, "(A)")
call lib%compute_md5sum ()

write (u, "(A)")  "* Write makefile (no-op)"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .true.)

write (u, "(A)")  "* Write driver source code (no-op)"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code (no-op)"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(A)")  "* Compile (no-op)"
write (u, "(A)")
call lib%make_compile (os_data)

write (u, "(A)")  "* Link (no-op)"
write (u, "(A)")
call lib%make_link (os_data)

write (u, "(A)")  "* Load (no-op)"
write (u, "(A)")
call lib%load (os_data)

```

```

call lib%write (u)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_4"
end subroutine process_libraries_4

```

Build workflow for test matrix element

Test 5: We write source code for a dummy process.

We define another trivial type for the process variant. The test type contains just no variable data, but produces code on file.

```

<Process libraries: test types>+≡
  type, extends (prc_core_def_t) :: prcdef_5_t
  contains
    <Process libraries: prcdef 5: TBP>
  end type prcdef_5_t

```

The process variant is named `test_file`.

```

<Process libraries: prcdef 5: TBP>≡
  procedure, nopass :: type_string => prcdef_5_type_string

<Process libraries: test auxiliary>+≡
  function prcdef_5_type_string () result (string)
    type(string_t) :: string
    string = "test_file"
  end function prcdef_5_type_string

```

We reuse the writer `test_writer_4` from the previous module.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure :: init => prcdef_5_init

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_init (object)
    class(prcdef_5_t), intent(out) :: object
    allocate (test_writer_4_t :: object%writer)
  end subroutine prcdef_5_init

```

Nothing to write.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure :: write => prcdef_5_write

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_write (object, unit)
    class(prcdef_5_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_5_write

```

Nothing to read.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure :: read => prcdef_5_read

```

```

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_read (object, unit)
    class(prcdef_5_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_5_read

```

Allocate the driver with the appropriate type.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure :: allocate_driver => prcdef_5_allocate_driver

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_allocate_driver (object, driver, basename)
    class(prcdef_5_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (prctest_5_t :: driver)
  end subroutine prcdef_5_allocate_driver

```

This time we need code:

```

<Process libraries: prcdef 5: TBP>+≡
  procedure, nopass :: needs_code => prcdef_5_needs_code

<Process libraries: test auxiliary>+≡
  function prcdef_5_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function prcdef_5_needs_code

```

For the test case, we implement a single feature proc1.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure, nopass :: get_features => prcdef_5_get_features

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (1))
    features = [ var_str ("proc1") ]
  end subroutine prcdef_5_get_features

```

Nothing to connect.

```

<Process libraries: prcdef 5: TBP>+≡
  procedure :: connect => prcdef_5_connect

<Process libraries: test auxiliary>+≡
  subroutine prcdef_5_connect (def, lib_driver, i, proc_driver)
    class(prcdef_5_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
  end subroutine prcdef_5_connect

```

The driver type.

```

(Process libraries: test types)+≡
  type, extends (prc_core_driver_t) :: prctest_5_t
  contains
    (Process libraries: prctest 5: TBP)
  end type prctest_5_t

```

Return the type name.

```

(Process libraries: prctest 5: TBP)≡
  procedure, nopass :: type_name => prctest_5_type_name

(Process libraries: test auxiliary)+≡
  function prctest_5_type_name () result (type)
    type(string_t) :: type
    type = "test_file"
  end function prctest_5_type_name

```

Here is the actual test:

```

(Process libraries: execute tests)+≡
  call test (process_libraries_5, "process_libraries_5", &
    "build external process library", &
    u, results)

(Process libraries: test declarations)+≡
  public :: process_libraries_5

(Process libraries: tests)+≡
  subroutine process_libraries_5 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    type(process_def_entry_t), pointer :: entry
    class(prc_core_def_t), allocatable :: core_def
    type(os_data_t) :: os_data

    write (u, "(A)")  "* Test output: process_libraries_5"
    write (u, "(A)")  "* Purpose: build a process library with an &
      &external (pseudo) matrix element"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize a process library with one entry"
    write (u, "(A)")
    call lib%init (var_str ("proclibs5"))
    call os_data%init ()

    allocate (prcdef_5_t :: core_def)
    select type (core_def)
    type is (prcdef_5_t)
      call core_def%init ()
    end select

    allocate (entry)
    call entry%init (var_str ("proclibs5_a"), &
      model_name = var_str ("Test_Model"), &
      n_in = 1, n_components = 1)

```

```

call entry%import_component (1, n_out = 2, &
    prt_in  = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method  = var_str ("test"), &
    variant = core_def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Compute MD5 sum"
write (u, "(A)")
call lib%compute_md5sum ()

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Write driver source code"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(A)")  "* Compile"
write (u, "(A)")
call lib%make_compile (os_data)

write (u, "(A)")  "* Link"
write (u, "(A)")
call lib%make_link (os_data)

call lib%write (u, libpath = .false.)

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_5"
end subroutine process_libraries_5

```

Build and load library with test matrix element

Test 6: We write source code for a dummy process.

This process variant is identical to the previous case, but it supports a driver for the test procedure 'proc1'.

```

<Process libraries: test types> +=
type, extends (prc_core_def_t) :: prcdef_6_t
contains
<Process libraries: prcdef 6: TBP>

```

```
end type prcdef_6_t
```

The process variant is named `test_file`.

```
<Process libraries: prcdef 6: TBP>+≡
  procedure, nopass :: type_string => prcdef_6_type_string
<Process libraries: test auxiliary>+≡
  function prcdef_6_type_string () result (string)
    type(string_t) :: string
    string = "test_file"
  end function prcdef_6_type_string
```

We reuse the writer `test_writer_4` from the previous module.

```
<Process libraries: prcdef 6: TBP>+≡
  procedure :: init => prcdef_6_init
<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_init (object)
    class(prcdef_6_t), intent(out) :: object
    allocate (test_writer_4_t :: object%writer)
    call object%writer%init_test ()
  end subroutine prcdef_6_init
```

Nothing to write.

```
<Process libraries: prcdef 6: TBP>+≡
  procedure :: write => prcdef_6_write
<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_write (object, unit)
    class(prcdef_6_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_6_write
```

Nothing to read.

```
<Process libraries: prcdef 6: TBP>+≡
  procedure :: read => prcdef_6_read
<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_read (object, unit)
    class(prcdef_6_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_6_read
```

Allocate the driver with the appropriate type.

```
<Process libraries: prcdef 6: TBP>+≡
  procedure :: allocate_driver => prcdef_6_allocate_driver
<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_allocate_driver (object, driver, basename)
    class(prcdef_6_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (prctest_6_t :: driver)
  end subroutine prcdef_6_allocate_driver
```


This time we need code:

```
<Process libraries: prcdef 6: TBP>+≡
    procedure, nopass :: needs_code => prcdef_6_needs_code

<Process libraries: test auxiliary>+≡
    function prcdef_6_needs_code () result (flag)
        logical :: flag
        flag = .true.
    end function prcdef_6_needs_code
```

For the test case, we implement a single feature `proc1`.

```
<Process libraries: prcdef 6: TBP>+≡
    procedure, nopass :: get_features => prcdef_6_get_features

<Process libraries: test auxiliary>+≡
    subroutine prcdef_6_get_features (features)
        type(string_t), dimension(:), allocatable, intent(out) :: features
        allocate (features (1))
        features = [ var_str ("proc1") ]
    end subroutine prcdef_6_get_features
```

The interface of the only specific feature.

```
<Process libraries: test types>+≡
    abstract interface
        subroutine proc1_t (n) bind(C)
            import
            integer(c_int), intent(out) :: n
        end subroutine proc1_t
    end interface
```

Connect the feature `proc1` with the process driver.

```
<Process libraries: prcdef 6: TBP>+≡
    procedure :: connect => prcdef_6_connect

<Process libraries: test auxiliary>+≡
    subroutine prcdef_6_connect (def, lib_driver, i, proc_driver)
        class(prcdef_6_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
        integer(c_int) :: pid, fid
        type(c_funptr) :: fptr
        select type (proc_driver)
            type is (prctest_6_t)
                pid = i
                fid = 1
                call lib_driver%get_fptr (pid, fid, fptr)
                call c_f_procpointer (fptr, proc_driver%proc1)
            end select
    end subroutine prcdef_6_connect
```

The driver type.

```

<Process libraries: test types>+≡
  type, extends (prc_core_driver_t) :: prctest_6_t
    procedure(proc1_t), nopass, pointer :: proc1 => null ()
    contains
      <Process libraries: prctest 6: TBP>
    end type prctest_6_t

```

Return the type name.

```

<Process libraries: prctest 6: TBP>≡
  procedure, nopass :: type_name => prctest_6_type_name

<Process libraries: test auxiliary>+≡
  function prctest_6_type_name () result (type)
    type(string_t) :: type
    type = "test_file"
  end function prctest_6_type_name

```

Here is the actual test:

```

<Process libraries: execute tests>+≡
  call test (process_libraries_6, "process_libraries_6", &
    "build and load external process library", &
    u, results)

<Process libraries: test declarations>+≡
  public :: process_libraries_6

<Process libraries: tests>+≡
  subroutine process_libraries_6 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    type(process_def_entry_t), pointer :: entry
    class(prc_core_def_t), allocatable :: core_def
    type(os_data_t) :: os_data
    type(string_t), dimension(:), allocatable :: name_list
    type(process_constants_t) :: data
    class(prc_core_driver_t), allocatable :: proc_driver
    integer :: i
    integer(c_int) :: n

    write (u, "(A)")  "* Test output: process_libraries_6"
    write (u, "(A)")  "* Purpose: build and load a process library"
    write (u, "(A)")  "*           with an external (pseudo) matrix element"
    write (u, "(A)")  "*           Check single-call linking"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize a process library with one entry"
    write (u, "(A)")
    call lib%init (var_str ("proclibs6"))
    call os_data%init ()

    allocate (prcdef_6_t :: core_def)
    select type (core_def)
    type is (prcdef_6_t)

```

```

        call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs6_a"), &
    model_name = var_str ("Test_model"), &
    n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method = var_str ("test"), &
    variant = core_def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Write driver source code"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,A,A)")  "name                = '", &
    char (lib%get_name ()), "'"
write (u, "(1x,A,L1)")  "is active                = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes                = ", &
    lib%get_n_processes ()
write (u, "(1x,A)", advance="no")  "processes                ="
call lib%get_process_id_list (name_list)
do i = 1, size (name_list)
    write (u, "(1x,A)", advance="no")  char (name_list(i))
end do
write (u, *)
write (u, "(1x,A,L1)")  "proclibs6_a is process    = ", &
    lib%contains (var_str ("proclibs6_a"))
write (u, "(1x,A,I0)")  "proclibs6_a has index    = ", &
    lib%get_entry_index (var_str ("proclibs6_a"))
write (u, "(1x,A,L1)")  "foobar is process        = ", &
    lib%contains (var_str ("foobar"))

```

```

write (u, "(1x,A,I0)") "foobar has index          = ", &
    lib%get_entry_index (var_str ("foobar"))
write (u, "(1x,A,I0)") "n_in(proclibs6_a)          = ", &
    lib%get_n_in (var_str ("proclibs6_a"))
write (u, "(1x,A,A)") "model_name(proclibs6_a)      = ", &
    char (lib%get_model_name (var_str ("proclibs6_a")))
write (u, "(1x,A)", advance="no") "components(proclibs6_a) ="
call lib%get_component_list (var_str ("proclibs6_a"), name_list)
do i = 1, size (name_list)
    write (u, "(1x,A)", advance="no") char (name_list(i))
end do
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Constants of proclibs6_a.i1:"
write (u, "(A)")

call lib%connect_process (var_str ("proclibs6_a"), 1, data, proc_driver)

write (u, "(1x,A,A)") "component ID          = ", char (data%id)
write (u, "(1x,A,A)") "model name            = ", char (data%model_name)
write (u, "(1x,A,A,A)") "md5sum              = '", data%md5sum, "'"
write (u, "(1x,A,L1)") "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)") "n_in = ", data%n_in
write (u, "(1x,A,I0)") "n_out = ", data%n_out
write (u, "(1x,A,I0)") "n_flv = ", data%n_flv
write (u, "(1x,A,I0)") "n_hel = ", data%n_hel
write (u, "(1x,A,I0)") "n_col = ", data%n_col
write (u, "(1x,A,I0)") "n_cin = ", data%n_cin
write (u, "(1x,A,I0)") "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))") "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I0))") "hel state =", data%hel_state
write (u, "(1x,A,10(1x,I0))") "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))") "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))") "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))") "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Call feature of proclibs6_a:"
write (u, "(A)")

select type (proc_driver)
type is (prctest_6_t)
    call proc_driver%proc1 (n)
    write (u, "(1x,A,I0)") "proc1 = ", n
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_6"
end subroutine process_libraries_6

```

MD5 sums

Check MD5 sum calculation.

```
(Process libraries: execute tests)+≡
    call test (process_libraries_7, "process_libraries_7", &
              "process definition list", &
              u, results)

(Process libraries: test declarations)+≡
    public :: process_libraries_7

(Process libraries: tests)+≡
    subroutine process_libraries_7 (u)
        integer, intent(in) :: u
        type(prc_template_t), dimension(:), allocatable :: process_core_templates
        type(process_def_entry_t), target :: entry
        class(prc_core_def_t), allocatable :: test_def
        class(prc_core_def_t), pointer :: def

        write (u, "(A)")  "* Test output: process_libraries_7"
        write (u, "(A)")  "* Purpose: Construct a process definition list &
                           &and check MD5 sums"
        write (u, "(A)")
        write (u, "(A)")  "* Construct a process definition list"
        write (u, "(A)")  "*   Process: two components"
        write (u, "(A)")

        allocate (process_core_templates (1))
        allocate (prcdef_2_t :: process_core_templates(1)%core_def)

        call entry%init (var_str ("first"), model_name = var_str ("Test"), &
                        n_in = 1, n_components = 2)
        allocate (prcdef_2_t :: test_def)
        select type (test_def)
        type is (prcdef_2_t); test_def%data = 31
        end select
        call entry%import_component (1, n_out = 3, &
            prt_in  = new_prt_spec ([var_str ("a")]), &
            prt_out = new_prt_spec ([var_str ("b"), var_str ("c"), &
                                    var_str ("e")]), &
            method  = var_str ("test"), &
            variant = test_def)
        allocate (prcdef_2_t :: test_def)
        select type (test_def)
        type is (prcdef_2_t); test_def%data = 42
        end select
        call entry%import_component (2, n_out = 2, &
            prt_in  = new_prt_spec ([var_str ("a")]), &
            prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
            method  = var_str ("test"), &
            variant = test_def)
        call entry%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Compute MD5 sums"
```

```

write (u, "(A)")

call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recalculate MD5 sums (should be identical)"
write (u, "(A)")

call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Modify a component and recalculate MD5 sums"
write (u, "(A)")

def => entry%get_core_def_ptr (2)
select type (def)
type is (prcdef_2_t)
    def%data = 54
end select
call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Modify the model and recalculate MD5 sums"
write (u, "(A)")

call entry%set_model_name (var_str ("foo"))
call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_7"
end subroutine process_libraries_7

```

Here is the actual test:

```

<Process libraries: execute tests>+≡
    call test (process_libraries_8, "process_libraries_8", &
        "library status checks", &
        u, results)

<Process libraries: test declarations>+≡
    public :: process_libraries_8

<Process libraries: tests>+≡
    subroutine process_libraries_8 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        type(process_def_entry_t), pointer :: entry
        class(prc_core_def_t), allocatable :: core_def
        type(os_data_t) :: os_data

        write (u, "(A)")  "* Test output: process_libraries_8"
        write (u, "(A)")  "* Purpose: build and load a process library"
    end subroutine process_libraries_8

```

```

write (u, "(A)")  "*"          with an external (pseudo) matrix element"
write (u, "(A)")  "*"          Check status updates"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("proclibs8"))
call os_data%init ()

allocate (prcdef_6_t :: core_def)
select type (core_def)
type is (prcdef_6_t)
    call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs8_a"), &
    model_name = var_str ("Test_model"), &
    n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method = var_str ("test"), &
    variant = core_def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")

call lib%configure (os_data)
call lib%compute_md5sum ()

call lib%test_transfer_md5sum (1, 1, 1)

write (u, "(1x,A,L1)")  "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)")  "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)")  "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)")  "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)")  "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)")  "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Write driver source code"
write (u, "(A)")

```

```

call lib%write_driver (force = .false.)

write (u, "(A)")  "* Write process source code"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Compile and load"
write (u, "(A)")

call lib%load (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Append process and reconfigure"
write (u, "(A)")

allocate (prcdef_6_t :: core_def)
select type (core_def)
type is (prcdef_6_t)
    call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs8_b"), &
    model_name = var_str ("Test_model"), &
    n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
    prt_in  = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("d")]), &
    method  = var_str ("test"), &
    variant = core_def)
call lib%append (entry)

call lib%configure(os_data)
call lib%compute_md5sum ()
call lib%test_transfer_md5sum (2, 2, 1)
call lib%write_makefile (os_data, force = .false., verbose = .false.)
call lib%write_driver (force = .false.)

write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

```



```

call lib%update_status (os_data)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)" "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)" "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)" "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Write source code"
write (u, "(A)")

call lib%make_source (os_data)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)" "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)" "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)" "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Reset status"
write (u, "(A)")

call lib%set_status (STAT_CONFIGURED, entries=.true.)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)" "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)" "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)" "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)" "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)" "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)" "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Partial cleanup"
write (u, "(A)")

call lib%clean (os_data, distclean = .false.)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)" "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)" "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)" "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)" "library loaded = ", lib%is_loaded ()

```

```

write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "** Complete cleanup"

call lib%clean (os_data, distclean = .true.)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: process_libraries_8"
end subroutine process_libraries_8

```

14.5 Process Library Stacks

For storing and handling multiple libraries, we define process library stacks. These are ordinary stacks where new entries are pushed onto the top.

```

⟨prclib_stacks.f90⟩≡
  ⟨File header⟩

  module prclib_stacks

    ⟨Use strings⟩
    use process_libraries

    ⟨Standard module head⟩

    ⟨Prclib stacks: public⟩

    ⟨Prclib stacks: types⟩

    interface
    ⟨Prclib stacks: sub interfaces⟩
    end interface

  end module prclib_stacks

⟨prclib_stacks_sub.f90⟩≡
  ⟨File header⟩

  submodule (prclib_stacks) prclib_stacks_s

    use io_units
    use format_utils, only: write_separator

    implicit none

  contains

  ⟨Prclib stacks: procedures⟩

```

```
end submodule prclib_stacks_s
```

14.5.1 The stack entry type

A stack entry is a process library object, augmented by a pointer to the next entry. We do not need specific methods, all relevant methods are inherited.

On higher level, process libraries should be prepared as process entry objects.

```
<Prclib_stacks: public>≡
  public :: prclib_entry_t
<Prclib_stacks: types>≡
  type, extends (process_library_t) :: prclib_entry_t
    type(prclib_entry_t), pointer :: next => null ()
  end type prclib_entry_t
```

14.5.2 The prclib stack type

For easy conversion and lookup it is useful to store the filling number in the object. The content is stored as a linked list.

```
<Prclib_stacks: public>+≡
  public :: prclib_stack_t
<Prclib_stacks: types>+≡
  type :: prclib_stack_t
    integer :: n = 0
    type(prclib_entry_t), pointer :: first => null ()
  contains
    <Prclib_stacks: prclib_stack: TBP>
  end type prclib_stack_t
```

Finalizer. Iteratively deallocate the stack entries. The resulting empty stack can be immediately recycled, if necessary.

```
<Prclib_stacks: prclib_stack: TBP>≡
  procedure :: final => prclib_stack_final
<Prclib_stacks: sub interfaces>≡
  module subroutine prclib_stack_final (object)
    class(prclib_stack_t), intent(inout) :: object
  end subroutine prclib_stack_final
<Prclib_stacks: procedures>≡
  module subroutine prclib_stack_final (object)
    class(prclib_stack_t), intent(inout) :: object
    type(prclib_entry_t), pointer :: lib
    do while (associated (object%first))
      lib => object%first
      object%first => lib%next
      call lib%final ()
      deallocate (lib)
    end do
    object%n = 0
  end subroutine prclib_stack_final
```

Output. The entries on the stack will be ordered LIFO, i.e., backwards.

```

<Prclib stacks: prclib stack: TBP>+≡
    procedure :: write => prclib_stack_write

<Prclib stacks: sub interfaces>+≡
    module subroutine prclib_stack_write (object, unit, libpath)
        class(prclib_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
    end subroutine prclib_stack_write

<Prclib stacks: procedures>+≡
    module subroutine prclib_stack_write (object, unit, libpath)
        class(prclib_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
        type(prclib_entry_t), pointer :: lib
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        select case (object%n)
        case (0)
            write (u, "(1x,A)") "Process library stack: [empty]"
        case default
            write (u, "(1x,A)") "Process library stack:"
            lib => object%first
            do while (associated (lib))
                call write_separator (u)
                call lib%write (u, libpath)
                lib => lib%next
            end do
        end select
        call write_separator (u, 2)
    end subroutine prclib_stack_write

```

14.5.3 Operating on Stacks

We take a library entry pointer and push it onto the stack. The previous pointer is nullified. Subsequently, the library entry is ‘owned’ by the stack and will be finalized when the stack is deleted.

```

<Prclib stacks: prclib stack: TBP>+≡
    procedure :: push => prclib_stack_push

<Prclib stacks: sub interfaces>+≡
    module subroutine prclib_stack_push (stack, lib)
        class(prclib_stack_t), intent(inout) :: stack
        type(prclib_entry_t), intent(inout), pointer :: lib
    end subroutine prclib_stack_push

<Prclib stacks: procedures>+≡
    module subroutine prclib_stack_push (stack, lib)
        class(prclib_stack_t), intent(inout) :: stack
        type(prclib_entry_t), intent(inout), pointer :: lib
        lib%next => stack%first
    end subroutine prclib_stack_push

```

```

stack%first => lib
lib => null ()
stack%n = stack%n + 1
end subroutine prclib_stack_push

```

14.5.4 Accessing Contents

Return a pointer to the topmost stack element. The result type is just the bare `process_library_t`. There is no `target` attribute required since the stack elements are allocated via pointers.

```

<Prclib stacks: prclib stack: TBP>+≡
  procedure :: get_first_ptr => prclib_stack_get_first_ptr

<Prclib stacks: sub interfaces>+≡
  module function prclib_stack_get_first_ptr (stack) result (ptr)
    class(prclib_stack_t), intent(in) :: stack
    type(process_library_t), pointer :: ptr
  end function prclib_stack_get_first_ptr

<Prclib stacks: procedures>+≡
  module function prclib_stack_get_first_ptr (stack) result (ptr)
    class(prclib_stack_t), intent(in) :: stack
    type(process_library_t), pointer :: ptr
    if (associated (stack%first)) then
      ptr => stack%first%process_library_t
    else
      ptr => null ()
    end if
  end function prclib_stack_get_first_ptr

```

Return a complete list of the libraries (names) in the stack. The list is in the order in which the elements got pushed onto the stack, so the 'first' entry is listed last.

```

<Prclib stacks: prclib stack: TBP>+≡
  procedure :: get_names => prclib_stack_get_names

<Prclib stacks: sub interfaces>+≡
  module subroutine prclib_stack_get_names (stack, libname)
    class(prclib_stack_t), intent(in) :: stack
    type(string_t), dimension(:), allocatable, intent(out) :: libname
  end subroutine prclib_stack_get_names

<Prclib stacks: procedures>+≡
  module subroutine prclib_stack_get_names (stack, libname)
    class(prclib_stack_t), intent(in) :: stack
    type(string_t), dimension(:), allocatable, intent(out) :: libname
    type(prclib_entry_t), pointer :: lib
    integer :: i
    allocate (libname (stack%n))
    i = stack%n
    lib => stack%first
    do while (associated (lib))
      libname(i) = lib%get_name ()
    end do
  end subroutine prclib_stack_get_names

```

```

        i = i - 1
        lib => lib%next
    end do
end subroutine prclib_stack_get_names

```

Return a pointer to the library with given name.

```

<Prclib stacks: prclib_stack: TBP>+≡
    procedure :: get_library_ptr => prclib_stack_get_library_ptr

<Prclib stacks: sub interfaces>+≡
    module function prclib_stack_get_library_ptr (stack, libname) result (ptr)
        class(prclib_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: libname
        type(process_library_t), pointer :: ptr
    end function prclib_stack_get_library_ptr

<Prclib stacks: procedures>+≡
    module function prclib_stack_get_library_ptr (stack, libname) result (ptr)
        class(prclib_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: libname
        type(process_library_t), pointer :: ptr
        type(prclib_entry_t), pointer :: current
        current => stack%first
        do while (associated (current))
            if (current%get_name () == libname) then
                ptr => current%process_library_t
                return
            end if
            current => current%next
        end do
        ptr => null ()
    end function prclib_stack_get_library_ptr

```

14.5.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<prclib_stacks_ut.f90>≡
<File header>

module prclib_stacks_ut
    use unit_tests
    use prclib_stacks_uti

<Standard module head>

<Prclib stacks: public test>

contains

<Prclib stacks: test driver>

end module prclib_stacks_ut

```

```

<prclib_stacks_uti.f90>≡
  <File header>

  module prclib_stacks_uti

    <Use strings>

    use prclib_stacks

    <Standard module head>

    <Prclib stacks: test declarations>

    contains

    <Prclib stacks: tests>

  end module prclib_stacks_uti
API: driver for the unit tests below.
<Prclib stacks: public test>≡
  public :: prclib_stacks_test
<Prclib stacks: test driver>≡
  subroutine prclib_stacks_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Prclib stacks: execute tests>
  end subroutine prclib_stacks_test

```

Write an empty process library stack

The most trivial test is to write an uninitialized process library stack.

```

<Prclib stacks: execute tests>≡
  call test (prclib_stacks_1, "prclib_stacks_1", &
    "write an empty process library stack", &
    u, results)
<Prclib stacks: test declarations>≡
  public :: prclib_stacks_1
<Prclib stacks: tests>≡
  subroutine prclib_stacks_1 (u)
    integer, intent(in) :: u
    type(prclib_stack_t) :: stack

    write (u, "(A)")  "* Test output: prclib_stacks_1"
    write (u, "(A)")  "* Purpose: display an empty process library stack"
    write (u, "(A)")

    call stack%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: prclib_stacks_1"

```

```
end subroutine prclib_stacks_1
```

Fill a process library stack

Fill a process library stack with two (identical) processes.

```
<Prclib_stacks: execute tests>+≡
  call test (prclib_stacks_2, "prclib_stacks_2", &
    "fill a process library stack", &
    u, results)

<Prclib_stacks: test declarations>+≡
  public :: prclib_stacks_2

<Prclib_stacks: tests>+≡
  subroutine prclib_stacks_2 (u)
    integer, intent(in) :: u
    type(prclib_stack_t) :: stack
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: prclib_stacks_2"
    write (u, "(A)")  "* Purpose: fill a process library stack"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize two (empty) libraries &
      &and push them on the stack"
    write (u, "(A)")

    allocate (lib)
    call lib%init (var_str ("lib1"))
    call stack%push (lib)

    allocate (lib)
    call lib%init (var_str ("lib2"))
    call stack%push (lib)

    call stack%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call stack%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: prclib_stacks_2"

  end subroutine prclib_stacks_2
```

14.6 Trivial matrix element for tests

For the purpose of testing the workflow, we implement here two matrix elements with the simplest possible structure.

This matrix element generator can only generate a single scattering process and a single decay process. The scattering process is a quartic interaction of a massless, neutral and colorless scalar s with unit coupling results in a trivial $2 \rightarrow 2$ scattering process. The matrix element is implemented internally, so we do not need the machinery of external process libraries. The decay process is a decay of s into a pair of colored fermions f .

```

<prc_test.f90>≡
  <File header>

  module prc_test

    use, intrinsic :: iso_c_binding !NODEP!

    <Use kinds>
    <Use strings>
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def
    use process_libraries

    <Standard module head>

    <Test ME: public>

    <Test ME: types>

    interface
    <Test ME: sub interfaces>
    end interface

    contains

    <Test ME: main procedures>

  end module prc_test

<prc_test_sub.f90>≡
  <File header>

  submodule (prc_test) prc_test_s

    implicit none

    contains

    <Test ME: procedures>

  end submodule prc_test_s

```

14.6.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```
<Test ME: public>≡
    public :: prc_test_def_t

<Test ME: types>≡
    type, extends (prc_core_def_t) :: prc_test_def_t
        type(string_t) :: model_name
        type(string_t), dimension(:), allocatable :: prt_in
        type(string_t), dimension(:), allocatable :: prt_out
    contains
        <Test ME: test me def: TBP>
    end type prc_test_def_t

<Test ME: test me def: TBP>≡
    procedure, nopass :: type_string => prc_test_def_type_string

<Test ME: sub interfaces>≡
    module function prc_test_def_type_string () result (string)
        type(string_t) :: string
    end function prc_test_def_type_string

<Test ME: procedures>≡
    module function prc_test_def_type_string () result (string)
        type(string_t) :: string
        string = "test_me"
    end function prc_test_def_type_string
```

There is no 'feature' here since there is no external code.

```
<Test ME: test me def: TBP>+≡
    procedure, nopass :: get_features => prc_test_def_get_features

<Test ME: sub interfaces>+≡
    module subroutine prc_test_def_get_features (features)
        type(string_t), dimension(:), allocatable, intent(out) :: features
    end subroutine prc_test_def_get_features

<Test ME: procedures>+≡
    module subroutine prc_test_def_get_features (features)
        type(string_t), dimension(:), allocatable, intent(out) :: features
        allocate (features(0))
    end subroutine prc_test_def_get_features
```

Initialization: set some data (not really useful).

```
<Test ME: test me def: TBP>+≡
    procedure :: init => prc_test_def_init

<Test ME: sub interfaces>+≡
    module subroutine prc_test_def_init (object, model_name, prt_in, prt_out)
        class(prc_test_def_t), intent(out) :: object
        type(string_t), intent(in) :: model_name
        type(string_t), dimension(:), intent(in) :: prt_in
        type(string_t), dimension(:), intent(in) :: prt_out
    end subroutine prc_test_def_init
```

<Test ME: procedures>+≡

```

module subroutine prc_test_def_init (object, model_name, prt_in, prt_out)
  class(prc_test_def_t), intent(out) :: object
  type(string_t), intent(in) :: model_name
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  object%model_name = model_name
  allocate (object%prt_in (size (prt_in)))
  object%prt_in = prt_in
  allocate (object%prt_out (size (prt_out)))
  object%prt_out = prt_out
end subroutine prc_test_def_init

```

Write/read process- and method-specific data. (No-op)

<Test ME: test me def: TBP>+≡

```

procedure :: write => prc_test_def_write

```

<Test ME: sub interfaces>+≡

```

module subroutine prc_test_def_write (object, unit)
  class(prc_test_def_t), intent(in) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_write

```

<Test ME: procedures>+≡

```

module subroutine prc_test_def_write (object, unit)
  class(prc_test_def_t), intent(in) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_write

```

<Test ME: test me def: TBP>+≡

```

procedure :: read => prc_test_def_read

```

<Test ME: sub interfaces>+≡

```

module subroutine prc_test_def_read (object, unit)
  class(prc_test_def_t), intent(out) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_read

```

<Test ME: procedures>+≡

```

module subroutine prc_test_def_read (object, unit)
  class(prc_test_def_t), intent(out) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_read

```

Allocate the driver for test ME matrix elements. We get the actual component ID (basename), and we can transfer all process-specific data from the process definition. Due to a bug of bind(C) features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

<Test ME: test me def: TBP>+≡

```

procedure :: allocate_driver => prc_test_def_allocate_driver

```

```

<Test ME: main procedures>≡
subroutine prc_test_def_allocate_driver (object, driver, basename)
  class(prc_test_def_t), intent(in) :: object
  class(prc_core_driver_t), intent(out), allocatable :: driver
  type(string_t), intent(in) :: basename
  allocate (prc_test_t :: driver)
  select type (driver)
  type is (prc_test_t)
    driver%id = basename
    driver%model_name = object%model_name
    select case (size (object%prt_in))
    case (1); driver%scattering = .false.
    case (2); driver%scattering = .true.
    end select
  end select
end subroutine prc_test_def_allocate_driver

```

Nothing to connect. This subroutine will not be called.

```

<Test ME: test me def: TBP>+≡
procedure :: connect => prc_test_def_connect

<Test ME: sub interfaces>+≡
module subroutine prc_test_def_connect (def, lib_driver, i, proc_driver)
  class(prc_test_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
end subroutine prc_test_def_connect

<Test ME: procedures>+≡
module subroutine prc_test_def_connect (def, lib_driver, i, proc_driver)
  class(prc_test_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
end subroutine prc_test_def_connect

```

14.6.2 Driver

```

<Test ME: public>+≡
public :: prc_test_t

<Test ME: types>+≡
type, extends (process_driver_internal_t) :: prc_test_t
  type(string_t) :: id
  type(string_t) :: model_name
  logical :: scattering = .true.
contains
  <Test ME: test me driver: TBP>
end type prc_test_t

```

In contrast to generic matrix-element implementations, we can hard-wire the amplitude method as a type-bound procedure.

```

<Test ME: test me driver: TBP>≡
    procedure, nopass :: get_amplitude => prc_test_get_amplitude

<Test ME: sub interfaces>+≡
    module function prc_test_get_amplitude (p) result (amp)
        complex(default) :: amp
        real(default), dimension(:,:), intent(in) :: p
    end function prc_test_get_amplitude

<Test ME: procedures>+≡
    module function prc_test_get_amplitude (p) result (amp)
        complex(default) :: amp
        real(default), dimension(:,:), intent(in) :: p
        amp = 1
    end function prc_test_get_amplitude

```

The reported type is the same as for the `prc_test_def_t` type.

```

<Test ME: test me driver: TBP>+≡
    procedure, nopass :: type_name => prc_test_type_name

<Test ME: sub interfaces>+≡
    module function prc_test_type_name () result (string)
        type(string_t) :: string
    end function prc_test_type_name

<Test ME: procedures>+≡
    module function prc_test_type_name () result (string)
        type(string_t) :: string
        string = "test_me"
    end function prc_test_type_name

```

Fill process constants.

```

<Test ME: test me driver: TBP>+≡
    procedure :: fill_constants => prc_test_fill_constants

<Test ME: sub interfaces>+≡
    module subroutine prc_test_fill_constants (driver, data)
        class(prc_test_t), intent(in) :: driver
        type(process_constants_t), intent(out) :: data
    end subroutine prc_test_fill_constants

<Test ME: procedures>+≡
    module subroutine prc_test_fill_constants (driver, data)
        class(prc_test_t), intent(in) :: driver
        type(process_constants_t), intent(out) :: data
        data%id = driver%id
        data%model_name = driver%model_name
        if (driver%scattering) then
            data%n_in = 2
            data%n_out = 2
            data%n_flv = 1
            data%n_hel = 1
            data%n_col = 1
            data%n_cin = 2

```

```

      data%n_cf = 1
      allocate (data%flv_state (4, 1))
      data%flv_state = 25
      allocate (data%hel_state (4, 1))
      data%hel_state = 0
      allocate (data%col_state (2, 4, 1))
      data%col_state = 0
      allocate (data%ghost_flag (4, 1))
      data%ghost_flag = .false.
      allocate (data%color_factors (1))
      data%color_factors = 1
      allocate (data%cf_index (2, 1))
      data%cf_index = 1
    else
      data%n_in = 1
      data%n_out = 2
      data%n_flv = 1
      data%n_hel = 2
      data%n_col = 1
      data%n_cin = 2
      data%n_cf = 1
      allocate (data%flv_state (3, 1))
      data%flv_state(:,1) = [25, 6, -6]
      allocate (data%hel_state (3, 2))
      data%hel_state(:,1) = [0, 1, -1]
      data%hel_state(:,2) = [0, -1, 1]
      allocate (data%col_state (2, 3, 1))
      data%col_state = reshape ([0,0, 1,0, 0,-1], [2,3,1])
      allocate (data%ghost_flag (3, 1))
      data%ghost_flag = .false.
      allocate (data%color_factors (1))
      data%color_factors = 3
      allocate (data%cf_index (2, 1))
      data%cf_index = 1
    end if
  end subroutine prc_test_fill_constants

```

14.6.3 Shortcut

Since this module is there for testing purposes, we set up a subroutine that does all the work at once: create a library with the two processes (scattering and decay), configure and load, and set up the driver. Due to a bug of bind(C) features with submodules in gfortran 7/8/9 (and maybe together with MPI) this needs to be in the module, not the submodule.

```

<Test ME: public>+≡
  public :: prc_test_create_library

<Test ME: main procedures>+≡
  subroutine prc_test_create_library &
    (libname, lib, scattering, decay, procname1, procname2)
    type(string_t), intent(in) :: libname
    type(process_library_t), intent(out) :: lib

```

```

logical, intent(in), optional :: scattering, decay
type(string_t), intent(in), optional :: procname1, procname2
type(string_t) :: model_name, procname
type(string_t), dimension(:), allocatable :: prt_in, prt_out
class(prc_core_def_t), allocatable :: def
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
logical :: sca, dec
sca = .true.; if (present (scattering)) sca = scattering
dec = .false.; if (present (decay)) dec = decay

call os_data%init ()
call lib%init (libname)
model_name = "Test"

if (sca) then
  if (present (procname1)) then
    procname = procname1
  else
    procname = libname
  end if
  allocate (prt_in (2), prt_out (2))
  prt_in = [var_str ("s"), var_str ("s")]
  prt_out = [var_str ("s"), var_str ("s")]
  allocate (prc_test_def_t :: def)
  select type (def)
  type is (prc_test_def_t)
    call def%init (model_name, prt_in, prt_out)
  end select
  allocate (entry)
  call entry%init (procname, model_name = model_name, &
    n_in = 2, n_components = 1)
  call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("test_me"), &
    variant = def)
  call lib%append (entry)
end if

if (dec) then
  if (present (procname2)) then
    procname = procname2
  else
    procname = libname
  end if
  if (allocated (prt_in)) deallocate (prt_in, prt_out)
  allocate (prt_in (1), prt_out (2))
  prt_in = [var_str ("s")]
  prt_out = [var_str ("f"), var_str ("fbar")]
  allocate (prc_test_def_t :: def)
  select type (def)
  type is (prc_test_def_t)
    call def%init (model_name, prt_in, prt_out)

```

```

        end select
        allocate (entry)
        call entry%init (procname, model_name = model_name, &
            n_in = 1, n_components = 1)
        call entry%import_component (1, n_out = size (prt_out), &
            prt_in = new_prt_spec (prt_in), &
            prt_out = new_prt_spec (prt_out), &
            method = var_str ("test_decay"), &
            variant = def)
        call lib%append (entry)
    end if

    call lib%configure (os_data)
    call lib%load (os_data)
end subroutine prc_test_create_library

```

14.6.4 Unit Test

Test module, followed by the corresponding implementation module.

```

<prc_test_ut.f90>≡
  <File header>

  module prc_test_ut
    use unit_tests
    use prc_test_uti

    <Standard module head>

    <Test ME: public test>

    contains

    <Test ME: test driver>

  end module prc_test_ut
<prc_test_uti.f90>≡
  <File header>

  module prc_test_uti

    <Use kinds>
    <Use strings>
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prc_core_def
    use process_libraries

    use prc_test

    <Standard module head>

```



```

    <Test ME: test declarations>

contains

    <Test ME: tests>

    end module prc_test_util

API: driver for the unit tests below.
<Test ME: public test>≡
    public :: prc_test_test
<Test ME: test driver>≡
    subroutine prc_test_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Test ME: execute tests>
    end subroutine prc_test_test

```

Generate and load the scattering process

The process is $ss \rightarrow ss$, where s is a trivial scalar particle, for vanishing mass and unit coupling. We initialize the process, build the library, and compute the particular matrix element for momenta of unit energy and right-angle scattering. (The scattering is independent of angle.) The matrix element is equal to unity.

```

<Test ME: execute tests>≡
    call test (prc_test_1, "prc_test_1", &
        "build and load trivial process", &
        u, results)

<Test ME: test declarations>≡
    public :: prc_test_1

<Test ME: tests>≡
    subroutine prc_test_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t) :: lib
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(string_t) :: model_name
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_constants_t) :: data
        class(prc_core_driver_t), allocatable :: driver
        real(default), dimension(0:3,4) :: p
        integer :: i

        write (u, "(A)")  "* Test output: prc_test_1"
        write (u, "(A)")  "*   Purpose: create a trivial process"
        write (u, "(A)")  "*               build a library and &
            &access the matrix element"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library with one entry"
    end subroutine prc_test_1

```

```

write (u, "(A)")
call os_data%init ()
call lib%init (var_str ("prc_test1"))

model_name = "Test"
allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("s"), var_str ("s")]
prt_out = [var_str ("s"), var_str ("s")]

allocate (prc_test_def_t :: def)
select type (def)
type is (prc_test_def_t)
    call def%init (model_name, prt_in, prt_out)
end select
allocate (entry)
call entry%init (var_str ("prc_test1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("test_me"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Load library"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of prc_test1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("prc_test1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID" = ", char (data%id)
write (u, "(1x,A,A)")  "model name" = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum" = ', data%md5sum, "'
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in

```

```

write (u, "(1x,A,I0)") "n_out = ", data%n_out
write (u, "(1x,A,I0)") "n_flv = ", data%n_flv
write (u, "(1x,A,I0)") "n_hel = ", data%n_hel
write (u, "(1x,A,I0)") "n_col = ", data%n_col
write (u, "(1x,A,I0)") "n_cin = ", data%n_cin
write (u, "(1x,A,I0)") "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))") "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))") "hel state =", data%hel_state(:,1)
write (u, "(1x,A,10(1x,I0))") "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))") "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))") "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))") "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_default, 0.0_default, 0.0_default, 1.0_default, &
    1.0_default, 0.0_default, 0.0_default, -1.0_default, &
    1.0_default, 1.0_default, 0.0_default, 0.0_default, &
    1.0_default, -1.0_default, 0.0_default, 0.0_default &
], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)
    write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_1"

end subroutine prc_test_1

```

Shortcut

This is identical to the previous test, but we create the library be a single command. This is handy for other modules which use the test process.

```

<Test ME: execute tests>+≡
call test (prc_test_2, "prc_test_2", &
    "build and load trivial process using shortcut", &
    u, results)

```

```

<Test ME: test declarations>+≡
    public :: prc_test_2
<Test ME: tests>+≡
    subroutine prc_test_2 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_driver_t), allocatable :: driver
        type(process_constants_t) :: data
        real(default), dimension(0:3,4) :: p

        write (u, "(A)")  "* Test output: prc_test_2"
        write (u, "(A)")  "*   Purpose: create a trivial process"
        write (u, "(A)")  "*               build a library and &
                        &access the matrix element"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a process library with one entry"

        call prc_test_create_library (var_str ("prc_test2"), lib)
        call lib%connect_process (var_str ("prc_test2"), 1, data, driver)

        p = reshape ([ &
            1.0_default, 0.0_default, 0.0_default, 1.0_default, &
            1.0_default, 0.0_default, 0.0_default, -1.0_default, &
            1.0_default, 1.0_default, 0.0_default, 0.0_default, &
            1.0_default, -1.0_default, 0.0_default, 0.0_default &
            ], [4,4])

        write (u, "(A)")
        write (u, "(A)")  "* Compute matrix element:"
        write (u, "(A)")

        select type (driver)
        type is (prc_test_t)
            write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
        end select

        call lib%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: prc_test_2"

    end subroutine prc_test_2

```

Generate and load the decay process

The process is $s \rightarrow f\bar{f}$, where s is a trivial scalar particle and f is a colored fermion. We initialize the process, build the library, and compute the particular matrix element for a fixed momentum configuration. (The decay is independent of angle.) The matrix element is equal to unity.

```

<Test ME: execute tests>+≡
    call test (prc_test_3, "prc_test_3", &

```

```

        "build and load trivial decay", &
        u, results)
<Test ME: test declarations>+≡
    public :: prc_test_3
<Test ME: tests>+≡
    subroutine prc_test_3 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t) :: lib
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(string_t) :: model_name
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_constants_t) :: data
        class(prc_core_driver_t), allocatable :: driver
        real(default), dimension(0:3,3) :: p
        integer :: i

        write (u, "(A)")  "* Test output: prc_test_3"
        write (u, "(A)")  "* Purpose: create a trivial decay process"
        write (u, "(A)")  "*          build a library and &
            &access the matrix element"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library with one entry"
        write (u, "(A)")
        call os_data%init ()
        call lib%init (var_str ("prc_test3"))

        model_name = "Test"
        allocate (prt_in (1), prt_out (2))
        prt_in = [var_str ("s")]
        prt_out = [var_str ("f"), var_str ("F")]

        allocate (prc_test_def_t :: def)
        select type (def)
        type is (prc_test_def_t)
            call def%init (model_name, prt_in, prt_out)
        end select
        allocate (entry)
        call entry%init (var_str ("prc_test3_a"), model_name = model_name, &
            n_in = 1, n_components = 1)
        call entry%import_component (1, n_out = size (prt_out), &
            prt_in = new_prt_spec (prt_in), &
            prt_out = new_prt_spec (prt_out), &
            method = var_str ("test_me"), &
            variant = def)
        call lib%append (entry)

        write (u, "(A)")  "* Configure library"
        write (u, "(A)")
        call lib%configure (os_data)

```

```

write (u, "(A)")  "* Load library"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of prc_test3_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("prc_test3_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID" = ", char (data%id)
write (u, "(1x,A,A)")  "model name" = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum" = ', data%md5sum, "'
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,2)
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
125._default, 0.0_default, 0.0_default, 0.0_default, &
62.5_default, 0.0_default, 0.0_default, 62.5_default, &
62.5_default, 0.0_default, 0.0_default, -62.5_default &
], [4,3])
do i = 1, 3
write (u, "(2x,A,I0,A,4(1x,F8.4))")  "p", i, " =", p(:,i)
end do

write (u, "(A)")

```

```

write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)
  write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_3"

end subroutine prc_test_3

```

Shortcut

This is identical to the previous test, but we create the library be a single command. This is handy for other modules which use the test process.

```

<Test ME: execute tests>+≡
  call test (prc_test_4, "prc_test_4", &
    "build and load trivial decay using shortcut", &
    u, results)

<Test ME: test declarations>+≡
  public :: prc_test_4

<Test ME: tests>+≡
  subroutine prc_test_4 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    class(prc_core_driver_t), allocatable :: driver
    type(process_constants_t) :: data
    real(default), dimension(0:3,3) :: p

    write (u, "(A)")  "* Test output: prc_test_4"
    write (u, "(A)")  "* Purpose: create a trivial decay process"
    write (u, "(A)")  "* build a library and &
      &access the matrix element"
    write (u, "(A)")

    write (u, "(A)")  "* Build and load a process library with one entry"

    call prc_test_create_library (var_str ("prc_test4"), lib, &
      scattering=.false., decay=.true.)
    call lib%connect_process (var_str ("prc_test4"), 1, data, driver)

    p = reshape ([ &
      125._default, 0.0_default, 0.0_default, 0.0_default, &
      62.5_default, 0.0_default, 0.0_default, 62.5_default, &
      62.5_default, 0.0_default, 0.0_default, -62.5_default &
      ], [4,3])

```

```

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)
    write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_4"

end subroutine prc_test_4

```


Chapter 15

Particles

This chapter collects modules that implement particle objects, for use in event records.

While within interactions, all correlations are manifest, a particle array is derived by selecting a particular quantum number set. This involves tracing over all other particles, as far as polarization is concerned. Thus, a particle has definite flavor, color, and a single-particle density matrix for polarization.

su_algebra We make use of $su(N)$ generators as the basis for representing polarization matrices. This module defines the basis and provides the necessary transformation routines.

bloch_vectors This defines polarization objects in Bloch representation. The object describes the spin density matrix of a particle, currently restricted to spin $0 \dots 2$.

polarizations This extends the basic polarization object such that it supports properties of physical particles and appropriate constructors.

particles Particle objects and particle lists, as the base of event records.

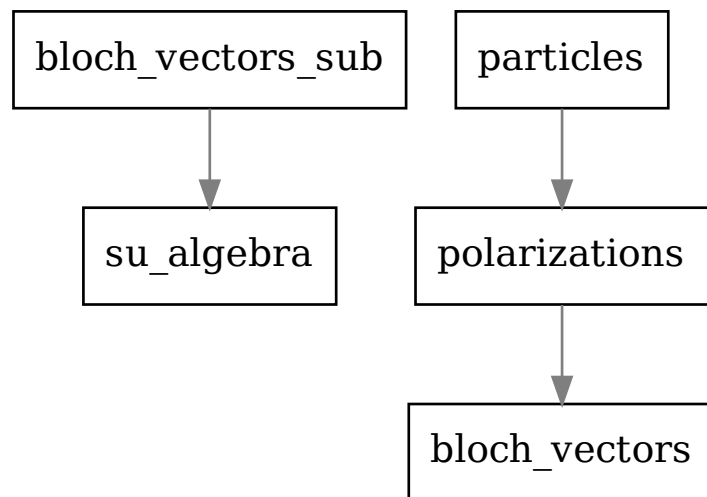


Figure 15.1: Module dependencies in `src/particles`.

15.1 $su(N)$ Algebra

We need a specific choice of basis for a well-defined component representation. The matrix elements of T^a are ordered as $m = \ell, \ell - 1, \dots - \ell$, i.e., from highest down to lowest weight, for both row and column.

We list first the generators of the $su(2)$ subalgebras which leave $|m|$ invariant ($|m| \neq 0$):

$$T^{b+1, b+2, b+3} \equiv \sigma^{1,2,3} \quad (15.1)$$

acting on the respective subspace $|m| = \ell, \ell - 1, \dots$ for $b = 0, 1, \dots$. This defines generators T^a for $a = 1, \dots, 3N/2$ ($\dots 3(N-1)/2$) for N even (odd), respectively.

The following generators successively extend this to $su(4)$, $su(6)$, \dots until $su(N)$ by adding first the missing off-diagonal and then diagonal generators. The phase conventions are analogous.

(It should be possible to code these conventions for generic spin, but in the current implementation we restrict ourselves to $s \leq 2$, i.e., $N \leq 5$.)

```

<su_algebra.f90>≡
  <File header>

  module su_algebra

    <Use kinds>

    <Standard module head>

    <SU algebra: public>

    interface
    <SU algebra: sub interfaces>
    end interface

  end module su_algebra

<su_algebra_sub.f90>≡
  <File header>

  submodule (su_algebra) su_algebra_s

    use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR

    implicit none

    contains

    <SU algebra: procedures>

  end submodule su_algebra_s

```

15.1.1 $su(N)$ fundamental representation

The dimension of the basis for a given spin type. consecutively, starting at SCALAR=1.

```

<SU algebra: public>≡
  public :: algebra_dimension

<SU algebra: sub interfaces>≡
  module function algebra_dimension (s) result (n)
    integer :: n
    integer, intent(in) :: s
  end function algebra_dimension

<SU algebra: procedures>≡
  module function algebra_dimension (s) result (n)
    integer :: n
    integer, intent(in) :: s
    n = fundamental_dimension (s) ** 2 - 1
  end function algebra_dimension

```

The dimension of the fundamental (defining) representation that we use. This implementation assumes that the spin type is numerically equal to the fundamental dimension.

```

<SU algebra: public>+≡
  public :: fundamental_dimension

<SU algebra: sub interfaces>+≡
  module function fundamental_dimension (s) result (d)
    integer :: d
    integer, intent(in) :: s
  end function fundamental_dimension

<SU algebra: procedures>+≡
  module function fundamental_dimension (s) result (d)
    integer :: d
    integer, intent(in) :: s
    d = s
  end function fundamental_dimension

```

15.1.2 Mapping between helicity and matrix index

Return the helicity that corresponds to a particular entry in the polarization matrix representation. Helicities are counted downwards, in integers, and zero helicity is included (omitted) for odd (even) spin, respectively.

```

<SU algebra: public>+≡
  public :: helicity_value

<SU algebra: sub interfaces>+≡
  module function helicity_value (s, i) result (h)
    integer :: h
    integer, intent(in) :: s, i
  end function helicity_value

<SU algebra: procedures>+≡
  module function helicity_value (s, i) result (h)
    integer :: h
    integer, intent(in) :: s, i
    integer, dimension(1), parameter :: hh1 = [0]
    integer, dimension(2), parameter :: hh2 = [1, -1]

```

```

integer, dimension(3), parameter :: hh3 = [1, 0, -1]
integer, dimension(4), parameter :: hh4 = [2, 1, -1, -2]
integer, dimension(5), parameter :: hh5 = [2, 1, 0, -1, -2]
h = 0
select case (s)
case (SCALAR)
  select case (i)
  case (1:1); h = hh1(i)
  end select
case (SPINOR)
  select case (i)
  case (1:2); h = hh2(i)
  end select
case (VECTOR)
  select case (i)
  case (1:3); h = hh3(i)
  end select
case (VECTORSPINOR)
  select case (i)
  case (1:4); h = hh4(i)
  end select
case (TENSOR)
  select case (i)
  case (1:5); h = hh5(i)
  end select
end select
end function helicity_value

```

Inverse: return the index that corresponds to a certain helicity value in the chosen representation.

```

<SU algebra: public>+≡
public :: helicity_index

<SU algebra: sub interfaces>+≡
module function helicity_index (s, h) result (i)
  integer, intent(in) :: s, h
  integer :: i
end function helicity_index

<SU algebra: procedures>+≡
module function helicity_index (s, h) result (i)
  integer, intent(in) :: s, h
  integer :: i
  integer, dimension(0:0), parameter :: hi1 = [1]
  integer, dimension(-1:1), parameter :: hi2 = [2, 0, 1]
  integer, dimension(-1:1), parameter :: hi3 = [3, 2, 1]
  integer, dimension(-2:2), parameter :: hi4 = [4, 3, 0, 2, 1]
  integer, dimension(-2:2), parameter :: hi5 = [5, 4, 3, 2, 1]
  select case (s)
  case (SCALAR)
    i = hi1(h)
  case (SPINOR)
    i = hi2(h)
  case (VECTOR)
    i = hi3(h)

```

```

    case (VECTORSPINOR)
        i = hi4(h)
    case (TENSOR)
        i = hi5(h)
    end select
end function helicity_index

```

15.1.3 Generator Basis: Cartan Generators

For each supported spin type, we return specific properties of the set of generators via inquiry functions. This is equivalent to using explicit representations of the generators.

For easy access, the properties are hard-coded and selected via case expressions.

Return true if the generator #i is in the Cartan subalgebra, i.e., a diagonal matrix for spin type s.

```

<SU algebra: public>+≡
    public :: is_cartan_generator

<SU algebra: sub interfaces>+≡
    elemental module function is_cartan_generator (s, i) result (cartan)
        logical :: cartan
        integer, intent(in) :: s, i
    end function is_cartan_generator

<SU algebra: procedures>+≡
    elemental module function is_cartan_generator (s, i) result (cartan)
        logical :: cartan
        integer, intent(in) :: s, i
        select case (s)
        case (SCALAR)
        case (SPINOR)
            select case (i)
            case (3); cartan = .true.
            case default
                cartan = .false.
            end select
        case (VECTOR)
            select case (i)
            case (3,8); cartan = .true.
            case default
                cartan = .false.
            end select
        case (VECTORSPINOR)
            select case (i)
            case (3,6,15); cartan = .true.
            case default
                cartan = .false.
            end select
        case (TENSOR)
            select case (i)
            case (3,6,15,24); cartan = .true.
            case default

```

```

        cartan = .false.
    end select
case default
    cartan = .false.
end select
end function is_cartan_generator

```

Return the index of Cartan generator #k in the chosen representation. This has to conform to `cartan` above.

```

<SU algebra: public>+≡
    public :: cartan_index

<SU algebra: sub interfaces>+≡
    elemental module function cartan_index (s, k) result (ci)
        integer :: ci
        integer, intent(in) :: s, k
    end function cartan_index

<SU algebra: procedures>+≡
    elemental module function cartan_index (s, k) result (ci)
        integer :: ci
        integer, intent(in) :: s, k
        integer, dimension(1), parameter :: ci2 = [3]
        integer, dimension(2), parameter :: ci3 = [3,8]
        integer, dimension(3), parameter :: ci4 = [3,6,15]
        integer, dimension(4), parameter :: ci5 = [3,6,15,24]
        select case (s)
        case (SPINOR)
            ci = ci2(k)
        case (VECTOR)
            ci = ci3(k)
        case (VECTORSPINOR)
            ci = ci4(k)
        case (TENSOR)
            ci = ci5(k)
        case default
            ci = 0
        end select
    end function cartan_index

```

The element #k of the result vector `a` is equal to the (h, h) diagonal entry of the generator matrix T^k . That is, evaluating this for all allowed values of `h`, we recover the set of Cartan generator matrices.

```

<SU algebra: public>+≡
    public :: cartan_element

<SU algebra: sub interfaces>+≡
    module function cartan_element (s, h) result (a)
        real(default), dimension(:), allocatable :: a
        integer, intent(in) :: s, h
    end function cartan_element

<SU algebra: procedures>+≡
    module function cartan_element (s, h) result (a)
        real(default), dimension(:), allocatable :: a

```

```

integer, intent(in) :: s, h
real(default), parameter :: sqrt2 = sqrt (2._default)
real(default), parameter :: sqrt3 = sqrt (3._default)
real(default), parameter :: sqrt10 = sqrt (10._default)
allocate (a (algebra_dimension (s)), source = 0._default)
select case (s)
case (SCALAR)
case (SPINOR)
    select case (h)
    case (1)
        a(3) = 1._default / 2
    case (-1)
        a(3) = -1._default / 2
    end select
case (VECTOR)
    select case (h)
    case (1)
        a(3) = 1._default / 2
        a(8) = 1._default / (2 * sqrt3)
    case (-1)
        a(3) = -1._default / 2
        a(8) = 1._default / (2 * sqrt3)
    case (0)
        a(8) = -1._default / sqrt3
    end select
case (VECTORSPINOR)
    select case (h)
    case (2)
        a(3) = 1._default / 2
        a(15) = 1._default / (2 * sqrt2)
    case (-2)
        a(3) = -1._default / 2
        a(15) = 1._default / (2 * sqrt2)
    case (1)
        a(6) = 1._default / 2
        a(15) = -1._default / (2 * sqrt2)
    case (-1)
        a(6) = -1._default / 2
        a(15) = -1._default / (2 * sqrt2)
    end select
case (TENSOR)
    select case (h)
    case (2)
        a(3) = 1._default / 2
        a(15) = 1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)
    case (-2)
        a(3) = -1._default / 2
        a(15) = 1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)
    case (1)
        a(6) = 1._default / 2
        a(15) = -1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)

```



```

        case (-1)
            a(6) = -1._default / 2
            a(15) = -1._default / (2 * sqrt2)
            a(24) = 1._default / (2 * sqrt10)
        case (0)
            a(24) = -4._default / (2 * sqrt10)
        end select
    end select
end function cartan_element

```

Given an array of diagonal matrix elements `rd` of a generator, compute the array `a` of basis coefficients. The array must be ordered as defined by `helicity_value`, i.e., highest weight first. The calculation is organized such that the trace of the generator, i.e., the sum of `rd` values, drops out. The result array `a` has coefficients for all basis generators, but only Cartan generators can get a nonzero coefficient.

<SU algebra: public>+≡

```
public :: cartan_coeff
```

<SU algebra: sub interfaces>+≡

```

module function cartan_coeff (s, rd) result (a)
    real(default), dimension(:), allocatable :: a
    integer, intent(in) :: s
    real(default), dimension(:), intent(in) :: rd
end function cartan_coeff

```

<SU algebra: procedures>+≡

```

module function cartan_coeff (s, rd) result (a)
    real(default), dimension(:), allocatable :: a
    integer, intent(in) :: s
    real(default), dimension(:), intent(in) :: rd
    real(default), parameter :: sqrt2 = sqrt (2._default)
    real(default), parameter :: sqrt3 = sqrt (3._default)
    real(default), parameter :: sqrt10 = sqrt (10._default)
    integer :: n
    n = algebra_dimension (s)
    allocate (a (n), source = 0._default)
    select case (s)
    case (SPINOR)
        a(3) = rd(1) - rd(2)
    case (VECTOR)
        a(3) = rd(1) - rd(3)
        a(8) = (rd(1) - 2 * rd(2) + rd(3)) / sqrt3
    case (VECTORSPINOR)
        a(3) = rd(1) - rd(4)
        a(6) = rd(2) - rd(3)
        a(15) = (rd(1) - rd(2) - rd(3) + rd(4)) / sqrt2
    case (TENSOR)
        a(3) = rd(1) - rd(5)
        a(6) = rd(2) - rd(4)
        a(15) = (rd(1) - rd(2) - rd(4) + rd(5)) / sqrt2
        a(24) = (rd(1) + rd(2) - 4 * rd(3) + rd(4) + rd(5)) / sqrt10
    end select
end function cartan_coeff

```

15.1.4 Roots (Off-Diagonal Generators)

Return the appropriate generator index for a given off-diagonal helicity combination. We require $h_1 > h_2$. We return the index of the appropriate real-valued generator if `r` is true, else the complex-valued one.

This is separate from the `cartan_coeff` function above. The reason is that the off-diagonal generators have only a single nonzero matrix element, so there is a one-to-one correspondence of helicity and index.

```
<SU algebra: public>+≡
  public :: root_index

<SU algebra: sub interfaces>+≡
  module function root_index (s, h1, h2, r) result (ai)
    integer :: ai
    integer, intent(in) :: s, h1, h2
    logical :: r
  end function root_index

<SU algebra: procedures>+≡
  module function root_index (s, h1, h2, r) result (ai)
    integer :: ai
    integer, intent(in) :: s, h1, h2
    logical :: r
    ai = 0
    select case (s)
    case (SCALAR)
    case (SPINOR)
      select case (h1)
      case (1)
        select case (h2)
        case (-1); ai = 1
        end select
      end select
    case (VECTOR)
      select case (h1)
      case (1)
        select case (h2)
        case (-1); ai = 1
        case (0); ai = 4
        end select
      case (0)
        select case (h2)
        case (-1); ai = 6
        end select
      end select
    case (VECTORSPINOR)
      select case (h1)
      case (2)
        select case (h2)
        case (-2); ai = 1
        case (1); ai = 7
        case (-1); ai = 11
```

```

        end select
    case (1)
        select case (h2)
            case (-1); ai = 4
            case (-2); ai = 13
        end select
    case (-1)
        select case (h2)
            case (-2); ai = 9
        end select
    end select
case (TENSOR)
    select case (h1)
        case (2)
            select case (h2)
                case (-2); ai = 1
                case (1); ai = 7
                case (-1); ai = 11
                case (0); ai = 16
            end select
        case (1)
            select case (h2)
                case (-1); ai = 4
                case (-2); ai = 13
                case (0); ai = 20
            end select
        case (-1)
            select case (h2)
                case (-2); ai = 9
            end select
        case (0)
            select case (h2)
                case (-2); ai = 18
                case (-1); ai = 22
            end select
        end select
    end select
    if (ai /= 0 .and. .not. r) ai = ai + 1
end function root_index

```

Inverse: return the helicity values ($h_2 > h_1$) for an off-diagonal generator. The flag *r* tells whether this is a real or diagonal generator. The others are Cartan generators.

```

<SU algebra: public>+≡
    public :: root_helicity

<SU algebra: sub interfaces>+≡
    module subroutine root_helicity (s, i, h1, h2, r)
        integer, intent(in) :: s, i
        integer, intent(out) :: h1, h2
        logical, intent(out) :: r
    end subroutine root_helicity

<SU algebra: procedures>+≡

```

```

module subroutine root_helicity (s, i, h1, h2, r)
  integer, intent(in) :: s, i
  integer, intent(out) :: h1, h2
  logical, intent(out) :: r
  h1 = 0
  h2 = 0
  r = .false.
  select case (s)
  case (SCALAR)
  case (SPINOR)
    select case (i)
    case ( 1, 2); h1 = 1; h2 = -1; r = i == 1
    end select
  case (VECTOR)
    select case (i)
    case ( 1, 2); h1 = 1; h2 = -1; r = i == 1
    case ( 4, 5); h1 = 1; h2 = 0; r = i == 4
    case ( 6, 7); h1 = 0; h2 = -1; r = i == 6
    end select
  case (VECTORSPINOR)
    select case (i)
    case ( 1, 2); h1 = 2; h2 = -2; r = i == 1
    case ( 4, 5); h1 = 1; h2 = -1; r = i == 4
    case ( 7, 8); h1 = 2; h2 = 1; r = i == 7
    case ( 9,10); h1 = -1; h2 = -2; r = i == 9
    case (11,12); h1 = 2; h2 = -1; r = i ==11
    case (13,14); h1 = 1; h2 = -2; r = i ==13
    end select
  case (TENSOR)
    select case (i)
    case ( 1, 2); h1 = 2; h2 = -2; r = i == 1
    case ( 4, 5); h1 = 1; h2 = -1; r = i == 4
    case ( 7, 8); h1 = 2; h2 = 1; r = i == 7
    case ( 9,10); h1 = -1; h2 = -2; r = i == 9
    case (11,12); h1 = 2; h2 = -1; r = i ==11
    case (13,14); h1 = 1; h2 = -2; r = i ==13
    case (16,17); h1 = 2; h2 = 0; r = i ==16
    case (18,19); h1 = 0; h2 = -2; r = i ==18
    case (20,21); h1 = 1; h2 = 0; r = i ==20
    case (22,23); h1 = 0; h2 = -1; r = i ==22
    end select
  end select
end subroutine root_helicity

```

15.1.5 Unit tests

Test module, followed by the corresponding implementation module.

`<su_algebra_ut.f90>`≡
<File header>

```

module su_algebra_ut
  use unit_tests

```

```

        use su_algebra_uti

        <Standard module head>

        <SU algebra: public test>

        contains

        <SU algebra: test driver>

        end module su_algebra_ut
    <su_algebra_uti.f90>≡
    <File header>

    module su_algebra_uti

    <Use kinds>
        use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
        use su_algebra

    <Standard module head>

    <SU algebra: test declarations>

    contains

    <SU algebra: tests>

    end module su_algebra_uti
API: driver for the unit tests below.
    <SU algebra: public test>≡
        public :: su_algebra_test
    <SU algebra: test driver>≡
        subroutine su_algebra_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <SU algebra: execute tests>
        end subroutine su_algebra_test

```

Generator Ordering

Show the position of Cartan generators in the sequence of basis generators.

```

    <SU algebra: execute tests>≡
        call test (su_algebra_1, "su_algebra_1", &
            "generator ordering", &
            u, results)
    <SU algebra: test declarations>≡
        public :: su_algebra_1

```

```

<SU algebra: tests>≡
subroutine su_algebra_1 (u)
  integer, intent(in) :: u

  write (u, "(A)")  "* Test output: su_algebra_1"
  write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
  write (u, "(A)")

  write (u, "(A)")  "* su(N) generators: &
    &list and mark Cartan subalgebra"

  write (u, "(A)")
  write (u, "(A)")  "* s = 0"
  call cartan_check (SCALAR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 1/2"
  call cartan_check (SPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 1"
  call cartan_check (VECTOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 3/2"
  call cartan_check (VECTORSPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 2"
  call cartan_check (TENSOR)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: su_algebra_1"

contains

subroutine cartan_check (s)
  integer, intent(in) :: s
  integer :: i
  write (u, *)
  do i = 1, algebra_dimension (s)
    write (u, "(1x,L1)", advance="no") is_cartan_generator (s, i)
  end do
  write (u, *)

end subroutine cartan_check

end subroutine su_algebra_1

```

Cartan Generator Basis

Show the explicit matrix representation for all Cartan generators and check their traces and Killing products.

Also test helicity index mappings.

```

<SU algebra: execute tests>+≡
  call test (su_algebra_2, "su_algebra_2", &
    "Cartan generator representation", &
    u, results)

<SU algebra: test declarations>+≡
  public :: su_algebra_2

<SU algebra: tests>+≡
  subroutine su_algebra_2 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: su_algebra_2"
    write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
    write (u, "(A)")

    write (u, "(A)")  "* diagonal su(N) generators: &
      &show explicit representation"
    write (u, "(A)")  "* and check trace and Killing form"

    write (u, "(A)")
    write (u, "(A)")  "* s = 1/2"
    call cartan_show (SPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1"
    call cartan_show (VECTOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 3/2"
    call cartan_show (VECTORSPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 2"
    call cartan_show (TENSOR)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: su_algebra_2"

```

contains

```

subroutine cartan_show (s)
  integer, intent(in) :: s
  real(default), dimension(:,:), allocatable :: rd
  integer, dimension(:), allocatable :: ci
  integer :: n, d, h, i, j, k, l

  n = algebra_dimension (s)
  d = fundamental_dimension (s)

  write (u, *)
  write (u, "(A2,5X)", advance="no")  "h:"
  do i = 1, d
    j = helicity_index (s, helicity_value (s, i))

```

```

        write (u, "(1x,I2,5X)", advance="no") helicity_value (s, j)
    end do
    write (u, "(8X)", advance="no")
    write (u, "(1X,A)" "tr"

    allocate (rd (n,d), source = 0._default)
    do i = 1, d
        h = helicity_value (s, i)
        rd(:,i) = cartan_element (s, h)
    end do

    allocate (ci (d-1), source = 0)
    do k = 1, d-1
        ci(k) = cartan_index (s, k)
    end do

    write (u, *)
    do k = 1, d-1
        write (u, "('T',I2,':',1X)", advance="no") ci(k)
        do i = 1, d
            write (u, 1, advance="no") rd(ci(k),i)
        end do
        write (u, "(8X)", advance="no")
        write (u, 1) sum (rd(ci(k),:))
    end do

    write (u, *)
    write (u, "(6X)", advance="no")
    do k = 1, d-1
        write (u, "(2X,'T',I2,3X)", advance="no") ci(k)
    end do
    write (u, *)

    do k = 1, d-1
        write (u, "('T',I2,2X)", advance="no") ci(k)
        do l = 1, d-1
            write (u, 1, advance="no") dot_product (rd(ci(k),:), rd(ci(l),:))
        end do
        write (u, *)
    end do

1    format (1x,F7.4)

    end subroutine cartan_show

    end subroutine su_algebra_2

```

Bloch Representation: Cartan Generators

Transform from Bloch vectors to matrix and back, considering Cartan generators only.

(SU algebra: execute tests) $\vdash \equiv$


```

call test (su_algebra_3, "su_algebra_3", &
  "Cartan generator mapping", &
  u, results)
<SU algebra: test declarations>+≡
public :: su_algebra_3
<SU algebra: tests>+≡
subroutine su_algebra_3 (u)
  integer, intent(in) :: u

  write (u, "(A)")  "* Test output: su_algebra_3"
  write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
  write (u, "(A)")

  write (u, "(A)")  "* diagonal su(N) generators: &
    &transform to matrix and back"

  write (u, "(A)")
  write (u, "(A)")  "* s = 1/2"
  call cartan_expand (SPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 1"
  call cartan_expand (VECTOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 3/2"
  call cartan_expand (VECTORSPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 2"
  call cartan_expand (TENSOR)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: su_algebra_3"

contains

subroutine cartan_expand (s)
  integer, intent(in) :: s
  real(default), dimension(:,:), allocatable :: rd
  integer, dimension(:), allocatable :: ci
  real(default), dimension(:), allocatable :: a
  logical, dimension(:), allocatable :: mask
  integer :: n, d, h, i, k, l

  n = algebra_dimension (s)
  d = fundamental_dimension (s)

  allocate (rd (n,d), source = 0._default)
  do i = 1, d
    h = helicity_value (s, i)
    rd(:,i) = cartan_element (s, h)
  end do

```

```

allocate (ci (d-1), source = 0)
do k = 1, d-1
    ci(k) = cartan_index (s, k)
end do

allocate (a (n))

write (u, *)
do k = 1, d-1
    a(:) = cartan_coeff (s, rd(ci(k),:))
    write (u, "('T',I2,':',1X)", advance="no") ci(k)
    do i = 1, n
        if (is_cartan_generator (s, i)) then
            write (u, 1, advance="no") a(i)
        else if (a(i) /= 0) then
            ! this should not happen (nonzero non-Cartan entry)
            write (u, "(1X,':',I2,':',3X)", advance="no") i
        end if
    end do
    write (u, *)
end do

1    format (1X,F7.4)

end subroutine cartan_expand

end subroutine su_algebra_3

```

Bloch Representation: Roots

List the mapping between helicity transitions and (real) off-diagonal generators.

```

<SU algebra: execute tests>+≡
    call test (su_algebra_4, "su_algebra_4", &
        "Root-helicity mapping", &
        u, results)

<SU algebra: test declarations>+≡
    public :: su_algebra_4

<SU algebra: tests>+≡
    subroutine su_algebra_4 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: su_algebra_4"
        write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
        write (u, "(A)")

        write (u, "(A)")  "* off-diagonal su(N) generators: &
            &mapping from/to helicity pair"

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call root_expand (SPINOR)
    end subroutine su_algebra_4

```

```

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call root_expand (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call root_expand (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call root_expand (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: su_algebra_4"

contains

subroutine root_expand (s)
  integer, intent(in) :: s
  integer :: n, d, i, j, h1, h2
  logical :: r

  n = algebra_dimension (s)

  write (u, *)
  do i = 1, n
    if (is_cartan_generator (s, i)) cycle
    call root_helicity (s, i, h1, h2, r)
    j = root_index (s, h1, h2, r)
    write (u, "('T',I2,':')", advance="no") j
    write (u, "(2(1x,I2))", advance="no") h1, h2
    if (r) then
      write (u, *)
    else
      write (u, "('*')")
    end if
  end do

end subroutine root_expand

end subroutine su_algebra_4

```

15.2 Bloch Representation

Particle polarization is determined by a particular quantum state which has just helicity information. Physically, this is the spin density matrix ρ , where we do not restrict ourselves to pure states.

We adopt the phase convention for a spin-1/2 particle that

$$\rho = \frac{1}{2}(1 + \vec{\alpha} \cdot \vec{\sigma}) \quad (15.2)$$

with the polarization axis $\vec{\alpha}$. For a particle with arbitrary spin s , and thus $N = 2s + 1$ spin states, we extend the above definition to generalized Bloch form

$$\rho = \frac{1}{N} \left(1 + \sqrt{2N(N-1)} \alpha^a T^a \right) \quad (15.3)$$

where the T^a ($a = 1, \dots, N^2 - 1$) are a basis of $su(N)$ algebra generators. These $N \times N$ matrices are hermitean, traceless, and orthogonal via

$$\text{Tr } T^a T^b = \frac{1}{2} \delta^{ab} \quad (15.4)$$

In the spin-1/2 case, this reduces to the above (standard Bloch) representation since $T^a = \sigma^a/2$, $a = 1, 2, 3$. For the spin-1 case, we could use $T^a = \lambda^a/2$ with the Gell-Mann matrices,

$$\rho = \frac{1}{3} \left(1 + \sqrt{3} \alpha^a \lambda^a \right), \quad (15.5)$$

The normalization is chosen that $|\alpha| \leq 1$ for allowed density matrix, where $|\alpha| = 1$ is a necessary, but not sufficient, condition for a pure state.

We need a specific choice of basis for a well-defined component representation. The matrix elements of T^a are ordered as $m = \ell, \ell - 1, \dots, -\ell$, i.e., from highest down to lowest weight, for both row and column.

We list first the generators of the $su(2)$ subalgebras which leave $|m|$ invariant ($|m| \neq 0$):

$$T^{b+1, b+2, b+3} \equiv \sigma^{1, 2, 3} \quad (15.6)$$

acting on the respective subspace $|m| = \ell, \ell - 1, \dots$ for $b = 0, 1, \dots$. This defines generators T^a for $a = 1, \dots, 3N/2$ ($\dots 3(N-1)/2$) for N even (odd), respectively.

The following generators successively extend this to $su(4)$, $su(6)$, \dots until $su(N)$ by adding first the missing off-diagonal and then diagonal generators. The phase conventions are analogous.

(It should be possible to code these conventions for generic spin, but in the current implementation we restrict ourselves to $s \leq 2$, i.e., $N \leq 5$.)

Particle polarization is determined by a particular quantum state which has just helicity information. Physically, this is the spin density matrix ρ , where we do not restrict ourselves to pure states.

We adopt the phase convention for a spin-1/2 particle that

$$\rho = \frac{1}{2}(1 + \vec{\alpha} \cdot \vec{\sigma}) \quad (15.7)$$

with the polarization axis $\vec{\alpha}$. For a particle with arbitrary spin s , and thus $N = 2s + 1$ spin states, we extend the above definition to generalized Bloch form

$$\rho = \frac{1}{N} \left(1 + \sqrt{2N(N-1)} \alpha^a T^a \right) \quad (15.8)$$

where the T^a ($a = 1, \dots, N^2 - 1$) are a basis of $su(N)$ algebra generators. These $N \times N$ matrices are hermitean, traceless, and orthogonal via

$$\text{Tr } T^a T^b = \frac{1}{2} \delta^{ab} \quad (15.9)$$

In the spin-1/2 case, this reduces to the above (standard Bloch) representation since $T^a = \sigma^a/2$, $a = 1, 2, 3$. For the spin-1 case, we could use $T^a = \lambda^a/2$ with the Gell-Mann matrices,

$$\rho = \frac{1}{3} \left(1 + \sqrt{3} \alpha^a \lambda^a \right), \quad (15.10)$$

The normalization is chosen that $|\alpha| \leq 1$ for allowed density matrix, where $|\alpha| = 1$ is a necessary, but not sufficient, condition for a pure state.

```

<bloch_vectors.f90>≡
  <File header>

  module bloch_vectors

    <Use kinds>
    use physics_defs, only: UNKNOWN

    <Standard module head>

    <Bloch vectors: public>

    <Bloch vectors: types>

    interface
    <Bloch vectors: sub interfaces>
    end interface

  end module bloch_vectors

<bloch_vectors_sub.f90>≡
  <File header>

  submodule (bloch_vectors) bloch_vectors_s

    use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
    use su_algebra

    implicit none

  contains

    <Bloch vectors: procedures>

  end submodule bloch_vectors_s

```

15.2.1 Preliminaries

The normalization factor $\sqrt{2N(N-1)}/N$ that enters the Bloch representation.

```

<Bloch vectors: procedures>≡

```

```

function bloch_factor (s) result (f)
  real(default) :: f
  integer, intent(in) :: s
  select case (s)
    case (SCALAR)
      f = 0
    case (SPINOR)
      f = 1
    case (VECTOR)
      f = 2 * sqrt (3._default) / 3
    case (VECTORSPINOR)
      f = 2 * sqrt (6._default) / 4
    case (TENSOR)
      f = 2 * sqrt (10._default) / 5
    case default
      f = 0
  end select
end function bloch_factor

```

15.2.2 The basic polarization type

The basic polarization object holds just the entries of the Bloch vector as an allocatable array.

Bloch is active whenever the coefficient array is allocated. For convenience, we store the spin type ($2s$) and the multiplicity (N) together with the coefficient array (α). We have to allow for the massless case where s is arbitrary > 0 but $N = 2$, and furthermore the chiral massless case where $N = 1$. In the latter case, the array remains deallocated but the chirality is set to ± 1 .

In the Bloch vector implementation, we do not distinguish between particle and antiparticle. If the distinction applies, it must be made by the caller when transforming between density matrix and Bloch vector.

```

<Bloch vectors: public>≡
  public :: bloch_vector_t

<Bloch vectors: types>≡
  type :: bloch_vector_t
    private
    integer :: spin_type = UNKNOWN
    real(default), dimension(:), allocatable :: a
  contains
    <Bloch vectors: bloch vector: TBP>
  end type bloch_vector_t

```

15.2.3 Direct Access

This basic initializer just sets the spin type, leaving the Bloch vector unallocated. The object therefore does not support nonzero polarization.

```

<Bloch vectors: bloch vector: TBP>≡
  procedure :: init_unpolarized => bloch_vector_init_unpolarized

```

```

<Bloch vectors: sub interfaces>+=
  module subroutine bloch_vector_init_unpolarized (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
  end subroutine bloch_vector_init_unpolarized

```

```

<Bloch vectors: procedures>+=
  module subroutine bloch_vector_init_unpolarized (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    pol%spin_type = spin_type
  end subroutine bloch_vector_init_unpolarized

```

The standard initializer allocates the Bloch vector and initializes with zeros, so we can define a polarization later. We make sure that this works only for the supported spin type. Initializing with UNKNOWN spin type resets the Bloch vector to undefined, i.e., unpolarized state.

```

<Bloch vectors: bloch vector: TBP>+=
  generic :: init => bloch_vector_init
  procedure, private :: bloch_vector_init

<Bloch vectors: sub interfaces>+=
  module subroutine bloch_vector_init (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
  end subroutine bloch_vector_init

<Bloch vectors: procedures>+=
  module subroutine bloch_vector_init (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    pol%spin_type = spin_type
    select case (spin_type)
    case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
      allocate (pol%a (algebra_dimension (spin_type)), source = 0._default)
    end select
  end subroutine bloch_vector_init

```

Fill the Bloch vector from an array, no change of normalization. No initialization and no check, we assume that the shapes do match.

```

<Bloch vectors: bloch vector: TBP>+=
  procedure :: from_array => bloch_vector_from_array

<Bloch vectors: sub interfaces>+=
  module subroutine bloch_vector_from_array (pol, a)
    class(bloch_vector_t), intent(inout) :: pol
    real(default), dimension(:), allocatable, intent(in) :: a
  end subroutine bloch_vector_from_array

<Bloch vectors: procedures>+=
  module subroutine bloch_vector_from_array (pol, a)
    class(bloch_vector_t), intent(inout) :: pol
    real(default), dimension(:), allocatable, intent(in) :: a
    pol%a(:) = a
  end subroutine bloch_vector_from_array

```

Transform to an array of reals, i.e., extract the Bloch vector as-is.

```

<Bloch vectors: bloch vector: TBP>+=
  procedure :: to_array => bloch_vector_to_array

<Bloch vectors: sub interfaces>+=
  module subroutine bloch_vector_to_array (pol, a)
    class(bloch_vector_t), intent(in) :: pol
    real(default), dimension(:), allocatable, intent(out) :: a
  end subroutine bloch_vector_to_array

<Bloch vectors: procedures>+=
  module subroutine bloch_vector_to_array (pol, a)
    class(bloch_vector_t), intent(in) :: pol
    real(default), dimension(:), allocatable, intent(out) :: a
    if (pol%is_defined ()) allocate (a (size (pol%a)), source = pol%a)
  end subroutine bloch_vector_to_array

```

15.2.4 Raw I/O

```

<Bloch vectors: bloch vector: TBP>+=
  procedure :: write_raw => bloch_vector_write_raw
  procedure :: read_raw => bloch_vector_read_raw

<Bloch vectors: sub interfaces>+=
  module subroutine bloch_vector_write_raw (pol, u)
    class(bloch_vector_t), intent(in) :: pol
    integer, intent(in) :: u
  end subroutine bloch_vector_write_raw
  module subroutine bloch_vector_read_raw (pol, u, iostat)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: u
    integer, intent(out) :: iostat
  end subroutine bloch_vector_read_raw

<Bloch vectors: procedures>+=
  module subroutine bloch_vector_write_raw (pol, u)
    class(bloch_vector_t), intent(in) :: pol
    integer, intent(in) :: u
    write (u) pol%spin_type
    write (u) allocated (pol%a)
    if (allocated (pol%a)) then
      write (u) pol%a
    end if
  end subroutine bloch_vector_write_raw

  module subroutine bloch_vector_read_raw (pol, u, iostat)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: u
    integer, intent(out) :: iostat
    integer :: s
    logical :: polarized
    read (u, iostat=iostat) s
    read (u, iostat=iostat) polarized
    if (iostat /= 0) return
    if (polarized) then

```



```

        call pol%init (s)
        read (u, iostat=iostat) pol%a
    else
        call pol%init_unpolarized (s)
    end if
end subroutine bloch_vector_read_raw

```

15.2.5 Properties

Re-export algebra functions that depend on the spin type. These functions do not depend on the Bloch vector being allocated.

```

<Bloch vectors: bloch vector: TBP>+≡
    procedure :: get_n_states
    procedure :: get_length
    procedure :: hel_index => bv_helicity_index
    procedure :: hel_value => bv_helicity_value
    procedure :: bloch_factor => bv_factor

<Bloch vectors: sub interfaces>+≡
    module function get_n_states (pol) result (n)
        class(bloch_vector_t), intent(in) :: pol
        integer :: n
    end function get_n_states
    module function get_length (pol) result (n)
        class(bloch_vector_t), intent(in) :: pol
        integer :: n
    end function get_length
    module function bv_helicity_index (pol, h) result (i)
        class(bloch_vector_t), intent(in) :: pol
        integer, intent(in) :: h
        integer :: i
    end function bv_helicity_index
    module function bv_helicity_value (pol, i) result (h)
        class(bloch_vector_t), intent(in) :: pol
        integer, intent(in) :: i
        integer :: h
    end function bv_helicity_value
    module function bv_factor (pol) result (f)
        class(bloch_vector_t), intent(in) :: pol
        real(default) :: f
    end function bv_factor

<Bloch vectors: procedures>+≡
    module function get_n_states (pol) result (n)
        class(bloch_vector_t), intent(in) :: pol
        integer :: n
        n = fundamental_dimension (pol%spin_type)
    end function get_n_states

    module function get_length (pol) result (n)
        class(bloch_vector_t), intent(in) :: pol
        integer :: n
        n = algebra_dimension (pol%spin_type)

```

```

end function get_length

module function bv_helicity_index (pol, h) result (i)
  class(bloch_vector_t), intent(in) :: pol
  integer, intent(in) :: h
  integer :: i
  i = helicity_index (pol%spin_type, h)
end function bv_helicity_index

module function bv_helicity_value (pol, i) result (h)
  class(bloch_vector_t), intent(in) :: pol
  integer, intent(in) :: i
  integer :: h
  h = helicity_value (pol%spin_type, i)
end function bv_helicity_value

module function bv_factor (pol) result (f)
  class(bloch_vector_t), intent(in) :: pol
  real(default) :: f
  f = bloch_factor (pol%spin_type)
end function bv_factor

```

If the Bloch vector object is defined, the spin type is anything else but UNKNOWN. This allows us to provide the representation-specific functions above.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: is_defined => bloch_vector_is_defined

<Bloch vectors: sub interfaces>+≡
  module function bloch_vector_is_defined (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag
  end function bloch_vector_is_defined

<Bloch vectors: procedures>+≡
  module function bloch_vector_is_defined (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag
    flag = pol%spin_type /= UNKNOWN
  end function bloch_vector_is_defined

```

If the Bloch vector object is (technically) polarized, it is defined, and the vector coefficient array has been allocated. However, the vector value may be zero.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: is_polarized => bloch_vector_is_polarized

<Bloch vectors: sub interfaces>+≡
  module function bloch_vector_is_polarized (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag
  end function bloch_vector_is_polarized

<Bloch vectors: procedures>+≡
  module function bloch_vector_is_polarized (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag

```

```

        flag = allocated (pol%a)
    end function bloch_vector_is_polarized

```

Return true if the polarization is diagonal, i.e., all entries in the density matrix are on the diagonal. This is equivalent to requiring that only Cartan generator coefficients are nonzero in the Bloch vector.

```

<Bloch vectors: bloch vector: TBP>+=
    procedure :: is_diagonal => bloch_vector_is_diagonal

<Bloch vectors: sub interfaces>+=
    module function bloch_vector_is_diagonal (pol) result (diagonal)
        class(bloch_vector_t), intent(in) :: pol
        logical :: diagonal
    end function bloch_vector_is_diagonal

<Bloch vectors: procedures>+=
    module function bloch_vector_is_diagonal (pol) result (diagonal)
        class(bloch_vector_t), intent(in) :: pol
        logical :: diagonal
        integer :: s, i
        s = pol%spin_type
        diagonal = .true.
        if (pol%is_polarized ()) then
            do i = 1, size (pol%a)
                if (is_cartan_generator (s, i)) cycle
                if (pol%a(i) /= 0) then
                    diagonal = .false.
                end if
            end do
        end if
    end function bloch_vector_is_diagonal

```

Return the Euclidean norm of the Bloch vector. This is equal to the Killing form value of the corresponding algebra generator. We assume that the polarization object has been initialized.

For a pure state, the norm is unity. All other allowed states have a norm less than unity. (For $s \geq 1$, this is a necessary but not sufficient condition.)

```

<Bloch vectors: bloch vector: TBP>+=
    procedure :: get_norm => bloch_vector_get_norm

<Bloch vectors: sub interfaces>+=
    module function bloch_vector_get_norm (pol) result (norm)
        class(bloch_vector_t), intent(in) :: pol
        real(default) :: norm
    end function bloch_vector_get_norm

<Bloch vectors: procedures>+=
    module function bloch_vector_get_norm (pol) result (norm)
        class(bloch_vector_t), intent(in) :: pol
        real(default) :: norm
        select case (pol%spin_type)
            case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
                norm = sqrt (dot_product (pol%a, pol%a))

```

```

        case default
            norm = 1
        end select
    end function bloch_vector_get_norm

```

15.2.6 Diagonal density matrix

This initializer takes a diagonal density matrix, represented by a real-valued array. We assume that the trace is unity, and that the array has the correct shape for the given `spin_type`.

The `bloch_factor` renormalization is necessary such that a pure state maps to a Bloch vector with unit norm.

```

<Bloch vectors: bloch vector: TBP>+≡
    generic :: init => bloch_vector_init_diagonal
    procedure, private :: bloch_vector_init_diagonal

<Bloch vectors: sub interfaces>+≡
    module subroutine bloch_vector_init_diagonal (pol, spin_type, rd)
        class(bloch_vector_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        real(default), dimension(:), intent(in) :: rd
    end subroutine bloch_vector_init_diagonal

<Bloch vectors: procedures>+≡
    module subroutine bloch_vector_init_diagonal (pol, spin_type, rd)
        class(bloch_vector_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        real(default), dimension(:), intent(in) :: rd
        call pol%init (spin_type)
        call pol%set (rd)
    end subroutine bloch_vector_init_diagonal

```

Set a Bloch vector, given a diagonal density matrix as a real array. The Bloch vector must be initialized with correct characteristics.

```

<Bloch vectors: bloch vector: TBP>+≡
    generic :: set => bloch_vector_set_diagonal
    procedure, private :: bloch_vector_set_diagonal

<Bloch vectors: sub interfaces>+≡
    module subroutine bloch_vector_set_diagonal (pol, rd)
        class(bloch_vector_t), intent(inout) :: pol
        real(default), dimension(:), intent(in) :: rd
    end subroutine bloch_vector_set_diagonal

<Bloch vectors: procedures>+≡
    module subroutine bloch_vector_set_diagonal (pol, rd)
        class(bloch_vector_t), intent(inout) :: pol
        real(default), dimension(:), intent(in) :: rd
        integer :: s
        s = pol%spin_type
        select case (s)
        case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
            pol%a(:) = cartan_coeff (s, rd) / bloch_factor (s)

```

```

end select
end subroutine bloch_vector_set_diagonal

```

15.2.7 Massless density matrix

This is a specific variant which initializes an equipartition for the maximum helicity, corresponding to an unpolarized massless particle.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: init_max_weight => bloch_vector_init_max_weight

<Bloch vectors: sub interfaces>+≡
  module subroutine bloch_vector_init_max_weight (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
  end subroutine bloch_vector_init_max_weight

<Bloch vectors: procedures>+≡
  module subroutine bloch_vector_init_max_weight (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    call pol%init (spin_type)
    select case (spin_type)
    case (VECTOR)
      call pol%set ([0.5_default, 0._default, 0.5_default])
    case (VECTORSPINOR)
      call pol%set ([0.5_default, 0._default, 0._default, 0.5_default])
    case (TENSOR)
      call pol%set ([0.5_default, 0._default, 0._default, 0._default, 0.5_default])
    end select
  end subroutine bloch_vector_init_max_weight

```

Initialize the maximum-weight submatrix with a three-component Bloch vector. This is not as trivial as it seems because we need the above initialization for the generalized Bloch in order to remove the lower weights from the density matrix.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: init_vector => bloch_vector_init_vector
  procedure :: to_vector => bloch_vector_to_vector

<Bloch vectors: sub interfaces>+≡
  module subroutine bloch_vector_init_vector (pol, s, a)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: s
    real(default), dimension(3), intent(in) :: a
  end subroutine bloch_vector_init_vector
  module subroutine bloch_vector_to_vector (pol, a)
    class(bloch_vector_t), intent(in) :: pol
    real(default), dimension(3), intent(out) :: a
  end subroutine bloch_vector_to_vector

<Bloch vectors: procedures>+≡
  module subroutine bloch_vector_init_vector (pol, s, a)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: s

```

```

    real(default), dimension(3), intent(in) :: a
    call pol%init_max_weight (s)
    select case (s)
    case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
        pol%a(1:3) = a / bloch_factor (s)
    end select
end subroutine bloch_vector_init_vector

module subroutine bloch_vector_to_vector (pol, a)
    class(bloch_vector_t), intent(in) :: pol
    real(default), dimension(3), intent(out) :: a
    integer :: s
    s = pol%spin_type
    select case (s)
    case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
        a = pol%a(1:3) * bloch_factor (s)
    case default
        a = 0
    end select
end subroutine bloch_vector_to_vector

```

15.2.8 Arbitrary density matrix

Initialize the Bloch vector from a density matrix. We assume that the density is valid. In particular, the shape should match, the matrix should be hermitian, and the trace should be unity.

We first fill the diagonal, then add the off-diagonal parts.

```

<Bloch vectors: bloch vector: TBP>+=
    generic :: init => bloch_vector_init_matrix
    procedure, private :: bloch_vector_init_matrix

<Bloch vectors: sub interfaces>+=
    module subroutine bloch_vector_init_matrix (pol, spin_type, r)
        class(bloch_vector_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        complex(default), dimension(:,:), intent(in) :: r
    end subroutine bloch_vector_init_matrix

<Bloch vectors: procedures>+=
    module subroutine bloch_vector_init_matrix (pol, spin_type, r)
        class(bloch_vector_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        complex(default), dimension(:,:), intent(in) :: r
        select case (spin_type)
        case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
            call pol%init (spin_type)
            call pol%set (r)
        case default
            call pol%init (UNKNOWN)
        end select
    end subroutine bloch_vector_init_matrix

```

Set a Bloch vector, given an arbitrary density matrix as a real array. The Bloch vector must be initialized with correct characteristics.

```

(Bloch vectors: bloch vector: TBP)+≡
    generic :: set => bloch_vector_set_matrix
    procedure, private :: bloch_vector_set_matrix

(Bloch vectors: sub interfaces)+≡
    module subroutine bloch_vector_set_matrix (pol, r)
        class(bloch_vector_t), intent(inout) :: pol
        complex(default), dimension(:,:), intent(in) :: r
    end subroutine bloch_vector_set_matrix

(Bloch vectors: procedures)+≡
    module subroutine bloch_vector_set_matrix (pol, r)
        class(bloch_vector_t), intent(inout) :: pol
        complex(default), dimension(:,:), intent(in) :: r
        real(default), dimension(:), allocatable :: rd
        integer :: s, d, i, j, h1, h2, ir, ii
        s = pol%spin_type
        select case (s)
        case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
            d = fundamental_dimension (s)
            allocate (rd (d))
            do i = 1, d
                rd(i) = r(i,i)
            end do
            call pol%set (rd)
            do i = 1, d
                h1 = helicity_value (s, i)
                do j = i+1, d
                    h2 = helicity_value (s, j)
                    ir = root_index (s, h1, h2, .true.)
                    ii = root_index (s, h1, h2, .false.)
                    pol%a(ir) = real (r(j,i) + r(i,j)) / bloch_factor (s)
                    pol%a(ii) = aimag (r(j,i) - r(i,j)) / bloch_factor (s)
                end do
            end do
        end select
    end subroutine bloch_vector_set_matrix

```

Allocate and fill the density matrix *r* (with the index ordering as defined in *su_algebra*) that corresponds to a given Bloch vector.

If the optional *only_max_weight* is set, the resulting matrix has entries only for $\pm h_{\max}$, as appropriate for a massless particle (for $\text{spin} \geq 1$). Note that we always add the unit matrix, as this is part of the Bloch-vector definition.

```

(Bloch vectors: bloch vector: TBP)+≡
    procedure :: to_matrix => bloch_vector_to_matrix

(Bloch vectors: sub interfaces)+≡
    module subroutine bloch_vector_to_matrix (pol, r, only_max_weight)
        class(bloch_vector_t), intent(in) :: pol
        complex(default), dimension(:,:), intent(out), allocatable :: r
        logical, intent(in), optional :: only_max_weight
    end subroutine bloch_vector_to_matrix

```

(Bloch vectors: procedures)+≡

```

module subroutine bloch_vector_to_matrix (pol, r, only_max_weight)
  class(bloch_vector_t), intent(in) :: pol
  complex(default), dimension(:, :), intent(out), allocatable :: r
  logical, intent(in), optional :: only_max_weight
  integer :: d, s, h0, ng, ai, h, h1, h2, i, j
  logical :: is_real, only_max
  complex(default) :: val
  if (.not. pol%is_polarized ()) return
  s = pol%spin_type
  only_max = .false.
  select case (s)
  case (VECTOR, VECTORSPINOR, TENSOR)
    if (present (only_max_weight)) only_max = only_max_weight
  end select
  if (only_max) then
    ng = 2
    h0 = helicity_value (s, 1)
  else
    ng = algebra_dimension (s)
    h0 = 0
  end if
  d = fundamental_dimension (s)
  allocate (r (d, d), source = (0._default, 0._default))
  do i = 1, d
    h = helicity_value (s, i)
    if (abs (h) < h0) cycle
    r(i,i) = 1._default / d &
      + dot_product (cartan_element (s, h), pol%a) * bloch_factor (s)
  end do
  do ai = 1, ng
    if (is_cartan_generator (s, ai)) cycle
    call root_helicity (s, ai, h1, h2, is_real)
    i = helicity_index (s, h1)
    j = helicity_index (s, h2)
    if (is_real) then
      val = cmplx (pol%a(ai) / 2 * bloch_factor (s), 0._default, &
        kind=default)
      r(i,j) = r(i,j) + val
      r(j,i) = r(j,i) + val
    else
      val = cmplx (0._default, pol%a(ai) / 2 * bloch_factor (s), &
        kind=default)
      r(i,j) = r(i,j) - val
      r(j,i) = r(j,i) + val
    end if
  end do
end subroutine bloch_vector_to_matrix

```

15.2.9 Unit tests

Test module, followed by the corresponding implementation module.


```

<bloch_vectors_ut.f90>≡
  <File header>

  module bloch_vectors_ut
    use unit_tests
    use bloch_vectors_uti

    <Standard module head>

    <Bloch vectors: public test>

    contains

    <Bloch vectors: test driver>

  end module bloch_vectors_ut
<bloch_vectors_uti.f90>≡
  <File header>

  module bloch_vectors_uti

    <Use kinds>
    use physics_defs, only: UNKNOWN, SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
    use su_algebra, only: algebra_dimension, fundamental_dimension, helicity_value

    use bloch_vectors

    <Standard module head>

    <Bloch vectors: test declarations>

    contains

    <Bloch vectors: tests>

  end module bloch_vectors_uti
API: driver for the unit tests below.
<Bloch vectors: public test>≡
  public :: bloch_vectors_test
<Bloch vectors: test driver>≡
  subroutine bloch_vectors_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Bloch vectors: execute tests>
  end subroutine bloch_vectors_test

```

Initialization

Initialize the Bloch vector for any spin type. First as unpolarized (no array), then as polarized but with zero polarization.

```

<Bloch vectors: execute tests>≡

```

```

call test (bloch_vectors_1, "bloch_vectors_1", &
  "initialization", &
  u, results)
<Bloch vectors: test declarations>≡
public :: bloch_vectors_1
<Bloch vectors: tests>≡
subroutine bloch_vectors_1 (u)
  integer, intent(in) :: u

  write (u, "(A)")  "* Test output: bloch_vectors_1"
  write (u, "(A)")  "* Purpose: test Bloch-vector &
    &polarization implementation"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization (unpolarized)"

  write (u, "(A)")
  write (u, "(A)")  "* unknown"
  call bloch_init (UNKNOWN)

  write (u, "(A)")
  write (u, "(A)")  "* s = 0"
  call bloch_init (SCALAR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 1/2"
  call bloch_init (SPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 1"
  call bloch_init (VECTOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 3/2"
  call bloch_init (VECTORSPINOR)

  write (u, "(A)")
  write (u, "(A)")  "* s = 2"
  call bloch_init (TENSOR)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: bloch_vectors_1"

contains

subroutine bloch_init (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(:), allocatable :: a
  integer :: i
  write (u, *)
  write (u, "(1X,L1,L1)", advance="no") &
    pol%is_defined (), pol%is_polarized ()

```

```

    call pol%init_unpolarized (s)
    write (u, "(1X,L1,L1)", advance="no") &
        pol%is_defined (), pol%is_polarized ()
    call pol%init (s)
    write (u, "(1X,L1,L1)", advance="no") &
        pol%is_defined (), pol%is_polarized ()
    write (u, *)
    call pol%to_array (a)
    if (allocated (a)) then
        write (u, "(*(F7.4))") a
        a(:) = [(real (mod (i, 10), kind=default), i = 1, size (a))]
        call pol%from_array (a)
        call pol%to_array (a)
        write (u, "(*(F7.4))") a
    else
        write (u, *)
        write (u, *)
    end if
end subroutine bloch_init

end subroutine bloch_vectors_1

```

Pure state (diagonal)

Initialize the Bloch vector with a pure state of definite helicity and check the normalization.

```

<Bloch vectors: execute tests>+≡
    call test (bloch_vectors_2, "bloch_vectors_2", &
        "pure state (diagonal)", &
        u, results)

<Bloch vectors: test declarations>+≡
    public :: bloch_vectors_2

<Bloch vectors: tests>+≡
    subroutine bloch_vectors_2 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_2"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization (polarized, diagonal): &
            &display vector and norm"
        write (u, "(A)")  "* transform back"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_diagonal (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
    end subroutine

```

```

call bloch_diagonal (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_diagonal (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_diagonal (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_diagonal (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_2"

contains

subroutine bloch_diagonal (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(:), allocatable :: a
  real(default), dimension(:), allocatable :: rd
  complex(default), dimension(:,:), allocatable :: r
  integer :: i, j, d
  real(default) :: rj
  real, parameter :: tolerance = 1.E-14_default
  d = fundamental_dimension (s)
  do i = 1, d
    allocate (rd (d), source = 0._default)
    rd(i) = 1
    call pol%init (s, rd)
    call pol%to_array (a)
    write (u, *)
    write (u, "(A,1X,I2)")  "h:", helicity_value (s, i)
    write (u, 1, advance="no") a
    write (u, "(1X,L1)")  pol%is_diagonal ()
    write (u, 1)  pol%get_norm ()
    call pol%to_matrix (r)
    do j = 1, d
      rj = real (r(j,j))
      if (abs (rj) < tolerance)  rj = 0
      write (u, 1, advance="no")  rj
    end do
    write (u, "(1X,L1)")  matrix_is_diagonal (r)
    deallocate (a, rd, r)
  end do
1  format (99(1X,F7.4,:))
end subroutine bloch_diagonal

function matrix_is_diagonal (r) result (diagonal)
  complex(default), dimension(:,:), intent(in) :: r
  logical :: diagonal

```

```

integer :: i, j
diagonal = .true.
do j = 1, size (r, 2)
  do i = 1, size (r, 1)
    if (i == j) cycle
    if (r(i,j) /= 0) then
      diagonal = .false.
      return
    end if
  end do
end do
end function matrix_is_diagonal

end subroutine bloch_vectors_2

```

Pure state (arbitrary)

Initialize the Bloch vector with an arbitrarily chosen pure state, check the normalization, and transform back to the density matrix.

```

<Bloch vectors: execute tests>+≡
  call test (bloch_vectors_3, "bloch_vectors_3", &
    "pure state (arbitrary)", &
    u, results)

<Bloch vectors: test declarations>+≡
  public :: bloch_vectors_3

<Bloch vectors: tests>+≡
  subroutine bloch_vectors_3 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: bloch_vectors_3"
    write (u, "(A)")  "* Purpose: test Bloch-vector &
      &polarization implementation"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization (pure polarized, arbitrary):"
    write (u, "(A)")  "* input matrix, transform, display norm, transform back"

    write (u, "(A)")
    write (u, "(A)")  "* s = 0"
    call bloch_arbitrary (SCALAR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1/2"
    call bloch_arbitrary (SPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1"
    call bloch_arbitrary (VECTOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 3/2"

```

```

call bloch_arbitrary (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_arbitrary (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_3"

contains

subroutine bloch_arbitrary (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  complex(default), dimension(:,:), allocatable :: r
  integer :: d
  d = fundamental_dimension (s)
  write (u, *)
  call init_matrix (d, r)
  where (abs (aimag (r)) < 1.e-14_default) &
    r = cmplx (real(r, kind=default), 0._default, kind=default)
  call write_matrix (d, r)
  call pol%init (s, r)
  write (u, *)
  write (u, 2)  pol%get_norm (), pol%is_diagonal ()
  write (u, *)
  call pol%to_matrix (r)
  call write_matrix (d, r)
2  format (1X,F7.4,1X,L1)
end subroutine bloch_arbitrary

subroutine init_matrix (d, r)
  integer, intent(in) :: d
  complex(default), dimension(:,:), allocatable, intent(out) :: r
  complex(default), dimension(:), allocatable :: a
  real(default) :: norm
  integer :: i, j
  allocate (a (d))
  norm = 0
  do i = 1, d
    a(i) = cmplx (2*i-1, 2*i, kind=default)
    norm = norm + conjg (a(i)) * a(i)
  end do
  a = a / sqrt (norm)
  allocate (r (d,d))
  do i = 1, d
    do j = 1, d
      r(i,j) = conjg (a(i)) * a(j)
    end do
  end do
end subroutine init_matrix

subroutine write_matrix (d, r)
  integer, intent(in) :: d

```

```

        complex(default), dimension(:,:), intent(in) :: r
        integer :: i, j
        do i = 1, d
            do j = 1, d
                write (u, 1, advance="no") r(i,j)
            end do
            write (u, *)
        end do
1      format (99(1X,'(',F7.4,',',F7.4,')',:))
      end subroutine write_matrix

      end subroutine bloch_vectors_3

```

Raw I/O

Check correct input/output in raw format.

```

<Bloch vectors: execute tests>+≡
      call test (bloch_vectors_4, "bloch_vectors_4", &
        "raw I/O", &
        u, results)

<Bloch vectors: test declarations>+≡
      public :: bloch_vectors_4

<Bloch vectors: tests>+≡
      subroutine bloch_vectors_4 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_4"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
          &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Raw I/O"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_io (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call bloch_io (SPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1"
        call bloch_io (VECTOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 3/2"
        call bloch_io (VECTORSPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 2"
        call bloch_io (TENSOR)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_4"

contains

subroutine bloch_io (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(:), allocatable :: a
  integer :: n, i, utmp, iostat
  n = algebra_dimension (s)
  allocate (a (n))
  a(:) = [(real (mod (i, 10), kind=default), i = 1, size (a))]
  write (u, *)
  write (u, "(*(F7.4))") a
  call pol%init (s)
  call pol%from_array (a)
  open (newunit = utmp, status = "scratch", action = "readwrite", &
    form = "unformatted")
  call pol%write_raw (utmp)
  rewind (utmp)
  call pol%read_raw (utmp, iostat=iostat)
  close (utmp)
  call pol%to_array (a)
  write (u, "(*(F7.4))") a
end subroutine bloch_io

end subroutine bloch_vectors_4

```

Convenience Methods

Check some further TBP that are called by the `polarizations` module.

```

<Bloch vectors: execute tests>+≡
  call test (bloch_vectors_5, "bloch_vectors_5", &
    "massless state (unpolarized)", &
    u, results)

<Bloch vectors: test declarations>+≡
  public :: bloch_vectors_5

<Bloch vectors: tests>+≡
  subroutine bloch_vectors_5 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: bloch_vectors_5"
    write (u, "(A)")  "* Purpose: test Bloch-vector &
      &polarization implementation"
    write (u, "(A)")

    write (u, "(A)")  "* Massless states: equipartition"

    write (u, "(A)")
    write (u, "(A)")  "* s = 0"
  end subroutine bloch_vectors_5

```



```

call bloch_massless_unpol (SCALAR)

write (u, "(A)")
write (u, "(A)")  "* s = 1/2"
call bloch_massless_unpol (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_massless_unpol (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_massless_unpol (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_massless_unpol (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_5"

contains

subroutine bloch_massless_unpol (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  complex(default), dimension(:,:), allocatable :: r
  real(default), dimension(:), allocatable :: a
  integer :: d
  d = fundamental_dimension (s)
  call pol%init_max_weight (s)
  call pol%to_matrix (r, only_max_weight = .false.)
  write (u, *)
  where (abs (r) < 1.e-14_default) r = 0
  call write_matrix (d, r)
  call pol%to_matrix (r, only_max_weight = .true.)
  write (u, *)
  call write_matrix (d, r)
end subroutine bloch_massless_unpol

subroutine write_matrix (d, r)
  integer, intent(in) :: d
  complex(default), dimension(:,:), intent(in) :: r
  integer :: i, j
  do i = 1, d
    do j = 1, d
      write (u, 1, advance="no") r(i,j)
    end do
    write (u, *)
  end do
1  format (99(1X,'(',F7.4,',',F7.4,')',:))
end subroutine write_matrix

end subroutine bloch_vectors_5

```

Massless state (arbitrary)

Initialize the Bloch vector with an arbitrarily chosen pure state which consists only of highest-weight components. Transform back to the density matrix.

```
<Bloch vectors: execute tests>+≡
  call test (bloch_vectors_6, "bloch_vectors_6", &
    "massless state (arbitrary)", &
    u, results)

<Bloch vectors: test declarations>+≡
  public :: bloch_vectors_6

<Bloch vectors: tests>+≡
  subroutine bloch_vectors_6 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: bloch_vectors_6"
    write (u, "(A)")  "* Purpose: test Bloch-vector &
      &polarization implementation"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization (pure polarized massless, arbitrary):"
    write (u, "(A)")  "* input matrix, transform, display norm, transform back"

    write (u, "(A)")
    write (u, "(A)")  "* s = 0"
    call bloch_massless (SCALAR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1/2"
    call bloch_massless (SPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1"
    call bloch_massless (VECTOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 3/2"
    call bloch_massless (VECTORSPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 2"
    call bloch_massless (TENSOR)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: bloch_vectors_6"

contains

    subroutine bloch_massless (s)
      integer, intent(in) :: s
      type(bloch_vector_t) :: pol
```

```

complex(default), dimension(:,:), allocatable :: r
integer :: d
d = fundamental_dimension (s)
write (u, *)
call init_matrix (d, r)
where (abs (aimag (r)) < 1.e-14_default) &
    r = cmplx (real(r, kind=default), 0._default, kind=default)
call write_matrix (d, r)
call pol%init (s, r)
write (u, *)
write (u, 2) pol%get_norm (), pol%is_diagonal ()
write (u, *)
call pol%to_matrix (r, only_max_weight = .true.)
call write_matrix (d, r)
2   format (1X,F7.4,1X,L1)
end subroutine bloch_massless

subroutine init_matrix (d, r)
integer, intent(in) :: d
complex(default), dimension(:,:), allocatable, intent(out) :: r
complex(default), dimension(:), allocatable :: a
real(default) :: norm
integer :: i, j
allocate (a (d), source = (0._default, 0._default))
norm = 0
do i = 1, d, max (d-1, 1)
    a(i) = cmplx (2*i-1, 2*i, kind=default)
    norm = norm + conjg (a(i)) * a(i)
end do
a = a / sqrt (norm)
allocate (r (d,d), source = (0._default, 0._default))
do i = 1, d, max (d-1, 1)
    do j = 1, d, max (d-1, 1)
        r(i,j) = conjg (a(i)) * a(j)
    end do
end do
end subroutine init_matrix

subroutine write_matrix (d, r)
integer, intent(in) :: d
complex(default), dimension(:,:), intent(in) :: r
integer :: i, j
do i = 1, d
    do j = 1, d
        write (u, 1, advance="no") r(i,j)
    end do
    write (u, *)
end do
1   format (99(1X,'(',F7.4,',',F7.4,')',:))
end subroutine write_matrix

end subroutine bloch_vectors_6

```

Massless state (Bloch vector)

Initialize the (generalized) Bloch vector with an ordinary three-component Bloch vector that applies to the highest-weight part only.

```
(Bloch vectors: execute tests)+≡
    call test (bloch_vectors_7, "bloch_vectors_7", &
        "massless state (vector)", &
        u, results)

(Bloch vectors: test declarations)+≡
    public :: bloch_vectors_7

(Bloch vectors: tests)+≡
    subroutine bloch_vectors_7 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_7"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization &
            &(pure polarized massless, arbitrary Bloch vector):"
        write (u, "(A)")  "* input vector, transform, display norm, &
            &transform back"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_massless_vector (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call bloch_massless_vector (SPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1"
        call bloch_massless_vector (VECTOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 3/2"
        call bloch_massless_vector (VECTORSPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 2"
        call bloch_massless_vector (TENSOR)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: bloch_vectors_7"

contains

    subroutine bloch_massless_vector (s)
        integer, intent(in) :: s
        type(bloch_vector_t) :: pol
        real(default), dimension(3) :: a
```

```

        complex(default), dimension(:,:), allocatable :: r
        write (u, *)
        a = [1._default, 2._default, 4._default]
        a = a / sqrt (sum (a ** 2))
        write (u, 2) a
        call pol%init_vector (s, a)
        write (u, 2) pol%get_norm ()
        call pol%to_vector (a)
        write (u, 2) a
        call pol%to_matrix (r, only_max_weight = .false.)
        write (u, *)
        where (abs (r) < 1.e-14_default) r = 0
        call write_matrix (r)
        call pol%to_matrix (r, only_max_weight = .true.)
        write (u, *)
        call write_matrix (r)
2      format (99(1X,F7.4,:))
end subroutine bloch_massless_vector

subroutine write_matrix (r)
    complex(default), dimension(:,:), intent(in) :: r
    integer :: i, j
    do i = 1, size (r, 1)
        do j = 1, size (r, 2)
            write (u, 1, advance="no") r(i,j)
        end do
        write (u, *)
    end do
1    format (99(1X,'(,F7.4,',',F7.4,')',:))
end subroutine write_matrix

end subroutine bloch_vectors_7

```

15.3 Polarization

Using generalized Bloch vectors and the $su(N)$ algebra (see above) for the internal representation, we can define various modes of polarization. For spin-1/2, and analogously for massless spin- s particles, we introduce

1. Trivial polarization: $\vec{\alpha} = 0$. [This is unpolarized, but distinct from the particular undefined polarization matrix which has the same meaning.]
2. Circular polarization: $\vec{\alpha}$ points in $\pm z$ direction.
3. Transversal polarization: $\vec{\alpha}$ points orthogonal to the z direction, with a phase ϕ that is 0 for the x axis, and $\pi/2 = 90^\circ$ for the y axis. For antiparticles, the phase switches sign, corresponding to complex conjugation.
4. Axis polarization, where we explicitly give $\vec{\alpha}$.

For higher spin, we retain this definition, but apply it to the two components with maximum and minimum weight. In effect, we concentrate on the first three entries in the α^a array. For massless particles, this is sufficient. For massive particles, we then add the possibilities:

5. Longitudinal polarization: Only the 0-component is set. This is possible only for bosons.
6. Diagonal polarization: Explicitly specify all components in the helicity basis. The $su(N)$ representation consists of diagonal generators only, the Cartan subalgebra.

Obviously, this does not exhaust the possible density matrices for higher spin, but it should cover practical applications.

`<polarizations.f90>≡`
<File header>

`module polarizations`

<Use kinds>

`use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR`
`use flavors`
`use quantum_numbers`
`use state_matrices`
`use bloch_vectors`

<Standard module head>

<Polarizations: public>

<Polarizations: types>

<Polarizations: interfaces>

`interface`

<Polarizations: sub interfaces>

`end interface`

`end module polarizations`

```

<polarizations_sub.f90>≡
  <File header>

  submodule (polarizations) polarizations_s

    use io_units
    use format_defs, only: FMT_19
    use diagnostics
    use helicities

    implicit none

  contains

  <Polarizations: procedures>

end submodule polarizations_s

```

15.3.1 The polarization type

Polarization is active whenever the coefficient array is allocated. For convenience, we store the spin type ($2s$) and the multiplicity (N) together with the coefficient array (α). We have to allow for the massless case where s is arbitrary > 0 but $N = 2$, and furthermore the chiral massless case where $N = 1$. In the latter case, the array remains deallocated but the chirality is set to ± 1 .

There is a convention that an antiparticle transforms according to the complex conjugate representation. We apply this only when transforming from/to polarization defined by a three-vector. For antiparticles, the two-component flips sign in that case. When transforming from/to a state matrix or `pmatrix` representation, we do not apply this sign flip.

```

<Polarizations: public>≡
  public :: polarization_t

<Polarizations: types>≡
  type :: polarization_t
    private
    integer :: spin_type = SCALAR
    integer :: multiplicity = 1
    integer :: chirality = 0
    logical :: anti = .false.
    type(bloch_vector_t) :: bv
  contains
  <Polarizations: polarization: TBP>
end type polarization_t

```

15.3.2 Basic initializer and finalizer

We need the particle flavor for determining the allowed helicity values. The Bloch vector is left undefined, so this initializer (in two versions) creates an unpolarized particle. Exception: a chiral particle is always polarized with definite helicity, it doesn't need a Bloch vector.

This is private.

```

(Polarizations: polarization: TBP)≡
  generic, private :: init => polarization_init, polarization_init_flv
  procedure, private :: polarization_init
  procedure, private :: polarization_init_flv

(Polarizations: sub interfaces)≡
  module subroutine polarization_init (pol, spin_type, multiplicity, &
    anti, left_handed, right_handed)
    class(polarization_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    integer, intent(in) :: multiplicity
    logical, intent(in) :: anti
    logical, intent(in) :: left_handed
    logical, intent(in) :: right_handed
  end subroutine polarization_init
  module subroutine polarization_init_flv (pol, flv)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
  end subroutine polarization_init_flv

(Polarizations: procedures)≡
  module subroutine polarization_init (pol, spin_type, multiplicity, &
    anti, left_handed, right_handed)
    class(polarization_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    integer, intent(in) :: multiplicity
    logical, intent(in) :: anti
    logical, intent(in) :: left_handed
    logical, intent(in) :: right_handed
    pol%spin_type = spin_type
    pol%multiplicity = multiplicity
    pol%anti = anti
    select case (pol%multiplicity)
    case (1)
      if (left_handed) then
        pol%chirality = -1
      else if (right_handed) then
        pol%chirality = 1
      end if
    end select
    select case (pol%chirality)
    case (0)
      call pol%bv%init_unpolarized (spin_type)
    end select
  end subroutine polarization_init

  module subroutine polarization_init_flv (pol, flv)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    call pol%init ( &
      spin_type = flv%get_spin_type (), &
      multiplicity = flv%get_multiplicity (), &
      anti = flv%is_antiparticle (), &
      left_handed = flv%is_left_handed (), &

```



```

        right_handed = flv%is_right_handed ()
    end subroutine polarization_init_flv

```

Generic polarization: as before, but create a polarized particle (Bloch vector defined) with initial polarization zero.

```

(Polarizations: polarization: TBP)+≡
    generic :: init_generic => &
        polarization_init_generic, &
        polarization_init_generic_flv
    procedure, private :: polarization_init_generic
    procedure, private :: polarization_init_generic_flv

(Polarizations: sub interfaces)+≡
    module subroutine polarization_init_generic (pol, spin_type, multiplicity, &
        anti, left_handed, right_handed)
        class(polarization_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        integer, intent(in) :: multiplicity
        logical, intent(in) :: anti
        logical, intent(in) :: left_handed
        logical, intent(in) :: right_handed
    end subroutine polarization_init_generic
    module subroutine polarization_init_generic_flv (pol, flv)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
    end subroutine polarization_init_generic_flv

(Polarizations: procedures)+≡
    module subroutine polarization_init_generic (pol, spin_type, multiplicity, &
        anti, left_handed, right_handed)
        class(polarization_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        integer, intent(in) :: multiplicity
        logical, intent(in) :: anti
        logical, intent(in) :: left_handed
        logical, intent(in) :: right_handed
        call pol%init (spin_type, multiplicity, &
            anti, left_handed, right_handed)
        select case (pol%chirality)
        case (0)
            if (pol%multiplicity == pol%bv%get_n_states ()) then
                call pol%bv%init (spin_type)
            else
                call pol%bv%init_max_weight (spin_type)
            end if
        end select
    end subroutine polarization_init_generic

    module subroutine polarization_init_generic_flv (pol, flv)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        call pol%init_generic ( &
            spin_type = flv%get_spin_type (), &
            multiplicity = flv%get_multiplicity (), &
            anti = flv%is_antiparticle (), &

```

```

        left_handed = flv%is_left_handed (), &
        right_handed = flv%is_right_handed ()
    end subroutine polarization_init_generic_flv

```

A finalizer is no longer necessary.

15.3.3 I/O

The default setting produces a tabular output of the polarization vector entries. Optionally, we can create a state matrix and write its contents, emulating the obsolete original implementation.

If `all_states` is true (default), we generate all helicity combinations regardless of the matrix-element value. Otherwise, skip helicities with zero entry, or absolute value less than `tolerance`, if also given.

```

(Polarizations: polarization: TBP)+≡
    procedure :: write => polarization_write

(Polarizations: sub interfaces)+≡
    module subroutine polarization_write (pol, unit, state_matrix, all_states, tolerance)
        class(polarization_t), intent(in) :: pol
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: state_matrix, all_states
        real(default), intent(in), optional :: tolerance
    end subroutine polarization_write

(Polarizations: procedures)+≡
    module subroutine polarization_write (pol, unit, state_matrix, all_states, tolerance)
        class(polarization_t), intent(in) :: pol
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: state_matrix, all_states
        real(default), intent(in), optional :: tolerance
        logical :: state_m
        type(state_matrix_t) :: state
        real(default), dimension(:), allocatable :: a
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        state_m = .false.; if (present (state_matrix)) state_m = state_matrix
        if (pol%anti) then
            write (u, "(1x,A,I1,A,I1,A,L1,A)") &
                "Polarization: [spin_type = ", pol%spin_type, &
                ", mult = ", pol%multiplicity, ", anti = ", pol%anti, "]"
        else
            write (u, "(1x,A,I1,A,I1,A)") &
                "Polarization: [spin_type = ", pol%spin_type, &
                ", mult = ", pol%multiplicity, "]"
        end if
        if (state_m) then
            call pol%to_state (state, all_states, tolerance)
            call state%write (unit=unit)
            call state%final ()
        else if (pol%chirality == 1) then
            write (u, "(1x,A)") "chirality = +"
        else if (pol%chirality == -1) then
            write (u, "(1x,A)") "chirality = -"
        end if
    end subroutine polarization_write

```

```

else if (pol%bv%is_polarized ()) then
  call pol%bv%to_array (a)
  do i = 1, size (a)
    write (u, "(1x,I2,':',1x,F10.7)" i, a(i)
  end do
else
  write (u, "(1x,A)" "[unpolarized]"
end if
end subroutine polarization_write

```

Binary I/O.

(Polarizations: polarization: TBP)+≡

```

procedure :: write_raw => polarization_write_raw
procedure :: read_raw => polarization_read_raw

```

(Polarizations: sub interfaces)+≡

```

module subroutine polarization_write_raw (pol, u)
  class(polarization_t), intent(in) :: pol
  integer, intent(in) :: u
end subroutine polarization_write_raw
module subroutine polarization_read_raw (pol, u, iostat)
  class(polarization_t), intent(out) :: pol
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
end subroutine polarization_read_raw

```

(Polarizations: procedures)+≡

```

module subroutine polarization_write_raw (pol, u)
  class(polarization_t), intent(in) :: pol
  integer, intent(in) :: u
  write (u) pol%spin_type
  write (u) pol%multiplicity
  write (u) pol%chirality
  write (u) pol%anti
  call pol%bv%write_raw (u)
end subroutine polarization_write_raw

module subroutine polarization_read_raw (pol, u, iostat)
  class(polarization_t), intent(out) :: pol
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
  read (u, iostat=iostat) pol%spin_type
  read (u, iostat=iostat) pol%multiplicity
  read (u, iostat=iostat) pol%chirality
  read (u, iostat=iostat) pol%anti
  call pol%bv%read_raw (u, iostat)
end subroutine polarization_read_raw

```

15.3.4 Accessing contents

Return true if the particle is technically polarized. The particle is either chiral, or its Bloch vector has been defined. The function returns true even if the Bloch

vector is zero or the particle is scalar.

```

(Polarizations: polarization: TBP)+≡
  procedure :: is_polarized => polarization_is_polarized

(Polarizations: sub interfaces)+≡
  module function polarization_is_polarized (pol) result (polarized)
    class(polarization_t), intent(in) :: pol
    logical :: polarized
  end function polarization_is_polarized

(Polarizations: procedures)+≡
  module function polarization_is_polarized (pol) result (polarized)
    class(polarization_t), intent(in) :: pol
    logical :: polarized
    polarized = pol%chirality /= 0 .or. pol%bv%is_polarized ()
  end function polarization_is_polarized

```

Return true if the polarization is diagonal, i.e., all entries in the density matrix are diagonal. For an unpolarized particle, we also return `.true.` since the density matrix is proportional to the unit matrix.

```

(Polarizations: polarization: TBP)+≡
  procedure :: is_diagonal => polarization_is_diagonal

(Polarizations: sub interfaces)+≡
  module function polarization_is_diagonal (pol) result (diagonal)
    class(polarization_t), intent(in) :: pol
    logical :: diagonal
  end function polarization_is_diagonal

(Polarizations: procedures)+≡
  module function polarization_is_diagonal (pol) result (diagonal)
    class(polarization_t), intent(in) :: pol
    logical :: diagonal
    select case (pol%chirality)
    case (0)
      diagonal = pol%bv%is_diagonal ()
    case default
      diagonal = .true.
    end select
  end function polarization_is_diagonal

```

15.3.5 Mapping between polarization and state matrix

Create the polarization object that corresponds to a state matrix. The state matrix is not necessarily normalized. The result will be either unpolarized, or a generalized Bloch vector that we compute in terms of the appropriate spin generator basis. To this end, we first construct the complete density matrix, then set the Bloch vector with this input.

For a naturally chiral particle (i.e., neutrino), we do not set the polarization vector, it is implied.

Therefore, we cannot account for any sign flip and transform as-is.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_state_matrix => polarization_init_state_matrix

```

```

<Polarizations: sub interfaces>+≡
    module subroutine polarization_init_state_matrix (pol, state)
        class(polarization_t), intent(out) :: pol
        type(state_matrix_t), intent(in), target :: state
    end subroutine polarization_init_state_matrix

<Polarizations: procedures>+≡
    module subroutine polarization_init_state_matrix (pol, state)
        class(polarization_t), intent(out) :: pol
        type(state_matrix_t), intent(in), target :: state
        type(state_iterator_t) :: it
        type(flavor_t) :: flv
        type(helicity_t) :: hel
        integer :: d, h1, h2, i, j
        complex(default), dimension(:,,:), allocatable :: r
        complex(default) :: me
        real(default) :: trace
        call it%init (state)
        flv = it%get_flavor (1)
        hel = it%get_helicity (1)
        if (hel%is_defined ()) then
            call pol%init_generic (flv)
            select case (pol%chirality)
            case (0)
                trace = 0
                d = pol%bv%get_n_states ()
                allocate (r (d, d), source = (0._default, 0._default))
                do while (it%is_valid ())
                    hel = it%get_helicity (1)
                    call hel%get_indices (h1, h2)
                    i = pol%bv%hel_index (h1)
                    j = pol%bv%hel_index (h2)
                    me = it%get_matrix_element ()
                    r(i,j) = me
                    if (i == j) trace = trace + real (me)
                    call it%advance ()
                end do
                if (trace /= 0) call pol%bv%set (r / trace)
            end select
        else
            call pol%init (flv)
        end if
    end subroutine polarization_init_state_matrix

```

Create the state matrix that corresponds to a given polarization. We make use of the polarization iterator as defined below, which should iterate according to the canonical helicity ordering.

```

<Polarizations: polarization: TBP>+≡
    procedure :: to_state => polarization_to_state_matrix

<Polarizations: sub interfaces>+≡
    module subroutine polarization_to_state_matrix (pol, state, all_states, tolerance)
        class(polarization_t), intent(in), target :: pol
        type(state_matrix_t), intent(out) :: state

```

```

        logical, intent(in), optional :: all_states
        real(default), intent(in), optional :: tolerance
    end subroutine polarization_to_state_matrix

<Polarizations: procedures>+≡
    module subroutine polarization_to_state_matrix (pol, state, all_states, tolerance)
        class(polarization_t), intent(in), target :: pol
        type(state_matrix_t), intent(out) :: state
        logical, intent(in), optional :: all_states
        real(default), intent(in), optional :: tolerance
        type(polarization_iterator_t) :: it
        type(quantum_numbers_t), dimension(1) :: qn
        complex(default) :: value
        call it%init (pol, all_states, tolerance)
        call state%init (store_values = .true.)
        do while (it%is_valid ())
            value = it%get_value ()
            qn(1) = it%get_quantum_numbers ()
            call state%add_state (qn, value = value)
            call it%advance ()
        end do
        call state%freeze ()
    end subroutine polarization_to_state_matrix

```

15.3.6 Specific initializers

Unpolarized particle, no nontrivial entries in the density matrix. This is the default initialization mode.

```

<Polarizations: polarization: TBP>+≡
    procedure :: init_unpolarized => polarization_init_unpolarized

<Polarizations: sub interfaces>+≡
    module subroutine polarization_init_unpolarized (pol, flv)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
    end subroutine polarization_init_unpolarized

<Polarizations: procedures>+≡
    module subroutine polarization_init_unpolarized (pol, flv)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        call pol%init (flv)
    end subroutine polarization_init_unpolarized

```

The following three modes are useful mainly for spin-1/2 particle and massless particles of any nonzero spin. Only the highest-weight components are filled.

Circular polarization: The density matrix of the two highest-weight states is

$$\rho(f) = \frac{1 - |f|}{2} \mathbf{1} + |f| \times \begin{cases} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & f > 0; \\ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, & f < 0, \end{cases}$$

In the generalized Bloch representation, this is an entry for the T^3 generator only, regardless of the spin representation.

A chiral particle is not affected.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_circular => polarization_init_circular

(Polarizations: sub interfaces)+≡
  module subroutine polarization_init_circular (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
  end subroutine polarization_init_circular

(Polarizations: procedures)+≡
  module subroutine polarization_init_circular (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
    call pol%init (flv)
    select case (pol%chirality)
    case (0)
      call pol%bv%init_vector (pol%spin_type, &
        [0._default, 0._default, f])
    end select
  end subroutine polarization_init_circular

```

Transversal polarization is analogous to circular, but we get a density matrix

$$\rho(f, \phi) = \frac{1 - |f|}{2} \mathbf{1} + \frac{|f|}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}.$$

for the highest-weight subspace. The lower weights are unaffected. The phase is $\phi = 0$ for the x -axis, $\phi = 90^\circ$ for the y axis as polarization vector.

For an antiparticle, the phase switches sign, and for $f < 0$, the off-diagonal elements switch sign.

A chiral particle is not affected.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_transversal => polarization_init_transversal

(Polarizations: sub interfaces)+≡
  module subroutine polarization_init_transversal (pol, flv, phi, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: phi, f
  end subroutine polarization_init_transversal

(Polarizations: procedures)+≡
  module subroutine polarization_init_transversal (pol, flv, phi, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: phi, f
    call pol%init (flv)
    select case (pol%chirality)
    case (0)
      if (pol%anti) then

```

```

        call pol%bv%init_vector (pol%spin_type, &
            [f * cos (phi), f * sin (phi), 0._default])
    else
        call pol%bv%init_vector (pol%spin_type, &
            [f * cos (phi), -f * sin (phi), 0._default])
    end if
end select
end subroutine polarization_init_transversal

```

For axis polarization, we again set only the entries with maximum weight, which for spin 1/2 means

$$\rho(f, \phi) = \frac{1}{2} \begin{pmatrix} 1 + \alpha_3 & \alpha_1 - i\alpha_2 \\ \alpha_1 + i\alpha_2 & 1 - \alpha_3 \end{pmatrix}.$$

For an antiparticle, the imaginary part proportional to α_2 switches sign (complex conjugate). A chiral particle is not affected.

In the generalized Bloch representation, this translates into coefficients for $T^{1,2,3}$, all others stay zero.

```

<Polarizations: polarization: TBP> +=
    procedure :: init_axis => polarization_init_axis
<Polarizations: sub interfaces> +=
    module subroutine polarization_init_axis (pol, flv, alpha)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        real(default), dimension(3), intent(in) :: alpha
    end subroutine polarization_init_axis
<Polarizations: procedures> +=
    module subroutine polarization_init_axis (pol, flv, alpha)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        real(default), dimension(3), intent(in) :: alpha
        call pol%init (flv)
        select case (pol%chirality)
        case (0)
            if (pol%anti) then
                call pol%bv%init_vector (pol%spin_type, &
                    [alpha(1), alpha(2), alpha(3)])
            else
                call pol%bv%init_vector (pol%spin_type, &
                    [alpha(1), -alpha(2), alpha(3)])
            end if
        end select
    end subroutine polarization_init_axis

```

This version specifies the polarization axis in terms of r (polarization degree) and θ, ϕ (polar and azimuthal angles).

If one of the angles is a nonzero multiple of π , roundoff errors typically will result in tiny contributions to unwanted components. Therefore, include a catch for small numbers.

```

<Polarizations: polarization: TBP> +=
    procedure :: init_angles => polarization_init_angles

```



```

<Polarizations: sub interfaces>+≡
  module subroutine polarization_init_angles (pol, flv, r, theta, phi)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: r, theta, phi
  end subroutine polarization_init_angles

<Polarizations: procedures>+≡
  module subroutine polarization_init_angles (pol, flv, r, theta, phi)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: r, theta, phi
    real(default), dimension(3) :: alpha
    real(default), parameter :: eps = 10 * epsilon (1._default)

    alpha(1) = r * sin (theta) * cos (phi)
    alpha(2) = r * sin (theta) * sin (phi)
    alpha(3) = r * cos (theta)
    where (abs (alpha) < eps) alpha = 0
    call pol%init_axis (flv, alpha)
  end subroutine polarization_init_angles

```

Longitudinal polarization is defined only for massive bosons. Only the zero component is filled. Otherwise, unpolarized.

In the generalized Bloch representation, the zero component corresponds to a linear combination of all diagonal (Cartan) generators.

```

<Polarizations: polarization: TBP>+≡
  procedure :: init_longitudinal => polarization_init_longitudinal

<Polarizations: sub interfaces>+≡
  module subroutine polarization_init_longitudinal (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
  end subroutine polarization_init_longitudinal

<Polarizations: procedures>+≡
  module subroutine polarization_init_longitudinal (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
    real(default), dimension(:), allocatable :: rd
    integer :: s, d
    s = flv%get_spin_type ()
    select case (s)
    case (VECTOR, TENSOR)
      call pol%init_generic (flv)
      if (pol%bv%is_polarized ()) then
        d = pol%bv%get_n_states ()
        allocate (rd (d), source = 0._default)
        rd(pol%bv%hel_index (0)) = f
        call pol%bv%set (rd)
      end if
    case default
      call pol%init_unpolarized (flv)
    end select
  end subroutine polarization_init_longitudinal

```

```

        end select
    end subroutine polarization_init_longitudinal

```

This is diagonal polarization: we specify all components explicitly. `rd` is the array of diagonal elements of the density matrix. We assume that the length of `rd` is equal to the particle multiplicity.

```

<Polarizations: polarization: TBP>+=
    procedure :: init_diagonal => polarization_init_diagonal

<Polarizations: sub interfaces>+=
    module subroutine polarization_init_diagonal (pol, flv, rd)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        real(default), dimension(:), intent(in) :: rd
    end subroutine polarization_init_diagonal

<Polarizations: procedures>+=
    module subroutine polarization_init_diagonal (pol, flv, rd)
        class(polarization_t), intent(out) :: pol
        type(flavor_t), intent(in) :: flv
        real(default), dimension(:), intent(in) :: rd
        real(default) :: trace
        call pol%init_generic (flv)
        if (pol%bv%is_polarized ()) then
            trace = sum (rd)
            if (trace /= 0) call pol%bv%set (rd / trace)
        end if
    end subroutine polarization_init_diagonal

```

15.3.7 Operations

Combine polarization states by computing the outer product of the state matrices.

```

<Polarizations: public>+=
    public :: combine_polarization_states

<Polarizations: sub interfaces>+=
    module subroutine combine_polarization_states (pol, state)
        type(polarization_t), dimension(:), intent(in), target :: pol
        type(state_matrix_t), intent(out) :: state
    end subroutine combine_polarization_states

<Polarizations: procedures>+=
    module subroutine combine_polarization_states (pol, state)
        type(polarization_t), dimension(:), intent(in), target :: pol
        type(state_matrix_t), intent(out) :: state
        type(state_matrix_t), dimension(size(pol)), target :: pol_state
        integer :: i
        do i = 1, size (pol)
            call pol(i)%to_state (pol_state(i))
        end do
        call outer_multiply (pol_state, state)
        do i = 1, size (pol)

```

```

        call pol_state(i)%final ()
    end do
end subroutine combine_polarization_states

```

Transform a polarization density matrix into a polarization vector. This is possible without information loss only for spin-1/2 and for massless particles. To get a unique answer in all cases, we consider only the components with highest weight. Obviously, this loses the longitudinal component of a massive vector, for instance. The norm of the returned axis is the polarization fraction for the highest-weight subspace. For a scalar particle, we return a zero vector. The same result applies if the highest-weight component vanishes.

This is the inverse operation of `polarization_init_axis` above, where the polarization fraction is set to unity.

For an antiparticle, the `alpha(2)` coefficient flips sign.

```

<Polarizations: polarization: TBP>+≡
    procedure :: get_axis => polarization_get_axis

<Polarizations: sub interfaces>+≡
    module function polarization_get_axis (pol) result (alpha)
        class(polarization_t), intent(in), target :: pol
        real(default), dimension(3) :: alpha
    end function polarization_get_axis

<Polarizations: procedures>+≡
    module function polarization_get_axis (pol) result (alpha)
        class(polarization_t), intent(in), target :: pol
        real(default), dimension(3) :: alpha
        select case (pol%chirality)
        case (0)
            call pol%bv%to_vector (alpha)
            if (.not. pol%anti) alpha(2) = - alpha(2)
        case (-1)
            alpha = [0._default, 0._default, -1._default]
        case (1)
            alpha = [0._default, 0._default, 1._default]
        end select
    end function polarization_get_axis

```

This function returns polarization degree and polar and azimuthal angles (θ, ϕ) of the polarization axis. The same restrictions apply as above.

Since we call the `get_axis` method, the phase flips sign for an antiparticle.

```

<Polarizations: polarization: TBP>+≡
    procedure :: to_angles => polarization_to_angles

<Polarizations: sub interfaces>+≡
    module subroutine polarization_to_angles (pol, r, theta, phi)
        class(polarization_t), intent(in) :: pol
        real(default), intent(out) :: r, theta, phi
    end subroutine polarization_to_angles

<Polarizations: procedures>+≡
    module subroutine polarization_to_angles (pol, r, theta, phi)
        class(polarization_t), intent(in) :: pol
        real(default), intent(out) :: r, theta, phi
    end subroutine polarization_to_angles

```

```

real(default), dimension(3) :: alpha
real(default) :: norm, r12
alpha = pol%get_axis ()
norm = sum (alpha**2)
r = sqrt (norm)
if (norm > 0) then
  r12 = sqrt (alpha(1)**2 + alpha(2)**2)
  theta = atan2 (r12, alpha(3))
  if (any (alpha(1:2) /= 0)) then
    phi = atan2 (alpha(2), alpha(1))
  else
    phi = 0
  end if
else
  theta = 0
  phi = 0
end if
end subroutine polarization_to_angles

```

15.3.8 Polarization Iterator

The iterator acts like a state matrix iterator, i.e., it points to one helicity combination at a time and can return the corresponding helicity object and matrix-element value.

Since the polarization is stored as a Bloch vector, we recover the whole density matrix explicitly upon initialization, store it inside the iterator object, and then just return its elements one at a time.

For an unpolarized particle, the iterator returns a single state with undefined helicity. The value is the value of any diagonal density matrix element, $1/n$ where n is the multiplicity.

```

<Polarizations: public>+≡
  public :: polarization_iterator_t

<Polarizations: types>+≡
  type :: polarization_iterator_t
  private
  type(polarization_t), pointer :: pol => null ()
  logical :: polarized = .false.
  integer :: h1 = 0
  integer :: h2 = 0
  integer :: i = 0
  integer :: j = 0
  complex(default), dimension(:,,:), allocatable :: r
  complex(default) :: value = 1._default
  real(default) :: tolerance = -1._default
  logical :: valid = .false.
  contains
  <Polarizations: polarization iterator: TBP>
end type polarization_iterator_t

```

Output for debugging purposes only, therefore no format for real/complex.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: write => polarization_iterator_write

(Polarizations: sub interfaces)+≡
  module subroutine polarization_iterator_write (it, unit)
    class(polarization_iterator_t), intent(in) :: it
    integer, intent(in), optional :: unit
  end subroutine polarization_iterator_write

(Polarizations: procedures)+≡
  module subroutine polarization_iterator_write (it, unit)
    class(polarization_iterator_t), intent(in) :: it
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1X,A)") "Polarization iterator:"
    write (u, "(3X,A,L1)") "assigned = ", associated (it%pol)
    write (u, "(3X,A,L1)") "valid    = ", it%valid
    if (it%valid) then
      write (u, "(3X,A,2(1X,I2))") "i, j    = ", it%i, it%j
      write (u, "(3X,A,2(1X,I2))") "h1, h2  = ", it%h1, it%h2
      write (u, "(3X,A)", advance="no") "value    = "
      write (u, *) it%value
      if (allocated (it%r)) then
        do i = 1, size (it%r, 2)
          write (u, *) it%r(i,:)
        end do
      end if
    end if
  end subroutine polarization_iterator_write

```

Initialize, i.e., (virtually) point to the first helicity state supported by the polarization object. If the density matrix is nontrivial, we calculate it here.

Following the older state-matrix conventions, the iterator sequence starts at the lowest helicity value. In the current internal representation, this corresponds to the highest index value.

If the current matrix-element value is zero, advance the iterator. Advancing will stop at a nonzero value or if the iterator becomes invalid.

If *tolerance* is given, any state matrix entry less or equal will be treated as zero, causing the iterator to skip an entry. By default, the value is negative, so no entry is skipped.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: init => polarization_iterator_init

(Polarizations: sub interfaces)+≡
  module subroutine polarization_iterator_init (it, pol, all_states, tolerance)
    class(polarization_iterator_t), intent(out) :: it
    type(polarization_t), intent(in), target :: pol
    logical, intent(in), optional :: all_states
    real(default), intent(in), optional :: tolerance
  end subroutine polarization_iterator_init

```

<Polarizations: procedures>+≡

```

module subroutine polarization_iterator_init (it, pol, all_states, tolerance)
  class(polarization_iterator_t), intent(out) :: it
  type(polarization_t), intent(in), target :: pol
  logical, intent(in), optional :: all_states
  real(default), intent(in), optional :: tolerance
  integer :: d
  logical :: only_max_weight
  it%pol => pol
  if (present (all_states)) then
    if (.not. all_states) then
      if (present (tolerance)) then
        it%tolerance = tolerance
      else
        it%tolerance = 0
      end if
    end if
  end if
  select case (pol%chirality)
  case (0)
    d = pol%bv%get_n_states ()
    only_max_weight = pol%multiplicity < d
    it%polarized = pol%bv%is_polarized ()
    if (it%polarized) then
      it%i = d
      it%j = it%i
      it%h1 = pol%bv%hel_value (it%i)
      it%h2 = it%h1
      call pol%bv%to_matrix (it%r, only_max_weight)
      it%value = it%r(it%i, it%j)
    else
      it%value = 1._default / d
    end if
    it%valid = .true.
  case (1,-1)
    it%polarized = .true.
    select case (pol%spin_type)
    case (SPINOR)
      it%h1 = pol%chirality
    case (VECTORSPINOR)
      it%h1 = 2 * pol%chirality
    end select
    it%h2 = it%h1
    it%valid = .true.
  end select
  if (it%valid .and. abs (it%value) <= it%tolerance) call it%advance ()
end subroutine polarization_iterator_init

```

Advance to the next valid helicity state. Repeat if the returned value is zero.

For an unpolarized object, we iterate through the diagonal helicity states with a constant value.

<Polarizations: polarization iterator: TBP>+≡

```

procedure :: advance => polarization_iterator_advance

```

```

<Polarizations: sub interfaces>+≡
    recursive module subroutine polarization_iterator_advance (it)
        class(polarization_iterator_t), intent(inout) :: it
        end subroutine polarization_iterator_advance
<Polarizations: procedures>+≡
    recursive module subroutine polarization_iterator_advance (it)
        class(polarization_iterator_t), intent(inout) :: it
        if (it%valid) then
            select case (it%pol%chirality)
            case (0)
                if (it%polarized) then
                    if (it%j > 1) then
                        it%j = it%j - 1
                        it%h2 = it%pol%bv%hel_value (it%j)
                        it%value = it%r(it%i, it%j)
                    else if (it%i > 1) then
                        it%j = it%pol%bv%get_n_states ()
                        it%h2 = it%pol%bv%hel_value (it%j)
                        it%i = it%i - 1
                        it%h1 = it%pol%bv%hel_value (it%i)
                        it%value = it%r(it%i, it%j)
                    else
                        it%valid = .false.
                    end if
                else
                    it%valid = .false.
                end if
            case default
                it%valid = .false.
            end select
            if (it%valid .and. abs (it%value) <= it%tolerance) call it%advance ()
        end if
    end subroutine polarization_iterator_advance

```

This is true as long as the iterator points to a valid helicity state.

```

<Polarizations: polarization iterator: TBP>+≡
    procedure :: is_valid => polarization_iterator_is_valid
<Polarizations: sub interfaces>+≡
    module function polarization_iterator_is_valid (it) result (is_valid)
        logical :: is_valid
        class(polarization_iterator_t), intent(in) :: it
        end function polarization_iterator_is_valid
<Polarizations: procedures>+≡
    module function polarization_iterator_is_valid (it) result (is_valid)
        logical :: is_valid
        class(polarization_iterator_t), intent(in) :: it
        is_valid = it%valid
    end function polarization_iterator_is_valid

```

Return the matrix element value for the helicity that we are currently pointing at.

```

<Polarizations: polarization iterator: TBP>+≡

```

```

    procedure :: get_value => polarization_iterator_get_value
<Polarizations: sub interfaces>+≡
    module function polarization_iterator_get_value (it) result (value)
        complex(default) :: value
        class(polarization_iterator_t), intent(in) :: it
    end function polarization_iterator_get_value
<Polarizations: procedures>+≡
    module function polarization_iterator_get_value (it) result (value)
        complex(default) :: value
        class(polarization_iterator_t), intent(in) :: it
        if (it%valid) then
            value = it%value
        else
            value = 0
        end if
    end function polarization_iterator_get_value

```

Return a quantum number object for the helicity that we are currently pointing at. This is a single quantum number object, not an array.

Note that the `init` method of the helicity object has the order reversed.

```

<Polarizations: polarization iterator: TBP>+≡
    procedure :: get_quantum_numbers => polarization_iterator_get_quantum_numbers
<Polarizations: sub interfaces>+≡
    module function polarization_iterator_get_quantum_numbers (it) result (qn)
        class(polarization_iterator_t), intent(in) :: it
        type(quantum_numbers_t) :: qn
    end function polarization_iterator_get_quantum_numbers
<Polarizations: procedures>+≡
    module function polarization_iterator_get_quantum_numbers (it) result (qn)
        class(polarization_iterator_t), intent(in) :: it
        type(helicity_t) :: hel
        type(quantum_numbers_t) :: qn
        if (it%polarized) then
            call hel%init (it%h2, it%h1)
        end if
        call qn%init (hel)
    end function polarization_iterator_get_quantum_numbers

```

15.3.9 Sparse Matrix

We introduce a simple implementation of a sparse matrix that can represent polarization (or similar concepts) for transfer to I/O within the program. It consists of an integer array that represents the index values, and a complex array that represents the nonvanishing entries. The number of nonvanishing entries must be known for initialization, but the entries are filled one at a time.

Here is a base type without the special properties of a spin-density matrix.

```

<Polarizations: public>+≡
    public :: smatrix_t

```



```

<Polarizations: types>+=
  type :: smatrix_t
    private
    integer :: dim = 0
    integer :: n_entry = 0
    integer, dimension(:,:), allocatable :: index
    complex(default), dimension(:), allocatable :: value
    contains
    <Polarizations: smatrix: TBP>
  end type smatrix_t

```

Output.

```

<Polarizations: smatrix: TBP>=
  procedure :: write => smatrix_write

<Polarizations: sub interfaces>+=
  module subroutine smatrix_write (object, unit, indent)
    class(smatrix_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
  end subroutine smatrix_write

<Polarizations: procedures>+=
  module subroutine smatrix_write (object, unit, indent)
    class(smatrix_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, i, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    if (allocated (object%value)) then
      if (size (object%value) > 0) then
        do i = 1, object%n_entry
          write (u, "(1x,A,'@(')", advance="no") repeat (" ", ind)
          write (u, "(SP,9999(I2.1,':',1x))", advance="no") &
            object%index(:,i)
          write (u, "('(', " // FMT_19 // ",','," // FMT_19 // &
            ",')')'") object%value(i)
        end do
      else
        write (u, "(1x,A)", advance="no") repeat (" ", ind)
        write (u, "(A)" "[empty matrix]"
      end if
    else
      write (u, "(1x,A)", advance="no") repeat (" ", ind)
      write (u, "(A)" "[undefined matrix]"
    end if
  end subroutine smatrix_write

```

Initialization: allocate arrays to the correct size. We specify both the dimension of the matrix (if different from two, this is rather a generic tensor) and the number of nonvanishing entries.

```

<Polarizations: smatrix: TBP>+=
  procedure :: init => smatrix_init

```

```

(Polarizations: sub interfaces)+≡
    module subroutine smatrix_init (smatrix, dim, n_entry)
        class(smatrix_t), intent(out) :: smatrix
        integer, intent(in) :: dim
        integer, intent(in) :: n_entry
    end subroutine smatrix_init

(Polarizations: procedures)+≡
    module subroutine smatrix_init (smatrix, dim, n_entry)
        class(smatrix_t), intent(out) :: smatrix
        integer, intent(in) :: dim
        integer, intent(in) :: n_entry
        smatrix%dim = dim
        smatrix%n_entry = n_entry
        allocate (smatrix%index (dim, n_entry))
        allocate (smatrix%value (n_entry))
    end subroutine smatrix_init

Fill: one entry at a time.

(Polarizations: smatrix: TBP)+≡
    procedure :: set_entry => smatrix_set_entry

(Polarizations: sub interfaces)+≡
    module subroutine smatrix_set_entry (smatrix, i, index, value)
        class(smatrix_t), intent(inout) :: smatrix
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: index
        complex(default), intent(in) :: value
    end subroutine smatrix_set_entry

(Polarizations: procedures)+≡
    module subroutine smatrix_set_entry (smatrix, i, index, value)
        class(smatrix_t), intent(inout) :: smatrix
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: index
        complex(default), intent(in) :: value
        smatrix%index(:,i) = index
        smatrix%value(i) = value
    end subroutine smatrix_set_entry

(Polarizations: smatrix: TBP)+≡
    procedure :: exists => smatrix_exists

(Polarizations: sub interfaces)+≡
    elemental module function smatrix_exists (smatrix) result (exist)
        logical :: exist
        class(smatrix_t), intent(in) :: smatrix
    end function smatrix_exists

(Polarizations: procedures)+≡
    elemental module function smatrix_exists (smatrix) result (exist)
        logical :: exist
        class(smatrix_t), intent(in) :: smatrix
        exist = .not. all (smatrix%value == 0)
    end function smatrix_exists

```

15.3.10 Polarization Matrix

As an extension of the more generic `smatrix` type, we implement a proper spin-density matrix. After the matrix has been filled, we can fix spin type and multiplicity for a particle, check the matrix for consistency, and normalize it if necessary.

This implementation does not have an antiparticle flag, just like the state matrix object. We therefore cannot account for sign flips when using this object.

TODO: The `pure` flag is for informational purposes only, and it only represents a necessary condition if spin is greater than 1/2. We may either check purity for all spins or drop this.

```

(Polarizations: public)+≡
    public :: pmatrix_t

(Polarizations: types)+≡
    type, extends (smatrix_t) :: pmatrix_t
        private
            integer :: spin_type = 0
            integer :: multiplicity = 0
            logical :: massive = .true.
            integer :: chirality = 0
            real(default) :: degree = 1
            logical :: pure = .false.
        contains
            (Polarizations: pmatrix: TBP)
        end type pmatrix_t

```

Output, including extra data. (The `indent` argument is ignored.)

```

(Polarizations: pmatrix: TBP)≡
    procedure :: write => pmatrix_write

(Polarizations: sub interfaces)+≡
    module subroutine pmatrix_write (object, unit, indent)
        class(pmatrix_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
    end subroutine pmatrix_write

(Polarizations: procedures)+≡
    module subroutine pmatrix_write (object, unit, indent)
        class(pmatrix_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Polarization: spin density matrix"
        write (u, "(3x,A,I0)") "spin type      = ", object%spin_type
        write (u, "(3x,A,I0)") "multiplicity = ", object%multiplicity
        write (u, "(3x,A,L1)") "massive      = ", object%massive
        write (u, "(3x,A,I0)") "chirality    = ", object%chirality
        write (u, "(3x,A,F10.7)") "pol.degree   = ", object%degree
        write (u, "(3x,A,L1)") "pure state    = ", object%pure
        call object%smatrix_t%write (u, 1)
    end subroutine pmatrix_write

```

This assignment is trivial, but must be coded explicitly.

```

(Polarizations: pmatrix: TBP)+≡
  generic :: assignment(=) => pmatrix_assign_from_smatrix
  procedure, private :: pmatrix_assign_from_smatrix

(Polarizations: sub interfaces)+≡
  module subroutine pmatrix_assign_from_smatrix (pmatrix, smatrix)
    class(pmatrix_t), intent(out) :: pmatrix
    type(smatrix_t), intent(in) :: smatrix
  end subroutine pmatrix_assign_from_smatrix

(Polarizations: procedures)+≡
  module subroutine pmatrix_assign_from_smatrix (pmatrix, smatrix)
    class(pmatrix_t), intent(out) :: pmatrix
    type(smatrix_t), intent(in) :: smatrix
    pmatrix%smatrix_t = smatrix
  end subroutine pmatrix_assign_from_smatrix

```

Declare spin, multiplicity, and polarization degree. Check whether all entries fit, and whether this is a valid matrix.

The required properties are:

1. all entries apply to the given spin and mass type
2. the diagonal is real
3. only the upper of corresponding off-diagonal elements is specified, i.e., the row index is less than the column index
4. the trace is nonnegative and equal to the polarization degree (the remainder, proportional to the unit matrix, is understood to be present)
5. the trace of the matrix square is positive and less or equal to the trace of the matrix itself, which is the polarization degree.
6. If the trace of the matrix square and the trace of the matrix are unity, we may have a pure state. (For spin up to 1/2, this is actually sufficient.)

```

(Polarizations: pmatrix: TBP)+≡
  procedure :: normalize => pmatrix_normalize

(Polarizations: sub interfaces)+≡
  module subroutine pmatrix_normalize (pmatrix, flv, degree, tolerance)
    class(pmatrix_t), intent(inout) :: pmatrix
    type(flavor_t), intent(in) :: flv
    real(default), intent(in), optional :: degree
    real(default), intent(in), optional :: tolerance
  end subroutine pmatrix_normalize

(Polarizations: procedures)+≡
  module subroutine pmatrix_normalize (pmatrix, flv, degree, tolerance)
    class(pmatrix_t), intent(inout) :: pmatrix
    type(flavor_t), intent(in) :: flv
    real(default), intent(in), optional :: degree
    real(default), intent(in), optional :: tolerance
    integer :: i, hmax
    logical :: fermion, ok

```

```

real(default) :: trace, trace_sq
real(default) :: tol
tol = 0; if (present (tolerance)) tol = tolerance
pmatrix%spin_type = flv%get_spin_type ()
pmatrix%massive = flv%get_mass () /= 0
if (.not. pmatrix%massive) then
    if (flv%is_left_handed ()) then
        pmatrix%chirality = -1
    else if (flv%is_right_handed ()) then
        pmatrix%chirality = +1
    end if
end if
if (pmatrix%spin_type == SCALAR) then
    pmatrix%multiplicity = 1
else if (pmatrix%massive) then
    pmatrix%multiplicity = pmatrix%spin_type
else if (pmatrix%chirality == 0) then
    pmatrix%multiplicity = 2
else
    pmatrix%multiplicity = 1
end if
if (present (degree)) then
    if (degree < 0 .or. degree > 1) &
        call msg_error ("polarization degree must be between 0 and 1")
    pmatrix%degree = degree
end if
if (size (pmatrix%index, 1) /= 2) call error ("wrong array rank")
fermion = mod (pmatrix%spin_type, 2) == 0
hmax = pmatrix%spin_type / 2
if (pmatrix%n_entry > 0) then
    if (fermion) then
        if (pmatrix%massive) then
            ok = all (pmatrix%index /= 0) &
                .and. all (abs (pmatrix%index) <= hmax)
        else if (pmatrix%chirality == -1) then
            ok = all (pmatrix%index == -hmax)
        else if (pmatrix%chirality == +1) then
            ok = all (pmatrix%index == +hmax)
        else
            ok = all (abs (pmatrix%index) == hmax)
        end if
    else
        if (pmatrix%massive) then
            ok = all (abs (pmatrix%index) <= hmax)
        else
            ok = all (abs (pmatrix%index) == hmax)
        end if
    end if
    if (.not. ok) call error ("illegal index value")
else
    pmatrix%degree = 0
    pmatrix%pure = pmatrix%multiplicity == 1
    return
end if

```

```

trace = 0
do i = 1, pmatrix%n_entry
  associate (index => pmatrix%index(:,i), value => pmatrix%value(i))
    if (index(1) == index(2)) then
      if (abs (aimag (value)) > tol) call error ("diagonal must be real")
      value = real (value, kind=default)
      trace = trace + value

      else if (any (pmatrix%index(1,:) == index(2) &
        .and. pmatrix%index(2,:) == index(1))) then
        call error ("redundant off-diagonal entry")
      else if (index(2) < index (1)) then
        index = index([2,1])
        value = conjg (value)
      end if
    end associate
  end do
  if (abs (trace) <= tol) call error ("trace must not vanish")
  trace = real (trace, kind=default)
  pmatrix%value = pmatrix%value / trace * pmatrix%degree
  trace_sq = (1 - pmatrix%degree ** 2) / pmatrix%multiplicity
  do i = 1, pmatrix%n_entry
    associate (index => pmatrix%index(:,i), value => pmatrix%value(i))
      if (index(1) == index(2)) then
        trace_sq = trace_sq + abs (value) ** 2
      else
        trace_sq = trace_sq + 2 * abs (value) ** 2
      end if
    end associate
  end do
  if (pmatrix%multiplicity == 1) then
    pmatrix%pure = .true.
  else if (abs (trace_sq - 1) <= tol) then
    pmatrix%pure = .true.
  else if (trace_sq - 1 > tol .or. trace_sq < -tol) then
    print *, "Trace of matrix square = ", trace_sq
    call error ("not permissible as density matrix")
  end if
contains
  subroutine error (msg)
    character(*), intent(in) :: msg
    call pmatrix%write ()
    call msg_fatal ("Spin density matrix: " // msg)
  end subroutine error
end subroutine pmatrix_normalize

```

A polarized matrix is defined as one with a positive polarization degree, even if the actual matrix is trivial.

<Polarizations: pmatrix: TBP>+≡

```
procedure :: is_polarized => pmatrix_is_polarized
```

<Polarizations: sub interfaces>+≡

```
elemental module function pmatrix_is_polarized (pmatrix) result (flag)
  class(pmatrix_t), intent(in) :: pmatrix

```

```

        logical :: flag
    end function pmatrix_is_polarized
<Polarizations: procedures>+≡
    elemental module function pmatrix_is_polarized (pmatrix) result (flag)
        class(pmatrix_t), intent(in) :: pmatrix
        logical :: flag
        flag = pmatrix%degree > 0
    end function pmatrix_is_polarized

```

Check if there are only diagonal entries.

```

<Polarizations: pmatrix: TBP>+≡
    procedure :: is_diagonal => pmatrix_is_diagonal
<Polarizations: sub interfaces>+≡
    elemental module function pmatrix_is_diagonal (pmatrix) result (flag)
        class(pmatrix_t), intent(in) :: pmatrix
        logical :: flag
        end function pmatrix_is_diagonal
<Polarizations: procedures>+≡
    elemental module function pmatrix_is_diagonal (pmatrix) result (flag)
        class(pmatrix_t), intent(in) :: pmatrix
        logical :: flag
        flag = all (pmatrix%index(1,:) == pmatrix%index(2,:))
    end function pmatrix_is_diagonal

```

Check if there are only diagonal entries.

```

<Polarizations: pmatrix: TBP>+≡
    procedure :: get_simple_pol => pmatrix_get_simple_pol
<Polarizations: sub interfaces>+≡
    elemental module function pmatrix_get_simple_pol (pmatrix) result (pol)
        class(pmatrix_t), intent(in) :: pmatrix
        real(default) :: pol
        end function pmatrix_get_simple_pol
<Polarizations: procedures>+≡
    elemental module function pmatrix_get_simple_pol (pmatrix) result (pol)
        class(pmatrix_t), intent(in) :: pmatrix
        real(default) :: pol
        if (pmatrix%is_polarized ()) then
            select case (size (pmatrix%value))
            case (0)
                pol = 0
            case (1)
                pol = pmatrix%index (1,1) * pmatrix%degree
            case (2)
                pol = 42
            end select
        else
            pol = 0
        end if
    end function pmatrix_get_simple_pol

```

15.3.11 Data Transformation

Create a `polarization_t` object from the contents of a normalized `pmatrix_t` object. We scan the entries as present in `pmatrix` and transform them into a density matrix, if necessary. The density matrix then initializes the Bloch vector. This is analogous to `polarization_init_state_matrix`.

There is a subtlety associated with massless particles. Since the `pmatrix` doesn't contain the full density matrix but just the nontrivial part, we have to initialize the polarization object with the massless equipartition, which contains nonzero entries for the Cartan generators. The `set` method therefore should not erase those initial contents. This is a constraint for the implementation of `set`, as applied to the Bloch vector.

As mentioned above, `pmatrix_t` does not support an antiparticle flag.

```

(Polarizations: polarization: TBP)+≡
    procedure :: init_pmatrix => polarization_init_pmatrix

(Polarizations: sub interfaces)+≡
    module subroutine polarization_init_pmatrix (pol, pmatrix)
        class(polarization_t), intent(out) :: pol
        type(pmatrix_t), intent(in) :: pmatrix
    end subroutine polarization_init_pmatrix

(Polarizations: procedures)+≡
    module subroutine polarization_init_pmatrix (pol, pmatrix)
        class(polarization_t), intent(out) :: pol
        type(pmatrix_t), intent(in) :: pmatrix
        integer :: d, i, j, k, h1, h2
        complex(default), dimension(:,,:), allocatable :: r
        call pol%init_generic ( &
            spin_type = pmatrix%spin_type, &
            multiplicity = pmatrix%multiplicity, &
            anti = .false., &                                     !!! SUFFICIENT?
            left_handed = pmatrix%chirality < 0, &
            right_handed = pmatrix%chirality > 0)
        if (pol%bv%is_polarized ()) then
            d = pol%bv%get_n_states ()
            allocate (r (d, d), source = (0._default, 0._default))
            if (d == pmatrix%multiplicity) then
                do i = 1, d
                    r(i,i) = (1 - pmatrix%degree) / d
                end do
            else if (d > pmatrix%multiplicity) then
                r(1,1) = (1 - pmatrix%degree) / 2
                r(d,d) = r(1,1)
            end if
            do k = 1, size (pmatrix%value)
                h1 = pmatrix%index(1,k)
                h2 = pmatrix%index(2,k)
                i = pol%bv%hel_index (h1)
                j = pol%bv%hel_index (h2)
                r(i,j) = r(i,j) + pmatrix%value(k)
                r(j,i) = conjg (r(i,j))
            end do
            call pol%bv%set (r)
        end if
    end subroutine polarization_init_pmatrix

```



```

        end if
    end subroutine polarization_init_pmatrix

```

15.3.12 Unit tests

Test module, followed by the corresponding implementation module.

<polarizations_ut.f90>≡
<File header>

```

module polarizations_ut
    use unit_tests
    use polarizations_uti

```

<Standard module head>

<Polarizations: public test>

contains

<Polarizations: test driver>

```

end module polarizations_ut

```

<polarizations_uti.f90>≡
<File header>

```

module polarizations_uti

```

<Use kinds>
 use flavors
 use model_data

```

    use polarizations

```

<Standard module head>

<Polarizations: test declarations>

contains

<Polarizations: tests>

```

end module polarizations_uti

```

API: driver for the unit tests below.

<Polarizations: public test>≡
 public :: polarizations_test

<Polarizations: test driver>≡
 subroutine polarizations_test (u, results)
 integer, intent(in) :: u
 type(test_results_t), intent(inout) :: results
<Polarizations: execute tests>
 end subroutine polarizations_test

Polarization type

Checking the setup for polarization.

```
<Polarizations: execute tests>≡
  call test (polarization_1, "polarization_1", &
    "check polarization setup", &
    u, results)

<Polarizations: test declarations>≡
  public :: polarization_1

<Polarizations: tests>≡
  subroutine polarization_1 (u)
    use os_interface
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(polarization_t) :: pol
    type(flavor_t) :: flv
    real(default), dimension(3) :: alpha
    real(default) :: r, theta, phi
    real(default), parameter :: tolerance = 1.E-14_default

    write (u, "(A)")  "* Test output: polarization_1"
    write (u, "(A)")  "* Purpose: test polarization setup"
    write (u, "(A)")

    write (u, "(A)")  "* Reading model file"
    write (u, "(A)")

    call model%init_sm_test ()

    write (u, "(A)")  "* Unpolarized fermion"
    write (u, "(A)")

    call flv%init (1, model)
    call pol%init_unpolarized (flv)
    call pol%write (u, state_matrix = .true.)
    write (u, "(A,L1)")  " diagonal =", pol%is_diagonal ()

    write (u, "(A)")
    write (u, "(A)")  "* Unpolarized fermion"
    write (u, "(A)")

    call pol%init_circular (flv, 0._default)
    call pol%write (u, state_matrix = .true., all_states = .false.)

    write (u, "(A)")
    write (u, "(A)")  "* Transversally polarized fermion, phi=0"
    write (u, "(A)")

    call pol%init_transversal (flv, 0._default, 1._default)
    call pol%write (u, state_matrix = .true.)
    write (u, "(A,L1)")  " diagonal =", pol%is_diagonal ()
```

```

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0.9, frac=0.8"
write (u, "(A)")

call pol%init_transversal (flv, 0.9_default, 0.8_default)
call pol%write (u, state_matrix = .true.)
write (u, "(A,L1)")  "   diagonal =", pol%is_diagonal ()

write (u, "(A)")
write (u, "(A)")  "* All polarization directions of a fermion"
write (u, "(A)")

call pol%init_generic (flv)
call pol%write (u, state_matrix = .true.)

call flv%init (21, model)

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized gluon, frac=0.3"
write (u, "(A)")

call pol%init_circular (flv, 0.3_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

call flv%init (23, model)

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector, frac=-0.7"
write (u, "(A)")

call pol%init_circular (flv, -0.7_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector"
write (u, "(A)")

call pol%init_circular (flv, 1._default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector, frac=0.4"
write (u, "(A)")

call pol%init_longitudinal (flv, 0.4_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

```

```

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector"
write (u, "(A)")

call pol%init_longitudinal (flv, 1._default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Diagonally polarized massive vector"
write (u, "(A)")

call pol%init_diagonal &
      (flv, [2._default, 1._default, 0._default])
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* All polarization directions of a massive vector"
write (u, "(A)")

call pol%init_generic (flv)
call pol%write (u, state_matrix = .true.)
call flv%init (21, model)

write (u, "(A)")
write (u, "(A)")  "* Axis polarization (0.2, 0.4, 0.6)"
write (u, "(A)")

alpha = [0.2_default, 0.4_default, 0.6_default]
call pol%init_axis (flv, alpha)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(1X,A)")  "Recovered axis:"
alpha = pol%get_axis ()
write (u, "(3(1X,F10.7))")  alpha

write (u, "(A)")
write (u, "(A)")  "* Angle polarization (0.5, 0.6, -1)"
r = 0.5_default
theta = 0.6_default
phi = -1._default
call pol%init_angles (flv, r, theta, phi)
write (u, "(A)")
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(1X,A)")  "Recovered parameters (r, theta, phi):"
call pol%to_angles (r, theta, phi)
write (u, "(3(1x,F10.7))")  r, theta, phi

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: polarization_1"

end subroutine polarization_1

```

Sparse-Matrix type

Use a sparse density matrix universally as the input for setting up polarization.

```

<Polarizations: execute tests>+≡
call test (polarization_2, "polarization_2", &
  "matrix polarization setup", &
  u, results)

<Polarizations: test declarations>+≡
public :: polarization_2

<Polarizations: tests>+≡
subroutine polarization_2 (u)
  use os_interface
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(polarization_t) :: pol
  real(default), dimension(3) :: alpha
  type(pmatrix_t) :: pmatrix
  real(default), parameter :: tolerance = 1e-8_default

  write (u, "(A)")  "* Test output: polarization_2"
  write (u, "(A)")  "* Purpose: matrix polarization setup"
  write (u, "(A)")

  write (u, "(A)")  "* Reading model file"
  write (u, "(A)")

  call model%init_sm_test ()

  write (u, "(A)")  "* Unpolarized fermion"
  write (u, "(A)")

  call flv%init (1, model)
  call pmatrix%init (2, 0)
  call pmatrix%normalize (flv, 0._default, tolerance)
  call pmatrix%write (u)
  write (u, *)
  write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
  write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
  write (u, *)

  call pol%init_pmatrix (pmatrix)
  call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0"
write (u, "(A)")

call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%set_entry (2, [+1,+1], (1._default, 0._default))
call pmatrix%set_entry (3, [-1,+1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)") "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)") "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0.9, frac=0.8"
write (u, "(A)")

call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%set_entry (2, [+1,+1], (1._default, 0._default))
call pmatrix%set_entry (3, [-1,+1], exp ((0._default, -0.9_default)))
call pmatrix%normalize (flv, 0.8_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massive fermion, frac=1"
write (u, "(A)")

call flv%init (11, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)") "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)") "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)

```

```

! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massive fermion, frac=0.8"
write (u, "(A)")

call flv%init (11, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.8_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massless fermion"
write (u, "(A)")

call flv%init (12, model)
call pmatrix%init (2, 0)
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Right-handed massless fermion, frac=0.5"
write (u, "(A)")

call flv%init (-12, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.5_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized gluon, frac=0.3"
write (u, "(A)")

call flv%init (21, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))

```

```

call pmatrix%normalize (flv, 0.3_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)") "* Circularly polarized massive vector, frac=0.7"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.7_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)") "* Circularly polarized massive vector"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)") "* Longitudinally polarized massive vector, frac=0.4"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [0,0], (1._default, 0._default))
call pmatrix%normalize (flv, 0.4_default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)") "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)") "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

```



```

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [0,0], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Axis polarization (0.2, 0.4, 0.6)"
write (u, "(A)")

call flv%init (11, model)
alpha = [0.2_default, 0.4_default, 0.6_default]
alpha = alpha / sqrt (sum (alpha**2))
call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], cmplx (1 - alpha(3), kind=default))
call pmatrix%set_entry (2, [1,-1], &
    cmplx (alpha(1),-alpha(2), kind=default))
call pmatrix%set_entry (3, [1,1], cmplx (1 + alpha(3), kind=default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: polarization_2"

end subroutine polarization_2

```

15.4 Particles

This module defines the `particle_t` object type, and the methods and operations that deal with it.

```
<particles.f90>≡
  <File header>

  module particles

    <Use kinds with double>
    <Use strings>
    <Use debug>
    use lorentz
    use phs_points, only: phs_point_t, assignment(=)
    use model_data
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices
    use interactions
    use subevents
    use polarizations

    <Standard module head>

    <Particles: public>

    <Particles: parameters>

    <Particles: types>

    <Particles: interfaces>

    interface
    <Particles: sub interfaces>
    end interface

  end module particles

<particles_sub.f90>≡
  <File header>

  submodule (particles) particles_s

    use io_units
    use format_utils, only: write_compressed_integer_array, write_separator
    use format_utils, only: pac_fmt
    use format_defs, only: FMT_16, FMT_19
    use numeric_utils
    use diagnostics
    use pdg_arrays, only: is_quark, is_gluon

    implicit none
```

```
contains

⟨Particles: procedures⟩

end submodule particles_s
```

15.4.1 The particle type

Particle status codes

The overall status codes (incoming/outgoing etc.) are inherited from the module `subevents`.

Polarization status:

```
⟨Particles: parameters⟩≡
  integer, parameter, public :: PRT_UNPOLARIZED = 0
  integer, parameter, public :: PRT_DEFINITE_HELICITY = 1
  integer, parameter, public :: PRT_GENERIC_POLARIZATION = 2
```

Definition

The quantum numbers are flavor (from which invariant particle properties can be derived), color, and polarization. The particle may be unpolarized. In this case, `hel` and `pol` are unspecified. If it has a definite helicity, the `hel` component is defined. If it has a generic polarization, the `pol` component is defined. For each particle we store the four-momentum and the invariant mass squared, i.e., the squared norm of the four-momentum. There is also an optional list of parent and child particles, for bookkeeping in physical events. The `vertex` is an optional component that consists of a Lorentz 4-vector, denoting the position and time of the vertex (displaced vertex/time). `lifetime` is an optional component that accounts for the finite lifetime τ of a decaying particle. In case there is no magnetic field etc., the true decay vertex of a particle in the detector would be $\vec{v}' = \vec{v} + \tau \times \vec{p}/p^0$, where p^0 and \vec{p} are the energy and 3-momentum of the particle.

```
⟨Particles: public⟩≡
  public :: particle_t

⟨Particles: types⟩≡
  type :: particle_t
    !private
    integer :: status = PRT_UNDEFINED
    integer :: polarization = PRT_UNPOLARIZED
    type(flavor_t) :: flv
    type(color_t) :: col
    type(helicity_t) :: hel
    type(polarization_t) :: pol
    type(vector4_t) :: p = vector4_null
    real(default) :: p2 = 0
    type(vector4_t), allocatable :: vertex
    real(default), allocatable :: lifetime
```

```

        integer, dimension(:), allocatable :: parent
        integer, dimension(:), allocatable :: child
contains
<Particles: particle: TBP>
end type particle_t

```

Copy a particle. (Deep copy) This excludes the parent-child relations.

```

<Particles: particle: TBP>≡
    generic :: init => init_particle
    procedure :: init_particle => particle_init_particle

<Particles: sub interfaces>≡
    module subroutine particle_init_particle (prt_out, prt_in)
        class(particle_t), intent(out) :: prt_out
        type(particle_t), intent(in) :: prt_in
    end subroutine particle_init_particle

<Particles: procedures>≡
    module subroutine particle_init_particle (prt_out, prt_in)
        class(particle_t), intent(out) :: prt_out
        type(particle_t), intent(in) :: prt_in
        prt_out%status = prt_in%status
        prt_out%polarization = prt_in%polarization
        prt_out%flv = prt_in%flv
        prt_out%col = prt_in%col
        prt_out%hel = prt_in%hel
        prt_out%pol = prt_in%pol
        prt_out%p = prt_in%p
        prt_out%p2 = prt_in%p2
        if (allocated (prt_in%vertex)) &
            allocate (prt_out%vertex, source=prt_in%vertex)
        if (allocated (prt_in%lifetime)) &
            allocate (prt_out%lifetime, source=prt_in%lifetime)
    end subroutine particle_init_particle

```

Initialize a particle using external information.

```

<Particles: particle: TBP>+≡
    generic :: init => init_external
    procedure :: init_external => particle_init_external

<Particles: sub interfaces>+≡
    module subroutine particle_init_external &
        (particle, status, pdg, model, col, anti_col, mom)
        class(particle_t), intent(out) :: particle
        integer, intent(in) :: status, pdg, col, anti_col
        class(model_data_t), pointer, intent(in) :: model
        type(vector4_t), intent(in) :: mom
    end subroutine particle_init_external

<Particles: procedures>+≡
    module subroutine particle_init_external &
        (particle, status, pdg, model, col, anti_col, mom)
        class(particle_t), intent(out) :: particle
        integer, intent(in) :: status, pdg, col, anti_col
        class(model_data_t), pointer, intent(in) :: model

```

```

type(vector4_t), intent(in) :: mom
type(flavor_t) :: flavor
type(color_t) :: color
call flavor%init (pdg, model)
call particle%set_flavor (flavor)
call color%init_col_acl (col, anti_col)
call particle%set_color (color)
call particle%set_status (status)
call particle%set_momentum (mom)
end subroutine particle_init_external

```

Initialize a particle using a single-particle state matrix which determines flavor, color, and polarization. The state matrix must have unique flavor and color. The factorization mode determines whether the particle is unpolarized, has definite helicity, or generic polarization. This mode is translated into the polarization status.

```

⟨Particles: particle: TBP⟩+=
  generic :: init => init_state
  procedure :: init_state => particle_init_state

⟨Particles: sub interfaces⟩+=
  module subroutine particle_init_state (prt, state, status, mode)
    class(particle_t), intent(out) :: prt
    type(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: status, mode
  end subroutine particle_init_state

⟨Particles: procedures⟩+=
  module subroutine particle_init_state (prt, state, status, mode)
    class(particle_t), intent(out) :: prt
    type(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: status, mode
    type(state_iterator_t) :: it
    prt%status = status
    call it%init (state)
    prt%flv = it%get_flavor (1)
    if (prt%flv%is_radiated ()) prt%status = PRT_BEAM_REMNANT
    prt%col = it%get_color (1)
    select case (mode)
    case (FM_SELECT_HELICITY)
      prt%hel = it%get_helicity (1)
      if (prt%hel%is_defined ()) then
        prt%polarization = PRT_DEFINITE_HELICITY
      end if
    case (FM_FACTOR_HELICITY)
      call prt%pol%init_state_matrix (state)
      prt%polarization = PRT_GENERIC_POLARIZATION
    end select
  end subroutine particle_init_state

```

Finalizer.

```

⟨Particles: particle: TBP⟩+=
  procedure :: final => particle_final

```

<Particles: sub interfaces>+≡

```
module subroutine particle_final (prt)
  class(particle_t), intent(inout) :: prt
end subroutine particle_final
```

<Particles: procedures>+≡

```
module subroutine particle_final (prt)
  class(particle_t), intent(inout) :: prt
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  if (allocated (prt%lifetime)) deallocate (prt%lifetime)
end subroutine particle_final
```

I/O

<Particles: particle: TBP>+≡

```
procedure :: write => particle_write
```

<Particles: sub interfaces>+≡

```
module subroutine particle_write (prt, unit, testflag, compressed, polarization)
  class(particle_t), intent(in) :: prt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag, compressed, polarization
end subroutine particle_write
```

<Particles: procedures>+≡

```
module subroutine particle_write (prt, unit, testflag, compressed, polarization)
  class(particle_t), intent(in) :: prt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag, compressed, polarization
  logical :: comp, pacified, pol
  integer :: u, h1, h2
  real(default) :: pp2
  character(len=7) :: fmt
  character(len=20) :: buffer
  comp = .false.; if (present (compressed)) comp = compressed
  pacified = .false.; if (present (testflag)) pacified = testflag
  pol = .true.; if (present (polarization)) pol = polarization
  call pac_fmt (fmt, FMT_19, FMT_16, testflag)
  u = given_output_unit (unit); if (u < 0) return
  pp2 = prt%p2
  if (pacified) call pacify (pp2, tolerance = 1E-10_default)
  select case (prt%status)
  case (PRT_UNDEFINED); write (u, "(1x, A)", advance="no") "[-]"
  case (PRT_BEAM); write (u, "(1x, A)", advance="no") "[b]"
  case (PRT_INCOMING); write (u, "(1x, A)", advance="no") "[i]"
  case (PRT_OUTGOING); write (u, "(1x, A)", advance="no") "[o]"
  case (PRT_VIRTUAL); write (u, "(1x, A)", advance="no") "[v]"
  case (PRT_RESONANT); write (u, "(1x, A)", advance="no") "[r]"
  case (PRT_BEAM_REMNANT); write (u, "(1x, A)", advance="no") "[x]"
  end select
  write (u, "(1x)", advance="no")
  if (comp) then
    write (u, "(A7,1X)", advance="no") char (prt%flv%get_name ())
    if (pol) then
      select case (prt%polarization)
```

```

case (PRT_DEFINITE_HELICITY)
  ! Integer helicity, assumed diagonal
  call prt%hel%get_indices (h1, h2)
  write (u, "(I2,1X)", advance="no") h1
case (PRT_GENERIC_POLARIZATION)
  ! No space for full density matrix here
  write (u, "(A2,1X)", advance="no") "*"
case default
  ! Blank entry if helicity is undefined
  write (u, "(A2,1X)", advance="no") " "
end select
end if
write (u, "(2(I4,1X))", advance="no") &
  prt%col%get_col (), prt%col%get_acl ()
call write_compressed_integer_array (buffer, prt%parent)
write (u, "(A,1X)", advance="no") buffer
call write_compressed_integer_array (buffer, prt%child)
write (u, "(A,1X)", advance="no") buffer
call prt%p%write(u, testflag = testflag, compressed = comp)
write (u, "(F12.3)") pp2
else
  call prt%flv%write (unit)
  if (prt%col%is_nonzero ()) then
    call color_write (prt%col, unit)
  end if
  if (pol) then
    select case (prt%polarization)
    case (PRT_DEFINITE_HELICITY)
      call prt%hel%write (unit)
      write (u, *)
    case (PRT_GENERIC_POLARIZATION)
      write (u, *)
      call prt%pol%write (unit, state_matrix = .true.)
    case default
      write (u, *)
    end select
  else
    write (u, *)
  end if
  call prt%p%write (unit, testflag = testflag)
  write (u, "(1x,A,1x," // fmt // ")") "T = ", pp2
  if (allocated (prt%parent)) then
    if (size (prt%parent) /= 0) then
      write (u, "(1x,A,40(1x,I0))") "Parents: ", prt%parent
    end if
  end if
  if (allocated (prt%child)) then
    if (size (prt%child) /= 0) then
      write (u, "(1x,A,40(1x,I0))") "Children:", prt%child
    end if
  end if
  if (allocated (prt%vertex)) then
    write (u, "(1x,A,1x," // fmt // ")") "Vtx t = ", prt%vertex%p(0)
    write (u, "(1x,A,1x," // fmt // ")") "Vtx x = ", prt%vertex%p(1)
  end if
end if

```

```

        write (u, "(1x,A,1x," // fmt // ")") "Vtx y = ", prt%vertex%p(2)
        write (u, "(1x,A,1x," // fmt // ")") "Vtx z = ", prt%vertex%p(3)
    end if
    if (allocated (prt%lifetime)) then
        write (u, "(1x,A,1x," // fmt // ")") "Lifetime = ", &
            prt%lifetime
    end if
end if
end subroutine particle_write

```

Binary I/O:

```

(Particles: particle: TBP)+≡
    procedure :: write_raw => particle_write_raw
    procedure :: read_raw => particle_read_raw

(Particles: sub interfaces)+≡
    module subroutine particle_write_raw (prt, u)
        class(particle_t), intent(in) :: prt
        integer, intent(in) :: u
    end subroutine particle_write_raw
    module subroutine particle_read_raw (prt, u, iostat)
        class(particle_t), intent(out) :: prt
        integer, intent(in) :: u
        integer, intent(out) :: iostat
    end subroutine particle_read_raw

(Particles: procedures)+≡
    module subroutine particle_write_raw (prt, u)
        class(particle_t), intent(in) :: prt
        integer, intent(in) :: u
        write (u) prt%status, prt%polarization
        call prt%flv%write_raw (u)
        call prt%col%write_raw (u)
        select case (prt%polarization)
        case (PRT_DEFINITE_HELICITY)
            call prt%hel%write_raw (u)
        case (PRT_GENERIC_POLARIZATION)
            call prt%pol%write_raw (u)
        end select
        call vector4_write_raw (prt%p, u)
        write (u) prt%p2
        write (u) allocated (prt%parent)
        if (allocated (prt%parent)) then
            write (u) size (prt%parent)
            write (u) prt%parent
        end if
        write (u) allocated (prt%child)
        if (allocated (prt%child)) then
            write (u) size (prt%child)
            write (u) prt%child
        end if
        write (u) allocated (prt%vertex)
        if (allocated (prt%vertex)) then
            call vector4_write_raw (prt%vertex, u)
        end if
    end if
end if

```



```

write (u) allocated (prt%lifetime)
if (allocated (prt%lifetime)) then
    write (u) prt%lifetime
end if
end subroutine particle_write_raw

module subroutine particle_read_raw (prt, u, iostat)
    class(particle_t), intent(out) :: prt
    integer, intent(in) :: u
    integer, intent(out) :: iostat
    logical :: allocated_parent, allocated_child
    logical :: allocated_vertex, allocated_lifetime
    integer :: size_parent, size_child
    read (u, iostat=iostat) prt%status, prt%polarization
    call prt%flv%read_raw (u, iostat=iostat)
    call prt%col%read_raw (u, iostat=iostat)
    select case (prt%polarization)
    case (PRT_DEFINITE_HELICITY)
        call prt%hel%read_raw (u, iostat=iostat)
    case (PRT_GENERIC_POLARIZATION)
        call prt%pol%read_raw (u, iostat=iostat)
    end select
    call vector4_read_raw (prt%p, u, iostat=iostat)
    read (u, iostat=iostat) prt%p2
    read (u, iostat=iostat) allocated_parent
    if (allocated_parent) then
        read (u, iostat=iostat) size_parent
        allocate (prt%parent (size_parent))
        read (u, iostat=iostat) prt%parent
    end if
    read (u, iostat=iostat) allocated_child
    if (allocated_child) then
        read (u, iostat=iostat) size_child
        allocate (prt%child (size_child))
        read (u, iostat=iostat) prt%child
    end if
    read (u, iostat=iostat) allocated_vertex
    if (allocated_vertex) then
        allocate (prt%vertex)
        read (u, iostat=iostat) prt%vertex%p
    end if
    read (u, iostat=iostat) allocated_lifetime
    if (allocated_lifetime) then
        allocate (prt%lifetime)
        read (u, iostat=iostat) prt%lifetime
    end if
end subroutine particle_read_raw

```

Setting contents

Reset the status code. Where applicable, set p^2 assuming that the particle is on-shell.

```

<Particles: particle: TBP>+≡
    procedure :: reset_status => particle_reset_status

<Particles: sub interfaces>+≡
    elemental module subroutine particle_reset_status (prt, status)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: status
    end subroutine particle_reset_status

<Particles: procedures>+≡
    elemental module subroutine particle_reset_status (prt, status)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: status
        prt%status = status
        select case (status)
        case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING)
            prt%p2 = prt%flv%get_mass () ** 2
        end select
    end subroutine particle_reset_status

```

The color can be given explicitly.

```

<Particles: particle: TBP>+≡
    procedure :: set_color => particle_set_color

<Particles: sub interfaces>+≡
    elemental module subroutine particle_set_color (prt, col)
        class(particle_t), intent(inout) :: prt
        type(color_t), intent(in) :: col
    end subroutine particle_set_color

<Particles: procedures>+≡
    elemental module subroutine particle_set_color (prt, col)
        class(particle_t), intent(inout) :: prt
        type(color_t), intent(in) :: col
        prt%col = col
    end subroutine particle_set_color

```

The flavor can be given explicitly.

```

<Particles: particle: TBP>+≡
    procedure :: set_flavor => particle_set_flavor

<Particles: sub interfaces>+≡
    module subroutine particle_set_flavor (prt, flv)
        class(particle_t), intent(inout) :: prt
        type(flavor_t), intent(in) :: flv
    end subroutine particle_set_flavor

<Particles: procedures>+≡
    module subroutine particle_set_flavor (prt, flv)
        class(particle_t), intent(inout) :: prt
        type(flavor_t), intent(in) :: flv
        prt%flv = flv
    end subroutine particle_set_flavor

```

As can the helicity.

```

(Particles: particle: TBP)+≡
    procedure :: set_helicity => particle_set_helicity

(Particles: sub interfaces)+≡
    module subroutine particle_set_helicity (prt, hel)
        class(particle_t), intent(inout) :: prt
        type(helicity_t), intent(in) :: hel
    end subroutine particle_set_helicity

(Particles: procedures)+≡
    module subroutine particle_set_helicity (prt, hel)
        class(particle_t), intent(inout) :: prt
        type(helicity_t), intent(in) :: hel
        prt%hel = hel
    end subroutine particle_set_helicity

```

And the polarization.

```

(Particles: particle: TBP)+≡
    procedure :: set_pol => particle_set_pol

(Particles: sub interfaces)+≡
    module subroutine particle_set_pol (prt, pol)
        class(particle_t), intent(inout) :: prt
        type(polarization_t), intent(in) :: pol
    end subroutine particle_set_pol

(Particles: procedures)+≡
    module subroutine particle_set_pol (prt, pol)
        class(particle_t), intent(inout) :: prt
        type(polarization_t), intent(in) :: pol
        prt%pol = pol
    end subroutine particle_set_pol

```

Manually set the model for the particle flavor. This is required, e.g., if the particle has been read from file.

```

(Particles: particle: TBP)+≡
    procedure :: set_model => particle_set_model

(Particles: sub interfaces)+≡
    module subroutine particle_set_model (prt, model)
        class(particle_t), intent(inout) :: prt
        class(model_data_t), intent(in), target :: model
    end subroutine particle_set_model

(Particles: procedures)+≡
    module subroutine particle_set_model (prt, model)
        class(particle_t), intent(inout) :: prt
        class(model_data_t), intent(in), target :: model
        call prt%flv%set_model (model)
    end subroutine particle_set_model

```

The momentum is set independent of the quantum numbers.

```

(Particles: particle: TBP)+≡
    procedure :: set_momentum => particle_set_momentum

```

```

<Particles: sub interfaces>+≡
    elemental module subroutine particle_set_momentum (prt, p, p2, on_shell)
        class(particle_t), intent(inout) :: prt
        type(vector4_t), intent(in) :: p
        real(default), intent(in), optional :: p2
        logical, intent(in), optional :: on_shell
    end subroutine particle_set_momentum

<Particles: procedures>+≡
    elemental module subroutine particle_set_momentum (prt, p, p2, on_shell)
        class(particle_t), intent(inout) :: prt
        type(vector4_t), intent(in) :: p
        real(default), intent(in), optional :: p2
        logical, intent(in), optional :: on_shell
        prt%p = p
        if (present (on_shell)) then
            if (on_shell) then
                if (prt%flv%is_associated ()) then
                    prt%p2 = prt%flv%get_mass () ** 2
                    return
                end if
            end if
        end if
        if (present (p2)) then
            prt%p2 = p2
        else
            prt%p2 = p ** 2
        end if
    end subroutine particle_set_momentum

```

Set resonance information. This should be done after momentum assignment, because we need to know whether the particle is spacelike or timelike. The resonance flag is defined only for virtual particles.

```

<Particles: particle: TBP>+≡
    procedure :: set_resonance_flag => particle_set_resonance_flag

<Particles: sub interfaces>+≡
    elemental module subroutine particle_set_resonance_flag (prt, resonant)
        class(particle_t), intent(inout) :: prt
        logical, intent(in) :: resonant
    end subroutine particle_set_resonance_flag

<Particles: procedures>+≡
    elemental module subroutine particle_set_resonance_flag (prt, resonant)
        class(particle_t), intent(inout) :: prt
        logical, intent(in) :: resonant
        select case (prt%status)
            case (PRT_VIRTUAL)
                if (resonant) prt%status = PRT_RESONANT
            end select
    end subroutine particle_set_resonance_flag

```

Set children and parents information.

```

<Particles: particle: TBP>+≡

```

```

    procedure :: set_children => particle_set_children
    procedure :: set_parents => particle_set_parents

    <Particles: sub interfaces>+=
        module subroutine particle_set_children (prt, idx)
            class(particle_t), intent(inout) :: prt
            integer, dimension(:), intent(in) :: idx
        end subroutine particle_set_children
        module subroutine particle_set_parents (prt, idx)
            class(particle_t), intent(inout) :: prt
            integer, dimension(:), intent(in) :: idx
        end subroutine particle_set_parents

    <Particles: procedures>+=
        module subroutine particle_set_children (prt, idx)
            class(particle_t), intent(inout) :: prt
            integer, dimension(:), intent(in) :: idx
            if (allocated (prt%child)) deallocate (prt%child)
            allocate (prt%child (count (idx /= 0)))
            prt%child = pack (idx, idx /= 0)
        end subroutine particle_set_children

        module subroutine particle_set_parents (prt, idx)
            class(particle_t), intent(inout) :: prt
            integer, dimension(:), intent(in) :: idx
            if (allocated (prt%parent)) deallocate (prt%parent)
            allocate (prt%parent (count (idx /= 0)))
            prt%parent = pack (idx, idx /= 0)
        end subroutine particle_set_parents

    <Particles: particle: TBP>+=
        procedure :: add_child => particle_add_child

    <Particles: sub interfaces>+=
        module subroutine particle_add_child (prt, new_child)
            class(particle_t), intent(inout) :: prt
            integer, intent(in) :: new_child
        end subroutine particle_add_child

    <Particles: procedures>+=
        module subroutine particle_add_child (prt, new_child)
            class(particle_t), intent(inout) :: prt
            integer, intent(in) :: new_child
            integer, dimension(:), allocatable :: idx
            integer :: n, i
            n = prt%get_n_children()
            if (n == 0) then
                call prt%set_children ([new_child])
            else
                do i = 1, n
                    if (prt%child(i) == new_child) then
                        return
                    end if
                end do
                allocate (idx (1:n+1))
                idx(1:n) = prt%get_children ()
            end if
        end subroutine particle_add_child

```

```

        idx(n+1) = new_child
        call prt%set_children (idx)
    end if
end subroutine particle_add_child

<Particles: particle: TBP>+≡
    procedure :: add_children => particle_add_children

<Particles: sub interfaces>+≡
    module subroutine particle_add_children (prt, new_child)
        class(particle_t), intent(inout) :: prt
        integer, dimension(:), intent(in) :: new_child
    end subroutine particle_add_children

<Particles: procedures>+≡
    module subroutine particle_add_children (prt, new_child)
        class(particle_t), intent(inout) :: prt
        integer, dimension(:), intent(in) :: new_child
        integer, dimension(:), allocatable :: idx
        integer :: n
        n = prt%get_n_children()
        if (n == 0) then
            call prt%set_children (new_child)
        else
            allocate (idx (1:n+size(new_child)))
            idx(1:n) = prt%get_children ()
            idx(n+1:n+size(new_child)) = new_child
            call prt%set_children (idx)
        end if
    end subroutine particle_add_children

<Particles: particle: TBP>+≡
    procedure :: set_status => particle_set_status

<Particles: sub interfaces>+≡
    elemental module subroutine particle_set_status (prt, status)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: status
    end subroutine particle_set_status

<Particles: procedures>+≡
    elemental module subroutine particle_set_status (prt, status)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: status
        prt%status = status
    end subroutine particle_set_status

<Particles: particle: TBP>+≡
    procedure :: set_polarization => particle_set_polarization

<Particles: sub interfaces>+≡
    module subroutine particle_set_polarization (prt, polarization)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: polarization
    end subroutine particle_set_polarization

```

<Particles: procedures>+≡

```

module subroutine particle_set_polarization (prt, polarization)
  class(particle_t), intent(inout) :: prt
  integer, intent(in) :: polarization
  prt%polarization = polarization
end subroutine particle_set_polarization

```

<Particles: particle: TBP>+≡

```

generic :: set_vertex => set_vertex_from_vector3, set_vertex_from_xyz, &
  set_vertex_from_vector4, set_vertex_from_xyzt
procedure :: set_vertex_from_vector4 => particle_set_vertex_from_vector4
procedure :: set_vertex_from_vector3 => particle_set_vertex_from_vector3
procedure :: set_vertex_from_xyzt => particle_set_vertex_from_xyzt
procedure :: set_vertex_from_xyz => particle_set_vertex_from_xyz

```

<Particles: sub interfaces>+≡

```

module subroutine particle_set_vertex_from_vector4 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector4_t), intent(in) :: vertex
end subroutine particle_set_vertex_from_vector4
module subroutine particle_set_vertex_from_vector3 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector3_t), intent(in) :: vertex
end subroutine particle_set_vertex_from_vector3
module subroutine particle_set_vertex_from_xyzt (prt, vx, vy, vz, t)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: vx, vy, vz, t
end subroutine particle_set_vertex_from_xyzt
module subroutine particle_set_vertex_from_xyz (prt, vx, vy, vz)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: vx, vy, vz
end subroutine particle_set_vertex_from_xyz

```

<Particles: procedures>+≡

```

module subroutine particle_set_vertex_from_vector4 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector4_t), intent(in) :: vertex
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  allocate (prt%vertex, source=vertex)
end subroutine particle_set_vertex_from_vector4

```

```

module subroutine particle_set_vertex_from_vector3 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector3_t), intent(in) :: vertex
  type(vector4_t) :: vtx
  vtx = vector4_moving (0._default, vertex)
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  allocate (prt%vertex, source=vtx)
end subroutine particle_set_vertex_from_vector3

```

```

module subroutine particle_set_vertex_from_xyzt (prt, vx, vy, vz, t)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: vx, vy, vz, t
  type(vector4_t) :: vertex
  if (allocated (prt%vertex)) deallocate (prt%vertex)

```

```

        vertex = vector4_moving (t, vector3_moving ([vx, vy, vz]))
        allocate (prt%vertex, source=vertex)
    end subroutine particle_set_vertex_from_xyz

    module subroutine particle_set_vertex_from_xyz (prt, vx, vy, vz)
        class(particle_t), intent(inout) :: prt
        real(default), intent(in) :: vx, vy, vz
        type(vector4_t) :: vertex
        if (allocated (prt%vertex)) deallocate (prt%vertex)
        vertex = vector4_moving (0._default, vector3_moving ([vx, vy, vz]))
        allocate (prt%vertex, source=vertex)
    end subroutine particle_set_vertex_from_xyz

```

Set the lifetime of a particle.

```

<Particles: particle: TBP>+≡
    procedure :: set_lifetime => particle_set_lifetime

<Particles: sub interfaces>+≡
    elemental module subroutine particle_set_lifetime (prt, lifetime)
        class(particle_t), intent(inout) :: prt
        real(default), intent(in) :: lifetime
    end subroutine particle_set_lifetime

<Particles: procedures>+≡
    elemental module subroutine particle_set_lifetime (prt, lifetime)
        class(particle_t), intent(inout) :: prt
        real(default), intent(in) :: lifetime
        if (allocated (prt%lifetime)) deallocate (prt%lifetime)
        allocate (prt%lifetime, source=lifetime)
    end subroutine particle_set_lifetime

```

Accessing contents

The status code.

```

<Particles: particle: TBP>+≡
    procedure :: get_status => particle_get_status

<Particles: sub interfaces>+≡
    elemental module function particle_get_status (prt) result (status)
        integer :: status
        class(particle_t), intent(in) :: prt
    end function particle_get_status

<Particles: procedures>+≡
    elemental module function particle_get_status (prt) result (status)
        integer :: status
        class(particle_t), intent(in) :: prt
        status = prt%status
    end function particle_get_status

```

Return true if the status is either INCOMING, OUTGOING or RESONANT. BEAM is kept, if keep_beams is set true.

```

<Particles: particle: TBP>+≡
    procedure :: is_real => particle_is_real

```



```

(Particles: sub interfaces)+≡
    elemental module function particle_is_real (prt, keep_beams) result (flag)
        logical :: flag, kb
        class(particle_t), intent(in) :: prt
        logical, intent(in), optional :: keep_beams
    end function particle_is_real

```

```

(Particles: procedures)+≡
    elemental module function particle_is_real (prt, keep_beams) result (flag)
        logical :: flag, kb
        class(particle_t), intent(in) :: prt
        logical, intent(in), optional :: keep_beams
        kb = .false.
        if (present (keep_beams)) kb = keep_beams
        select case (prt%status)
        case (PRT_INCOMING, PRT_OUTGOING, PRT_RESONANT)
            flag = .true.
        case (PRT_BEAM)
            flag = kb
        case default
            flag = .false.
        end select
    end function particle_is_real

```

```

(Particles: particle: TBP)+≡
    procedure :: is_colored => particle_is_colored

```

```

(Particles: sub interfaces)+≡
    elemental module function particle_is_colored (particle) result (flag)
        logical :: flag
        class(particle_t), intent(in) :: particle
    end function particle_is_colored

```

```

(Particles: procedures)+≡
    elemental module function particle_is_colored (particle) result (flag)
        logical :: flag
        class(particle_t), intent(in) :: particle
        flag = particle%col%is_nonzero ()
    end function particle_is_colored

```

[90,100] hopefully catches all of them and not too many.

```

(Particles: particle: TBP)+≡
    procedure :: is_hadronic_beam_remnant => particle_is_hadronic_beam_remnant

```

```

(Particles: sub interfaces)+≡
    elemental module function particle_is_hadronic_beam_remnant (particle) result (flag)
        class(particle_t), intent(in) :: particle
        logical :: flag
    end function particle_is_hadronic_beam_remnant

```

```

(Particles: procedures)+≡
    elemental module function particle_is_hadronic_beam_remnant (particle) result (flag)
        class(particle_t), intent(in) :: particle
        logical :: flag
        integer :: pdg
        pdg = particle%flv%get_pdg ()

```

```

        flag = particle%status == PRT_BEAM_REMNANT .and. &
              abs(pdg) >= 90 .and. abs(pdg) <= 100
    end function particle_is_hadronic_beam_remnant

```

<Particles: particle: TBP>+≡

```

    procedure :: is_beam_remnant => particle_is_beam_remnant

```

<Particles: sub interfaces>+≡

```

    elemental module function particle_is_beam_remnant (particle) result (flag)
        class(particle_t), intent(in) :: particle
        logical :: flag
    end function particle_is_beam_remnant

```

<Particles: procedures>+≡

```

    elemental module function particle_is_beam_remnant (particle) result (flag)
        class(particle_t), intent(in) :: particle
        logical :: flag
        flag = particle%status == PRT_BEAM_REMNANT
    end function particle_is_beam_remnant

```

Polarization status.

<Particles: particle: TBP>+≡

```

    procedure :: get_polarization_status => particle_get_polarization_status

```

<Particles: sub interfaces>+≡

```

    elemental module function particle_get_polarization_status (prt) result (status)
        integer :: status
        class(particle_t), intent(in) :: prt
    end function particle_get_polarization_status

```

<Particles: procedures>+≡

```

    elemental module function particle_get_polarization_status (prt) result (status)
        integer :: status
        class(particle_t), intent(in) :: prt
        status = prt%polarization
    end function particle_get_polarization_status

```

Return the PDG code from the flavor component directly.

<Particles: particle: TBP>+≡

```

    procedure :: get_pdg => particle_get_pdg

```

<Particles: sub interfaces>+≡

```

    elemental module function particle_get_pdg (prt) result (pdg)
        integer :: pdg
        class(particle_t), intent(in) :: prt
    end function particle_get_pdg

```

<Particles: procedures>+≡

```

    elemental module function particle_get_pdg (prt) result (pdg)
        integer :: pdg
        class(particle_t), intent(in) :: prt
        pdg = prt%flv%get_pdg ()
    end function particle_get_pdg

```

Return the color and anticolor quantum numbers.

```

(Particles: particle: TBP)+≡
  procedure :: get_color => particle_get_color

(Particles: sub interfaces)+≡
  pure module function particle_get_color (prt) result (col)
    integer, dimension(2) :: col
    class(particle_t), intent(in) :: prt
  end function particle_get_color

(Particles: procedures)+≡
  pure module function particle_get_color (prt) result (col)
    integer, dimension(2) :: col
    class(particle_t), intent(in) :: prt
    col(1) = prt%col%get_col ()
    col(2) = prt%col%get_acl ()
  end function particle_get_color

```

Return a copy of the polarization density matrix.

```

(Particles: particle: TBP)+≡
  procedure :: get_polarization => particle_get_polarization

(Particles: sub interfaces)+≡
  module function particle_get_polarization (prt) result (pol)
    class(particle_t), intent(in) :: prt
    type(polarization_t) :: pol
  end function particle_get_polarization

(Particles: procedures)+≡
  module function particle_get_polarization (prt) result (pol)
    class(particle_t), intent(in) :: prt
    type(polarization_t) :: pol
    pol = prt%pol
  end function particle_get_polarization

```

Return the flavor, color and helicity.

```

(Particles: particle: TBP)+≡
  procedure :: get_flv => particle_get_flv
  procedure :: get_col => particle_get_col
  procedure :: get_hel => particle_get_hel

(Particles: sub interfaces)+≡
  module function particle_get_flv (prt) result (flv)
    class(particle_t), intent(in) :: prt
    type(flavor_t) :: flv
  end function particle_get_flv
  module function particle_get_col (prt) result (col)
    class(particle_t), intent(in) :: prt
    type(color_t) :: col
  end function particle_get_col
  module function particle_get_hel (prt) result (hel)
    class(particle_t), intent(in) :: prt
    type(helicity_t) :: hel
  end function particle_get_hel

```

```

<Particles: procedures>+≡
module function particle_get_flv (prt) result (flv)
  class(particle_t), intent(in) :: prt
  type(flavor_t) :: flv
  flv = prt%flv
end function particle_get_flv

module function particle_get_col (prt) result (col)
  class(particle_t), intent(in) :: prt
  type(color_t) :: col
  col = prt%col
end function particle_get_col

module function particle_get_hel (prt) result (hel)
  class(particle_t), intent(in) :: prt
  type(helicity_t) :: hel
  hel = prt%hel
end function particle_get_hel

```

Return the helicity (if defined and diagonal).

```

<Particles: particle: TBP>+≡
  procedure :: get_helicity => particle_get_helicity

<Particles: sub interfaces>+≡
  elemental module function particle_get_helicity (prt) result (hel)
    integer :: hel
    class(particle_t), intent(in) :: prt
  end function particle_get_helicity

<Particles: procedures>+≡
  elemental module function particle_get_helicity (prt) result (hel)
    integer :: hel
    integer, dimension(2) :: hel_arr
    class(particle_t), intent(in) :: prt
    hel = 0
    if (prt%hel%is_defined () .and. prt%hel%is_diagonal ()) then
      hel_arr = prt%hel%to_pair ()
      hel = hel_arr (1)
    end if
  end function particle_get_helicity

```

Return the number of children/parents

```

<Particles: particle: TBP>+≡
  procedure :: get_n_parents => particle_get_n_parents
  procedure :: get_n_children => particle_get_n_children

<Particles: sub interfaces>+≡
  elemental module function particle_get_n_parents (prt) result (n)
    integer :: n
    class(particle_t), intent(in) :: prt
  end function particle_get_n_parents
  elemental module function particle_get_n_children (prt) result (n)
    integer :: n
    class(particle_t), intent(in) :: prt
  end function particle_get_n_children

```

```

(Particles: procedures) +=
  elemental module function particle_get_n_parents (prt) result (n)
    integer :: n
    class(particle_t), intent(in) :: prt
    if (allocated (prt%parent)) then
      n = size (prt%parent)
    else
      n = 0
    end if
  end function particle_get_n_parents

  elemental module function particle_get_n_children (prt) result (n)
    integer :: n
    class(particle_t), intent(in) :: prt
    if (allocated (prt%child)) then
      n = size (prt%child)
    else
      n = 0
    end if
  end function particle_get_n_children

```

Return the array of parents/children.

```

(Particles: particle: TBP) +=
  procedure :: get_parents => particle_get_parents
  procedure :: get_children => particle_get_children

(Particles: sub interfaces) +=
  module function particle_get_parents (prt) result (parent)
    class(particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: parent
  end function particle_get_parents
  module function particle_get_children (prt) result (child)
    class(particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: child
  end function particle_get_children

(Particles: procedures) +=
  module function particle_get_parents (prt) result (parent)
    class(particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: parent
    if (allocated (prt%parent)) then
      allocate (parent (size (prt%parent)))
      parent = prt%parent
    else
      allocate (parent (0))
    end if
  end function particle_get_parents

  module function particle_get_children (prt) result (child)
    class(particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: child
    if (allocated (prt%child)) then
      allocate (child (size (prt%child)))
      child = prt%child
    else

```

```

        allocate (child (0))
    end if
end function particle_get_children

<Particles: particle: TBP>+≡
    procedure :: has_children => particle_has_children

<Particles: sub interfaces>+≡
    elemental module function particle_has_children (prt) result (has_children)
        logical :: has_children
        class(particle_t), intent(in) :: prt
    end function particle_has_children

<Particles: procedures>+≡
    elemental module function particle_has_children (prt) result (has_children)
        logical :: has_children
        class(particle_t), intent(in) :: prt
        has_children = .false.
        if (allocated (prt%child)) then
            has_children = size (prt%child) > 0
        end if
    end function particle_has_children

<Particles: particle: TBP>+≡
    procedure :: has_parents => particle_has_parents

<Particles: sub interfaces>+≡
    elemental module function particle_has_parents (prt) result (has_parents)
        logical :: has_parents
        class(particle_t), intent(in) :: prt
    end function particle_has_parents

<Particles: procedures>+≡
    elemental module function particle_has_parents (prt) result (has_parents)
        logical :: has_parents
        class(particle_t), intent(in) :: prt
        has_parents = .false.
        if (allocated (prt%parent)) then
            has_parents = size (prt%parent) > 0
        end if
    end function particle_has_parents

Return momentum and momentum squared.

<Particles: particle: TBP>+≡
    procedure :: get_momentum => particle_get_momentum
    procedure :: get_p2 => particle_get_p2

<Particles: sub interfaces>+≡
    elemental module function particle_get_momentum (prt) result (p)
        type(vector4_t) :: p
        class(particle_t), intent(in) :: prt
    end function particle_get_momentum
    elemental module function particle_get_p2 (prt) result (p2)
        real(default) :: p2
        class(particle_t), intent(in) :: prt
    end function particle_get_p2

```

```

<Particles: procedures>+≡
  elemental module function particle_get_momentum (prt) result (p)
    type(vector4_t) :: p
    class(particle_t), intent(in) :: prt
    p = prt%p
  end function particle_get_momentum

  elemental module function particle_get_p2 (prt) result (p2)
    real(default) :: p2
    class(particle_t), intent(in) :: prt
    p2 = prt%p2
  end function particle_get_p2

```

Return the particle vertex, if allocated.

```

<Particles: particle: TBP>+≡
  procedure :: get_vertex => particle_get_vertex

<Particles: sub interfaces>+≡
  elemental module function particle_get_vertex (prt) result (vtx)
    type(vector4_t) :: vtx
    class(particle_t), intent(in) :: prt
  end function particle_get_vertex

<Particles: procedures>+≡
  elemental module function particle_get_vertex (prt) result (vtx)
    type(vector4_t) :: vtx
    class(particle_t), intent(in) :: prt
    if (allocated (prt%vertex)) then
      vtx = prt%vertex
    else
      vtx = vector4_null
    end if
  end function particle_get_vertex

```

Return the lifetime of a particle.

```

<Particles: particle: TBP>+≡
  procedure :: get_lifetime => particle_get_lifetime

<Particles: sub interfaces>+≡
  elemental module function particle_get_lifetime (prt) result (lifetime)
    real(default) :: lifetime
    class(particle_t), intent(in) :: prt
  end function particle_get_lifetime

<Particles: procedures>+≡
  elemental module function particle_get_lifetime (prt) result (lifetime)
    real(default) :: lifetime
    class(particle_t), intent(in) :: prt
    if (allocated (prt%lifetime)) then
      lifetime = prt%lifetime
    else
      lifetime = 0
    end if
  end function particle_get_lifetime

```

```

⟨Particles: particle: TBP⟩+≡
    procedure :: momentum_to_pythia6 => particle_momentum_to_pythia6

⟨Particles: sub interfaces⟩+≡
    pure module function particle_momentum_to_pythia6 (prt) result (p)
        real(double), dimension(1:5) :: p
        class(particle_t), intent(in) :: prt
    end function particle_momentum_to_pythia6

⟨Particles: procedures⟩+≡
    pure module function particle_momentum_to_pythia6 (prt) result (p)
        real(double), dimension(1:5) :: p
        class(particle_t), intent(in) :: prt
        p = prt%p%to_pythia6 (sqrt (prt%p2))
    end function particle_momentum_to_pythia6

```

15.4.2 Particle sets

A particle set is what is usually called an event: an array of particles. The individual particle entries carry momentum, quantum numbers, polarization, and optionally connections. There is (also optionally) a correlated state-density matrix that maintains spin correlations that are lost in the individual particle entries.

```

⟨Particles: public⟩+≡
    public :: particle_set_t

⟨Particles: types⟩+≡
    type :: particle_set_t
        ! private !!!
        integer :: n_beam = 0
        integer :: n_in = 0
        integer :: n_vir = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        integer :: factorization_mode = FM_IGNORE_HELICITY
        type(particle_t), dimension(:), allocatable :: prt
        type(state_matrix_t) :: correlated_state
    contains
        ⟨Particles: particle set: TBP⟩
    end type particle_set_t

```

A particle set can be initialized from an interaction or from a HepMC event record.

```

⟨Particles: particle set: TBP⟩≡
    generic :: init => init_interaction
    procedure :: init_interaction => particle_set_init_interaction

```

When a particle set is initialized from a given interaction, we have to determine the branch within the original state matrix that fixes the particle quantum numbers. This is done with the appropriate probabilities, based on a random number `x`. The `mode` determines whether the individual particles become unpolarized, or take a definite (diagonal) helicity, or acquire single-particle polarization matrices. The flag `keep_correlations` tells whether the spin-correlation matrix is

to be calculated and stored in addition to the particles. The flag `keep_virtual` tells whether virtual particles should be dropped. Note that if virtual particles are dropped, the spin-correlation matrix makes no sense, and parent-child relations are not set.

For a correct disentangling of color and flavor (in the presence of helicity), we consider two interactions. `int` has no color information, and is used to select a flavor state. Consequently, we trace over helicities here. `int_flows` contains color-flow and potentially helicity information, but is useful only after the flavor combination has been chosen. So this interaction is used to select helicity and color, but restricted to the selected flavor combination.

`int` and `int_flows` may be identical if there is only a single (or no) color flow. If there is just a single flavor combination, `x(1)` can be set to zero.

The current algorithm of evaluator convolution requires that the beam particles are assumed outgoing (in the beam interaction) and become virtual in all derived interactions. In the particle set they should be re-identified as incoming. The optional integer `n_incoming` can be used to perform this correction.

The flag `is_valid` is false if factorization of the state is not possible, in particular if the squared matrix element is zero.

(Particles: sub interfaces)+≡

```

module subroutine particle_set_init_interaction &
  (particle_set, is_valid, int, int_flows, mode, x, &
   keep_correlations, keep_virtual, n_incoming, qn_select)
class(particle_set_t), intent(out) :: particle_set
logical, intent(out) :: is_valid
type(interaction_t), intent(in), target :: int, int_flows
integer, intent(in) :: mode
real(default), dimension(2), intent(in) :: x
logical, intent(in) :: keep_correlations, keep_virtual
integer, intent(in), optional :: n_incoming
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
end subroutine particle_set_init_interaction

```

(Particles: procedures)+≡

```

module subroutine particle_set_init_interaction &
  (particle_set, is_valid, int, int_flows, mode, x, &
   keep_correlations, keep_virtual, n_incoming, qn_select)
class(particle_set_t), intent(out) :: particle_set
logical, intent(out) :: is_valid
type(interaction_t), intent(in), target :: int, int_flows
integer, intent(in) :: mode
real(default), dimension(2), intent(in) :: x
logical, intent(in) :: keep_correlations, keep_virtual
integer, intent(in), optional :: n_incoming
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
type(state_matrix_t), dimension(:), allocatable, target :: flavor_state
type(state_matrix_t), dimension(:), allocatable, target :: single_state
integer :: n_in, n_vir, n_out, n_tot
type(quantum_numbers_t), dimension(:,:), allocatable :: qn
logical :: ok
integer :: i, j
if (present (n_incoming)) then
  n_in = n_incoming
  n_vir = int%get_n_vir () - n_incoming

```

```

else
  n_in = int%get_n_in ()
  n_vir = int%get_n_vir ()
end if
n_out = int%get_n_out ()
n_tot = int%get_n_tot ()
particle_set%n_in = n_in
particle_set%n_out = n_out
if (keep_virtual) then
  particle_set%n_vir = n_vir
  particle_set%n_tot = n_tot
else
  particle_set%n_vir = 0
  particle_set%n_tot = n_in + n_out
end if
particle_set%factorization_mode = mode
allocate (qn (n_tot, 1))
if (.not. present (qn_select)) then
  call int%factorize &
    (FM_IGNORE_HELICITY, x(1), is_valid, flavor_state)
  do i = 1, n_tot
    qn(i,:) = flavor_state(i)%get_quantum_number (1)
  end do
else
  do i = 1, n_tot
    qn(i,:) = qn_select(i)
  end do
  is_valid = .true.
end if
if (keep_correlations .and. keep_virtual) then
  call particle_set%correlated_state%final ()
  call int_flows%factorize (mode, x(2), ok, &
    single_state, particle_set%correlated_state, qn(:,1))
else
  call int_flows%factorize (mode, x(2), ok, &
    single_state, qn_in=qn(:,1))
end if
is_valid = is_valid .and. ok
allocate (particle_set%prt (particle_set%n_tot))
j = 1
do i = 1, n_tot
  if (i <= n_in) then
    call particle_set%prt(j)%init (single_state(i), PRT_INCOMING, mode)
    call particle_set%prt(j)%set_momentum (int%get_momentum (i))
  else if (i <= n_in + n_vir) then
    if (.not. keep_virtual) cycle
    call particle_set%prt(j)%init &
      (single_state(i), PRT_VIRTUAL, mode)
    call particle_set%prt(j)%set_momentum (int%get_momentum (i))
  else
    call particle_set%prt(j)%init (single_state(i), PRT_OUTGOING, mode)
    call particle_set%prt(j)%set_momentum &
      (int%get_momentum (i), on_shell = .true.)
  end if
  j = j + 1
end do
end if

```

```

        if (keep_virtual) then
            call particle_set%prt(j)%set_children (int%get_children (i))
            call particle_set%prt(j)%set_parents (int%get_parents (i))
        end if
        j = j + 1
    end do
    if (keep_virtual) then
        call particle_set_resonance_flag &
            (particle_set%prt, int%get_resonance_flags ())
    end if
    if (allocated (flavor_state)) then
        do i = 1, size(flavor_state)
            call flavor_state(i)%final ()
        end do
    end if
    do i = 1, size(single_state)
        call single_state(i)%final ()
    end do
end subroutine particle_set_init_interaction

```

Duplicate generic binding, to make sure that assignment works as it should.

```

⟨Particles: particle set: TBP⟩+≡
    generic :: assignment(=) => init_particle_set
    generic :: init => init_particle_set
    procedure :: init_particle_set => particle_set_init_particle_set

⟨Particles: sub interfaces⟩+≡
    module subroutine particle_set_init_particle_set (pset_out, pset_in)
        class(particle_set_t), intent(out) :: pset_out
        type(particle_set_t), intent(in) :: pset_in
    end subroutine particle_set_init_particle_set

⟨Particles: procedures⟩+≡
    module subroutine particle_set_init_particle_set (pset_out, pset_in)
        class(particle_set_t), intent(out) :: pset_out
        type(particle_set_t), intent(in) :: pset_in
        integer :: i
        pset_out%n_beam = pset_in%n_beam
        pset_out%n_in   = pset_in%n_in
        pset_out%n_vir  = pset_in%n_vir
        pset_out%n_out  = pset_in%n_out
        pset_out%n_tot  = pset_in%n_tot
        pset_out%factorization_mode = pset_in%factorization_mode
        if (allocated (pset_in%prt)) then
            allocate (pset_out%prt (size (pset_in%prt)))
            do i = 1, size (pset_in%prt)
                pset_out%prt(i) = pset_in%prt(i)
            end do
        end if
        pset_out%correlated_state = pset_in%correlated_state
    end subroutine particle_set_init_particle_set

```

Manually set the model for the stored particles.

```

⟨Particles: particle set: TBP⟩+≡

```

```

    procedure :: set_model => particle_set_set_model
  <Particles: sub interfaces>+≡
    module subroutine particle_set_set_model (particle_set, model)
      class(particle_set_t), intent(inout) :: particle_set
      class(model_data_t), intent(in), target :: model
    end subroutine particle_set_set_model
  <Particles: procedures>+≡
    module subroutine particle_set_set_model (particle_set, model)
      class(particle_set_t), intent(inout) :: particle_set
      class(model_data_t), intent(in), target :: model
      integer :: i
      do i = 1, particle_set%n_tot
        call particle_set%prt(i)%set_model (model)
      end do
      call particle_set%correlated_state%set_model (model)
    end subroutine particle_set_set_model

```

Pointer components are hidden inside the particle polarization, and in the correlated state matrix.

```

  <Particles: particle set: TBP>+≡
    procedure :: final => particle_set_final
  <Particles: sub interfaces>+≡
    module subroutine particle_set_final (particle_set)
      class(particle_set_t), intent(inout) :: particle_set
    end subroutine particle_set_final
  <Particles: procedures>+≡
    module subroutine particle_set_final (particle_set)
      class(particle_set_t), intent(inout) :: particle_set
      integer :: i
      if (allocated (particle_set%prt)) then
        do i = 1, size(particle_set%prt)
          call particle_set%prt(i)%final ()
        end do
        deallocate (particle_set%prt)
      end if
      call particle_set%correlated_state%final ()
    end subroutine particle_set_final

```

15.4.3 Manual build

Basic initialization. Just allocate with a given number of beam, incoming, virtual, and outgoing particles.

```

  <Particles: particle set: TBP>+≡
    procedure :: basic_init => particle_set_basic_init
  <Particles: sub interfaces>+≡
    module subroutine particle_set_basic_init (particle_set, n_beam, n_in, n_vir, n_out)
      class(particle_set_t), intent(out) :: particle_set
      integer, intent(in) :: n_beam, n_in, n_vir, n_out
    end subroutine particle_set_basic_init

```

<Particles: procedures>+≡

```

module subroutine particle_set_basic_init (particle_set, n_beam, n_in, n_vir, n_out)
  class(particle_set_t), intent(out) :: particle_set
  integer, intent(in) :: n_beam, n_in, n_vir, n_out
  particle_set%n_beam = n_beam
  particle_set%n_in = n_in
  particle_set%n_vir = n_vir
  particle_set%n_out = n_out
  particle_set%n_tot = n_beam + n_in + n_vir + n_out
  allocate (particle_set%prt (particle_set%n_tot))
end subroutine particle_set_basic_init

```

Build a particle set from scratch. This is used for testing purposes. The ordering of particles in the result is beam-incoming-remnant-virtual-outgoing.

Parent-child relations:

- Beams are parents of incoming and beam remnants. The assignment is alternating (first beam, second beam).
- Incoming are parents of virtual and outgoing, collectively.

More specific settings, such as resonance histories, cannot be set this way.

Beam-remnant particles are counted as virtual, but have a different status code.

We assume that the `pdg` array has the correct size.

<Particles: particle set: TBP>+≡

```

procedure :: init_direct => particle_set_init_direct

```

<Particles: sub interfaces>+≡

```

module subroutine particle_set_init_direct (particle_set, &
  n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
  class(particle_set_t), intent(out) :: particle_set
  integer, intent(in) :: n_beam
  integer, intent(in) :: n_in
  integer, intent(in) :: n_rem
  integer, intent(in) :: n_vir
  integer, intent(in) :: n_out
  integer, dimension(:), intent(in) :: pdg
  class(model_data_t), intent(in), target :: model
end subroutine particle_set_init_direct

```

<Particles: procedures>+≡

```

module subroutine particle_set_init_direct (particle_set, &
  n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
  class(particle_set_t), intent(out) :: particle_set
  integer, intent(in) :: n_beam
  integer, intent(in) :: n_in
  integer, intent(in) :: n_rem
  integer, intent(in) :: n_vir
  integer, intent(in) :: n_out
  integer, dimension(:), intent(in) :: pdg
  class(model_data_t), intent(in), target :: model
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: i, k, n
  call particle_set%basic_init (n_beam, n_in, n_rem+n_vir, n_out)

```

```

n = 0
call particle_set%prt(n+1:n+n_beam)%reset_status (PRT_BEAM)
do i = n+1, n+n_beam
    call particle_set%prt(i)%set_children &
        ([[k, k=i+n_beam, n+n_beam+n_in+n_rem, 2]])
end do
n = n + n_beam
call particle_set%prt(n+1:n+n_in)%reset_status (PRT_INCOMING)
do i = n+1, n+n_in
    if (n_beam > 0) then
        call particle_set%prt(i)%set_parents &
            ([i-n_beam])
    end if
    call particle_set%prt(i)%set_children &
        ([[k, k=n+n_in+n_rem+1, n+n_in+n_rem+n_vir+n_out]])
end do
n = n + n_in
call particle_set%prt(n+1:n+n_rem)%reset_status (PRT_BEAM_REMNANT)
do i = n+1, n+n_rem
    if (n_beam > 0) then
        call particle_set%prt(i)%set_parents &
            ([i-n_in-n_beam])
    end if
end do
n = n + n_rem
call particle_set%prt(n+1:n+n_vir)%reset_status (PRT_VIRTUAL)
do i = n+1, n+n_vir
    call particle_set%prt(i)%set_parents &
        ([[k, k=n-n_rem-n_in+1, n-n_rem]])
end do
n = n + n_vir
call particle_set%prt(n+1:n+n_out)%reset_status (PRT_OUTGOING)
do i = n+1, n+n_out
    call particle_set%prt(i)%set_parents &
        ([[k, k=n-n_vir-n_rem-n_in+1, n-n_vir-n_rem]])
end do
allocate (flv (particle_set%n_tot))
call flv%init (pdg, model)
do k = n_beam+n_in+1, n_beam+n_in+n_rem
    call flv(k)%tag_radiated ()
end do
do i = 1, particle_set%n_tot
    call particle_set%prt(i)%set_flavor (flv(i))
end do
end subroutine particle_set_init_direct

```

Copy a particle set into a new, extended one. Use the mapping array to determine the new positions of particles. The new set contains **n_new** additional entries. Count the new, undefined particles as virtual.

<Particles: particle set: TBP>+≡

procedure :: transfer => particle_set_transfer

<Particles: sub interfaces>+≡

module subroutine particle_set_transfer (pset, source, n_new, map)

```

        class(particle_set_t), intent(out) :: pset
        class(particle_set_t), intent(in) :: source
        integer, intent(in) :: n_new
        integer, dimension(:), intent(in) :: map
    end subroutine particle_set_transfer
<Particles: procedures>+≡
    module subroutine particle_set_transfer (pset, source, n_new, map)
        class(particle_set_t), intent(out) :: pset
        class(particle_set_t), intent(in) :: source
        integer, intent(in) :: n_new
        integer, dimension(:), intent(in) :: map
        integer :: i
        call pset%basic_init &
            (source%n_beam, source%n_in, source%n_vir + n_new, source%n_out)
        pset%factorization_mode = source%factorization_mode
        do i = 1, source%n_tot
            call pset%prt(map(i))%reset_status (source%prt(i)%get_status ())
            call pset%prt(map(i))%set_flavor (source%prt(i)%get_flv ())
            call pset%prt(map(i))%set_color (source%prt(i)%get_col ())
            call pset%prt(map(i))%set_parents (map (source%prt(i)%get_parents ()))
            call pset%prt(map(i))%set_children (map (source%prt(i)%get_children ()))
            call pset%prt(map(i))%set_polarization &
                (source%prt(i)%get_polarization_status ())
            select case (source%prt(i)%get_polarization_status ())
            case (PRT_DEFINITE_HELICITY)
                call pset%prt(map(i))%set_helicity (source%prt(i)%get_hel ())
            case (PRT_GENERIC_POLARIZATION)
                call pset%prt(map(i))%set_pol (source%prt(i)%get_polarization ())
            end select
        end do
    end subroutine particle_set_transfer

```

Insert a new particle as an intermediate into a previously empty position.

Flavor and status are just set. Color is not set (but see below). The complicated part is reassigning parent-child relations. The inserted particle comes with an array `child` of its children which are supposed to be existing particles.

We first scan all particles that come before the new insertion. Whenever a particle has children that coincide with the children of the new particle, those child entries are removed. (a) If the new particle has no parent entry yet, those child entries are replaced by the index of the new particle and simultaneously, the particle is registered as a parent of the new particle. (b) If the current particle already has a parent entry, those child entries are removed.

When this is done, the new particle is registered as the (only) parent of its children.

```

<Particles: particle set: TBP>+≡
    procedure :: insert => particle_set_insert
<Particles: sub interfaces>+≡
    module subroutine particle_set_insert (pset, i, status, flv, child)
        class(particle_set_t), intent(inout) :: pset
        integer, intent(in) :: i
        integer, intent(in) :: status
        type(flavor_t), intent(in) :: flv

```

```

        integer, dimension(:), intent(in) :: child
    end subroutine particle_set_insert

    <Particles: procedures>+≡
    module subroutine particle_set_insert (pset, i, status, flv, child)
        class(particle_set_t), intent(inout) :: pset
        integer, intent(in) :: i
        integer, intent(in) :: status
        type(flavor_t), intent(in) :: flv
        integer, dimension(:), intent(in) :: child
        integer, dimension(:), allocatable :: p_child, parent
        integer :: j, k, c, n_parent
        logical :: no_match
        call pset%prt(i)%reset_status (status)
        call pset%prt(i)%set_flavor (flv)
        call pset%prt(i)%set_children (child)
        n_parent = pset%prt(i)%get_n_parents ()
        do j = 1, i - 1
            p_child = pset%prt(j)%get_children ()
            no_match = .true.
            do k = 1, size (p_child)
                if (any (p_child(k) == child)) then
                    if (n_parent == 0 .and. no_match) then
                        if (.not. allocated (parent)) then
                            parent = [j]
                        else
                            parent = [parent, j]
                        end if
                        p_child(k) = i
                    else
                        p_child(k) = 0
                    end if
                    no_match = .false.
                end if
            end do
            if (.not. no_match) then
                p_child = pack (p_child, p_child /= 0)
                call pset%prt(j)%set_children (p_child)
            end if
        end do
        if (n_parent == 0) then
            call pset%prt(i)%set_parents (parent)
        end if
        do j = 1, size (child)
            c = child(j)
            call pset%prt(c)%set_parents ([i])
        end do
    end subroutine particle_set_insert

```

This should be done after completing all insertions: recover color assignments for the inserted particles, working backwards from children to parents. A single call to the routine recovers the color and anticolor line indices for a single particle.

```

    <Particles: particle set: TBP>+≡
    procedure :: recover_color => particle_set_recover_color

```



```

(Particles: sub interfaces) +=
    module subroutine particle_set_recover_color (pset, i)
        class(particle_set_t), intent(inout) :: pset
        integer, intent(in) :: i
    end subroutine particle_set_recover_color

```

```

(Particles: procedures) +=
    module subroutine particle_set_recover_color (pset, i)
        class(particle_set_t), intent(inout) :: pset
        integer, intent(in) :: i
        type(color_t) :: col
        integer, dimension(:), allocatable :: child
        integer :: j
        child = pset%prt(i)%get_children ()
        if (size (child) > 0) then
            col = pset%prt(child(1))%get_col ()
            do j = 2, size (child)
                col = col .fuse. pset%prt(child(j))%get_col ()
            end do
            call pset%prt(i)%set_color (col)
        end if
    end subroutine particle_set_recover_color

```

15.4.4 Extract/modify contents

```

(Particles: particle set: TBP) +=
    generic :: get_color => get_color_all
    generic :: get_color => get_color_indices
    procedure :: get_color_all => particle_set_get_color_all
    procedure :: get_color_indices => particle_set_get_color_indices

```

```

(Particles: sub interfaces) +=
    module function particle_set_get_color_all (particle_set) result (col)
        class(particle_set_t), intent(in) :: particle_set
        type(color_t), dimension(:), allocatable :: col
    end function particle_set_get_color_all

```

```

(Particles: procedures) +=
    module function particle_set_get_color_all (particle_set) result (col)
        class(particle_set_t), intent(in) :: particle_set
        type(color_t), dimension(:), allocatable :: col
        allocate (col (size (particle_set%prt)))
        col = particle_set%prt%col
    end function particle_set_get_color_all

```

```

(Particles: sub interfaces) +=
    module function particle_set_get_color_indices (particle_set, indices) result (col)
        type(color_t), dimension(:), allocatable :: col
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in), dimension(:), allocatable :: indices
    end function particle_set_get_color_indices

```

<Particles: procedures>+≡

```

module function particle_set_get_color_indices (particle_set, indices) result (col)
  type(color_t), dimension(:), allocatable :: col
  class(particle_set_t), intent(in) :: particle_set
  integer, intent(in), dimension(:), allocatable :: indices
  integer :: i
  allocate (col (size (indices)))
  do i = 1, size (indices)
    col(i) = particle_set%prt(indices(i))%col
  end do
end function particle_set_get_color_indices

```

Set a single or all color components. This is a wrapper around the corresponding `particle_t` method, with the same options. We assume that the particle array is allocated.

<Particles: particle set: TBP>+≡

```

generic :: set_color => set_color_single
generic :: set_color => set_color_indices
generic :: set_color => set_color_all
procedure :: set_color_single => particle_set_set_color_single
procedure :: set_color_indices => particle_set_set_color_indices
procedure :: set_color_all => particle_set_set_color_all

```

<Particles: sub interfaces>+≡

```

module subroutine particle_set_set_color_single (particle_set, i, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, intent(in) :: i
  type(color_t), intent(in) :: col
end subroutine particle_set_set_color_single
module subroutine particle_set_set_color_indices (particle_set, indices, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, dimension(:), intent(in) :: indices
  type(color_t), dimension(:), intent(in) :: col
end subroutine particle_set_set_color_indices
module subroutine particle_set_set_color_all (particle_set, col)
  class(particle_set_t), intent(inout) :: particle_set
  type(color_t), dimension(:), intent(in) :: col
end subroutine particle_set_set_color_all

```

<Particles: procedures>+≡

```

module subroutine particle_set_set_color_single (particle_set, i, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, intent(in) :: i
  type(color_t), intent(in) :: col
  call particle_set%prt(i)%set_color (col)
end subroutine particle_set_set_color_single

module subroutine particle_set_set_color_indices (particle_set, indices, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, dimension(:), intent(in) :: indices
  type(color_t), dimension(:), intent(in) :: col
  integer :: i
  do i = 1, size (indices)
    call particle_set%prt(indices(i))%set_color (col(i))
  end do
end subroutine particle_set_set_color_indices

```

```

        end do
    end subroutine particle_set_set_color_indices

    module subroutine particle_set_set_color_all (particle_set, col)
        class(particle_set_t), intent(inout) :: particle_set
        type(color_t), dimension(:), intent(in) :: col
        call particle_set%prt%set_color (col)
    end subroutine particle_set_set_color_all

```

Assigning particles manually may result in color mismatches. This is checked here for all particles in the set. The color object is compared against the color type that belongs to the flavor object. The return value is an allocatable array which consists of the particles with invalid color assignments. If the array size is zero, all is fine.

(Particles: particle set: TBP)+≡

```

    procedure :: find_prt_invalid_color => particle_set_find_prt_invalid_color

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_find_prt_invalid_color (particle_set, index, prt)
        class(particle_set_t), intent(in) :: particle_set
        integer, dimension(:), allocatable, intent(out) :: index
        type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
    end subroutine particle_set_find_prt_invalid_color

```

(Particles: procedures)+≡

```

    module subroutine particle_set_find_prt_invalid_color (particle_set, index, prt)
        class(particle_set_t), intent(in) :: particle_set
        integer, dimension(:), allocatable, intent(out) :: index
        type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
        type(flavor_t) :: flv
        type(color_t) :: col
        logical, dimension(:), allocatable :: mask
        integer :: i, n, n_invalid
        n = size (particle_set%prt)
        allocate (mask (n))
        do i = 1, n
            associate (prt => particle_set%prt(i))
                flv = prt%get_flv ()
                col = prt%get_col ()
                mask(i) = flv%get_color_type () /= col%get_type ()
            end associate
        end do
        index = pack ([(i, i = 1, n)], mask)
        if (present (prt)) prt = pack (particle_set%prt, mask)
    end subroutine particle_set_find_prt_invalid_color

```

(Particles: particle set: TBP)+≡

```

    generic :: get_momenta => get_momenta_all
    generic :: get_momenta => get_momenta_indices
    procedure :: get_momenta_all => particle_set_get_momenta_all
    procedure :: get_momenta_indices => particle_set_get_momenta_indices

```

(Particles: sub interfaces)+≡

```

    module function particle_set_get_momenta_all (particle_set) result (p)

```

```

        class(particle_set_t), intent(in) :: particle_set
        type(vector4_t), dimension(:), allocatable :: p
    end function particle_set_get_momenta_all

<Particles: procedures>+≡
module function particle_set_get_momenta_all (particle_set) result (p)
    class(particle_set_t), intent(in) :: particle_set
    type(vector4_t), dimension(:), allocatable :: p
    allocate (p (size (particle_set%prt)))
    p = particle_set%prt%p
end function particle_set_get_momenta_all

<Particles: sub interfaces>+≡
module function particle_set_get_momenta_indices (particle_set, indices) result (p)
    type(vector4_t), dimension(:), allocatable :: p
    class(particle_set_t), intent(in) :: particle_set
    integer, intent(in), dimension(:), allocatable :: indices
end function particle_set_get_momenta_indices

<Particles: procedures>+≡
module function particle_set_get_momenta_indices (particle_set, indices) result (p)
    type(vector4_t), dimension(:), allocatable :: p
    class(particle_set_t), intent(in) :: particle_set
    integer, intent(in), dimension(:), allocatable :: indices
    integer :: i
    allocate (p (size (indices)))
    do i = 1, size (indices)
        p(i) = particle_set%prt(indices(i))%p
    end do
end function particle_set_get_momenta_indices

```

Replace a single or all momenta. This is a wrapper around the corresponding `particle_t` method, with the same options. We assume that the particle array is allocated.

```

<Particles: particle set: TBP>+≡
generic :: set_momentum => set_momentum_single
generic :: set_momentum => set_momentum_indices
generic :: set_momentum => set_momentum_all
procedure :: set_momentum_single => particle_set_set_momentum_single
procedure :: set_momentum_indices => particle_set_set_momentum_indices
procedure :: set_momentum_all => particle_set_set_momentum_all

<Particles: sub interfaces>+≡
module subroutine particle_set_set_momentum_single &
    (particle_set, i, p, p2, on_shell)
    class(particle_set_t), intent(inout) :: particle_set
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    real(default), intent(in), optional :: p2
    logical, intent(in), optional :: on_shell
end subroutine particle_set_set_momentum_single
module subroutine particle_set_set_momentum_indices &
    (particle_set, indices, p, p2, on_shell)
    class(particle_set_t), intent(inout) :: particle_set

```

```

integer, dimension(:), intent(in) :: indices
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
end subroutine particle_set_set_momentum_indices
module subroutine particle_set_set_momentum_all (particle_set, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
end subroutine particle_set_set_momentum_all

```

(Particles: procedures)+≡

```

module subroutine particle_set_set_momentum_single &
  (particle_set, i, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
integer, intent(in) :: i
type(vector4_t), intent(in) :: p
real(default), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
call particle_set%prt(i)%set_momentum (p, p2, on_shell)
end subroutine particle_set_set_momentum_single

```

```

module subroutine particle_set_set_momentum_indices &
  (particle_set, indices, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
integer, dimension(:), intent(in) :: indices
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
integer :: i
if (present (p2)) then
  do i = 1, size (indices)
    call particle_set%prt(indices(i))%set_momentum (p(i), p2(i), on_shell)
  end do
else
  do i = 1, size (indices)
    call particle_set%prt(indices(i))%set_momentum &
      (p(i), on_shell=on_shell)
  end do
end if
end subroutine particle_set_set_momentum_indices

```

```

module subroutine particle_set_set_momentum_all (particle_set, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
call particle_set%prt%set_momentum (p, p2, on_shell)
end subroutine particle_set_set_momentum_all

```

Recover a momentum by recombining from children, assuming that this is possible. The reconstructed momentum is not projected on-shell.

(Particles: particle set: TBP)+≡

```

    procedure :: recover_momentum => particle_set_recover_momentum

    <Particles: sub interfaces>+≡
        module subroutine particle_set_recover_momentum (particle_set, i)
            class(particle_set_t), intent(inout) :: particle_set
            integer, intent(in) :: i
        end subroutine particle_set_recover_momentum

    <Particles: procedures>+≡
        module subroutine particle_set_recover_momentum (particle_set, i)
            class(particle_set_t), intent(inout) :: particle_set
            integer, intent(in) :: i
            type(vector4_t), dimension(:), allocatable :: p
            integer, dimension(:), allocatable :: index
            index = particle_set%prt(i)%get_children ()
            p = particle_set%get_momenta (index)
            call particle_set%set_momentum (i, sum (p))
        end subroutine particle_set_recover_momentum

    <Particles: particle set: TBP>+≡
        procedure :: replace_incoming_momenta => particle_set_replace_incoming_momenta

    <Particles: sub interfaces>+≡
        module subroutine particle_set_replace_incoming_momenta (particle_set, p)
            class(particle_set_t), intent(inout) :: particle_set
            type(vector4_t), intent(in), dimension(:) :: p
        end subroutine particle_set_replace_incoming_momenta

    <Particles: procedures>+≡
        module subroutine particle_set_replace_incoming_momenta (particle_set, p)
            class(particle_set_t), intent(inout) :: particle_set
            type(vector4_t), intent(in), dimension(:) :: p
            integer :: i, j
            i = 1
            do j = 1, particle_set%get_n_tot ()
                if (particle_set%prt(j)%get_status () == PRT_INCOMING) then
                    particle_set%prt(j)%p = p(i)
                    i = i + 1
                    if (i > particle_set%n_in) exit
                end if
            end do
        end subroutine particle_set_replace_incoming_momenta

    <Particles: particle set: TBP>+≡
        procedure :: replace_outgoing_momenta => particle_set_replace_outgoing_momenta

    <Particles: sub interfaces>+≡
        module subroutine particle_set_replace_outgoing_momenta (particle_set, p)
            class(particle_set_t), intent(inout) :: particle_set
            type(vector4_t), intent(in), dimension(:) :: p
        end subroutine particle_set_replace_outgoing_momenta

    <Particles: procedures>+≡
        module subroutine particle_set_replace_outgoing_momenta (particle_set, p)
            class(particle_set_t), intent(inout) :: particle_set
            type(vector4_t), intent(in), dimension(:) :: p

```

```

integer :: i, j
i = particle_set%n_in + 1
do j = 1, particle_set%n_tot
  if (particle_set%prt(j)%get_status () == PRT_OUTGOING) then
    particle_set%prt(j)%p = p(i)
    i = i + 1
  end if
end do
end subroutine particle_set_replace_outgoing_momenta

```

<Particles: particle set: TBP>+≡

```

procedure :: get_outgoing_momenta => particle_set_get_outgoing_momenta

```

<Particles: sub interfaces>+≡

```

module function particle_set_get_outgoing_momenta (particle_set) result (p)
  class(particle_set_t), intent(in) :: particle_set
  type(vector4_t), dimension(:), allocatable :: p
end function particle_set_get_outgoing_momenta

```

<Particles: procedures>+≡

```

module function particle_set_get_outgoing_momenta (particle_set) result (p)
  class(particle_set_t), intent(in) :: particle_set
  type(vector4_t), dimension(:), allocatable :: p
  integer :: i, k
  allocate (p (count (particle_set%prt%get_status () == PRT_OUTGOING)))
  k = 0
  do i = 1, size (particle_set%prt)
    if (particle_set%prt(i)%get_status () == PRT_OUTGOING) then
      k = k + 1
      p(k) = particle_set%prt(i)%get_momentum ()
    end if
  end do
end function particle_set_get_outgoing_momenta

```

<Particles: particle set: TBP>+≡

```

procedure :: parent_add_child => particle_set_parent_add_child

```

<Particles: sub interfaces>+≡

```

module subroutine particle_set_parent_add_child (particle_set, parent, child)
  class(particle_set_t), intent(inout) :: particle_set
  integer, intent(in) :: parent, child
end subroutine particle_set_parent_add_child

```

<Particles: procedures>+≡

```

module subroutine particle_set_parent_add_child (particle_set, parent, child)
  class(particle_set_t), intent(inout) :: particle_set
  integer, intent(in) :: parent, child
  call particle_set%prt(child)%set_parents ([parent])
  call particle_set%prt(parent)%add_child (child)
end subroutine particle_set_parent_add_child

```

Given the `particle_set` before radiation, the new momenta `p_radiated`, the emitter and the `flv_radiated` as well as the model and a random number `r_color` for choosing a color in ambiguous cases, we update the `particle_set`.

The reference for this procedure is [0709.2092], Sec. 4.5.1. We do not (yet) account for helicities and polarisations here nor do we update the beam remnant color and momenta.

(Particles: particle set: TBP)+≡

```
procedure :: build_radiation => particle_set_build_radiation
```

(Particles: sub interfaces)+≡

```
module subroutine particle_set_build_radiation (particle_set, p_radiated, &
    emitter, flv_radiated, model, r_color)
    class(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), intent(in), dimension(:) :: p_radiated
    integer, intent(in) :: emitter
    integer, intent(in), dimension(:) :: flv_radiated
    class(model_data_t), intent(in), target :: model
    real(default), intent(in) :: r_color
end subroutine particle_set_build_radiation
```

(Particles: procedures)+≡

```
module subroutine particle_set_build_radiation (particle_set, p_radiated, &
    emitter, flv_radiated, model, r_color)
    class(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), intent(in), dimension(:) :: p_radiated
    integer, intent(in) :: emitter
    integer, intent(in), dimension(:) :: flv_radiated
    class(model_data_t), intent(in), target :: model
    real(default), intent(in) :: r_color
    type(particle_set_t) :: new_particle_set
    type(particle_t) :: new_particle
    integer :: i, j, pdg_index_emitter, pdg_index_radiation, new_color_index
    integer, dimension(:), allocatable :: parents, children
    type(vector4_t) :: mom_sum_children
    type(flavor_t) :: new_flv, real_emitter_flavor
    logical, dimension(:), allocatable :: status_mask
    integer, dimension(:), allocatable :: &
        i_in1, i_beam1, i_remnant1, i_virt1, i_res1, i_out1
    integer, dimension(:), allocatable :: &
        i_in2, i_beam2, i_remnant2, i_virt2, i_res2, i_out2
    integer :: n_in1, n_beam1, n_remnant1, n_virt1, n_res1, n_out1
    integer :: n_in2, n_beam2, n_remnant2, n_virt2, n_res2, n_out2
    integer :: n, n_tot, i_emitter
    logical :: is_fsr

    n = particle_set%get_n_tot ()
    allocate (status_mask (n))
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_INCOMING
    end do
    n_in1 = count (status_mask)
    allocate (i_in1 (n_in1))
    i_in1 = particle_set%get_indices (status_mask)
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_BEAM
    end do
    n_beam1 = count (status_mask)
    allocate (i_beam1 (n_beam1))
```



```

i_beam1 = particle_set%get_indices (status_mask)
do i = 1, n
    status_mask(i) = particle_set%prt(i)%get_status () == PRT_BEAM_REMNANT
end do
n_remnant1 = count (status_mask)
allocate (i_remnant1 (n_remnant1))
i_remnant1 = particle_set%get_indices (status_mask)
do i = 1, n
    status_mask(i) = particle_set%prt(i)%get_status () == PRT_VIRTUAL
end do
n_virt1 = count (status_mask)
allocate (i_virt1 (n_virt1))
i_virt1 = particle_set%get_indices (status_mask)
do i = 1, n
    status_mask(i) = particle_set%prt(i)%get_status () == PRT_RESONANT
end do
n_res1 = count (status_mask)
allocate (i_res1 (n_res1))
i_res1 = particle_set%get_indices (status_mask)
do i = 1, n
    status_mask(i) = particle_set%prt(i)%get_status () == PRT_OUTGOING
end do
n_out1 = count (status_mask)
allocate (i_out1 (n_out1))
i_out1 = particle_set%get_indices (status_mask)

n_in2 = n_in1; n_beam2 = n_beam1; n_remnant2 = n_remnant1; n_res2 = n_res1
n_virt2 = n_virt1
n_out2 = n_out1 + 1
n_tot = n_in2 + n_beam2 + n_remnant2 + n_virt2 + n_res2 + n_out2

allocate (i_in2 (n_in2), i_beam2 (n_beam2), i_remnant2 (n_remnant2), i_res2 (n_res2))
i_in2 = i_in1; i_beam2 = i_beam1; i_remnant2 = i_remnant1; i_res2 = i_res1

allocate (i_virt2 (n_virt2))
i_virt2(1 : n_virt1) = i_virt1

allocate (i_out2 (n_out2))
i_out2(1 : n_out1) = i_out1(1 : n_out1)
i_out2(n_out2) = n_tot

new_particle_set%n_beam = n_beam2
new_particle_set%n_in = n_in2
new_particle_set%n_vir = n_virt2 + n_res2
new_particle_set%n_out = n_out2
new_particle_set%n_tot = n_tot
new_particle_set%correlated_state = particle_set%correlated_state
allocate (new_particle_set%prt (n_tot))
if (size (i_beam1) > 0) new_particle_set%prt(i_beam2) = particle_set%prt(i_beam1)
if (size (i_remnant1) > 0) new_particle_set%prt(i_remnant2) = particle_set%prt(i_remnant1)
if (size (i_res1) > 0) new_particle_set%prt(i_res2) = particle_set%prt(i_res1)
do i = 1, n_virt1
    new_particle_set%prt(i_virt2(i)) = particle_set%prt(i_virt1(i))
end do

```

```

do i = 1, n_in2
  new_particle_set%prt(i_in2(i)) = particle_set%prt(i_in1(i))
  new_particle_set%prt(i_in2(i))%p = p_radiated (i)
end do

do i = 1, n_out2 - 1
  new_particle_set%prt(i_out2(i)) = particle_set%prt(i_out1(i))
  new_particle_set%prt(i_out2(i))%p = p_radiated(i + n_in2)
  call new_particle_set%prt(i_out2(i))%reset_status (PRT_OUTGOING)
end do

call new_particle%reset_status (PRT_OUTGOING)
call new_particle%set_momentum (p_radiated (n_in2 + n_out2))

!!! Helicity and polarization handling is missing at this point
!!! Also, no helicities or polarizations yet
pdg_index_emitter = flv_radiated (emitter)
pdg_index_radiation = flv_radiated (n_in2 + n_out2)
call new_flv%init (pdg_index_radiation, model)
is_fsr = emitter > n_in1
if (is_fsr) then
  i_emitter = emitter + n_virt2 + n_res2 + n_remnant2 + n_beam2
else
  i_emitter = emitter + n_beam2
end if

call real_emitter_flavor%init (pdg_index_emitter, model)
call new_particle_set%prt(i_emitter)%set_flavor(real_emitter_flavor)

new_color_index = 0
do i = 1, n_tot - 1
  new_color_index = max(maxval(abs(particle_set%prt(i)%get_color())), new_color_index)
end do
new_color_index = new_color_index + 1
call reassign_colors (new_particle, new_particle_set%prt(i_emitter), &
  pdg_index_radiation, pdg_index_emitter, new_color_index, is_fsr, r_color)

call new_particle%set_flavor (new_flv)
new_particle_set%prt(n_tot) = new_particle

!!! Set proper parents for outgoing particles
if (is_fsr) then
  call new_particle_set%prt(n_tot)%set_parents ( &
    new_particle_set%prt(i_emitter)%get_parents ())
else
  call new_particle_set%prt(n_tot)%set_parents (i_in2)
end if

do i = n_in2 + n_beam2 + n_remnant2 + n_virt1 + 1, &
  n_in2 + n_beam2 + n_remnant2 + n_virt2 + n_res2
  allocate(children(0))
  mom_sum_children = vector4_null
  do j = n_in2 + n_beam2 + n_remnant2, n_tot

```

```

        if (any(new_particle_set%prt(j)%get_parents() == i)) then
            children = [children, j]
            if (new_particle_set%prt(j)%get_status() == PRT_OUTGOING) then
                mom_sum_children = mom_sum_children &
                    + new_particle_set%prt(j)%get_momentum()
            end if
        end if
    end do
    call new_particle_set%prt(i)%set_children(children)
    if (mom_sum_children /= vector4_null) then
        call new_particle_set%set_momentum(i, mom_sum_children)
    end if
    deallocate(children)
end do
call particle_set%init(new_particle_set)
contains

```

<build radiation: set color offset>

```

subroutine reassign_colors(prt_radiated, prt_emitter, flv_rad, flv_em, &
    new_color_index, is_fsr, r_col)

```

```

    type(particle_t), intent(inout) :: prt_radiated, prt_emitter
    integer, intent(in) :: flv_rad, flv_em, new_color_index
    logical, intent(in) :: is_fsr
    real(default), intent(in) :: r_col
    type(color_t) :: col_rad, col_em
    if (is_fsr) then
        if (is_quark(flv_em) .and. is_gluon(flv_rad)) then
            call reassign_colors_q_to_qg_fsr(prt_emitter, new_color_index, col_rad, col_em)
        else if (is_gluon(flv_em) .and. is_gluon(flv_rad)) then
            call reassign_colors_g_to_gg_fsr(prt_emitter, r_col, new_color_index, col_rad, col_em)
        else if (is_quark(flv_em) .and. is_quark(flv_rad)) then
            call reassign_colors_g_to_qq_fsr(prt_emitter, flv_em, col_rad, col_em)
        else
            call msg_fatal("reassign_colors: invalid splitting")
        end if
    else
        if (is_quark(flv_em) .and. is_gluon(flv_rad)) then
            call reassign_colors_q_to_qg_isr(prt_emitter, new_color_index, col_rad, col_em)
        else if (is_quark(flv_em) .and. is_quark(flv_rad)) then
            call reassign_colors_g_to_qq_isr(prt_emitter, flv_rad, col_rad, col_em)
        else if (is_gluon(flv_em) .and. is_quark(flv_rad)) then
            call reassign_colors_q_to_gq_isr(prt_emitter, flv_rad, new_color_index, col_rad, col_em)
        else if (is_gluon(flv_em) .and. is_gluon(flv_rad)) then
            call reassign_colors_g_to_gg_isr(prt_emitter, r_col, new_color_index, col_rad, col_em)
        else
            call msg_fatal("reassign_colors: invalid splitting")
        end if
    end if
    call prt_emitter%set_color(col_em)
    call prt_radiated%set_color(col_rad)
end subroutine reassign_colors

```

```

subroutine reassign_colors_q_to_qg_fsr(prt_emitter, new_color_index, &
    col_rad, col_em)

```

```

type(particle_t), intent(in) :: prt_emitter
integer, intent(in) :: new_color_index
type(color_t), intent(out) :: col_rad, col_em
integer, dimension(2) :: color_rad, color_em
integer :: i1, i2
logical :: is_anti_quark

color_em = prt_emitter%get_color ()
i1 = 1; i2 = 2
is_anti_quark = color_em(2) /= 0
if (is_anti_quark) then
    i1 = 2; i2 = 1
end if
color_rad(i1) = color_em(i1)
color_rad(i2) = new_color_index
color_em(i1) = new_color_index
call col_em%init_col_acl (color_em(1), color_em(2))
call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_q_to_qg_fsr

subroutine reassign_colors_g_to_gg_fsr (prt_emitter, random, new_color_index, &
    col_rad, col_em)
type(particle_t), intent(in) :: prt_emitter
real(default), intent(in) :: random
integer, intent(in) :: new_color_index
type(color_t), intent(out) :: col_rad, col_em
integer, dimension(2) :: color_rad, color_em
integer :: i1, i2

color_em = prt_emitter%get_color ()
i1 = 1; i2 = 2
if (random < 0.5) then
    i1 = 2; i2 = 1
end if
color_rad(i1) = new_color_index
color_rad(i2) = color_em(i2)
color_em(i2) = new_color_index
call col_em%init_col_acl (color_em(1), color_em(2))
call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_g_to_gg_fsr

subroutine reassign_colors_g_to_qq_fsr (prt_emitter, pdg_emitter, col_rad, col_em)
type(particle_t), intent(in) :: prt_emitter
integer, intent(in) :: pdg_emitter
type(color_t), intent(out) :: col_rad, col_em
integer, dimension(2) :: color_rad, color_em
integer :: i1, i2
logical :: is_anti_quark

color_em = prt_emitter%get_color ()
i1 = 1; i2 = 2
is_anti_quark = pdg_emitter < 0
if (is_anti_quark) then
    i1 = 2; i1 = 1

```

```

end if
color_em(i2) = 0
color_rad(i1) = 0
color_rad(i2) = color_em(i1)
call col_em%init_col_acl (color_em(1), color_em(2))
call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_g_to_qq_fsr

subroutine reassign_colors_q_to_qg_isr (prt_emitter, new_color_index, &
    col_rad, col_em)
    type(particle_t), intent(in) :: prt_emitter
    integer, intent(in) :: new_color_index
    type(color_t), intent(out) :: col_rad, col_em
    integer, dimension(2) :: color_rad, color_em
    integer :: i1, i2
    logical :: is_anti_quark

    color_em = prt_emitter%get_color ()
    i1 = 1; i2 = 2
    is_anti_quark = color_em(2) /= 0
    if (is_anti_quark) then
        i1 = 2; i2 = 1
    end if
    color_rad(i2) = color_em(i1)
    color_rad(i1) = new_color_index
    color_em(i1) = new_color_index
    call col_em%init_col_acl (color_em(1), color_em(2))
    call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_q_to_qg_isr

subroutine reassign_colors_g_to_qq_isr (prt_emitter, pdg_rad, col_rad, col_em)
    type(particle_t), intent(in) :: prt_emitter
    integer, intent(in) :: pdg_rad
    type(color_t), intent(out) :: col_rad, col_em
    integer, dimension(2) :: color_rad, color_em
    integer :: i1, i2
    logical :: is_anti_quark

    color_em = prt_emitter%get_color ()
    i1 = 1; i2 = 2
    is_anti_quark = pdg_rad < 0
    if (is_anti_quark) then
        i1 = 2; i2 = 1
    end if
    color_rad(i1) = color_em(i2)
    color_rad(i2) = 0
    color_em(i2) = 0
    call col_em%init_col_acl (color_em(1), color_em(2))
    call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_g_to_qq_isr

subroutine reassign_colors_q_to_gq_isr (prt_emitter, pdg_rad, new_color_index, &
    col_rad, col_em)
    type(particle_t), intent(in) :: prt_emitter

```

```

integer, intent(in) :: pdg_rad, new_color_index
type(color_t), intent(out) :: col_rad, col_em
integer, dimension(2) :: color_rad, color_em
integer :: i1, i2
logical :: rad_is_quark

color_em = prt_emitter%get_color ()
i1 = 1; i2 = 2
rad_is_quark = pdg_rad > 0
if (rad_is_quark) then
    i1 = 2; i2 = 1
end if
color_rad(i1) = 0
color_rad(i2) = new_color_index
color_em(i2) = new_color_index
call col_em%init_col_acl (color_em(1), color_em(2))
call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_q_to_gq_isr

subroutine reassign_colors_g_to_gg_isr (prt_emitter, random, new_color_index, &
    col_rad, col_em)
    type(particle_t), intent(in) :: prt_emitter
    real(default), intent(in) :: random
    integer, intent(in) :: new_color_index
    type(color_t), intent(out) :: col_rad, col_em
    integer, dimension(2) :: color_rad, color_em
    integer :: i1, i2

    color_em = prt_emitter%get_color ()
    i1 = 1; i2 = 2
    if (random < 0.5) then
        i1 = 2; i2 = 1
    end if
    color_rad(i2) = new_color_index
    color_rad(i1) = color_em(i2)
    color_em(i2) = new_color_index
    call col_em%init_col_acl (color_em(1), color_em(2))
    call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_g_to_gg_isr
end subroutine particle_set_build_radiation

```

Increments the color indices of all particles by their maximal value to distinguish them from the record-keeping Born particles in the LHE-output if the virtual entries are kept.

```

<build radiation: set color offset>≡
subroutine set_color_offset (particle_set)
    type(particle_set_t), intent(inout) :: particle_set
    integer, dimension(2) :: color
    integer :: i, i_color_max
    type(color_t) :: new_color

    i_color_max = 0
    do i = 1, size (particle_set%prt)

```

```

        associate (prt => particle_set%prt(i))
            if (prt%get_status () <= PRT_INCOMING) cycle
            color = prt%get_color ()
            i_color_max = maxval([i_color_max, color(1), color(2)])
        end associate
    end do

    do i = 1, size (particle_set%prt)
        associate (prt => particle_set%prt(i))
            if (prt%get_status () /= PRT_OUTGOING) cycle
            color = prt%get_color ()
            where (color /= 0) color = color + i_color_max
            call new_color%init_col_acl (color(1), color(2))
            call prt%set_color (new_color)
        end associate
    end do
end subroutine set_color_offset

```

Output (default format)

(Particles: particle set: TBP)+≡

```

    procedure :: write => particle_set_write

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_write &
        (particle_set, unit, testflag, summary, compressed)
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, summary, compressed
    end subroutine particle_set_write

```

(Particles: procedures)+≡

```

    module subroutine particle_set_write &
        (particle_set, unit, testflag, summary, compressed)
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, summary, compressed
        logical :: summ, comp, pol
        type(vector4_t) :: sum_vec
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        summ = .false.; if (present (summary)) summ = summary
        comp = .false.; if (present (compressed)) comp = compressed
        pol = particle_set%factorization_mode /= FM_IGNORE_HELICITY
        write (u, "(1x,A)") "Particle set:"
        call write_separator (u)
        if (comp) then
            if (pol) then
                write (u, &
                    "((A4,1X),(A6,1X),(A7,1X),(A3),2(A4,1X),2(A20,1X),5(A12,1X)))" &
                    "Nr", "Status", "Flavor", "Hel", "Col", "ACol", &
                    "Parents", "Children", &
                    "P(0)", "P(1)", "P(2)", "P(3)", "P~2"
            else
                write (u, &

```

```

        ((A4,1X),(A6,1X),(A7,1X),2(A4,1X),2(A20,1X),5(A12,1X))) &
        "Nr", "Status", "Flavor", "Col", "ACol", &
        "Parents", "Children", &
        "P(0)", "P(1)", "P(2)", "P(3)", "P~2"
    end if
end if
if (particle_set%n_tot /= 0) then
    do i = 1, particle_set%n_tot
        if (comp) then
            write (u, "(I4,1X,2X)", advance="no") i
        else
            write (u, "(1x,A,1x,I0)", advance="no") "Particle", i
        end if
        call particle_set%prt(i)%write (u, testflag = testflag, &
            compressed = comp, polarization = pol)
    end do
    if (particle_set%correlated_state%is_defined ()) then
        call write_separator (u)
        write (u, *) "Correlated state density matrix:"
        call particle_set%correlated_state%write (u)
    end if
    if (summ) then
        call write_separator (u)
        write (u, "(A)", advance="no") &
            "Sum of incoming momenta: p(0:3) = "
        sum_vec = sum (particle_set%prt%p, &
            mask=particle_set%prt%get_status () == PRT_INCOMING)
        call pacify (sum_vec, tolerance = 1E-3_default)
        call sum_vec%write (u, compressed=.true.)
        write (u, *)
        write (u, "(A)", advance="no") &
            "Sum of beam remnant momenta: p(0:3) = "
        sum_vec = sum (particle_set%prt%p, &
            mask=particle_set%prt%get_status () == PRT_BEAM_REMNANT)
        call pacify (sum_vec, tolerance = 1E-3_default)
        call sum_vec%write (u, compressed=.true.)
        write (u, *)
        write (u, "(A)", advance="no") &
            "Sum of outgoing momenta: p(0:3) = "
        sum_vec = sum (particle_set%prt%p, &
            mask=particle_set%prt%get_status () == PRT_OUTGOING)
        call pacify (sum_vec, tolerance = 1E-3_default)
        call sum_vec%write (u, compressed=.true.)
        write (u, "(A)") ""
    end if
else
    write (u, "(3x,A)") "[empty]"
end if
end subroutine particle_set_write

```


15.4.5 I/O formats

Here, we define input/output of particle sets in various formats. This is the right place since particle sets contain most of the event information.

All write/read routines take as first argument the object, as second argument the I/O unit which in this case is a mandatory argument. Then follow further event data.

Internal binary format

This format is supposed to contain the complete information, so the particle data set can be fully reconstructed. The exception is the model part of the particle flavors; this is unassigned for the flavor values read from file.

(Particles: particle set: TBP)+≡

```
procedure :: write_raw => particle_set_write_raw
procedure :: read_raw => particle_set_read_raw
```

(Particles: sub interfaces)+≡

```
module subroutine particle_set_write_raw (particle_set, u)
  class(particle_set_t), intent(in) :: particle_set
  integer, intent(in) :: u
end subroutine particle_set_write_raw
module subroutine particle_set_read_raw (particle_set, u, iostat)
  class(particle_set_t), intent(out) :: particle_set
  integer, intent(in) :: u
  integer, intent(out) :: iostat
end subroutine particle_set_read_raw
```

(Particles: procedures)+≡

```
module subroutine particle_set_write_raw (particle_set, u)
  class(particle_set_t), intent(in) :: particle_set
  integer, intent(in) :: u
  integer :: i
  write (u) &
    particle_set%n_beam, particle_set%n_in, &
    particle_set%n_vir, particle_set%n_out
  write (u) particle_set%factorization_mode
  write (u) particle_set%n_tot
  do i = 1, particle_set%n_tot
    call particle_set%prt(i)%write_raw (u)
  end do
  call particle_set%correlated_state%write_raw (u)
end subroutine particle_set_write_raw

module subroutine particle_set_read_raw (particle_set, u, iostat)
  class(particle_set_t), intent(out) :: particle_set
  integer, intent(in) :: u
  integer, intent(out) :: iostat
  integer :: i
  read (u, iostat=iostat) &
    particle_set%n_beam, particle_set%n_in, &
    particle_set%n_vir, particle_set%n_out
  read (u, iostat=iostat) particle_set%factorization_mode
  read (u, iostat=iostat) particle_set%n_tot
  allocate (particle_set%prt (particle_set%n_tot))
```

```

do i = 1, size (particle_set%prt)
  call particle_set%prt(i)%read_raw (u, iostat=iostat)
end do
call particle_set%correlated_state%read_raw (u, iostat=iostat)
end subroutine particle_set_read_raw

```

Get contents

Find parents/children of a particular particle recursively; the search terminates if a parent/child has status BEAM, INCOMING, OUTGOING or RESONANT.

(Particles: particle set: TBP)+≡

```

procedure :: get_real_parents => particle_set_get_real_parents
procedure :: get_real_children => particle_set_get_real_children

```

(Particles: sub interfaces)+≡

```

module function particle_set_get_real_parents (pset, i, keep_beams) result (parent)
  integer, dimension(:), allocatable :: parent
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: i
  logical, intent(in), optional :: keep_beams
end function particle_set_get_real_parents
module function particle_set_get_real_children (pset, i, keep_beams) result (child)
  integer, dimension(:), allocatable :: child
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: i
  logical, intent(in), optional :: keep_beams
end function particle_set_get_real_children

```

(Particles: procedures)+≡

```

module function particle_set_get_real_parents (pset, i, keep_beams) result (parent)
  integer, dimension(:), allocatable :: parent
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: i
  logical, intent(in), optional :: keep_beams
  logical, dimension(:), allocatable :: is_real
  logical, dimension(:), allocatable :: is_parent, is_real_parent
  logical :: kb
  integer :: j, k
  kb = .false.
  if (present (keep_beams)) kb = keep_beams
  allocate (is_real (pset%n_tot))
  is_real = pset%prt%is_real (kb)
  allocate (is_parent (pset%n_tot), is_real_parent (pset%n_tot))
  is_real_parent = .false.
  is_parent = .false.
  is_parent(pset%prt(i)%get_parents()) = .true.
  do while (any (is_parent))
    where (is_real .and. is_parent)
      is_real_parent = .true.
      is_parent = .false.
    end where
    mark_next_parent: do j = size (is_parent), 1, -1
      if (is_parent(j)) then

```

```

        is_parent(pset%prt(j)%get_parents()) = .true.
        is_parent(j) = .false.
        exit mark_next_parent
    end if
end do mark_next_parent
end do
allocate (parent (count (is_real_parent)))
j = 0
do k = 1, size (is_parent)
    if (is_real_parent(k)) then
        j = j + 1
        parent(j) = k
    end if
end do
end function particle_set_get_real_parents

module function particle_set_get_real_children (pset, i, keep_beams) result (child)
    integer, dimension(:), allocatable :: child
    class(particle_set_t), intent(in) :: pset
    integer, intent(in) :: i
    logical, dimension(:), allocatable :: is_real
    logical, dimension(:), allocatable :: is_child, is_real_child
    logical, intent(in), optional :: keep_beams
    integer :: j, k
    logical :: kb
    kb = .false.
    if (present (keep_beams)) kb = keep_beams
    allocate (is_real (pset%n_tot))
    is_real = pset%prt%is_real (kb)
    is_real = pset%prt%is_real (kb)
    allocate (is_child (pset%n_tot), is_real_child (pset%n_tot))
    is_real_child = .false.
    is_child = .false.
    is_child(pset%prt(i)%get_children()) = .true.
    do while (any (is_child))
        where (is_real .and. is_child)
            is_real_child = .true.
            is_child = .false.
        end where
        mark_next_child: do j = 1, size (is_child)
            if (is_child(j)) then
                is_child(pset%prt(j)%get_children()) = .true.
                is_child(j) = .false.
                exit mark_next_child
            end if
        end do mark_next_child
    end do
    allocate (child (count (is_real_child)))
    j = 0
    do k = 1, size (is_child)
        if (is_real_child(k)) then
            j = j + 1
            child(j) = k
        end if
    end do
end module

```

```

end do
end function particle_set_get_real_children

```

Get the `n_tot`, `n_in`, and `n_out` values out of the particle set.

(Particles: particle set: TBP)+≡

```

procedure :: get_n_beam => particle_set_get_n_beam
procedure :: get_n_in  => particle_set_get_n_in
procedure :: get_n_vir => particle_set_get_n_vir
procedure :: get_n_out => particle_set_get_n_out
procedure :: get_n_tot => particle_set_get_n_tot
procedure :: get_n_remnants => particle_set_get_n_remnants

```

(Particles: sub interfaces)+≡

```

module function particle_set_get_n_beam (pset) result (n_beam)
  class(particle_set_t), intent(in) :: pset
  integer :: n_beam
end function particle_set_get_n_beam
module function particle_set_get_n_in (pset) result (n_in)
  class(particle_set_t), intent(in) :: pset
  integer :: n_in
end function particle_set_get_n_in
module function particle_set_get_n_vir (pset) result (n_vir)
  class(particle_set_t), intent(in) :: pset
  integer :: n_vir
end function particle_set_get_n_vir
module function particle_set_get_n_out (pset) result (n_out)
  class(particle_set_t), intent(in) :: pset
  integer :: n_out
end function particle_set_get_n_out
module function particle_set_get_n_tot (pset) result (n_tot)
  class(particle_set_t), intent(in) :: pset
  integer :: n_tot
end function particle_set_get_n_tot
module function particle_set_get_n_remnants (pset) result (n_remn)
  class(particle_set_t), intent(in) :: pset
  integer :: n_remn
end function particle_set_get_n_remnants

```

(Particles: procedures)+≡

```

module function particle_set_get_n_beam (pset) result (n_beam)
  class(particle_set_t), intent(in) :: pset
  integer :: n_beam
  n_beam = pset%n_beam
end function particle_set_get_n_beam

module function particle_set_get_n_in (pset) result (n_in)
  class(particle_set_t), intent(in) :: pset
  integer :: n_in
  n_in = pset%n_in
end function particle_set_get_n_in

module function particle_set_get_n_vir (pset) result (n_vir)
  class(particle_set_t), intent(in) :: pset
  integer :: n_vir
  n_vir = pset%n_vir

```

```

end function particle_set_get_n_vir

module function particle_set_get_n_out (pset) result (n_out)
  class(particle_set_t), intent(in) :: pset
  integer :: n_out
  n_out = pset%n_out
end function particle_set_get_n_out

module function particle_set_get_n_tot (pset) result (n_tot)
  class(particle_set_t), intent(in) :: pset
  integer :: n_tot
  n_tot = pset%n_tot
end function particle_set_get_n_tot

module function particle_set_get_n_remnants (pset) result (n_remn)
  class(particle_set_t), intent(in) :: pset
  integer :: n_remn
  if (allocated (pset%prt)) then
    n_remn = count (pset%prt%get_status () == PRT_BEAM_REMNANT)
  else
    n_remn = 0
  end if
end function particle_set_get_n_remnants

```

Return a pointer to the particle corresponding to the number

(Particles: particle set: TBP)+≡

```
procedure :: get_particle => particle_set_get_particle
```

(Particles: sub interfaces)+≡

```

module function particle_set_get_particle (pset, index) result (particle)
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: index
  type(particle_t) :: particle
end function particle_set_get_particle

```

(Particles: procedures)+≡

```

module function particle_set_get_particle (pset, index) result (particle)
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: index
  type(particle_t) :: particle
  particle = pset%prt(index)
end function particle_set_get_particle

```

(Particles: particle set: TBP)+≡

```
procedure :: get_indices => particle_set_get_indices
```

(Particles: sub interfaces)+≡

```

pure module function particle_set_get_indices (pset, mask) result (finals)
  integer, dimension(:), allocatable :: finals
  class(particle_set_t), intent(in) :: pset
  logical, dimension(:), intent(in) :: mask
end function particle_set_get_indices

```

```

<Particles: procedures>+≡
pure module function particle_set_get_indices (pset, mask) result (finals)
  integer, dimension(:), allocatable :: finals
  class(particle_set_t), intent(in) :: pset
  logical, dimension(:), intent(in) :: mask
  integer, dimension(size(mask)) :: indices
  integer :: i
  allocate (finals (count (mask)))
  indices = [(i, i=1, pset%n_tot)]
  finals = pack (indices, mask)
end function particle_set_get_indices

```

Copy the subset of physical momenta to a phs_point container.

```

<Particles: particle set: TBP>+≡
procedure :: get_in_and_out_momenta => particle_set_get_in_and_out_momenta

```

```

<Particles: sub interfaces>+≡
module function particle_set_get_in_and_out_momenta (pset) result (phs_point)
  type(phs_point_t) :: phs_point
  class(particle_set_t), intent(in) :: pset
end function particle_set_get_in_and_out_momenta

```

```

<Particles: procedures>+≡
module function particle_set_get_in_and_out_momenta (pset) result (phs_point)
  type(phs_point_t) :: phs_point
  class(particle_set_t), intent(in) :: pset
  logical, dimension(:), allocatable :: mask
  integer, dimension(:), allocatable :: indices
  type(vector4_t), dimension(:), allocatable :: p
  allocate (mask (pset%get_n_tot ()))
  allocate (p (size (pset%prt)))
  mask = pset%prt%status == PRT_INCOMING .or. &
    pset%prt%status == PRT_OUTGOING
  allocate (indices (count (mask)))
  indices = pset%get_indices (mask)
  phs_point = pset%get_momenta (indices)
end function particle_set_get_in_and_out_momenta

```

Tools

Build a new particles array without hadronic remnants but with `n_extra` additional spots. We also update the mother-daughter relations assuming the ordering b, i, r, x, o.

```

<Particles: particle set: TBP>+≡
procedure :: without_hadronic_remnants => &
  particle_set_without_hadronic_remnants

<Particles: sub interfaces>+≡
module subroutine particle_set_without_hadronic_remnants &
  (particle_set, particles, n_particles, n_extra)
  class(particle_set_t), intent(inout) :: particle_set
  type(particle_t), dimension(:), allocatable, intent(out) :: particles
  integer, intent(out) :: n_particles

```

```

        integer, intent(in) :: n_extra
    end subroutine particle_set_without_hadronic_remnants

    (Particles: procedures)+≡
    module subroutine particle_set_without_hadronic_remnants &
        (particle_set, particles, n_particles, n_extra)
        class(particle_set_t), intent(inout) :: particle_set
        type(particle_t), dimension(:), allocatable, intent(out) :: particles
        integer, intent(out) :: n_particles
        integer, intent(in) :: n_extra
        logical, dimension(:), allocatable :: no_hadronic_remnants, &
            no_hadronic_children
        integer, dimension(:), allocatable :: children, new_children
        integer :: i, j, k, first_remnant
        first_remnant = particle_set%n_tot
        do i = 1, particle_set%n_tot
            if (particle_set%prt(i)%is_hadronic_beam_remnant ()) then
                first_remnant = i
                exit
            end if
        end do
        n_particles = count (.not. particle_set%prt%is_hadronic_beam_remnant ())
        allocate (no_hadronic_remnants (particle_set%n_tot))
        no_hadronic_remnants = .not. particle_set%prt%is_hadronic_beam_remnant ()
        allocate (particles (n_particles + n_extra))
        k = 1
        do i = 1, particle_set%n_tot
            if (no_hadronic_remnants(i)) then
                particles(k) = particle_set%prt(i)
                k = k + 1
            end if
        end do
        if (n_particles /= particle_set%n_tot) then
            do i = 1, n_particles
                select case (particles(i)%get_status ())
                case (PRT_BEAM)
                    if (allocated (children)) deallocate (children)
                    allocate (children (particles(i)%get_n_children ()))
                    children = particles(i)%get_children ()
                    if (allocated (no_hadronic_children)) &
                        deallocate (no_hadronic_children)
                    allocate (no_hadronic_children (particles(i)%get_n_children ()))
                    no_hadronic_children = .not. &
                        particle_set%prt(children)%is_hadronic_beam_remnant ()
                    if (allocated (new_children)) deallocate (new_children)
                    allocate (new_children (count (no_hadronic_children)))
                    new_children = pack (children, no_hadronic_children)
                    call particles(i)%set_children (new_children)
                case (PRT_INCOMING, PRT_RESONANT)
                    (update children after remnant)
                case (PRT_OUTGOING, PRT_BEAM_REMNANT)
                case default
                end select
            end do
        end if
    end if

```

```
end subroutine particle_set_without_hadronic_remnants
```

```
<update children after remnant>≡
  if (allocated (children)) deallocate (children)
  allocate (children (particles(i)%get_n_children ()))
  children = particles(i)%get_children ()
  do j = 1, size (children)
    if (children(j) > first_remnant) then
      children(j) = children (j) - &
        (particle_set%n_tot - n_particles)
    end if
  end do
  call particles(i)%set_children (children)
```

Build a new particles array without remnants but with `n_extra` additional spots.
We also update the mother-daughter relations assuming the ordering `b, i, r, x, o`.

```
<Particles: particle set: TBP>+≡
  procedure :: without_remnants => particle_set_without_remnants

<Particles: sub interfaces>+≡
  module subroutine particle_set_without_remnants &
    (particle_set, particles, n_particles, n_extra)
    class(particle_set_t), intent(inout) :: particle_set
    type(particle_t), dimension(:), allocatable, intent(out) :: particles
    integer, intent(in) :: n_extra
    integer, intent(out) :: n_particles
  end subroutine particle_set_without_remnants

<Particles: procedures>+≡
  module subroutine particle_set_without_remnants &
    (particle_set, particles, n_particles, n_extra)
    class(particle_set_t), intent(inout) :: particle_set
    type(particle_t), dimension(:), allocatable, intent(out) :: particles
    integer, intent(in) :: n_extra
    integer, intent(out) :: n_particles
    logical, dimension(:), allocatable :: no_remnants, no_children
    integer, dimension(:), allocatable :: children, new_children
    integer :: i, j, k, first_remnant
    first_remnant = particle_set%n_tot
    do i = 1, particle_set%n_tot
      if (particle_set%prt(i)%is_beam_remnant ()) then
        first_remnant = i
        exit
      end if
    end do
    allocate (no_remnants (particle_set%n_tot))
    no_remnants = .not. (particle_set%prt%is_beam_remnant ())
    n_particles = count (no_remnants)
    allocate (particles (n_particles + n_extra))
    k = 1
    do i = 1, particle_set%n_tot
      if (no_remnants(i)) then
        particles(k) = particle_set%prt(i)
        k = k + 1
      end if
    end do
```



```

        end if
    end do
    if (n_particles /= particle_set%n_tot) then
        do i = 1, n_particles
            select case (particles(i)%get_status ())
            case (PRT_BEAM)
                if (allocated (children)) deallocate (children)
                allocate (children (particles(i)%get_n_children ()))
                children = particles(i)%get_children ()
                if (allocated (no_children)) deallocate (no_children)
                allocate (no_children (particles(i)%get_n_children ()))
                no_children = .not. (particle_set%prt(children)%is_beam_remnant ())
                if (allocated (new_children)) deallocate (new_children)
                allocate (new_children (count (no_children)))
                new_children = pack (children, no_children)
                call particles(i)%set_children (new_children)
            case (PRT_INCOMING, PRT_RESONANT)
                <update children after remnant>
            case (PRT_OUTGOING, PRT_BEAM_REMNANT)
            case default
            end select
        end do
    end if
end subroutine particle_set_without_remnants

```

<Particles: particle set: TBP>+≡

```

    procedure :: find_particle => particle_set_find_particle

```

<Particles: sub interfaces>+≡

```

    pure module function particle_set_find_particle (particle_set, pdg, &
        momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
    end function particle_set_find_particle

```

<Particles: procedures>+≡

```

    pure module function particle_set_find_particle (particle_set, pdg, &
        momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        integer :: i
        logical, dimension(0:3) :: equals
        idx = 0
        do i = 1, size (particle_set%prt)
            if (particle_set%prt(i)%flv%get_pdg () == pdg) then
                equals = nearly_equal (particle_set%prt(i)%p%p, momentum%p, &
                    abs_smallness, rel_smallness)
                if (all (equals)) then
                    idx = i

```

```

        return
    end if
end if
end do
end function particle_set_find_particle

```

(Particles: particle set: TBP)+≡

```

    procedure :: reverse_find_particle => particle_set_reverse_find_particle

```

(Particles: sub interfaces)+≡

```

    pure module function particle_set_reverse_find_particle &
        (particle_set, pdg, momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
    end function particle_set_reverse_find_particle

```

(Particles: procedures)+≡

```

    pure module function particle_set_reverse_find_particle &
        (particle_set, pdg, momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        integer :: i
        idx = 0
        do i = size (particle_set%prt), 1, -1
            if (particle_set%prt(i)%flv%get_pdg () == pdg) then
                if (all (nearly_equal (particle_set%prt(i)%p%p, momentum%p, &
                    abs_smallness, rel_smallness))) then
                    idx = i
                    return
                end if
            end if
        end if
    end do
end function particle_set_reverse_find_particle

```

This connects broken links of the form something $\rightarrow i \rightarrow$ none or j and none $\rightarrow j \rightarrow$ something or none where the particles i and j are *identical*. It also works if $i \rightarrow j$, directly, and thus removes duplicates. We are removing j and connect the possible daughters to i .

(Particles: particle set: TBP)+≡

```

    procedure :: remove_duplicates => particle_set_remove_duplicates

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_remove_duplicates (particle_set, smallness)
        class(particle_set_t), intent(inout) :: particle_set
        real(default), intent(in) :: smallness
    end subroutine particle_set_remove_duplicates

```

(Particles: procedures)+≡

```

    module subroutine particle_set_remove_duplicates (particle_set, smallness)

```

```

class(particle_set_t), intent(inout) :: particle_set
real(default), intent(in) :: smallness
integer :: n_removals
integer, dimension(particle_set%n_tot) :: to_remove
type(particle_t), dimension(:), allocatable :: particles
type(vector4_t) :: p_i
integer, dimension(:), allocatable :: map
to_remove = 0
call find_duplicates ()
n_removals = count (to_remove > 0)
if (n_removals > 0) then
    call strip_duplicates (particles)
    call particle_set%replace (particles)
end if

contains

<Particles: remove duplicates: procedures>

end subroutine particle_set_remove_duplicates

```

This does not catch all cases. Missing are splittings of the type $i \rightarrow \text{something and } j$.

```

<Particles: remove duplicates: procedures>≡
subroutine find_duplicates ()
    integer :: pdg_i, child_i, i, j
    OUTER: do i = 1, particle_set%n_tot
        if (particle_set%prt(i)%status == PRT_OUTGOING .or. &
            particle_set%prt(i)%status == PRT_VIRTUAL .or. &
            particle_set%prt(i)%status == PRT_RESONANT) then
            if (allocated (particle_set%prt(i)%child)) then
                if (size (particle_set%prt(i)%child) > 1) cycle OUTER
                if (size (particle_set%prt(i)%child) == 1) then
                    child_i = particle_set%prt(i)%child(1)
                else
                    child_i = 0
                end if
            else
                child_i = 0
            end if
            pdg_i = particle_set%prt(i)%flv%get_pdg ()
            p_i = particle_set%prt(i)%p
            do j = i + 1, particle_set%n_tot
                if (pdg_i == particle_set%prt(j)%flv%get_pdg ()) then
                    if (all (nearly_equal (particle_set%prt(j)%p%p, p_i%p, &
                        abs_smallness = smallness, &
                        rel_smallness = 1E4_default * smallness))) then
                        if (child_i == 0 .or. j == child_i) then
                            to_remove(j) = i
                            if (debug_on) call msg_debug2 (D_PARTICLES, &
                                "Particles: Will remove duplicate of i", i)
                            if (debug_on) call msg_debug2 (D_PARTICLES, &
                                "Particles: j", j)
                        end if
                    end if
                end if
            end do
        end if
    end do
end subroutine find_duplicates

```

```

        cycle OUTER
      end if
    end if
  end do
end if
end do OUTER
end subroutine find_duplicates

```

(Particles: remove duplicates: procedures)+≡

```

recursive function get_alive_index (try) result (alive)
  integer :: alive
  integer :: try
  if (map(try) > 0) then
    alive = map(try)
  else
    alive = get_alive_index (to_remove(try))
  end if
end function get_alive_index

```

(Particles: remove duplicates: procedures)+≡

```

subroutine strip_duplicates (particles)
  type(particle_t), dimension(:), allocatable, intent(out) :: particles
  integer :: kept, removed, i, j
  integer, dimension(:), allocatable :: old_children
  logical, dimension(:), allocatable :: parent_set
  if (debug_on) call msg_debug (D_PARTICLES, "Particles: Removing duplicates")
  if (debug_on) call msg_debug (D_PARTICLES, "Particles: n_removals", n_removals)
  if (debug2_active (D_PARTICLES)) then
    call msg_debug2 (D_PARTICLES, "Particles: Given set before removing:")
    call particle_set%write (summary=.true., compressed=.true.)
  end if
  allocate (particles (particle_set%n_tot - n_removals))
  allocate (map (particle_set%n_tot))
  allocate (parent_set (particle_set%n_tot))
  parent_set = .false.
  map = 0
  j = 0
  do i = 1, particle_set%n_tot
    if (to_remove(i) == 0) then
      j = j + 1
      map(i) = j
      call particles(j)%init (particle_set%prt(i))
    end if
  end do
  do i = 1, particle_set%n_tot
    if (map(i) /= 0) then
      if (.not. parent_set(map(i))) then
        call particles(map(i))%set_parents &
          (map (particle_set%prt(i)%get_parents ()))
      end if
      call particles(map(i))%set_children &
        (map (particle_set%prt(i)%get_children ()))
    else

```

```

        removed = i
        kept = to_remove(i)
        if (particle_set%prt(removed)%has_children ()) then
            old_children = particle_set%prt(removed)%get_children ()
            do j = 1, size (old_children)
                if (map(old_children(j)) > 0) then
                    call particles(map(old_children(j)))%set_parents &
                        ([get_alive_index (kept)])
                    parent_set(map(old_children(j))) = .true.
                    call particles(get_alive_index (kept))%add_child &
                        (map(old_children(j)))
                end if
            end do
            particles(get_alive_index (kept))%status = PRT_RESONANT
        else
            particles(get_alive_index (kept))%status = PRT_OUTGOING
        end if
    end if
end do
end subroutine strip_duplicates

```

Given a subevent, reset status codes. If the new status is beam, incoming, or outgoing, we also make sure that the stored p^2 value is equal to the on-shell mass squared.

(Particles: particle set: TBP)+≡

```

    procedure :: reset_status => particle_set_reset_status

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_reset_status (particle_set, index, status)
        class(particle_set_t), intent(inout) :: particle_set
        integer, dimension(:), intent(in) :: index
        integer, intent(in) :: status
    end subroutine particle_set_reset_status

```

(Particles: procedures)+≡

```

    module subroutine particle_set_reset_status (particle_set, index, status)
        class(particle_set_t), intent(inout) :: particle_set
        integer, dimension(:), intent(in) :: index
        integer, intent(in) :: status
        integer :: i
        if (allocated (particle_set%prt)) then
            do i = 1, size (index)
                call particle_set%prt(index(i))%reset_status (status)
            end do
        end if
        particle_set%n_beam = &
            count (particle_set%prt%get_status () == PRT_BEAM)
        particle_set%n_in = &
            count (particle_set%prt%get_status () == PRT_INCOMING)
        particle_set%n_out = &
            count (particle_set%prt%get_status () == PRT_OUTGOING)
        particle_set%n_vir = particle_set%n_tot &
            - particle_set%n_beam - particle_set%n_in - particle_set%n_out
    end subroutine particle_set_reset_status

```

Reduce a particle set to the essential entries. The entries kept are those with status INCOMING, OUTGOING or RESONANT. BEAM is kept if keep_beams is true. Other entries are skipped. The correlated state matrix, if any, is also ignored.

(Particles: particle set: TBP)+≡

```
procedure :: reduce => particle_set_reduce
```

(Particles: sub interfaces)+≡

```
module subroutine particle_set_reduce (pset_in, pset_out, keep_beams)
  class(particle_set_t), intent(in) :: pset_in
  type(particle_set_t), intent(out) :: pset_out
  logical, intent(in), optional :: keep_beams
end subroutine particle_set_reduce
```

(Particles: procedures)+≡

```
module subroutine particle_set_reduce (pset_in, pset_out, keep_beams)
  class(particle_set_t), intent(in) :: pset_in
  type(particle_set_t), intent(out) :: pset_out
  logical, intent(in), optional :: keep_beams
  integer, dimension(:), allocatable :: status, map
  integer :: i, j
  logical :: kb
  kb = .false.; if (present (keep_beams)) kb = keep_beams
  allocate (status (pset_in%n_tot))
  pset_out%factorization_mode = pset_in%factorization_mode
  status = pset_in%prt%get_status ()
  if (kb) pset_out%n_beam = count (status == PRT_BEAM)
  pset_out%n_in = count (status == PRT_INCOMING)
  pset_out%n_vir = count (status == PRT_RESONANT)
  pset_out%n_out = count (status == PRT_OUTGOING)
  pset_out%n_tot = &
    pset_out%n_beam + pset_out%n_in + pset_out%n_vir + pset_out%n_out
  allocate (pset_out%prt (pset_out%n_tot))
  allocate (map (pset_in%n_tot))
  map = 0
  j = 0
  if (kb) call copy_particles (PRT_BEAM)
  call copy_particles (PRT_INCOMING)
  call copy_particles (PRT_RESONANT)
  call copy_particles (PRT_OUTGOING)
  do i = 1, pset_in%n_tot
    if (map(i) == 0) cycle
    call pset_out%prt(map(i))%set_parents &
      (pset_in%get_real_parents (i, kb))
    call pset_out%prt(map(i))%set_parents &
      (map (pset_out%prt(map(i))%parent))
    call pset_out%prt(map(i))%set_children &
      (pset_in%get_real_children (i, kb))
    call pset_out%prt(map(i))%set_children &
      (map (pset_out%prt(map(i))%child))
  end do
contains
  subroutine copy_particles (stat)
    integer, intent(in) :: stat
    integer :: i
    do i = 1, pset_in%n_tot
```

```

        if (status(i) == stat) then
            j = j + 1
            map(i) = j
            call particle_init_particle (pset_out%prt(j), pset_in%prt(i))
        end if
    end do
end subroutine copy_particles
end subroutine particle_set_reduce

```

Remove the beam particles and beam remnants from the particle set if the keep beams flag is false. If keep beams is not given, the beam particles and the beam remnants are removed. The correlated state matrix, if any, is also ignored.

(Particles: particle set: TBP)+≡

```

    procedure :: filter_particles => particle_set_filter_particles

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_filter_particles &
        (pset_in, pset_out, keep_beams, real_parents, keep_virtinals)
        class(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), intent(out) :: pset_out
        logical, intent(in), optional :: keep_beams, real_parents, keep_virtinals
    end subroutine particle_set_filter_particles

```

(Particles: procedures)+≡

```

    module subroutine particle_set_filter_particles &
        (pset_in, pset_out, keep_beams, real_parents, keep_virtinals)
        class(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), intent(out) :: pset_out
        logical, intent(in), optional :: keep_beams, real_parents, keep_virtinals
        integer, dimension(:), allocatable :: status, map
        logical, dimension(:), allocatable :: filter
        integer :: i, j
        logical :: kb, rp, kv
        kb = .false.; if (present (keep_beams)) kb = keep_beams
        rp = .false.; if (present (real_parents)) rp = real_parents
        kv = .true.; if (present (keep_virtinals)) kv = keep_virtinals
        if (debug_on) call msg_debug (D_PARTICLES, "filter_particles")
        if (debug2_active (D_PARTICLES)) then
            print *, 'keep_beams = ', kb
            print *, 'real_parents = ', rp
            print *, 'keep_virtinals = ', kv
            print *, '»> pset_in : '
            call pset_in%write(compressed=.true.)
        end if
        call count_and_allocate()
        map = 0
        j = 0
        filter = .false.
        if (.not. kb) filter = status == PRT_BEAM .or. status == PRT_BEAM_REMNANT
        if (.not. kv) filter = filter .or. status == PRT_VIRTUAL
        call copy_particles ()
        do i = 1, pset_in%n_tot
            if (map(i) == 0) cycle
            if (rp) then

```

```

        call pset_out%prt(map(i))%set_parents &
            (map (pset_in%get_real_parents (i, kb)))
        call pset_out%prt(map(i))%set_children &
            (map (pset_in%get_real_children (i, kb)))
    else
        call pset_out%prt(map(i))%set_parents &
            (map (pset_in%prt(i)%get_parents ()))
        call pset_out%prt(map(i))%set_children &
            (map (pset_in%prt(i)%get_children ()))
    end if
end do
if (debug2_active (D_PARTICLES)) then
    print *, '»» pset_out : '
    call pset_out%write(compressed=.true.)
end if
contains
    <filter particles: procedures>
end subroutine particle_set_filter_particles

```

```

<filter particles: procedures>≡
subroutine copy_particles ()
    integer :: i
    do i = 1, pset_in%n_tot
        if (.not. filter(i)) then
            j = j + 1
            map(i) = j
            call particle_init_particle (pset_out%prt(j), pset_in%prt(i))
        end if
    end do
end subroutine copy_particles

```

```

<filter particles: procedures>+≡
subroutine count_and_allocate
    allocate (status (pset_in%n_tot))
    status = particle_get_status (pset_in%prt)
    if (kb) pset_out%n_beam = count (status == PRT_BEAM)
    pset_out%n_in = count (status == PRT_INCOMING)
    if (kb .and. kv) then
        pset_out%n_vir = count (status == PRT_VIRTUAL) + &
            count (status == PRT_RESONANT) + &
            count (status == PRT_BEAM_REMNANT)
    else if (kb .and. .not. kv) then
        pset_out%n_vir = count (status == PRT_RESONANT) + &
            count (status == PRT_BEAM_REMNANT)
    else if (.not. kb .and. kv) then
        pset_out%n_vir = count (status == PRT_VIRTUAL) + &
            count (status == PRT_RESONANT)
    else
        pset_out%n_vir = count (status == PRT_RESONANT)
    end if
    pset_out%n_out = count (status == PRT_OUTGOING)
    pset_out%n_tot = &
        pset_out%n_beam + pset_out%n_in + pset_out%n_vir + pset_out%n_out

```



```

        allocate (pset_out%prt (pset_out%n_tot))
        allocate (map (pset_in%n_tot))
        allocate (filter (pset_in%n_tot))
    end subroutine count_and_allocate

```

Transform a particle set into HEPEVT-compatible form. In this form, for each particle, the parents and the children are contiguous in the particle array. Usually, this requires to clone some particles.

We do not know in advance how many particles the canonical form will have. To be on the safe side, allocate four times the original size.

```

<Particles: types>+≡
    type :: particle_entry_t
        integer :: src = 0
        integer :: status = 0
        integer :: orig = 0
        integer :: copy = 0
    end type particle_entry_t

<Particles: particle set: TBP>+≡
    procedure :: to_hepevt_form => particle_set_to_hepevt_form

<Particles: sub interfaces>+≡
    module subroutine particle_set_to_hepevt_form (pset_in, pset_out)
        class(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), intent(out) :: pset_out
    end subroutine particle_set_to_hepevt_form

<Particles: procedures>+≡
    module subroutine particle_set_to_hepevt_form (pset_in, pset_out)
        class(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), intent(out) :: pset_out
        type(particle_entry_t), dimension(:), allocatable :: prt
        integer, dimension(:), allocatable :: map1, map2
        integer, dimension(:), allocatable :: parent, child
        integer :: n_tot, n_parents, n_children, i, j, c, n

        n_tot = pset_in%n_tot
        allocate (prt (4 * n_tot))
        allocate (map1(4 * n_tot))
        allocate (map2(4 * n_tot))
        map1 = 0
        map2 = 0
        allocate (child (n_tot))
        allocate (parent (n_tot))
        n = 0
        do i = 1, n_tot
            if (pset_in%prt(i)%get_n_parents () == 0) then
                call append (i)
            end if
        end do
        do i = 1, n_tot
            n_children = pset_in%prt(i)%get_n_children ()
            if (n_children > 0) then
                child(1:n_children) = pset_in%prt(i)%get_children ()

```

```

c = child(1)
if (map1(c) == 0) then
  n_parents = pset_in%prt(c)%get_n_parents ()
  if (n_parents > 1) then
    parent(1:n_parents) = pset_in%prt(c)%get_parents ()
    if (i == parent(1) .and. &
        any( [(map1(i)+j-1, j=1,n_parents)] /= &
            map1(parent(1:n_parents)))) then
      do j = 1, n_parents
        call append (parent(j))
      end do
    end if
  else if (map1(i) == 0) then
    call append (i)
  end if
  do j = 1, n_children
    call append (child(j))
  end do
end if
else if (map1(i) == 0) then
  call append (i)
end if
end do
do i = n, 1, -1
  if (prt(i)%status /= PRT_OUTGOING) then
    do j = 1, i-1
      if (prt(j)%status == PRT_OUTGOING) then
        call append(prt(j)%src)
      end if
    end do
  end if
end do
exit
end if
end do
pset_out%n_beam = count (prt(1:n)%status == PRT_BEAM)
pset_out%n_in   = count (prt(1:n)%status == PRT_INCOMING)
pset_out%n_vir  = count (prt(1:n)%status == PRT_RESONANT)
pset_out%n_out  = count (prt(1:n)%status == PRT_OUTGOING)
pset_out%n_tot = n
allocate (pset_out%prt (n))
do i = 1, n
  call particle_init_particle (pset_out%prt(i), pset_in%prt(prt(i)%src))
  call pset_out%prt(i)%reset_status (prt(i)%status)
  if (prt(i)%orig == 0) then
    call pset_out%prt(i)%set_parents &
      (map2 (pset_in%prt(prt(i)%src)%get_parents ()))
  else
    call pset_out%prt(i)%set_parents ([ prt(i)%orig ])
  end if
  if (prt(i)%copy == 0) then
    call pset_out%prt(i)%set_children &
      (map1 (pset_in%prt(prt(i)%src)%get_children ()))
  else
    call pset_out%prt(i)%set_children ([ prt(i)%copy ])
  end if
end if

```

```

end do
contains
subroutine append (i)
  integer, intent(in) :: i
  n = n + 1
  if (n > size (prt)) &
    call msg_bug ("Particle set transform to HEPEVT: insufficient space")
  prt(n)%src = i
  prt(n)%status = pset_in%prt(i)%get_status ()
  if (map1(i) == 0) then
    map1(i) = n
  else
    prt(map2(i))%status = PRT_VIRTUAL
    prt(map2(i))%copy = n
    prt(n)%orig = map2(i)
  end if
  map2(i) = n
end subroutine append
end subroutine particle_set_to_hepevt_form

```

This procedure aims at reconstructing the momenta of an interaction, given a particle set. The main task is to find the original hard process, by following the event history.

In-state: take those particles which are flagged as `PRT_INCOMING`

Out-state: try to be smart by checking the immediate children of the incoming particles. If the `state_flg` table is present, check any `PRT_RESONANT` particles that we get this way, whether they are potential out-particles by their PDG codes. If not, replace them by their children, recursively. (Resonances may have been inserted by the corresponding event transform.)

[WK 21-02-16] Revised the algorithm for the case `recover_beams` = false, i.e., the particle set contains beams and radiation. This does not mean that the particle set contains the complete radiation history. To make up for missing information, we follow the history in the interaction one step backwards and do a bit of guesswork to match this to the possibly incomplete history in the particle set. [The current implementation allows only for one stage of radiation; this could be improved by iterating the procedure!]

[WK 21-03-21] Amended the `find_hard_process_in_pset` algorithm as follows: Occasionally, PYTHIA adds a stepchild to the decay of a resonance that WHIZARD has inserted, a shower object that also has other particles in the event as parents. Such objects must not enter the hard-process record. Therefore, resonance child particle objects are ignored if they have more than one parent.

(Particles: particle set: TBP)+≡

```

procedure :: fill_interaction => particle_set_fill_interaction

```

(Particles: sub interfaces)+≡

```

module subroutine particle_set_fill_interaction &
  (pset, int, n_in, recover_beams, check_match, state_flg, success)
  class(particle_set_t), intent(in) :: pset
  type(interaction_t), intent(inout) :: int
  integer, intent(in) :: n_in
  logical, intent(in), optional :: recover_beams, check_match

```

```

        type(state_flv_content_t), intent(in), optional :: state_flv
        logical, intent(out), optional :: success
    end subroutine particle_set_fill_interaction

    (Particles: procedures)+≡
    module subroutine particle_set_fill_interaction &
        (pset, int, n_in, recover_beams, check_match, state_flv, success)
        class(particle_set_t), intent(in) :: pset
        type(interaction_t), intent(inout) :: int
        integer, intent(in) :: n_in
        logical, intent(in), optional :: recover_beams, check_match
        type(state_flv_content_t), intent(in), optional :: state_flv
        logical, intent(out), optional :: success
        integer, dimension(:), allocatable :: map, pdg
        integer, dimension(:), allocatable :: i_in, i_out, p_in, p_out
        logical, dimension(:), allocatable :: i_set
        integer :: n_out, i, p
        logical :: r_beams, check
        r_beams = .false.; if (present (recover_beams)) r_beams = recover_beams
        check = .true.; if (present (check_match)) check = check_match
        if (check) then
            call find_hard_process_in_int (i_in, i_out)
            call find_hard_process_in_pset (p_in, p_out, state_flv, success)
            if (present (success)) then
                if (size (i_in) /= n_in) success = .false.
                if (size (p_in) /= n_in) success = .false.
                if (size (p_out) /= n_out) success = .false.
                if (.not. success) return
            else
                if (size (i_in) /= n_in) call err_int_n_in
                if (size (p_in) /= n_in) call err_pset_n_in
                if (size (p_out) /= n_out) call err_pset_n_out
            end if
            call extract_hard_process_from_pset (pdg)
            call determine_map_for_hard_process (map, state_flv, success)
            if (present (success)) then
                if (.not. success) return
            end if
            call map_handle_duplicates (map)
            if (.not. r_beams) then
                call determine_map_for_beams (map)
                call map_handle_duplicates (map)
                call determine_map_for_radiation (map, i_in, p_in)
                call map_handle_duplicates (map)
            end if
        else
            allocate (map (int%get_n_tot ()))
            map = [(i, i = 1, size (map))]
            r_beams = .false.
        end if
        allocate (i_set (int%get_n_tot ()), source = .false.)
        do p = 1, size (map)
            if (map(p) /= 0) then
                if (.not. i_set(map(p))) then
                    call int%set_momentum (pset%prt(p)%get_momentum (), map(p))
                end if
            end if
        end do
    end module

```

```

        i_set(map(p)) = .true.
    end if
end if
end do
if (r_beams) then
    do i = 1, n_in
        call reconstruct_beam_and_radiation (i, i_set)
    end do
else
    do i = int%get_n_tot (), 1, -1
        if (.not. i_set(i)) call reconstruct_missing (i, i_set)
    end do
end if
if (any (.not. i_set)) then
    if (present (success)) then
        success = .false.
    else
        call err_map
    end if
end if
contains
subroutine find_hard_process_in_int (i_in, i_out)
    integer, dimension(:), allocatable, intent(out) :: i_in, i_out
    integer :: n_in_i
    integer :: i
    i = int%get_n_tot ()
    n_in_i = int%get_n_parents (i)
    if (n_in_i /= n_in) call err_int_n_in
    allocate (i_in (n_in))
    i_in = int%get_parents (i)
    i = i_in(1)
    n_out = int%get_n_children (i)
    allocate (i_out (n_out))
    i_out = int%get_children (i)
end subroutine find_hard_process_in_int
subroutine find_hard_process_in_pset (p_in, p_out, state_flg, success)
    integer, dimension(:), allocatable, intent(out) :: p_in, p_out
    type(state_flg_content_t), intent(in), optional :: state_flg
    logical, intent(out), optional :: success
    integer, dimension(:), allocatable :: p_status, p_idx, p_child
    integer :: n_out_p, n_child, n_shift
    integer :: i, k, c
    allocate (p_status (pset%n_tot), p_idx (pset%n_tot), p_child (pset%n_tot))
    p_status = pset%prt%get_status ()
    p_idx = [(i, i = 1, pset%n_tot)]
    allocate (p_in (n_in))
    p_in = pack (p_idx, p_status == PRT_INCOMING)
    if (size (p_in) == 0) call err_pset_hard
    i = p_in(1)
    allocate (p_out (n_out))
    n_out_p = pset%prt(i)%get_n_children ()
    p_out(1:n_out_p) = particle_get_children (pset%prt(i))
    do k = 1, size (p_out)
        i = p_out(k)

```

```

    if (present (state_flv)) then
      do while (pset%prt(i)%get_status () == PRT_RESONANT)
        if (state_flv%contains (pset%prt(i)%get_pdg ())) exit
        n_child = pset%prt(i)%get_n_children ()
        p_child(1:n_child) = particle_get_children (pset%prt(i))
        n_shift = -1
        do c = 1, n_child
          if (pset%prt(p_child(c))%get_n_parents () == 1) then
            n_shift = n_shift + 1
          else
            p_child(c) = 0
          end if
        end do
        if (n_shift < 0) then
          if (present (success)) then
            success = .false.
            return
          else
            call err_mismatch
          end if
        end if
        p_out(k+1+n_shift:n_out_p+n_shift) = p_out(k+1:n_out_p)
        n_out_p = n_out_p + n_shift
        do c = 1, n_child
          if (p_child(c) /= 0) then
            p_out(k+c-1) = p_child(c)
          end if
        end do
        i = p_out(k)
      end do
    end if
  end do
  if (present (success)) success = .true.
end subroutine find_hard_process_in_pset
subroutine extract_hard_process_from_pset (pdg)
  integer, dimension(:), allocatable, intent(out) :: pdg
  integer, dimension(:), allocatable :: pdg_p
  logical, dimension(:), allocatable :: mask_p
  integer :: i
  allocate (pdg_p (pset%n_tot))
  pdg_p = pset%prt%get_pdg ()
  allocate (mask_p (pset%n_tot), source = .false.)
  mask_p (p_in) = .true.
  mask_p (p_out) = .true.
  allocate (pdg (n_in + n_out))
  pdg = pack (pdg_p, mask_p)
end subroutine extract_hard_process_from_pset
subroutine determine_map_for_hard_process (map, state_flv, success)
  integer, dimension(:), allocatable, intent(out) :: map
  type(state_flv_content_t), intent(in), optional :: state_flv
  logical, intent(out), optional :: success
  integer, dimension(:), allocatable :: pdg_i, map_i
  integer :: n_tot
  logical, dimension(:), allocatable :: mask_i, mask_p

```

```

logical :: match
n_tot = int%get_n_tot ()
if (present (state_flv)) then
    allocate (mask_i (n_tot), source = .false.)
    mask_i (i_in) = .true.
    mask_i (i_out) = .true.
    allocate (pdg_i (n_tot), map_i (n_tot))
    pdg_i = unpack (pdg, mask_i, 0)
    call state_flv%match (pdg_i, match, map_i)
    if (present (success)) then
        success = match
    end if
    if (.not. match) then
        if (present (success)) then
            return
        else
            call err_mismatch
        end if
    end if
    allocate (mask_p (pset%n_tot), source = .false.)
    mask_p (p_in) = .true.
    mask_p (p_out) = .true.
    allocate (map (size (mask_p)), &
        source = unpack (pack (map_i, mask_i), mask_p, 0))
else
    allocate (map (n_tot), source = 0)
    map(p_in) = i_in
    map(p_out) = i_out
end if
end subroutine determine_map_for_hard_process
subroutine map_handle_duplicates (map)
    integer, dimension(:), intent(inout) :: map
    integer, dimension(1) :: p_parent, p_child
    integer :: p
    do p = 1, pset%n_tot
        if (map(p) == 0) then
            if (pset%prt(p)%get_n_parents () == 1) then
                p_parent = pset%prt(p)%get_parents ()
                if (map(p_parent(1)) /= 0) then
                    if (pset%prt(p_parent(1))%get_n_children () == 1) then
                        map(p) = map(p_parent(1))
                    end if
                end if
            end if
        end if
    end do
    do p = pset%n_tot, 1, -1
        if (map(p) == 0) then
            if (pset%prt(p)%get_n_children () == 1) then
                p_child = pset%prt(p)%get_children ()
                if (map(p_child(1)) /= 0) then
                    if (pset%prt(p_child(1))%get_n_parents () == 1) then
                        map(p) = map(p_child(1))
                    end if
                end if
            end if
        end if
    end do
end subroutine

```

```

        end if
    end if
end do
end subroutine map_handle_duplicates
subroutine determine_map_for_beams (map)
    integer, dimension(:), intent(inout) :: map
    select case (n_in)
    case (1); map(1) = 1
    case (2); map(1:2) = [1,2]
    end select
end subroutine determine_map_for_beams
subroutine determine_map_for_radiation (map, i_in, p_in)
    integer, dimension(:), intent(inout) :: map
    integer, dimension(:), intent(in) :: i_in
    integer, dimension(:), intent(in) :: p_in
    integer, dimension(:), allocatable :: i_cur, p_cur
    integer, dimension(:), allocatable :: i_par, p_par, i_rad, p_rad
    integer :: i, p
    integer :: b, r
    i_cur = i_in
    p_cur = p_in
    do b = 1, n_in
        i = i_cur(b)
        p = p_cur(b)
        i_par = int%get_parents (i)
        p_par = pset%prt(p)%get_parents ()
        if (size (i_par) == 0 .or. size (p_par) == 0) cycle
        if (size (p_par) == 1) then
            if (pset%prt(p_par(1))%get_n_children () == 1) then
                p_par = pset%prt(p_par(1))%get_parents () ! copy of entry
            end if
        end if
        i_rad = int%get_children (i_par(1))
        p_rad = pset%prt(p_par(1))%get_children ()
        do r = 1, size (i_rad)
            if (any (map == i_rad(r))) i_rad(r) = 0
        end do
        i_rad = pack (i_rad, i_rad /= 0)
        do r = 1, size (p_rad)
            if (map(p_rad(r)) /= 0) p_rad(r) = 0
        end do
        p_rad = pack (p_rad, p_rad /= 0)
        do r = 1, min (size (i_rad), size (p_rad))
            map(p_rad(r)) = i_rad(r)
        end do
    end do
    do b = 1, min (size (p_par), size (i_par))
        if (map(p_par(b)) == 0 .and. all (map /= i_par(b))) then
            map(p_par(b)) = i_par(b)
        end if
    end do
end subroutine determine_map_for_radiation
subroutine reconstruct_beam_and_radiation (k, i_set)

```



```

integer, intent(in) :: k
logical, dimension(:), intent(inout) :: i_set
integer :: k_src, k_pre, k_in, k_rad
type(interaction_t), pointer :: int_src
integer, dimension(2) :: i_child
logical, dimension(2) :: is_final
integer :: i
call int%find_source (k, int_src, k_src)
k_pre = 0
k_in = k
do while (.not. i_set (k_in))
  if (k_pre == 0) then
    call int%set_momentum (int_src%get_momentum (k_src), k_in)
  else
    call int%set_momentum (int%get_momentum (k_pre), k_in)
  end if
  i_set(k_in) = .true.
  if (n_in == 2) then
    k_pre = k_in
    i_child = int%get_children (k_pre)
    do i = 1, 2
      is_final(i) = int%get_n_children (i_child(i)) == 0
    end do
    if (all (.not. is_final)) then
      k_in = i_child(k); k_rad = 0
    else if (is_final(2)) then
      k_in = i_child(1); k_rad = i_child(2)
    else if (is_final(1)) then
      k_in = i_child(2); k_rad = i_child(1)
    else
      call err_beams
    end if
    if (k_rad /= 0) then
      if (i_set (k_in)) then
        call int%set_momentum &
          (int%get_momentum (k) - int%get_momentum (k_in), k_rad)
        i_set(k_rad) = .true.
      else
        call err_beams_norad
      end if
    end if
  end if
end do
end subroutine reconstruct_beam_and_radiation
subroutine reconstruct_missing (i, i_set)
integer, intent(in) :: i
logical, dimension(:), intent(inout) :: i_set
integer, dimension(:), allocatable :: i_child, i_parent, i_sibling
integer :: s
i_child = int%get_children (i)
i_parent = int%get_parents (i)
if (size (i_child) > 0 .and. all (i_set(i_child))) then
  call int%set_momentum (sum (int%get_momenta (i_child)), i)
else if (size (i_parent) > 0 .and. all (i_set(i_parent))) then

```

```

        i_sibling = int%get_children (i_parent(1))
        call int%set_momentum (sum (int%get_momenta (i_parent)), i)
        do s = 1, size (i_sibling)
            if (i_sibling(s) == i) cycle
            if (i_set(i_sibling(s))) then
                call int%set_momentum (int%get_momentum (i) &
                    - int%get_momentum (i_sibling(s)), i)
            else
                call err_beams_norad
            end if
        end do
    else
        call err_beams_norad
    end if
    i_set(i) = .true.
end subroutine reconstruct_missing
subroutine err_pset_hard
    call msg_fatal ("Reading particle set: no particles marked as incoming")
end subroutine err_pset_hard
subroutine err_int_n_in
    integer :: n
    if (allocated (i_in)) then
        n = size (i_in)
    else
        n = 0
    end if
    write (msg_buffer, "(A,IO,A,IO)") &
        "Filling hard process from particle set: expect ", n_in, &
        " incoming particle(s), found ", n
    call msg_bug
end subroutine err_int_n_in
subroutine err_pset_n_in
    write (msg_buffer, "(A,IO,A,IO)") &
        "Reading hard-process particle set: should contain ", n_in, &
        " incoming particle(s), found ", size (p_in)
    call msg_fatal
end subroutine err_pset_n_in
subroutine err_pset_n_out
    write (msg_buffer, "(A,IO,A,IO)") &
        "Reading hard-process particle set: should contain ", n_out, &
        " outgoing particle(s), found ", size (p_out)
    call msg_fatal
end subroutine err_pset_n_out
subroutine err_mismatch
    call pset%write ()
    call state_flv%write ()
    call msg_fatal ("Reading particle set: Flavor combination " &
        // "does not match requested process")
end subroutine err_mismatch
subroutine err_map
    call pset%write ()
    call int%basic_write ()
    call msg_fatal ("Reading hard-process particle set: " &
        // "Incomplete mapping from particle set to interaction")

```

```

end subroutine err_map
subroutine err_beams
  call pset%write ()
  call int%basic_write ()
  call msg_fatal ("Reading particle set: Beam structure " &
    // "does not match requested process")
end subroutine err_beams
subroutine err_beams_norad
  call pset%write ()
  call int%basic_write ()
  call msg_fatal ("Reading particle set: Beam structure " &
    // "cannot be reconstructed for this configuration")
end subroutine err_beams_norad
subroutine err_radiation
  call int%basic_write ()
  call msg_bug ("Reading particle set: Interaction " &
    // "contains inconsistent radiation pattern.")
end subroutine err_radiation
end subroutine particle_set_fill_interaction

```

This procedure reconstructs an array of vertex indices from the parent-child information in the particle entries, according to the HepMC scheme. For each particle, we determine which vertex it comes from and which vertex it goes to. We return the two arrays and the maximum vertex index.

For each particle in the list, we first check its parents. If for any parent the vertex where it goes to is already known, this vertex index is assigned as the current 'from' vertex. Otherwise, a new index is created, assigned as the current 'from' vertex, and as the 'to' vertex for all parents.

Then, the analogous procedure is done for the children.

Furthermore, we assign to each vertex the vertex position from the parent(s). We check that these vertex positions coincide, and if not return a null vector.

(Particles: particle set: TBP)+≡

```
procedure :: assign_vertices => particle_set_assign_vertices
```

(Particles: sub interfaces)+≡

```

module subroutine particle_set_assign_vertices &
  (particle_set, v_from, v_to, n_vertices)
  class(particle_set_t), intent(in) :: particle_set
  integer, dimension(:), intent(out) :: v_from, v_to
  integer, intent(out) :: n_vertices
end subroutine particle_set_assign_vertices

```

(Particles: procedures)+≡

```

module subroutine particle_set_assign_vertices &
  (particle_set, v_from, v_to, n_vertices)
  class(particle_set_t), intent(in) :: particle_set
  integer, dimension(:), intent(out) :: v_from, v_to
  integer, intent(out) :: n_vertices
  integer, dimension(:), allocatable :: parent, child
  integer :: n_parents, n_children, vf, vt
  integer :: i, j, v
  v_from = 0
  v_to = 0
  vf = 0

```

```

vt = 0
do i = 1, particle_set%n_tot
  n_parents = particle_set%prt(i)%get_n_parents ()
  if (n_parents /= 0) then
    allocate (parent (n_parents))
    parent = particle_set%prt(i)%get_parents ()
    SCAN_PARENTS: do j = 1, size (parent)
      v = v_to(parent(j))
      if (v /= 0) then
        v_from(i) = v; exit SCAN_PARENTS
      end if
    end do SCAN_PARENTS
    if (v_from(i) == 0) then
      vf = vf + 1; v_from(i) = vf
      v_to(parent) = vf
    end if
    deallocate (parent)
  end if
  n_children = particle_set%prt(i)%get_n_children ()
  if (n_children /= 0) then
    allocate (child (n_children))
    child = particle_set%prt(i)%get_children ()
    SCAN_CHILDREN: do j = 1, size (child)
      v = v_from(child(j))
      if (v /= 0) then
        v_to(i) = v; exit SCAN_CHILDREN
      end if
    end do SCAN_CHILDREN
    if (v_to(i) == 0) then
      vt = vt + 1; v_to(i) = vt
      v_from(child) = vt
    end if
    deallocate (child)
  end if
end do
n_vertices = max (vf, vt)
end subroutine particle_set_assign_vertices

```

15.4.6 Expression interface

This converts a `particle_set` object as defined here to a more concise `subevt` object that can be used as the event root of an expression. In particular, the latter lacks virtual particles, spin correlations and parent-child relations.

We keep beam particles, incoming partons, and outgoing partons. Furthermore, we keep radiated particles (a.k.a. beam remnants) if they have no children in the current particle set, and mark them as outgoing particles.

If `colorize` is set and true, mark all particles in the subevent as colorized, and set color/anticolor flow indices where they are defined. Colorless particles do not get indices but are still marked as colorized, for consistency.

(Particles: particle set: TBP)+≡

```
procedure :: to_subevt => particle_set_to_subevt
```

(Particles: sub interfaces)+≡

```

module subroutine particle_set_to_subevt (particle_set, subevt, colorize)
  class(particle_set_t), intent(in) :: particle_set
  type(subevt_t), intent(out) :: subevt
  logical, intent(in), optional :: colorize
end subroutine particle_set_to_subevt

```

(Particles: procedures)+≡

```

module subroutine particle_set_to_subevt (particle_set, subevt, colorize)
  class(particle_set_t), intent(in) :: particle_set
  type(subevt_t), intent(out) :: subevt
  logical, intent(in), optional :: colorize
  integer :: n_tot, n_beam, n_in, n_out, n_rad
  integer :: i, k, n_active
  integer, dimension(2) :: hel
  logical :: keep
  n_tot = particle_set_get_n_tot      (particle_set)
  n_beam = particle_set_get_n_beam    (particle_set)
  n_in   = particle_set_get_n_in     (particle_set)
  n_out  = particle_set_get_n_out     (particle_set)
  n_rad  = particle_set_get_n_remnants (particle_set)
  call subevt_init (subevt, n_beam + n_rad + n_in + n_out)
  k = 0
  do i = 1, n_tot
    associate (prt => particle_set%prt(i))
      keep = .false.
      select case (particle_get_status (prt))
        case (PRT_BEAM)
          k = k + 1
          call subevt%set_beam (k, &
                                particle_get_pdg (prt), &
                                particle_get_momentum (prt), &
                                particle_get_p2 (prt))
          keep = .true.
        case (PRT_INCOMING)
          k = k + 1
          call subevt%set_incoming (k, &
                                    particle_get_pdg (prt), &
                                    particle_get_momentum (prt), &
                                    particle_get_p2 (prt))
          keep = .true.
        case (PRT_OUTGOING)
          k = k + 1
          call subevt%set_outgoing (k, &
                                    particle_get_pdg (prt), &
                                    particle_get_momentum (prt), &
                                    particle_get_p2 (prt))
          keep = .true.
        case (PRT_BEAM_REMNANT)
          if (prt%get_n_children () == 0) then
            k = k + 1
            call subevt%set_outgoing (k, &
                                      particle_get_pdg (prt), &
                                      particle_get_momentum (prt), &
                                      particle_get_p2 (prt))
          end if
        end select
      end associate
    end do
  end do

```

```

        keep = .true.
    end if
end select
if (keep) then
    if (prt%polarization == PRT_DEFINITE_HELICITY) then
        if (prt%hel%is_diagonal ()) then
            hel = prt%hel%to_pair ()
            call subvt_polarize (subvt, k, hel(1))
        end if
    end if
end if
if (present (colorize)) then
    if (colorize) then
        call subvt_colorize &
            (subvt, i, prt%col%get_col (), prt%col%get_acl ())
    end if
end if
end associate
n_active = k
end do
call subvt%reset (n_active)
end subroutine particle_set_to_subvt

```

This replaces the `particle_set\%prt` array with a given array of particles

(Particles: particle set: TBP)+≡

```

    procedure :: replace => particle_set_replace

```

(Particles: sub interfaces)+≡

```

    module subroutine particle_set_replace (particle_set, newprt)
        class(particle_set_t), intent(inout) :: particle_set
        type(particle_t), intent(in), dimension(:), allocatable :: newprt
    end subroutine particle_set_replace

```

(Particles: procedures)+≡

```

    module subroutine particle_set_replace (particle_set, newprt)
        class(particle_set_t), intent(inout) :: particle_set
        type(particle_t), intent(in), dimension(:), allocatable :: newprt
        if (allocated (particle_set%prt)) deallocate (particle_set%prt)
        allocate (particle_set%prt(size (newprt)))
        particle_set%prt = newprt
        particle_set%n_tot = size (newprt)
        particle_set%n_beam = count (particle_get_status (newprt) == PRT_BEAM)
        particle_set%n_in = count (particle_get_status (newprt) == PRT_INCOMING)
        particle_set%n_out = count (particle_get_status (newprt) == PRT_OUTGOING)
        particle_set%n_vir = particle_set%n_tot &
            - particle_set%n_beam - particle_set%n_in - particle_set%n_out
    end subroutine particle_set_replace

```

This routine orders the outgoing particles into clusters of colorless particles and such of particles ordered corresponding to the indices of the color lines. All outgoing particles in the ordered set appear as child of the corresponding outgoing particle in the unordered set, including colored beam remnants. We always start continue via the anti-color line, such that color flows within each

Lund string system is always continued from the anticolor of one particle to the identical color index of another particle.

(Particles: particle set: TBP)+≡

```
procedure :: order_color_lines => particle_set_order_color_lines
```

(Particles: sub interfaces)+≡

```
module subroutine particle_set_order_color_lines (pset_out, pset_in)
  class(particle_set_t), intent(inout) :: pset_out
  type(particle_set_t), intent(in) :: pset_in
end subroutine particle_set_order_color_lines
```

(Particles: procedures)+≡

```
module subroutine particle_set_order_color_lines (pset_out, pset_in)
  class(particle_set_t), intent(inout) :: pset_out
  type(particle_set_t), intent(in) :: pset_in
  integer :: i, n, n_col_rem
  n_col_rem = 0
  do i = 1, pset_in%n_tot
    if (pset_in%prt(i)%get_status () == PRT_BEAM_REMNANT .and. &
        any (pset_in%prt(i)%get_color () /= 0)) then
      n_col_rem = n_col_rem + 1
    end if
  end do
  pset_out%n_beam = pset_in%n_beam
  pset_out%n_in = pset_in%n_in
  pset_out%n_vir = pset_in%n_vir + pset_in%n_out + n_col_rem
  pset_out%n_out = pset_in%n_out
  pset_out%n_tot = pset_in%n_tot + pset_in%n_out + n_col_rem
  pset_out%correlated_state = pset_in%correlated_state
  pset_out%factorization_mode = pset_in%factorization_mode
  allocate (pset_out%prt (pset_out%n_tot))
  do i = 1, pset_in%n_tot
    call pset_out%prt(i)%init (pset_in%prt(i))
    call pset_out%prt(i)%set_children (pset_in%prt(i)%child)
    call pset_out%prt(i)%set_parents (pset_in%prt(i)%parent)
  end do
  n = pset_in%n_tot
  do i = 1, pset_in%n_tot
    if (pset_out%prt(i)%get_status () == PRT_OUTGOING .and. &
        all (pset_out%prt(i)%get_color () == 0) .and. &
        .not. pset_out%prt(i)%has_children ()) then
      n = n + 1
      call pset_out%prt(n)%init (pset_out%prt(i))
      call pset_out%prt(i)%reset_status (PRT_VIRTUAL)
      call pset_out%prt(i)%add_child (n)
      call pset_out%prt(i)%set_parents ([i])
    end if
  end do
  if (n_col_rem > 0) then
    do i = 1, n_col_rem
    end do
  end if
end subroutine particle_set_order_color_lines
```

Eliminate numerical noise

```
<Particles: public>+≡
    public :: pacify

<Particles: interfaces>≡
    interface pacify
        module procedure pacify_particle
        module procedure pacify_particle_set
    end interface pacify

<Particles: sub interfaces>+≡
    module subroutine pacify_particle (prt)
        class(particle_t), intent(inout) :: prt
    end subroutine pacify_particle
    module subroutine pacify_particle_set (pset)
        class(particle_set_t), intent(inout) :: pset
    end subroutine pacify_particle_set

<Particles: procedures>+≡
    module subroutine pacify_particle (prt)
        class(particle_t), intent(inout) :: prt
        real(default) :: e
        e = epsilon (1._default) * energy (prt%p)
        call pacify (prt%p, 10 * e)
        call pacify (prt%p2, 1e4 * e)
    end subroutine pacify_particle

    module subroutine pacify_particle_set (pset)
        class(particle_set_t), intent(inout) :: pset
        integer :: i
        do i = 1, pset%n_tot
            call pacify (pset%prt(i))
        end do
    end subroutine pacify_particle_set
```

15.4.7 Unit tests

Test module, followed by the corresponding implementation module.

```
<particles_ut.f90>≡
    <File header>

    module particles_ut
        use unit_tests
        use particles_ut_i

    <Standard module head>

    <Particles: public test>

    contains

    <Particles: test driver>
```



```

    end module particles_ut
<particles_uti.f90>≡
  <File header>

  module particles_uti

    <Use kinds>
    use io_units
    use numeric_utils
    use constants, only: one, tiny_07
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices
    use interactions
    use evaluators
    use model_data
    use subevents

    use particles

    <Standard module head>

    <Particles: test declarations>

    contains

    <Particles: tests>

    <Particles: test auxiliary>

    end module particles_uti
API: driver for the unit tests below.
<Particles: public test>≡
  public :: particles_test
<Particles: test driver>≡
  subroutine particles_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Particles: execute tests>
  end subroutine particles_test

```

Check the basic setup of the `particle_set_t` type: Set up a chain of production and decay and factorize the result into particles. The process is $d\bar{d} \rightarrow Z \rightarrow q\bar{q}$.

```

<Particles: execute tests>≡
  call test (particles_1, "particles_1", &
    "check particle_set routines", &
    u, results)
<Particles: test declarations>≡
  public :: particles_1

```

```

(Particles: tests)≡
subroutine particles_1 (u)
  use os_interface
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t), dimension(3) :: flv
  type(color_t), dimension(3) :: col
  type(helicity_t), dimension(3) :: hel
  type(quantum_numbers_t), dimension(3) :: qn
  type(vector4_t), dimension(3) :: p
  type(interaction_t), target :: int1, int2
  type(quantum_numbers_mask_t) :: qn_mask_conn
  type(evaluator_t), target :: eval
  type(interaction_t) :: int
  type(particle_set_t) :: particle_set1, particle_set2
  type(particle_set_t) :: particle_set3, particle_set4
  type(subevt_t) :: subevt
  logical :: ok
  integer :: unit, iostat

  write (u, "(A)")  "* Test output: Particles"
  write (u, "(A)")  "* Purpose: test particle_set routines"
  write (u, "(A)")

  write (u, "(A)")  "* Reading model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* Initializing production process"

  call int1%basic_init (2, 0, 1, set_relations=.true.)
  call flv%init ([1, -1, 23], model)
  call col%init_col_acl ([0, 0, 0], [0, 0, 0])
  call hel(3)%init (1, 1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.25_default, 0._default))
  call hel(3)%init (1,-1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0._default, 0.25_default))
  call hel(3)%init (-1, 1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0._default,-0.25_default))
  call hel(3)%init (-1,-1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.25_default, 0._default))
  call hel(3)%init (0, 0)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.5_default, 0._default))
  call int1%freeze ()
  p(1) = vector4_moving (45._default, 45._default, 3)
  p(2) = vector4_moving (45._default,-45._default, 3)
  p(3) = p(1) + p(2)
  call int1%set_momenta (p)

```

```

write (u, "(A)")
write (u, "(A)")  "** Setup decay process"

call int2%basic_init (1, 0, 2, set_relations=.true.)
call flv%init ([23, 1, -1], model)
call col%init_col_acl ([0, 501, 0], [0, 0, 501])
call hel%init ([1, 1, 1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([1, 1, 1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default, 0.1_default))
call hel%init ([-1,-1,-1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default,-0.1_default))
call hel%init ([-1,-1,-1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call hel%init ([0,-1, 1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0, 1,-1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call flv%init ([23, 2, -2], model)
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call int2%freeze ()
p(2) = vector4_moving (45._default, 45._default, 2)
p(3) = vector4_moving (45._default,-45._default, 2)
call int2%set_momenta (p)
call int2%set_source_link (1, int1, 3)
call int1%basic_write (u)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "** Concatenate production and decay"

call eval%init_product (int1, int2, qn_mask_conn, &
    connections_are_resonant=.true.)
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, polarized)"
write (u, "(A)")

int = eval%interaction_t
call particle_set1%init &
      (ok, int, int, FM_FACTOR_HELICITY, &
       [0.2_default, 0.2_default], .false., .true.)
call particle_set1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (in/out only, selected helicity)"
write (u, "(A)")

int = eval%interaction_t
call particle_set2%init &
      (ok, int, int, FM_SELECT_HELICITY, &
       [0.9_default, 0.9_default], .false., .false.)
call particle_set2%write (u)
call particle_set2%final ()

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, selected helicity)"
write (u, "(A)")

int = eval%interaction_t
call particle_set2%init &
      (ok, int, int, FM_SELECT_HELICITY, &
       [0.7_default, 0.7_default], .false., .true.)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)") &
      "* Factorize (complete, polarized, correlated); write and read again"
write (u, "(A)")

int = eval%interaction_t
call particle_set3%init &
      (ok, int, int, FM_FACTOR_HELICITY, &
       [0.7_default, 0.7_default], .true., .true.)
call particle_set3%write (u)

unit = free_unit ()
open (unit, action="readwrite", form="unformatted", status="scratch")
call particle_set3%write_raw (unit)
rewind (unit)
call particle_set4%read_raw (unit, iostat=iostat)
call particle_set4%set_model (model)
close (unit)

write (u, "(A)")
write (u, "(A)")  "* Result from reading"
write (u, "(A)")

```

```

call particle_set4%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transform to a subevt object"
write (u, "(A)")

call particle_set4%to_subevt (subevt)
call subevt%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set1%final ()
call particle_set2%final ()
call particle_set3%final ()
call particle_set4%final ()
call eval%final ()
call int1%final ()
call int2%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_1"

end subroutine particles_1

```

Reconstruct a hard interaction from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_2, "particles_2", &
    "reconstruct hard interaction", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_2

<Particles: tests>+≡
  subroutine particles_2 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "* Purpose: reconstruct simple interaction"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 3 interaction"
    write (u, "(A)")  "    + incoming partons marked as virtual"
    write (u, "(A)")  "    + no quantum numbers"

```

```

write (u, "(A)")

call reset_interaction_counter ()
call int%basic_init (0, 2, 3)
do i = 1, 2
  do j = 3, 5
    call int%relate (i, j)
  end do
end do

allocate (qn (5))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [11, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 2
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 5
allocate (pset%prt (pset%n_tot))
do i = 1, 2
  call pset%prt(i)%reset_status (PRT_INCOMING)
  call pset%prt(i)%set_children ([3,4,5])
end do
do i = 3, 5
  call pset%prt(i)%reset_status (PRT_OUTGOING)
  call pset%prt(i)%set_parents ([1,2])
end do
call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (5._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))
call pset%prt(5)%set_momentum (vector4_at_rest (3._default))

allocate (flv (5))
call flv%init ([11,12,5,4,3])

```

```

do i = 1, 5
  call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_2"

end subroutine particles_2

```

Reconstruct an interaction with beam structure, e.g., a hadronic interaction, from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_3, "particles_3", &
    "reconstruct interaction with beam structure", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_3

<Particles: tests>+≡
  subroutine particles_3 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "*   Purpose: reconstruct simple interaction"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "      + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()
    call int%basic_init (0, 6, 3)
    call int%relate (1, 3)

```

```

call int%relate (1, 4)
call int%relate (2, 5)
call int%relate (2, 6)
do i = 4, 6, 2
  do j = 7, 9
    call int%relate (i, j)
  end do
end do

allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

call create_test_particle_set_1 (pset)

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_3"

end subroutine particles_3

```



```

(Particles: test auxiliary)≡
subroutine create_test_particle_set_1 (pset)
  type(particle_set_t), intent(out) :: pset
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: i
  pset%n_beam = 2
  pset%n_in   = 2
  pset%n_vir  = 2
  pset%n_out  = 3
  pset%n_tot  = 9

  allocate (pset%prt (pset%n_tot))
  call pset%prt(1)%reset_status (PRT_BEAM)
  call pset%prt(2)%reset_status (PRT_BEAM)
  call pset%prt(3)%reset_status (PRT_INCOMING)
  call pset%prt(4)%reset_status (PRT_INCOMING)
  call pset%prt(5)%reset_status (PRT_BEAM_REMNANT)
  call pset%prt(6)%reset_status (PRT_BEAM_REMNANT)
  call pset%prt(7)%reset_status (PRT_OUTGOING)
  call pset%prt(8)%reset_status (PRT_OUTGOING)
  call pset%prt(9)%reset_status (PRT_OUTGOING)

  call pset%prt(1)%set_children ([3,5])
  call pset%prt(2)%set_children ([4,6])
  call pset%prt(3)%set_children ([7,8,9])
  call pset%prt(4)%set_children ([7,8,9])

  call pset%prt(3)%set_parents ([1])
  call pset%prt(4)%set_parents ([2])
  call pset%prt(5)%set_parents ([1])
  call pset%prt(6)%set_parents ([2])
  call pset%prt(7)%set_parents ([3,4])
  call pset%prt(8)%set_parents ([3,4])
  call pset%prt(9)%set_parents ([3,4])

  call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
  call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
  call pset%prt(3)%set_momentum (vector4_at_rest (4._default))
  call pset%prt(4)%set_momentum (vector4_at_rest (6._default))
  call pset%prt(5)%set_momentum (vector4_at_rest (3._default))
  call pset%prt(6)%set_momentum (vector4_at_rest (5._default))
  call pset%prt(7)%set_momentum (vector4_at_rest (7._default))
  call pset%prt(8)%set_momentum (vector4_at_rest (8._default))
  call pset%prt(9)%set_momentum (vector4_at_rest (9._default))

  allocate (flv (9))
  call flv%init ([2011, 2012, 11, 12, 91, 92, 3, 4, 5])
  do i = 1, 9
    call pset%prt(i)%set_flavor (flv(i))
  end do
end subroutine create_test_particle_set_1

```

Reconstruct an interaction with beam structure, e.g., a hadronic interaction, from a particle set that is missing the beam information.

```

<Particles: execute tests>+≡
  call test (particles_4, "particles_4", &
    "reconstruct interaction with missing beams", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_4

<Particles: tests>+≡
  subroutine particles_4 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(interaction_t), target :: int_beams
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "* Purpose: reconstruct beams"
    write (u, "(A)")

    call reset_interaction_counter ()

    write (u, "(A)")  "* Set up an interaction that contains beams only"
    write (u, "(A)")

    call int_beams%basic_init (0, 0, 2)
    call int_beams%set_momentum (vector4_at_rest (1._default), 1)
    call int_beams%set_momentum (vector4_at_rest (2._default), 2)
    allocate (qn (2))
    call int_beams%add_state (qn)
    call int_beams%freeze ()

    call int_beams%basic_write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "    + no quantum numbers"
    write (u, "(A)")

    call int%basic_init (0, 6, 3)
    call int%relate (1, 3)
    call int%relate (1, 4)
    call int%relate (2, 5)
    call int%relate (2, 6)
    do i = 4, 6, 2
      do j = 7, 9
        call int%relate (i, j)
      end do
    end do
    do i = 1, 2
      call int%set_source_link (i, int_beams, i)
    end do
  end subroutine particles_4

```

```

end do

deallocate (qn)
allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
    map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 2
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 5

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_INCOMING)
call pset%prt(2)%reset_status (PRT_INCOMING)
call pset%prt(3)%reset_status (PRT_OUTGOING)
call pset%prt(4)%reset_status (PRT_OUTGOING)
call pset%prt(5)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,4,5])
call pset%prt(2)%set_children ([3,4,5])

call pset%prt(3)%set_parents ([1,2])
call pset%prt(4)%set_parents ([1,2])
call pset%prt(5)%set_parents ([1,2])

call pset%prt(1)%set_momentum (vector4_at_rest (6._default))
call pset%prt(2)%set_momentum (vector4_at_rest (6._default))
call pset%prt(3)%set_momentum (vector4_at_rest (3._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))
call pset%prt(5)%set_momentum (vector4_at_rest (5._default))

allocate (flv (5))
call flv%init ([11, 12, 3, 4, 5])

```

```

do i = 1, 5
  call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv, &
  recover_beams = .true.)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_4"

end subroutine particles_4

```

Reconstruct an interaction with beam structure and cloned particles (radiated particles repeated in the event record, to maintain some canonical ordering).

```

<Particles: execute tests>+≡
  call test (particles_5, "particles_5", &
    "reconstruct interaction with beams and duplicate entries", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_5

<Particles: tests>+≡
  subroutine particles_5 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "*   Purpose: reconstruct event with duplicate entries"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "      + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()

```

```

call int%basic_init (0, 6, 3)
call int%relate (1, 3)
call int%relate (1, 4)
call int%relate (2, 5)
call int%relate (2, 6)
do i = 4, 6, 2
  do j = 7, 9
    call int%relate (i, j)
  end do
end do

allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 2
pset%n_in   = 2
pset%n_vir  = 4
pset%n_out  = 5
pset%n_tot  = 13

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_BEAM)
call pset%prt(2)%reset_status (PRT_BEAM)
call pset%prt(3)%reset_status (PRT_VIRTUAL)
call pset%prt(4)%reset_status (PRT_VIRTUAL)
call pset%prt(5)%reset_status (PRT_VIRTUAL)
call pset%prt(6)%reset_status (PRT_VIRTUAL)
call pset%prt(7)%reset_status (PRT_INCOMING)
call pset%prt(8)%reset_status (PRT_INCOMING)
call pset%prt( 9)%reset_status (PRT_OUTGOING)
call pset%prt(10)%reset_status (PRT_OUTGOING)
call pset%prt(11)%reset_status (PRT_OUTGOING)
call pset%prt(12)%reset_status (PRT_OUTGOING)
call pset%prt(13)%reset_status (PRT_OUTGOING)

```

```

call pset%prt(1)%set_children ([3,4])
call pset%prt(2)%set_children ([5,6])
call pset%prt(3)%set_children ([ 7])
call pset%prt(4)%set_children ([ 9])
call pset%prt(5)%set_children ([ 8])
call pset%prt(6)%set_children ([10])
call pset%prt(7)%set_children ([11,12,13])
call pset%prt(8)%set_children ([11,12,13])

call pset%prt(3)%set_parents ([1])
call pset%prt(4)%set_parents ([1])
call pset%prt(5)%set_parents ([2])
call pset%prt(6)%set_parents ([2])
call pset%prt( 7)%set_parents ([3])
call pset%prt( 8)%set_parents ([5])
call pset%prt( 9)%set_parents ([4])
call pset%prt(10)%set_parents ([6])
call pset%prt(11)%set_parents ([7,8])
call pset%prt(12)%set_parents ([7,8])
call pset%prt(13)%set_parents ([7,8])

call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (4._default))
call pset%prt(4)%set_momentum (vector4_at_rest (3._default))
call pset%prt(5)%set_momentum (vector4_at_rest (6._default))
call pset%prt(6)%set_momentum (vector4_at_rest (5._default))
call pset%prt(7)%set_momentum (vector4_at_rest (4._default))
call pset%prt(8)%set_momentum (vector4_at_rest (6._default))
call pset%prt( 9)%set_momentum (vector4_at_rest (3._default))
call pset%prt(10)%set_momentum (vector4_at_rest (5._default))
call pset%prt(11)%set_momentum (vector4_at_rest (7._default))
call pset%prt(12)%set_momentum (vector4_at_rest (8._default))
call pset%prt(13)%set_momentum (vector4_at_rest (9._default))

allocate (flv (13))
call flv%init ([2011, 2012, 11, 91, 12, 92, 11, 12, 91, 92, 3, 4, 5])
do i = 1, 13
    call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*"  Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

```

```

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_5"

end subroutine particles_5

```

Reconstruct an interaction with pair spectrum, e.g., beamstrahlung from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_6, "particles_6", &
    "reconstruct interaction with pair spectrum", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_6

<Particles: tests>+≡
  subroutine particles_6 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "* Purpose: reconstruct interaction with pair spectrum"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "      + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()
    call int%basic_init (0, 6, 3)
    do i = 1, 2
      do j = 3, 6
        call int%relate (i, j)
      end do
    end do
    do i = 5, 6
      do j = 7, 9
        call int%relate (i, j)
      end do
    end do

    allocate (qn (9))
    call int%add_state (qn)
    call int%freeze ()

    call int%basic_write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [1011, 1012, 21, 22, 11, 12, 3, 4, 5], &
    map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 2
pset%n_in   = 2
pset%n_vir  = 2
pset%n_out  = 3
pset%n_tot  = 9

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_BEAM)
call pset%prt(2)%reset_status (PRT_BEAM)
call pset%prt(3)%reset_status (PRT_INCOMING)
call pset%prt(4)%reset_status (PRT_INCOMING)
call pset%prt(5)%reset_status (PRT_OUTGOING)
call pset%prt(6)%reset_status (PRT_OUTGOING)
call pset%prt(7)%reset_status (PRT_OUTGOING)
call pset%prt(8)%reset_status (PRT_OUTGOING)
call pset%prt(9)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,4,5,6])
call pset%prt(2)%set_children ([3,4,5,6])
call pset%prt(3)%set_children ([7,8,9])
call pset%prt(4)%set_children ([7,8,9])

call pset%prt(3)%set_parents ([1,2])
call pset%prt(4)%set_parents ([1,2])
call pset%prt(5)%set_parents ([1,2])
call pset%prt(6)%set_parents ([1,2])
call pset%prt(7)%set_parents ([3,4])
call pset%prt(8)%set_parents ([3,4])
call pset%prt(9)%set_parents ([3,4])

call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (5._default))
call pset%prt(4)%set_momentum (vector4_at_rest (6._default))
call pset%prt(5)%set_momentum (vector4_at_rest (3._default))
call pset%prt(6)%set_momentum (vector4_at_rest (4._default))

```



```

call pset%prt(7)%set_momentum (vector4_at_rest (7._default))
call pset%prt(8)%set_momentum (vector4_at_rest (8._default))
call pset%prt(9)%set_momentum (vector4_at_rest (9._default))

allocate (flv (9))
call flv%init ([1011, 1012, 11, 12, 21, 22, 3, 4, 5])
do i = 1, 9
  call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_6"

end subroutine particles_6

```

Reconstruct a hard decay interaction from a shuffled particle set.

```

<Particles: execute tests>+≡
  call test (particles_7, "particles_7", &
    "reconstruct decay interaction with reordering", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_7

<Particles: tests>+≡
  subroutine particles_7 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "*   Purpose: reconstruct decay interaction with reordering"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 1 -> 3 interaction"

```

```

write (u, "(A)") "      + no quantum numbers"
write (u, "(A)")

call reset_interaction_counter ()
call int%basic_init (0, 1, 3)
do j = 2, 4
    call int%relate (1, j)
end do

allocate (qn (4))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)") "* Manually set up a flavor-content record"
write (u, "(A)") "* assumed interaction: 6 12 5 -11"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [6, 5, -11, 12], &
    map = [1, 4, 2, 3])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)") "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 1
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 4
allocate (pset%prt (pset%n_tot))
do i = 1, 1
    call pset%prt(i)%reset_status (PRT_INCOMING)
    call pset%prt(i)%set_children ([2,3,4])
end do
do i = 2, 4
    call pset%prt(i)%reset_status (PRT_OUTGOING)
    call pset%prt(i)%set_parents ([1])
end do
call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (3._default))
call pset%prt(3)%set_momentum (vector4_at_rest (2._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))

allocate (flv (4))
call flv%init ([6,5,12,-11])
do i = 1, 4

```

```

        call pset%prt(i)%set_flavor (flv(i))
    end do

    call pset%write (u)

    write (u, "(A)")
    write (u, "(A)")  "*   Fill interaction from particle set"
    write (u, "(A)")

    call pset%fill_interaction (int, 1, state_flg=state_flg)
    call int%basic_write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call int%final ()
    call pset%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: particles_7"

end subroutine particles_7

```

<Particles: execute tests>+≡

```

    call test (particles_8, "particles_8", &
               "Test functions on particle sets", u, results)

```

<Particles: test declarations>+≡

```

    public :: particles_8

```

<Particles: tests>+≡

```

subroutine particles_8 (u)
    integer, intent(in) :: u
    type(particle_set_t) :: particle_set
    type(particle_t), dimension(:), allocatable :: particles
    integer, allocatable, dimension(:) :: children, parents
    integer :: n_particles, i
    write (u, "(A)")  "* Test output: particles_8"
    write (u, "(A)")  "*   Purpose: Test functions on particle sets"
    write (u, "(A)")

    call create_test_particle_set_1 (particle_set)
    call particle_set%write (u)
    call assert_equal (u, particle_set%n_tot, 9)
    call assert_equal (u, particle_set%n_beam, 2)
    allocate (children (particle_set%prt(3)%get_n_children ()))
    children = particle_set%prt(3)%get_children()
    call assert_equal (u, particle_set%prt(children(1))%get_pdg (), 3)
    call assert_equal (u, size (particle_set%prt(1)%get_children ()), 2)
    call assert_equal (u, size (particle_set%prt(2)%get_children ()), 2)

    call particle_set%without_hadronic_remnants &
        (particles, n_particles, 3)
    call particle_set%replace (particles)
    write (u, "(A)")

```

```

call particle_set%write (u)

call assert_equal (u, n_particles, 7)
call assert_equal (u, size(particles), 10)
call assert_equal (u, particle_set%n_tot, 10)
call assert_equal (u, particle_set%n_beam, 2)
do i = 3, 4
  if (allocated (children)) deallocate (children)
  allocate (children (particle_set%prt(i)%get_n_children ()))
  children = particle_set%prt(i)%get_children()
  call assert_equal (u, particle_set%prt(children(1))%get_pdg (), 3)
  call assert_equal (u, particle_set%prt(children(2))%get_pdg (), 4)
  call assert_equal (u, particle_set%prt(children(3))%get_pdg (), 5)
end do
do i = 5, 7
  if (allocated (parents)) deallocate (parents)
  allocate (parents (particle_set%prt(i)%get_n_parents ()))
  parents = particle_set%prt(i)%get_parents()
  call assert_equal (u, particle_set%prt(parents(1))%get_pdg (), 11)
  call assert_equal (u, particle_set%prt(parents(2))%get_pdg (), 12)
end do
call assert_equal (u, size (particle_set%prt(1)%get_children ()), &
  1, "get children of 1")
call assert_equal (u, size (particle_set%prt(2)%get_children ()), &
  1, "get children of 2")

call assert_equal (u, particle_set%find_particle &
  (particle_set%prt(1)%get_pdg (), particle_set%prt(1)%p), &
  1, "find 1st particle")
call assert_equal (u, particle_set%find_particle &
  (particle_set%prt(2)%get_pdg (), particle_set%prt(2)%p * &
    (one + tiny_07), rel_smallness=1.0E-6_default), &
  2, "find 2nd particle fuzzy")

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_8"
end subroutine particles_8

```

Order color lines into Lund string systems, without colored beam remnants first.

```

<Particles: execute tests>+≡
  call test (particles_9, "particles_9", &
    "order into Lund strings, uncolored beam remnants", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_9

<Particles: tests>+≡
  subroutine particles_9 (u)
    integer, intent(in) :: u
    write (u, "(A)")  "* Test output: particles_9"
    write (u, "(A)")  "* Purpose: Order into Lund strings, "
    write (u, "(A)")  "* uncolored beam remnants"
    write (u, "(A)")
  end subroutine particles_9

```


Chapter 16

Beams

These modules implement beam configuration and beam structure, the latter in abstract terms.

beam_structures The `beam_structure_t` type is a messenger type that communicates the user settings to the **WHIZARD** core.

beams Beam configuration.

sf_aux Tools for handling structure functions and splitting

sf_mappings Mapping functions, useful for structure function implementation

sf_base The abstract structure-function interaction and structure-function chain types.

These are the implementation modules, the concrete counterparts of **sf_base**:

sf_isr ISR structure function (photon radiation inclusive and resummed in collinear and IR regions).

sf_epa Effective Photon Approximation.

sf_ewa Effective W (and Z) approximation.

sf_escan Energy spectrum that emulates a uniform energy scan.

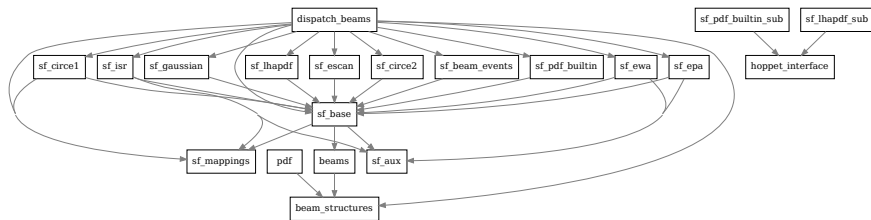


Figure 16.1: Module dependencies in `src/beams`.

sf_gaussian Gaussian beam spread

sf_beam_events Beam-event generator that reads its input from an external file.

sf_circe1 CIRCE1 beam spectra for electrons and photons.

sf_circe2 CIRCE2 beam spectra for electrons and photons.

hoppet_interface Support for *b*-quark matching, add-on to PDF modules.

sf_pdf_builtin Direct support for selected hadron PDFs.

sf_lhapdf LHAPDF library support.

16.1 Beam structure

This module stores the beam structure definition as it is declared in the SINDARIN script. The structure definition is not analyzed, just recorded for later use.

We do not capture any numerical parameters, just names of particles and structure functions.

```
(beam_structures.f90)≡
  <File header>

  module beam_structures

    <Use kinds>
    <Use strings>
    use lorentz
    use polarizations

    <Standard module head>

    <Beam structures: public>

    <Beam structures: types>

    <Beam structures: interfaces>

    interface
    <Beam structures: sub interfaces>
    end interface

  end module beam_structures

(beam_structures_sub.f90)≡
  <File header>

  submodule (beam_structures) beam_structures_s

    use io_units
    use format_defs, only: FMT_19
    use diagnostics

    implicit none

  contains

  <Beam structures: procedures>

  end submodule beam_structures_s
```

16.1.1 Beam structure elements

An entry in a beam-structure record consists of a string that denotes a type of structure function.


```

⟨Beam structures: types⟩≡
  type :: beam_structure_entry_t
    logical :: is_valid = .false.
    type(string_t) :: name
  contains
    ⟨Beam structures: beam structure entry: TBP⟩
  end type beam_structure_entry_t

```

Output.

```

⟨Beam structures: beam structure entry: TBP⟩≡
  procedure :: to_string => beam_structure_entry_to_string

⟨Beam structures: sub interfaces⟩≡
  module function beam_structure_entry_to_string (object) result (string)
    class (beam_structure_entry_t), intent(in) :: object
    type(string_t) :: string
  end function beam_structure_entry_to_string

⟨Beam structures: procedures⟩≡
  module function beam_structure_entry_to_string (object) result (string)
    class (beam_structure_entry_t), intent(in) :: object
    type(string_t) :: string
    if (object%is_valid) then
      string = object%name
    else
      string = "none"
    end if
  end function beam_structure_entry_to_string

```

A record in the beam-structure sequence denotes either a structure-function entry, a pair of such entries, or a pair spectrum.

```

⟨Beam structures: types⟩+≡
  type :: beam_structure_record_t
    type (beam_structure_entry_t), dimension(:), allocatable :: entry
  end type beam_structure_record_t

```

16.1.2 Beam structure type

The beam-structure object contains the beam particle(s) as simple strings. The sequence of records indicates the structure functions by name. No numerical parameters are stored.

```

⟨Beam structures: public⟩≡
  public :: beam_structure_t

⟨Beam structures: types⟩+≡
  type :: beam_structure_t
    private
    integer :: n_beam = 0
    type(string_t), dimension(:), allocatable :: prt
    type (beam_structure_record_t), dimension(:), allocatable :: record
    type (smatrix_t), dimension(:), allocatable :: smatrix
    real(default), dimension(:), allocatable :: pol_f

```

```

    real(default), dimension(:), allocatable :: p
    real(default), dimension(:), allocatable :: theta
    real(default), dimension(:), allocatable :: phi
contains
  <Beam structures: beam structure: TBP>≡
end type beam_structure_t

```

The finalizer deletes all contents explicitly, so we can continue with an empty beam record. (It is not needed for deallocation.) We have distinct finalizers for the independent parts of the beam structure.

```

<Beam structures: beam structure: TBP>≡
  procedure :: final_sf => beam_structure_final_sf

<Beam structures: sub interfaces>+≡
  module subroutine beam_structure_final_sf (object)
    class(beam_structure_t), intent(inout) :: object
    end subroutine beam_structure_final_sf

<Beam structures: procedures>+≡
  module subroutine beam_structure_final_sf (object)
    class(beam_structure_t), intent(inout) :: object
    if (allocated (object%prt)) deallocate (object%prt)
    if (allocated (object%record)) deallocate (object%record)
    object%n_beam = 0
  end subroutine beam_structure_final_sf

```

Output. The actual information fits in a single line, therefore we can provide a `to_string` method. The `show` method also lists the current values of relevant global variables.

```

<Beam structures: beam structure: TBP>+≡
  procedure :: write => beam_structure_write
  procedure :: to_string => beam_structure_to_string

<Beam structures: sub interfaces>+≡
  module subroutine beam_structure_write (object, unit)
    class(beam_structure_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine beam_structure_write
  module function beam_structure_to_string (object, sf_only) result (string)
    class(beam_structure_t), intent(in) :: object
    logical, intent(in), optional :: sf_only
    type(string_t) :: string
  end function beam_structure_to_string

<Beam structures: procedures>+≡
  module subroutine beam_structure_write (object, unit)
    class(beam_structure_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A,A)") "Beam structure: ", char (object%to_string ())
    if (allocated (object%smatrix)) then
      do i = 1, size (object%smatrix)
        write (u, "(3x,A,I0,A)") "polarization (beam ", i, "):"
        call object%smatrix(i)%write (u, indent=2)
      end do
    end if
  end subroutine beam_structure_write

```

```

        end do
    end if
    if (allocated (object%pol_f)) then
        write (u, "(3x,A,F10.7,:',',F10.7)") "polarization degree =", &
            object%pol_f
    end if
    if (allocated (object%p)) then
        write (u, "(3x,A," // FMT_19 // " ,:',','," // FMT_19 // &
            ")") "momentum =", object%p
    end if
    if (allocated (object%theta)) then
        write (u, "(3x,A," // FMT_19 // " ,:',','," // FMT_19 // &
            ")") "angle th =", object%theta
    end if
    if (allocated (object%phi)) then
        write (u, "(3x,A," // FMT_19 // " ,:',','," // FMT_19 // &
            ")") "angle ph =", object%phi
    end if
end subroutine beam_structure_write

module function beam_structure_to_string (object, sf_only) result (string)
    class(beam_structure_t), intent(in) :: object
    logical, intent(in), optional :: sf_only
    type(string_t) :: string
    integer :: i, j
    logical :: with_beams
    with_beams = .true.; if (present (sf_only)) with_beams = .not. sf_only
    select case (object%n_beam)
    case (1)
        if (with_beams) then
            string = object%prt(1)
        else
            string = ""
        end if
    case (2)
        if (with_beams) then
            string = object%prt(1) // ", " // object%prt(2)
        else
            string = ""
        end if
        if (allocated (object%record)) then
            if (size (object%record) > 0) then
                if (with_beams) string = string // " => "
                do i = 1, size (object%record)
                    if (i > 1) string = string // " => "
                    do j = 1, size (object%record(i)%entry)
                        if (j > 1) string = string // ", "
                        string = string // object%record(i)%entry(j)%to_string ()
                    end do
                end do
            end if
        end if
    case default
        string = "[any particles]"
    end select
end function beam_structure_to_string

```

```

        end select
    end function beam_structure_to_string

```

Initializer: dimension the beam structure record. Each array element denotes the number of entries for a record within the beam-structure sequence. The number of entries is either one or two, while the number of records is unlimited.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: init_sf => beam_structure_init_sf

<Beam structures: sub interfaces>+≡
    module subroutine beam_structure_init_sf (beam_structure, prt, dim_array)
        class(beam_structure_t), intent(inout) :: beam_structure
        type(string_t), dimension(:), intent(in) :: prt
        integer, dimension(:), intent(in), optional :: dim_array
    end subroutine beam_structure_init_sf

<Beam structures: procedures>+≡
    module subroutine beam_structure_init_sf (beam_structure, prt, dim_array)
        class(beam_structure_t), intent(inout) :: beam_structure
        type(string_t), dimension(:), intent(in) :: prt
        integer, dimension(:), intent(in), optional :: dim_array
        integer :: i
        call beam_structure%final_sf ()
        beam_structure%n_beam = size (prt)
        allocate (beam_structure%prt (size (prt)))
        beam_structure%prt = prt
        if (present (dim_array)) then
            allocate (beam_structure%record (size (dim_array)))
            do i = 1, size (dim_array)
                allocate (beam_structure%record(i)%entry (dim_array(i)))
            end do
        else
            allocate (beam_structure%record (0))
        end if
    end subroutine beam_structure_init_sf

```

Set an entry, specified by record number and entry number.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: set_sf => beam_structure_set_sf

<Beam structures: sub interfaces>+≡
    module subroutine beam_structure_set_sf (beam_structure, i, j, name)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i, j
        type(string_t), intent(in) :: name
    end subroutine beam_structure_set_sf

<Beam structures: procedures>+≡
    module subroutine beam_structure_set_sf (beam_structure, i, j, name)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i, j
        type(string_t), intent(in) :: name
        associate (entry => beam_structure%record(i)%entry(j))
            entry%name = name
            entry%is_valid = .true.
        end associate
    end subroutine beam_structure_set_sf

```

```

        end associate
    end subroutine beam_structure_set_sf

```

Expand the beam-structure object. (i) For a pair spectrum, keep the entry. (ii) For a single-particle structure function written as a single entry, replace this by a record with two entries. (ii) For a record with two nontrivial entries, separate this into two records with one trivial entry each.

To achieve this, we need a function that tells us whether an entry is a spectrum or a structure function. It returns 0 for a trivial entry, 1 for a single-particle structure function, and 2 for a two-particle spectrum.

(Beam structures: interfaces)≡

```

abstract interface
    function strfun_mode_fun (name) result (n)
    import
    type(string_t), intent(in) :: name
    integer :: n
    end function strfun_mode_fun
end interface

```

Algorithm: (1) Mark entries as invalid where necessary. (2) Count the number of entries that we will need. (3) Expand and copy entries to a new record array. (4) Replace the old array by the new one.

(Beam structures: beam structure: TBP)+≡

```

procedure :: expand => beam_structure_expand

```

(Beam structures: sub interfaces)+≡

```

module subroutine beam_structure_expand (beam_structure, strfun_mode)
    class(beam_structure_t), intent(inout) :: beam_structure
    procedure(strfun_mode_fun) :: strfun_mode
    end subroutine beam_structure_expand

```

(Beam structures: procedures)+≡

```

module subroutine beam_structure_expand (beam_structure, strfun_mode)
    class(beam_structure_t), intent(inout) :: beam_structure
    procedure(strfun_mode_fun) :: strfun_mode
    type(beam_structure_record_t), dimension(:), allocatable :: new
    integer :: n_record, i, j
    if (.not. allocated (beam_structure%record)) return
    do i = 1, size (beam_structure%record)
        associate (entry => beam_structure%record(i)%entry)
            do j = 1, size (entry)
                select case (strfun_mode (entry(j)%name))
                    case (0); entry(j)%is_valid = .false.
                end select
            end do
        end associate
    end do
    n_record = 0
    do i = 1, size (beam_structure%record)
        associate (entry => beam_structure%record(i)%entry)
            select case (size (entry))
                case (1)
                    if (entry(1)%is_valid) then

```

```

        select case (strfun_mode (entry(1)%name))
        case (1); n_record = n_record + 2
        case (2); n_record = n_record + 1
        end select
    end if
case (2)
do j = 1, 2
    if (entry(j)%is_valid) then
        select case (strfun_mode (entry(j)%name))
        case (1); n_record = n_record + 1
        case (2)
            call beam_structure%write ()
            call msg_fatal ("Pair spectrum used as &
                &single-particle structure function")
        end select
    end if
end do
end select
end associate
end do
allocate (new (n_record))
n_record = 0
do i = 1, size (beam_structure%record)
    associate (entry => beam_structure%record(i)%entry)
        select case (size (entry))
        case (1)
            if (entry(1)%is_valid) then
                select case (strfun_mode (entry(1)%name))
                case (1)
                    n_record = n_record + 1
                    allocate (new(n_record)%entry (2))
                    new(n_record)%entry(1) = entry(1)
                    n_record = n_record + 1
                    allocate (new(n_record)%entry (2))
                    new(n_record)%entry(2) = entry(1)
                case (2)
                    n_record = n_record + 1
                    allocate (new(n_record)%entry (1))
                    new(n_record)%entry(1) = entry(1)
                end select
            end if
        case (2)
            do j = 1, 2
                if (entry(j)%is_valid) then
                    n_record = n_record + 1
                    allocate (new(n_record)%entry (2))
                    new(n_record)%entry(j) = entry(j)
                end if
            end do
        end select
    end associate
end do
call move_alloc (from = new, to = beam_structure%record)
end subroutine beam_structure_expand

```

16.1.3 Polarization

To record polarization, we provide an allocatable array of `smatrix` objects, sparse matrices. The polarization structure is independent of the structure-function setup, they are combined only when an actual beam object is constructed.

```

(Beam structures: beam structure: TBP)+≡
  procedure :: final_pol => beam_structure_final_pol
  procedure :: init_pol => beam_structure_init_pol

(Beam structures: sub interfaces)+≡
  module subroutine beam_structure_final_pol (beam_structure)
    class(beam_structure_t), intent(inout) :: beam_structure
  end subroutine beam_structure_final_pol
  module subroutine beam_structure_init_pol (beam_structure, n)
    class(beam_structure_t), intent(inout) :: beam_structure
    integer, intent(in) :: n
  end subroutine beam_structure_init_pol

(Beam structures: procedures)+≡
  module subroutine beam_structure_final_pol (beam_structure)
    class(beam_structure_t), intent(inout) :: beam_structure
    if (allocated (beam_structure%smatrix)) deallocate (beam_structure%smatrix)
    if (allocated (beam_structure%pol_f)) deallocate (beam_structure%pol_f)
  end subroutine beam_structure_final_pol

  module subroutine beam_structure_init_pol (beam_structure, n)
    class(beam_structure_t), intent(inout) :: beam_structure
    integer, intent(in) :: n
    if (allocated (beam_structure%smatrix)) deallocate (beam_structure%smatrix)
    allocate (beam_structure%smatrix (n))
    if (.not. allocated (beam_structure%pol_f)) &
      allocate (beam_structure%pol_f (n), source = 1._default)
  end subroutine beam_structure_init_pol

```

Check if polarized beams are used.

```

(Beam structures: beam structure: TBP)+≡
  procedure :: has_polarized_beams => beam_structure_has_polarized_beams

(Beam structures: sub interfaces)+≡
  elemental module function beam_structure_has_polarized_beams &
    (beam_structure) result (pol)
    logical :: pol
    class(beam_structure_t), intent(in) :: beam_structure
  end function beam_structure_has_polarized_beams

(Beam structures: procedures)+≡
  elemental module function beam_structure_has_polarized_beams &
    (beam_structure) result (pol)
    logical :: pol
    class(beam_structure_t), intent(in) :: beam_structure
    if (allocated (beam_structure%pol_f)) then

```

```

        pol = any (beam_structure%pol_f /= 0)
    else
        pol = .false.
    end if
end function beam_structure_has_polarized_beams

```

Directly copy the spin density matrices.

```

<Beam structures: beam structure: TBP>+=
    procedure :: set_smatrix => beam_structure_set_smatrix

<Beam structures: sub interfaces>+=
    module subroutine beam_structure_set_smatrix (beam_structure, i, smatrix)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        type(smatrix_t), intent(in) :: smatrix
    end subroutine beam_structure_set_smatrix

<Beam structures: procedures>+=
    module subroutine beam_structure_set_smatrix (beam_structure, i, smatrix)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        type(smatrix_t), intent(in) :: smatrix
        beam_structure%smatrix(i) = smatrix
    end subroutine beam_structure_set_smatrix

```

Initialize one of the spin density matrices manually.

```

<Beam structures: beam structure: TBP>+=
    procedure :: init_smatrix => beam_structure_init_smatrix

<Beam structures: sub interfaces>+=
    module subroutine beam_structure_init_smatrix (beam_structure, i, n_entry)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: n_entry
    end subroutine beam_structure_init_smatrix

<Beam structures: procedures>+=
    module subroutine beam_structure_init_smatrix (beam_structure, i, n_entry)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: n_entry
        call beam_structure%smatrix(i)%init (2, n_entry)
    end subroutine beam_structure_init_smatrix

```

Set a polarization entry.

```

<Beam structures: beam structure: TBP>+=
    procedure :: set_sentry => beam_structure_set_sentry

<Beam structures: sub interfaces>+=
    module subroutine beam_structure_set_sentry &
        (beam_structure, i, i_entry, index, value)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: i_entry
        integer, dimension(:), intent(in) :: index

```



```

        complex(default), intent(in) :: value
    end subroutine beam_structure_set_sentry
<Beam structures: procedures>+≡
    module subroutine beam_structure_set_sentry &
        (beam_structure, i, i_entry, index, value)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: i_entry
        integer, dimension(:), intent(in) :: index
        complex(default), intent(in) :: value
        call beam_structure%smatrix(i)%set_entry (i_entry, index, value)
    end subroutine beam_structure_set_sentry

```

Set the array of polarization fractions.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: set_pol_f => beam_structure_set_pol_f
<Beam structures: sub interfaces>+≡
    module subroutine beam_structure_set_pol_f (beam_structure, f)
        class(beam_structure_t), intent(inout) :: beam_structure
        real(default), dimension(:), intent(in) :: f
    end subroutine beam_structure_set_pol_f
<Beam structures: procedures>+≡
    module subroutine beam_structure_set_pol_f (beam_structure, f)
        class(beam_structure_t), intent(inout) :: beam_structure
        real(default), dimension(:), intent(in) :: f
        if (allocated (beam_structure%pol_f)) deallocate (beam_structure%pol_f)
        allocate (beam_structure%pol_f (size (f)), source = f)
    end subroutine beam_structure_set_pol_f

```

16.1.4 Beam momenta

By default, beam momenta are deduced from the `sqrts` value or from the mass of the decaying particle, assuming a c.m. setup. Here we set them explicitly.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: final_mom => beam_structure_final_mom
<Beam structures: sub interfaces>+≡
    module subroutine beam_structure_final_mom (beam_structure)
        class(beam_structure_t), intent(inout) :: beam_structure
    end subroutine beam_structure_final_mom
<Beam structures: procedures>+≡
    module subroutine beam_structure_final_mom (beam_structure)
        class(beam_structure_t), intent(inout) :: beam_structure
        if (allocated (beam_structure%p)) deallocate (beam_structure%p)
        if (allocated (beam_structure%theta)) deallocate (beam_structure%theta)
        if (allocated (beam_structure%phi)) deallocate (beam_structure%phi)
    end subroutine beam_structure_final_mom

```

```

<Beam structures: beam structure: TBP>+≡
  procedure :: set_momentum => beam_structure_set_momentum
  procedure :: set_theta => beam_structure_set_theta
  procedure :: set_phi => beam_structure_set_phi

<Beam structures: sub interfaces>+≡
  module subroutine beam_structure_set_momentum (beam_structure, p)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: p
  end subroutine beam_structure_set_momentum
  module subroutine beam_structure_set_theta (beam_structure, theta)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: theta
  end subroutine beam_structure_set_theta
  module subroutine beam_structure_set_phi (beam_structure, phi)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: phi
  end subroutine beam_structure_set_phi

<Beam structures: procedures>+≡
  module subroutine beam_structure_set_momentum (beam_structure, p)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: p
    if (allocated (beam_structure%p)) deallocate (beam_structure%p)
    allocate (beam_structure%p (size (p)), source = p)
  end subroutine beam_structure_set_momentum

  module subroutine beam_structure_set_theta (beam_structure, theta)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: theta
    if (allocated (beam_structure%theta)) deallocate (beam_structure%theta)
    allocate (beam_structure%theta (size (theta)), source = theta)
  end subroutine beam_structure_set_theta

  module subroutine beam_structure_set_phi (beam_structure, phi)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: phi
    if (allocated (beam_structure%phi)) deallocate (beam_structure%phi)
    allocate (beam_structure%phi (size (phi)), source = phi)
  end subroutine beam_structure_set_phi

```

16.1.5 Get contents

Look at the incoming particles. We may also have the case that beam particles are not specified, but polarization.

```

<Beam structures: beam structure: TBP>+≡
  procedure :: is_set => beam_structure_is_set
  procedure :: get_n_beam => beam_structure_get_n_beam
  procedure :: get_prt => beam_structure_get_prt

<Beam structures: sub interfaces>+≡
  module function beam_structure_is_set (beam_structure) result (flag)
    class(beam_structure_t), intent(in) :: beam_structure
    logical :: flag

```

```

end function beam_structure_is_set
module function beam_structure_get_n_beam (beam_structure) result (n)
  class(beam_structure_t), intent(in) :: beam_structure
  integer :: n
end function beam_structure_get_n_beam
module function beam_structure_get_prt (beam_structure) result (prt)
  class(beam_structure_t), intent(in) :: beam_structure
  type(string_t), dimension(:), allocatable :: prt
end function beam_structure_get_prt
<Beam structures: procedures>+≡
module function beam_structure_is_set (beam_structure) result (flag)
  class(beam_structure_t), intent(in) :: beam_structure
  logical :: flag
  flag = beam_structure%n_beam > 0 .or. beam_structure%asymmetric ()
end function beam_structure_is_set

module function beam_structure_get_n_beam (beam_structure) result (n)
  class(beam_structure_t), intent(in) :: beam_structure
  integer :: n
  n = beam_structure%n_beam
end function beam_structure_get_n_beam

module function beam_structure_get_prt (beam_structure) result (prt)
  class(beam_structure_t), intent(in) :: beam_structure
  type(string_t), dimension(:), allocatable :: prt
  allocate (prt (size (beam_structure%prt)))
  prt = beam_structure%prt
end function beam_structure_get_prt

```

Return the number of records.

```

<Beam structures: beam structure: TBP>+≡
  procedure :: get_n_record => beam_structure_get_n_record
<Beam structures: sub interfaces>+≡
  module function beam_structure_get_n_record (beam_structure) result (n)
    class(beam_structure_t), intent(in) :: beam_structure
    integer :: n
  end function beam_structure_get_n_record
<Beam structures: procedures>+≡
module function beam_structure_get_n_record (beam_structure) result (n)
  class(beam_structure_t), intent(in) :: beam_structure
  integer :: n
  if (allocated (beam_structure%record)) then
    n = size (beam_structure%record)
  else
    n = 0
  end if
end function beam_structure_get_n_record

```

Return an array consisting of the beam indices affected by the valid entries within a record. After expansion, there should be exactly one valid entry per record.

```

<Beam structures: beam structure: TBP>+≡

```

```

        procedure :: get_i_entry => beam_structure_get_i_entry
    <Beam structures: sub interfaces>+≡
        module function beam_structure_get_i_entry &
            (beam_structure, i) result (i_entry)
            class(beam_structure_t), intent(in) :: beam_structure
            integer, intent(in) :: i
            integer, dimension(:), allocatable :: i_entry
        end function beam_structure_get_i_entry

```

```

    <Beam structures: procedures>+≡
        module function beam_structure_get_i_entry &
            (beam_structure, i) result (i_entry)
            class(beam_structure_t), intent(in) :: beam_structure
            integer, intent(in) :: i
            integer, dimension(:), allocatable :: i_entry
            associate (record => beam_structure%record(i))
                select case (size (record%entry))
                    case (1)
                        if (record%entry(1)%is_valid) then
                            allocate (i_entry (2), source = [1, 2])
                        else
                            allocate (i_entry (0))
                        end if
                    case (2)
                        if (all (record%entry%is_valid)) then
                            allocate (i_entry (2), source = [1, 2])
                        else if (record%entry(1)%is_valid) then
                            allocate (i_entry (1), source = [1])
                        else if (record%entry(2)%is_valid) then
                            allocate (i_entry (1), source = [2])
                        else
                            allocate (i_entry (0))
                        end if
                    end select
                end associate
            end function beam_structure_get_i_entry

```

Return the name of the first valid entry within a record. After expansion, there should be exactly one valid entry per record.

```

    <Beam structures: beam structure: TBP>+≡
        procedure :: get_name => beam_structure_get_name
    <Beam structures: sub interfaces>+≡
        module function beam_structure_get_name (beam_structure, i) result (name)
            type(string_t) :: name
            class(beam_structure_t), intent(in) :: beam_structure
            integer, intent(in) :: i
        end function beam_structure_get_name
    <Beam structures: procedures>+≡
        module function beam_structure_get_name (beam_structure, i) result (name)
            type(string_t) :: name
            class(beam_structure_t), intent(in) :: beam_structure
            integer, intent(in) :: i
            associate (record => beam_structure%record(i))

```

```

        if (record%entry(1)%is_valid) then
            name = record%entry(1)%name
        else if (size (record%entry) == 2) then
            name = record%entry(2)%name
        end if
    end associate
end function beam_structure_get_name

```

(Beam structures: beam structure: TBP)+≡

```

    procedure :: has_pdf => beam_structure_has_pdf

```

(Beam structures: sub interfaces)+≡

```

    module function beam_structure_has_pdf (beam_structure) result (has_pdf)
        logical :: has_pdf
        class(beam_structure_t), intent(in) :: beam_structure
    end function beam_structure_has_pdf

```

(Beam structures: procedures)+≡

```

    module function beam_structure_has_pdf (beam_structure) result (has_pdf)
        logical :: has_pdf
        class(beam_structure_t), intent(in) :: beam_structure
        integer :: i
        type(string_t) :: name
        has_pdf = .false.
        do i = 1, beam_structure%get_n_record ()
            name = beam_structure%get_name (i)
            has_pdf = has_pdf .or. name == var_str ("pdf_builtin") .or. name == var_str ("lhpdf")
        end do
    end function beam_structure_has_pdf

```

Return true if the beam structure contains a particular structure function identifier (such as lhpdf, isr, etc.)

(Beam structures: beam structure: TBP)+≡

```

    procedure :: contains => beam_structure_contains

```

(Beam structures: sub interfaces)+≡

```

    module function beam_structure_contains (beam_structure, name) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        character(*), intent(in) :: name
        logical :: flag
    end function beam_structure_contains

```

(Beam structures: procedures)+≡

```

    module function beam_structure_contains (beam_structure, name) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        character(*), intent(in) :: name
        logical :: flag
        integer :: i, j
        flag = .false.
        if (allocated (beam_structure%record)) then
            do i = 1, size (beam_structure%record)
                do j = 1, size (beam_structure%record(i)%entry)
                    flag = beam_structure%record(i)%entry(j)%name == name
                    if (flag) return
                end do
            end do
        end if
    end function beam_structure_contains

```

```

        end do
    end if
end function beam_structure_contains

```

Return polarization data.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: polarized => beam_structure_polarized
    procedure :: get_smatrix => beam_structure_get_smatrix
    procedure :: get_pol_f => beam_structure_get_pol_f
    procedure :: asymmetric => beam_structure_asymmetric

<Beam structures: sub interfaces>+≡
    module function beam_structure_polarized (beam_structure) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        logical :: flag
    end function beam_structure_polarized
    module function beam_structure_get_smatrix (beam_structure) result (smatrix)
        class(beam_structure_t), intent(in) :: beam_structure
        type(smatrixt_t), dimension(:), allocatable :: smatrix
    end function beam_structure_get_smatrix
    module function beam_structure_get_pol_f (beam_structure) result (pol_f)
        class(beam_structure_t), intent(in) :: beam_structure
        real(default), dimension(:), allocatable :: pol_f
    end function beam_structure_get_pol_f
    module function beam_structure_asymmetric (beam_structure) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        logical :: flag
    end function beam_structure_asymmetric

<Beam structures: procedures>+≡
    module function beam_structure_polarized (beam_structure) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        logical :: flag
        flag = allocated (beam_structure%smatrix)
    end function beam_structure_polarized

    module function beam_structure_get_smatrix (beam_structure) result (smatrix)
        class(beam_structure_t), intent(in) :: beam_structure
        type(smatrixt_t), dimension(:), allocatable :: smatrix
        allocate (smatrix (size (beam_structure%smatrix)), &
            source = beam_structure%smatrix)
    end function beam_structure_get_smatrix

    module function beam_structure_get_pol_f (beam_structure) result (pol_f)
        class(beam_structure_t), intent(in) :: beam_structure
        real(default), dimension(:), allocatable :: pol_f
        allocate (pol_f (size (beam_structure%pol_f)), &
            source = beam_structure%pol_f)
    end function beam_structure_get_pol_f

    module function beam_structure_asymmetric (beam_structure) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        logical :: flag
        flag = allocated (beam_structure%p) &
            .or. allocated (beam_structure%theta) &

```

```

.or. allocated (beam_structure%phi)
end function beam_structure_asymmetric

```

Return the beam momenta (the space part, i.e., three-momenta). This is meaningful only if momenta and, optionally, angles have been set.

```

<Beam structures: beam structure: TBP>+=
  procedure :: get_momenta => beam_structure_get_momenta

<Beam structures: sub interfaces>+=
  module function beam_structure_get_momenta (beam_structure) result (p)
    class(beam_structure_t), intent(in) :: beam_structure
    type(vector3_t), dimension(:), allocatable :: p
  end function beam_structure_get_momenta

<Beam structures: procedures>+=
  module function beam_structure_get_momenta (beam_structure) result (p)
    class(beam_structure_t), intent(in) :: beam_structure
    type(vector3_t), dimension(:), allocatable :: p
    real(default), dimension(:), allocatable :: theta, phi
    integer :: n, i
    if (allocated (beam_structure%p)) then
      n = size (beam_structure%p)
      if (allocated (beam_structure%theta)) then
        if (size (beam_structure%theta) == n) then
          allocate (theta (n), source = beam_structure%theta)
        else
          call msg_fatal ("Beam structure: mismatch in momentum vs. &
            &angle theta specification")
        end if
      else if
      allocate (theta (n), source = 0._default)
    end if
    if (allocated (beam_structure%phi)) then
      if (size (beam_structure%phi) == n) then
        allocate (phi (n), source = beam_structure%phi)
      else
        call msg_fatal ("Beam structure: mismatch in momentum vs. &
          &angle phi specification")
      end if
    else
      allocate (phi (n), source = 0._default)
    end if
    allocate (p (n))
    do i = 1, n
      p(i) = beam_structure%p(i) * vector3_moving ([ &
        sin (theta(i)) * cos (phi(i)), &
        sin (theta(i)) * sin (phi(i)), &
        cos (theta(i))]
    end do
    if (n == 2) p(2) = - p(2)
  else
    call msg_fatal ("Beam structure: angle theta/phi specified but &
      &momentum/a p undefined")
  end if
end function beam_structure_get_momenta

```

Check for a complete beam structure. The **applies** flag tells if the beam structure should actually be used for a process with the given **n_in** number of incoming particles.

It is set if the beam structure matches the process as either decay or scattering. It is unset if beam structure references a scattering setup but the process is a decay. It is also unset if the beam structure itself is empty.

If the beam structure cannot be used, terminate with fatal error.

```

<Beam structures: beam structure: TBP>+=
  procedure :: check_against_n_in => beam_structure_check_against_n_in

<Beam structures: sub interfaces>+=
  module subroutine beam_structure_check_against_n_in &
    (beam_structure, n_in, applies)
    class(beam_structure_t), intent(in) :: beam_structure
    integer, intent(in) :: n_in
    logical, intent(out) :: applies
  end subroutine beam_structure_check_against_n_in

<Beam structures: procedures>+=
  module subroutine beam_structure_check_against_n_in &
    (beam_structure, n_in, applies)
    class(beam_structure_t), intent(in) :: beam_structure
    integer, intent(in) :: n_in
    logical, intent(out) :: applies
    if (beam_structure%is_set ()) then
      if (n_in == beam_structure%get_n_beam ()) then
        applies = .true.
      else if (beam_structure%get_n_beam () == 0) then
        call msg_fatal &
          ("Asymmetric beams: missing beam particle specification")
        applies = .false.
      else
        call msg_fatal &
          ("Mismatch of process and beam setup (scattering/decay)")
        applies = .false.
      end if
    else
      applies = .false.
    end if
  end subroutine beam_structure_check_against_n_in

```

16.1.6 Unit Tests

Test module, followed by the corresponding implementation module.

```

<beam_structures_ut.f90>=
  <File header>

  module beam_structures_ut
    use unit_tests
    use beam_structures_ut

```



```

    <Standard module head>

    <Beam structures: public test>

    contains

    <Beam structures: test driver>

    end module beam_structures_ut
<beam_structures_uti.f90>≡
    <File header>

    module beam_structures_uti

    <Use kinds>
    <Use strings>

        use beam_structures

    <Standard module head>

    <Beam structures: test declarations>

    contains

    <Beam structures: tests>

    <Beam structures: test auxiliary>

    end module beam_structures_uti
API: driver for the unit tests below.
<Beam structures: public test>≡
    public :: beam_structures_test
<Beam structures: test driver>≡
    subroutine beam_structures_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Beam structures: execute tests>
    end subroutine beam_structures_test

```

Empty structure

```

<Beam structures: execute tests>≡
    call test (beam_structures_1, "beam_structures_1", &
        "empty beam structure record", &
        u, results)
<Beam structures: test declarations>≡
    public :: beam_structures_1

```

```

<Beam structures: tests>≡
subroutine beam_structures_1 (u)
  integer, intent(in) :: u
  type(beam_structure_t) :: beam_structure

  write (u, "(A)")  "* Test output: beam_structures_1"
  write (u, "(A)")  "* Purpose: display empty beam structure record"
  write (u, "(A)")

  call beam_structure%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: beam_structures_1"

end subroutine beam_structures_1

```

Nontrivial configurations

```

<Beam structures: execute tests>+≡
  call test (beam_structures_2, "beam_structures_2", &
    "beam structure records", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_2

<Beam structures: tests>+≡
subroutine beam_structures_2 (u)
  integer, intent(in) :: u
  type(beam_structure_t) :: beam_structure
  integer, dimension(0) :: empty_array
  type(string_t) :: s

  write (u, "(A)")  "* Test output: beam_structures_2"
  write (u, "(A)")  "* Purpose: setup beam structure records"
  write (u, "(A)")

  s = "s"

  call beam_structure%init_sf ([s], empty_array)
  call beam_structure%write (u)

  write (u, "(A)")

  call beam_structure%init_sf ([s, s], [1])
  call beam_structure%set_sf (1, 1, var_str ("a"))
  call beam_structure%write (u)

  write (u, "(A)")

  call beam_structure%init_sf ([s, s], [2])
  call beam_structure%set_sf (1, 1, var_str ("a"))
  call beam_structure%set_sf (1, 2, var_str ("b"))
  call beam_structure%write (u)

```

```

write (u, "(A)")

call beam_structure%init_sf ([s, s], [2, 1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%set_sf (1, 2, var_str ("b"))
call beam_structure%set_sf (2, 1, var_str ("c"))
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_structures_2"

end subroutine beam_structures_2

```

Expansion

Provide a function that tells, for the dummy structure function names used here, whether they are considered a two-particle spectrum or a single-particle structure function:

```

<Beam structures: test auxiliary>≡
function test_strfun_mode (name) result (n)
  type(string_t), intent(in) :: name
  integer :: n
  select case (char (name))
  case ("a");  n = 2
  case ("b");  n = 1
  case default; n = 0
  end select
end function test_strfun_mode

<Beam structures: execute tests>+≡
call test (beam_structures_3, "beam_structures_3", &
  "beam structure expansion", &
  u, results)

<Beam structures: test declarations>+≡
public :: beam_structures_3

<Beam structures: tests>+≡
subroutine beam_structures_3 (u)
  integer, intent(in) :: u
  type(beam_structure_t) :: beam_structure
  type(string_t) :: s

  write (u, "(A)")  "* Test output: beam_structures_3"
  write (u, "(A)")  "* Purpose: expand beam structure records"
  write (u, "(A)")

  s = "s"

  write (u, "(A)")  "* Pair spectrum (keep as-is)"
  write (u, "(A)")

```

```

call beam_structure%init_sf ([s, s], [1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%expand (test_strfun_mode)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure function pair (expand)"
write (u, "(A)")

call beam_structure%init_sf ([s, s], [2])
call beam_structure%set_sf (1, 1, var_str ("b"))
call beam_structure%set_sf (1, 2, var_str ("b"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%expand (test_strfun_mode)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure function (separate and expand)"
write (u, "(A)")

call beam_structure%init_sf ([s, s], [1])
call beam_structure%set_sf (1, 1, var_str ("b"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%expand (test_strfun_mode)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Combination"
write (u, "(A)")

call beam_structure%init_sf ([s, s], [1, 1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%set_sf (2, 1, var_str ("b"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%expand (test_strfun_mode)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_structures_3"

end subroutine beam_structures_3

```

Public methods

Check the methods that can be called to get the beam-structure contents.

```
<Beam structures: execute tests>+≡
  call test (beam_structures_4, "beam_structures_4", &
    "beam structure contents", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_4

<Beam structures: tests>+≡
  subroutine beam_structures_4 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    type(string_t) :: s
    type(string_t), dimension(2) :: prt
    integer :: i

    write (u, "(A)")  "* Test output: beam_structures_4"
    write (u, "(A)")  "* Purpose: check the API"
    write (u, "(A)")

    s = "s"

    write (u, "(A)")  "* Structure-function combination"
    write (u, "(A)")

    call beam_structure%init_sf ([s, s], [1, 2, 2])
    call beam_structure%set_sf (1, 1, var_str ("a"))
    call beam_structure%set_sf (2, 1, var_str ("b"))
    call beam_structure%set_sf (3, 2, var_str ("c"))
    call beam_structure%write (u)

    write (u, *)
    write (u, "(1x,A,I0)")  "n_beam = ", beam_structure%get_n_beam ()
    prt = beam_structure%get_prt ()
    write (u, "(1x,A,2(1x,A))")  "prt =", char (prt(1)), char (prt(2))

    write (u, *)
    write (u, "(1x,A,I0)")  "n_record = ", beam_structure%get_n_record ()

    do i = 1, 3
      write (u, "(A)")
      write (u, "(1x,A,I0,A,A)")  "name(", i, ") = ", &
        char (beam_structure%get_name (i))
      write (u, "(1x,A,I0,A,2(1x,I0))")  "i_entry(", i, ") =", &
        beam_structure%get_i_entry (i)
    end do

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: beam_structures_4"
```

```
end subroutine beam_structures_4
```

Polarization

The polarization properties are independent from the structure-function setup.

```
(Beam structures: execute tests)+≡
  call test (beam_structures_5, "beam_structures_5", &
    "polarization", &
    u, results)

(Beam structures: test declarations)+≡
  public :: beam_structures_5

(Beam structures: tests)+≡
  subroutine beam_structures_5 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    integer, dimension(0) :: empty_array
    type(string_t) :: s

    write (u, "(A)")  "* Test output: beam_structures_5"
    write (u, "(A)")  "* Purpose: setup polarization in beam structure records"
    write (u, "(A)")

    s = "s"

    call beam_structure%init_sf ([s], empty_array)
    call beam_structure%init_pol (1)
    call beam_structure%init_smatrix (1, 1)
    call beam_structure%set_sentry (1, 1, [0,0], (1._default, 0._default))
    call beam_structure%set_pol_f ([0.5_default])
    call beam_structure%write (u)

    write (u, "(A)")
    call beam_structure%final_sf ()
    call beam_structure%final_pol ()

    call beam_structure%init_sf ([s, s], [1])
    call beam_structure%set_sf (1, 1, var_str ("a"))
    call beam_structure%init_pol (2)
    call beam_structure%init_smatrix (1, 2)
    call beam_structure%set_sentry (1, 1, [-1,1], (0.5_default,-0.5_default))
    call beam_structure%set_sentry (1, 2, [ 1,1], (1._default, 0._default))
    call beam_structure%init_smatrix (2, 0)
    call beam_structure%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: beam_structures_5"

  end subroutine beam_structures_5
```

Momenta

The momenta are independent from the structure-function setup.

```
<Beam structures: execute tests>+≡
    call test (beam_structures_6, "beam_structures_6", &
              "momenta", &
              u, results)

<Beam structures: test declarations>+≡
    public :: beam_structures_6

<Beam structures: tests>+≡
    subroutine beam_structures_6 (u)
        integer, intent(in) :: u
        type(beam_structure_t) :: beam_structure
        integer, dimension(0) :: empty_array
        type(string_t) :: s

        write (u, "(A)")  "* Test output: beam_structures_6"
        write (u, "(A)")  "* Purpose: setup momenta in beam structure records"
        write (u, "(A)")

        s = "s"

        call beam_structure%init_sf ([s], empty_array)
        call beam_structure%set_momentum ([500._default])
        call beam_structure%write (u)

        write (u, "(A)")
        call beam_structure%final_sf ()
        call beam_structure%final_mom ()

        call beam_structure%init_sf ([s, s], [1])
        call beam_structure%set_momentum ([500._default, 700._default])
        call beam_structure%set_theta ([0._default, 0.1_default])
        call beam_structure%set_phi ([0._default, 1.51_default])
        call beam_structure%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: beam_structures_6"

    end subroutine beam_structures_6
```

16.2 Beams for collisions and decays

```
<beams.f90>≡
    <File header>

    module beams

        <Use kinds>
        <Use strings>
```

```

    use lorentz
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use interactions
    use polarizations
    use beam_structures

    <Standard module head>

    <Beams: public>

    <Beams: types>

    <Beams: interfaces>

    interface
    <Beams: sub interfaces>
    end interface

    end module beams

    <beams_sub.f90>≡
    <File header>

    submodule (beams) beams_s

        use io_units
        use format_defs, only: FMT_19
        use numeric_utils
        use diagnostics
        use md5

        implicit none

    contains

    <Beams: procedures>

    end submodule beams_s

```

16.2.1 Beam data

The beam data type contains beam data for one or two beams, depending on whether we are dealing with beam collisions or particle decay. In addition, it holds the c.m. energy `sqrts`, the Lorentz transformation `L` that transforms the c.m. system into the lab system, and the pair of c.m. momenta.

```

    <Beams: public>≡
        public :: beam_data_t

    <Beams: types>≡
        type :: beam_data_t

```



```

logical :: initialized = .false.
integer :: n = 0
type(flavor_t), dimension(:), allocatable :: flv
real(default), dimension(:), allocatable :: mass
type(pmatrix_t), dimension(:), allocatable :: pmatrix
logical :: lab_is_cm = .true.
type(vector4_t), dimension(:), allocatable :: p_cm
type(vector4_t), dimension(:), allocatable :: p
type(lorentz_transformation_t), allocatable :: L_cm_to_lab
real(default) :: sqrts = 0
character(32) :: md5sum = ""
contains
  <Beams: beam data: TBP>
end type beam_data_t

```

Generic initializer. This is called by the specific initializers below. Initialize either for decay or for collision.

```

<Beams: procedures>≡
  subroutine beam_data_init (beam_data, n)
    type(beam_data_t), intent(out) :: beam_data
    integer, intent(in) :: n
    beam_data%n = n
    allocate (beam_data%flv (n))
    allocate (beam_data%mass (n))
    allocate (beam_data%pmatrix (n))
    allocate (beam_data%p_cm (n))
    allocate (beam_data%p (n))
    beam_data%initialized = .true.
  end subroutine beam_data_init

```

Finalizer: needed for the polarization components of the beams.

```

<Beams: beam data: TBP>≡
  procedure :: final => beam_data_final

<Beams: sub interfaces>≡
  module subroutine beam_data_final (beam_data)
    class(beam_data_t), intent(inout) :: beam_data
  end subroutine beam_data_final

<Beams: procedures>+≡
  module subroutine beam_data_final (beam_data)
    class(beam_data_t), intent(inout) :: beam_data
    beam_data%initialized = .false.
  end subroutine beam_data_final

```

The verbose (default) version is for debugging. The short version is for screen output in the UI.

```

<Beams: beam data: TBP>+≡
  procedure :: write => beam_data_write

<Beams: sub interfaces>+≡
  module subroutine beam_data_write (beam_data, unit, verbose, write_md5sum)
    class(beam_data_t), intent(in) :: beam_data
    integer, intent(in), optional :: unit

```

```

        logical, intent(in), optional :: verbose, write_md5sum
    end subroutine beam_data_write

(Beams: procedures)+≡
module subroutine beam_data_write (beam_data, unit, verbose, write_md5sum)
    class(beam_data_t), intent(in) :: beam_data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, write_md5sum
    integer :: prt_name_len
    logical :: verb, write_md5
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    verb = .false.; if (present (verbose)) verb = verbose
    write_md5 = verb; if (present (write_md5sum)) write_md5 = write_md5sum
    if (.not. beam_data%initialized) then
        write (u, "(1x,A)") "Beam data: [undefined]"
        return
    end if
    prt_name_len = maxval (len (beam_data%flv%get_name ()))
    select case (beam_data%n)
    case (1)
        write (u, "(1x,A)") "Beam data (decay):"
        if (verb) then
            call write_prt (1)
            call beam_data%pmatrix(1)%write (u)
            write (u, *) "R.f. momentum:"
            call vector4_write (beam_data%p_cm(1), u)
            write (u, *) "Lab momentum:"
            call vector4_write (beam_data%p(1), u)
        else
            call write_prt (1)
        end if
    case (2)
        write (u, "(1x,A)") "Beam data (collision):"
        if (verb) then
            call write_prt (1)
            call beam_data%pmatrix(1)%write (u)
            call write_prt (2)
            call beam_data%pmatrix(2)%write (u)
            call write_sqrts
            write (u, *) "C.m. momenta:"
            call vector4_write (beam_data%p_cm(1), u)
            call vector4_write (beam_data%p_cm(2), u)
            write (u, *) "Lab momenta:"
            call vector4_write (beam_data%p(1), u)
            call vector4_write (beam_data%p(2), u)
        else
            call write_prt (1)
            call write_prt (2)
            call write_sqrts
        end if
    end select
    if (allocated (beam_data%L_cm_to_lab)) then
        if (verb) then
            call lorentz_transformation_write (beam_data%L_cm_to_lab, u)

```

```

        else
            write (u, "(1x,A)") "Beam structure: lab and c.m. frame differ"
        end if
    end if
    if (write_md5) then
        write (u, *) "MD5 sum: ", beam_data%md5sum
    end if
contains
    subroutine write_sqrts
        character(80) :: sqrts_str
        write (sqrts_str, "(" // FMT_19 // ")") beam_data%sqrts
        write (u, "(3x,A)") "sqrts = " // trim (adjustl (sqrts_str)) // " GeV"
    end subroutine write_sqrts
    subroutine write_prt (i)
        integer, intent(in) :: i
        character(80) :: name_str, mass_str
        write (name_str, "(A)") char (beam_data%flv(i)%get_name ())
        write (mass_str, "(ES13.7)") beam_data%mass(i)
        write (u, "(3x,A)", advance="no") &
            name_str(:prt_name_len) // " (mass = " &
            // trim (adjustl (mass_str)) // " GeV)"
        if (beam_data%pmatrix(i)%is_polarized ()) then
            write (u, "(2x,A)") "polarized"
        else
            write (u, *)
        end if
    end subroutine write_prt
end subroutine beam_data_write

```

Return initialization status:

```

(Beams: beam data: TBP)+≡
    procedure :: are_valid => beam_data_are_valid

(Beams: sub interfaces)+≡
    module function beam_data_are_valid (beam_data) result (flag)
        class(beam_data_t), intent(in) :: beam_data
        logical :: flag
    end function beam_data_are_valid

(Beams: procedures)+≡
    module function beam_data_are_valid (beam_data) result (flag)
        class(beam_data_t), intent(in) :: beam_data
        logical :: flag
        flag = beam_data%initialized
    end function beam_data_are_valid

```

Check whether beam data agree with the current values of relevant parameters.

```

(Beams: beam data: TBP)+≡
    procedure :: check_scattering => beam_data_check_scattering

(Beams: sub interfaces)+≡
    module subroutine beam_data_check_scattering (beam_data, sqrts)
        class(beam_data_t), intent(in) :: beam_data
        real(default), intent(in), optional :: sqrts
    end subroutine beam_data_check_scattering

```

```

(Beams: procedures)+≡
module subroutine beam_data_check_scattering (beam_data, sqrts)
  class(beam_data_t), intent(in) :: beam_data
  real(default), intent(in), optional :: sqrts
  if (beam_data_are_valid (beam_data)) then
    if (present (sqrts)) then
      if (.not. nearly_equal (sqrts, beam_data%sqrts)) then
        call msg_error ("Current setting of sqrts is inconsistent " &
          // "with beam setup (ignored).")
      end if
    end if
  else
    call msg_bug ("Beam setup: invalid beam data")
  end if
end subroutine beam_data_check_scattering

```

Return the number of beams (1 for decays, 2 for collisions).

```

(Beams: beam data: TBP)+≡
procedure :: get_n_in => beam_data_get_n_in

(Beams: sub interfaces)+≡
module function beam_data_get_n_in (beam_data) result (n_in)
  class(beam_data_t), intent(in) :: beam_data
  integer :: n_in
end function beam_data_get_n_in

(Beams: procedures)+≡
module function beam_data_get_n_in (beam_data) result (n_in)
  class(beam_data_t), intent(in) :: beam_data
  integer :: n_in
  n_in = beam_data%n
end function beam_data_get_n_in

```

Return the beam flavor

```

(Beams: beam data: TBP)+≡
procedure :: get_flavor => beam_data_get_flavor

(Beams: sub interfaces)+≡
module function beam_data_get_flavor (beam_data) result (flv)
  class(beam_data_t), intent(in) :: beam_data
  type(flavor_t), dimension(:), allocatable :: flv
end function beam_data_get_flavor

(Beams: procedures)+≡
module function beam_data_get_flavor (beam_data) result (flv)
  class(beam_data_t), intent(in) :: beam_data
  type(flavor_t), dimension(:), allocatable :: flv
  allocate (flv (beam_data%n))
  flv = beam_data%flv
end function beam_data_get_flavor

```

Return the beam energies

```

(Beams: beam data: TBP)+≡
procedure :: get_energy => beam_data_get_energy

```

<Beams: sub interfaces>+≡

```
module function beam_data_get_energy (beam_data) result (e)
  class(beam_data_t), intent(in) :: beam_data
  real(default), dimension(:), allocatable :: e
end function beam_data_get_energy
```

<Beams: procedures>+≡

```
module function beam_data_get_energy (beam_data) result (e)
  class(beam_data_t), intent(in) :: beam_data
  real(default), dimension(:), allocatable :: e
  integer :: i
  allocate (e (beam_data%n))
  if (beam_data%initialized) then
    do i = 1, beam_data%n
      e(i) = energy (beam_data%p(i))
    end do
  else
    e = 0
  end if
end function beam_data_get_energy
```

Return the c.m. energy.

<Beams: beam data: TBP>+≡

```
procedure :: get_sqrts => beam_data_get_sqrts
```

<Beams: sub interfaces>+≡

```
module function beam_data_get_sqrts (beam_data) result (sqrts)
  class(beam_data_t), intent(in) :: beam_data
  real(default) :: sqrts
end function beam_data_get_sqrts
```

<Beams: procedures>+≡

```
module function beam_data_get_sqrts (beam_data) result (sqrts)
  class(beam_data_t), intent(in) :: beam_data
  real(default) :: sqrts
  sqrts = beam_data%sqrts
end function beam_data_get_sqrts
```

Return the polarization in case it is just two degrees

<Beams: beam data: TBP>+≡

```
procedure :: get_polarization => beam_data_get_polarization
```

<Beams: sub interfaces>+≡

```
module function beam_data_get_polarization (beam_data) result (pol)
  class(beam_data_t), intent(in) :: beam_data
  real(default), dimension(beam_data%n) :: pol
end function beam_data_get_polarization
```

<Beams: procedures>+≡

```
module function beam_data_get_polarization (beam_data) result (pol)
  class(beam_data_t), intent(in) :: beam_data
  real(default), dimension(beam_data%n) :: pol
  pol = beam_data%pmatrx%get_simple_pol ()
end function beam_data_get_polarization
```

```

<Beams: beam data: TBP>+≡
    procedure :: get_helicity_state_matrix => beam_data_get_helicity_state_matrix

<Beams: sub interfaces>+≡
    module function beam_data_get_helicity_state_matrix &
        (beam_data) result (state_hel)
        type(state_matrix_t) :: state_hel
        class(beam_data_t), intent(in) :: beam_data
    end function beam_data_get_helicity_state_matrix

<Beams: procedures>+≡
    module function beam_data_get_helicity_state_matrix &
        (beam_data) result (state_hel)
        type(state_matrix_t) :: state_hel
        class(beam_data_t), intent(in) :: beam_data
        type(polarization_t), dimension(:), allocatable :: pol
        integer :: i
        allocate (pol (beam_data%n))
        do i = 1, beam_data%n
            call pol(i)%init_pmatrix (beam_data%pmatrix(i))
        end do
        call combine_polarization_states (pol, state_hel)
    end function beam_data_get_helicity_state_matrix

<Beams: beam data: TBP>+≡
    procedure :: is_initialized => beam_data_is_initialized

<Beams: sub interfaces>+≡
    module function beam_data_is_initialized (beam_data) result (initialized)
        logical :: initialized
        class(beam_data_t), intent(in) :: beam_data
    end function beam_data_is_initialized

<Beams: procedures>+≡
    module function beam_data_is_initialized (beam_data) result (initialized)
        logical :: initialized
        class(beam_data_t), intent(in) :: beam_data
        initialized = any (beam_data%pmatrix%exists ())
    end function beam_data_is_initialized

```

Return a MD5 checksum for beam data. If no checksum is present (because beams have not been initialized), compute the checksum of the sqrts value.

```

<Beams: beam data: TBP>+≡
    procedure :: get_md5sum => beam_data_get_md5sum

<Beams: sub interfaces>+≡
    module function beam_data_get_md5sum &
        (beam_data, sqrts) result (md5sum_beams)
        class(beam_data_t), intent(in) :: beam_data
        real(default), intent(in) :: sqrts
        character(32) :: md5sum_beams
    end function beam_data_get_md5sum

<Beams: procedures>+≡
    module function beam_data_get_md5sum &
        (beam_data, sqrts) result (md5sum_beams)

```

```

class(beam_data_t), intent(in) :: beam_data
real(default), intent(in) :: sqrts
character(32) :: md5sum_beams
character(80) :: buffer
if (beam_data%md5sum /= "") then
    md5sum_beams = beam_data%md5sum
else
    write (buffer, *) sqrts
    md5sum_beams = md5sum (buffer)
end if
end function beam_data_get_md5sum

```

16.2.2 Initializers: beam structure

Initialize the beam data object from a beam structure object, given energy and model.

(Beams: beam data: TBP)+≡

```

procedure :: init_structure => beam_data_init_structure

```

(Beams: sub interfaces)+≡

```

module subroutine beam_data_init_structure &
    (beam_data, structure, sqrts, model, decay_rest_frame)
class(beam_data_t), intent(out) :: beam_data
type(beam_structure_t), intent(in) :: structure
real(default), intent(in) :: sqrts
class(model_data_t), intent(in), target :: model
logical, intent(in), optional :: decay_rest_frame
end subroutine beam_data_init_structure

```

(Beams: procedures)+≡

```

module subroutine beam_data_init_structure &
    (beam_data, structure, sqrts, model, decay_rest_frame)
class(beam_data_t), intent(out) :: beam_data
type(beam_structure_t), intent(in) :: structure
integer :: n_beam
real(default), intent(in) :: sqrts
class(model_data_t), intent(in), target :: model
logical, intent(in), optional :: decay_rest_frame
type(flavor_t), dimension(:), allocatable :: flv
n_beam = structure%get_n_beam ()
allocate (flv (n_beam))
call flv%init (structure%get_prt (), model)
if (structure%asymmetric ()) then
    if (structure%polarized ()) then
        call beam_data%init_momenta (structure%get_momenta (), flv, &
            structure%get_smatrix (), structure%get_pol_f ())
    else
        call beam_data%init_momenta (structure%get_momenta (), flv)
    end if
else
    select case (n_beam)
    case (1)
        if (structure%polarized ()) then

```

```

        call beam_data%init_decay (flv, &
            structure%get_smatrix (), structure%get_pol_f (), &
            rest_frame = decay_rest_frame)
    else
        call beam_data%init_decay (flv, &
            rest_frame = decay_rest_frame)
    end if
case (2)
    if (structure%polarized ()) then
        call beam_data%init_sqrts (sqrts, flv, &
            structure%get_smatrix (), structure%get_pol_f ())
    else
        call beam_data%init_sqrts (sqrts, flv)
    end if
case default
    call msg_bug ("Beam data: invalid beam structure object")
end select
end if
end subroutine beam_data_init_structure

```

16.2.3 Initializers: collisions

This is the simplest one: just the two flavors, c.m. energy, polarization. Color is inferred from flavor. Beam momenta and c.m. momenta coincide.

(Beams: beam data: TBP)+≡

```

    procedure :: init_sqrts => beam_data_init_sqrts

```

(Beams: sub interfaces)+≡

```

    module subroutine beam_data_init_sqrts &
        (beam_data, sqrts, flv, smatrix, pol_f)
        class(beam_data_t), intent(out) :: beam_data
        real(default), intent(in) :: sqrts
        type(flavor_t), dimension(:), intent(in) :: flv
        type(smatrix_t), dimension(:), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
    end subroutine beam_data_init_sqrts

```

(Beams: procedures)+≡

```

    module subroutine beam_data_init_sqrts &
        (beam_data, sqrts, flv, smatrix, pol_f)
        class(beam_data_t), intent(out) :: beam_data
        real(default), intent(in) :: sqrts
        type(flavor_t), dimension(:), intent(in) :: flv
        type(smatrix_t), dimension(:), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
        real(default), dimension(size(flv)) :: E, p
        call beam_data_init (beam_data, size (flv))
        beam_data%sqrts = sqrts
        beam_data%lab_is_cm = .true.
        select case (beam_data%n)
        case (1)
            E = sqrts; p = 0
            beam_data%p_cm = vector4_moving (E, p, 3)

```



```

        beam_data%p = beam_data%p_cm
    case (2)
        beam_data%p_cm = colliding_momenta (sqrts, flv%get_mass ())
        beam_data%p = colliding_momenta (sqrts, flv%get_mass ())
    end select
    call beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
end subroutine beam_data_init_sqrts

```

This version sets beam momenta directly, assuming that they are asymmetric, i.e., lab frame and c.m. frame do not coincide. Polarization info is deferred to a common initializer.

The Lorentz transformation that we compute here is not actually used in the calculation; instead, it will be recomputed for each event in the subroutine `phs_set_incoming_momenta`. We compute it here for the nominal beam setup nevertheless, so we can print it and, in particular, include it in the MD5 sum.

```

(Beams: beam data: TBP)+≡
    procedure :: init_momenta => beam_data_init_momenta

(Beams: sub interfaces)+≡
    module subroutine beam_data_init_momenta &
        (beam_data, p3, flv, smatrix, pol_f)
        class(beam_data_t), intent(out) :: beam_data
        type(vector3_t), dimension(:), intent(in) :: p3
        type(flavor_t), dimension(:), intent(in) :: flv
        type(smatrix_t), dimension(:), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
    end subroutine beam_data_init_momenta

(Beams: procedures)+≡
    module subroutine beam_data_init_momenta &
        (beam_data, p3, flv, smatrix, pol_f)
        class(beam_data_t), intent(out) :: beam_data
        type(vector3_t), dimension(:), intent(in) :: p3
        type(flavor_t), dimension(:), intent(in) :: flv
        type(smatrix_t), dimension(:), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
        type(vector4_t) :: p0
        type(vector4_t), dimension(:), allocatable :: p, p_cm_rot
        real(default), dimension(size(p3)) :: e
        real(default), dimension(size(flv)) :: m
        type(lorentz_transformation_t) :: L_boost, L_rot
        call beam_data_init (beam_data, size (flv))
        m = flv%get_mass ()
        e = sqrt (p3 ** 2 + m ** 2)
        allocate (p (beam_data%n))
        p = vector4_moving (e, p3)
        p0 = sum (p)
        beam_data%p = p
        beam_data%lab_is_cm = .false.
        beam_data%sqrts = p0 ** 1
        L_boost = boost (p0, beam_data%sqrts)
        allocate (p_cm_rot (beam_data%n))
        p_cm_rot = inverse (L_boost) * p
        allocate (beam_data%L_cm_to_lab)

```

```

select case (beam_data%n)
case (1)
    beam_data%L_cm_to_lab = L_boost
    beam_data%p_cm = vector4_at_rest (beam_data%sqrts)
case (2)
    L_rot = rotation_to_2nd (3, space_part (p_cm_rot(1)))
    beam_data%L_cm_to_lab = L_boost * L_rot
    beam_data%p_cm = &
        colliding_momenta (beam_data%sqrts, flv%get_mass ())
end select
call beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
end subroutine beam_data_init_momenta

```

Final steps: If requested, rotate the beams in the lab frame, and set the beam-data components.

<Beams: procedures>+≡

```

subroutine beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
    type(beam_data_t), intent(inout) :: beam_data
    type(flavor_t), dimension(:), intent(in) :: flv
    type(smatrix_t), dimension(:), intent(in), optional :: smatrix
    real(default), dimension(:), intent(in), optional :: pol_f
    integer :: i
    do i = 1, beam_data%n
        beam_data%flv(i) = flv(i)
        beam_data%mass(i) = flv(i)%get_mass ()
        if (present (smatrix)) then
            if (size (smatrix) /= beam_data%n) &
                call msg_fatal ("Beam data: &
                    &polarization density array has wrong dimension")
            beam_data%pmatrix(i) = smatrix(i)
            if (present (pol_f)) then
                if (size (pol_f) /= size (smatrix)) &
                    call msg_fatal ("Beam data: &
                        &polarization fraction array has wrong dimension")
                call beam_data%pmatrix(i)%normalize (flv(i), pol_f(i))
            else
                call beam_data%pmatrix(i)%normalize (flv(i), 1._default)
            end if
        else
            call beam_data%pmatrix(i)%init (2, 0)
            call beam_data%pmatrix(i)%normalize (flv(i), 0._default)
        end if
    end do
    call beam_data%compute_md5sum ()
end subroutine beam_data_finish_initialization

```

The MD5 sum is stored within the beam-data record, so it can be checked for integrity in subsequent runs.

<Beams: beam data: TBP>+≡

```

procedure :: compute_md5sum => beam_data_compute_md5sum

```

<Beams: sub interfaces>+≡

```

module subroutine beam_data_compute_md5sum (beam_data)

```

```

        class(beam_data_t), intent(inout) :: beam_data
        integer :: unit
    end subroutine beam_data_compute_md5sum
<Beams: procedures>+≡
module subroutine beam_data_compute_md5sum (beam_data)
    class(beam_data_t), intent(inout) :: beam_data
    integer :: unit
    unit = free_unit ()
    open (unit = unit, status = "scratch", action = "readwrite")
    call beam_data%write (unit, write_md5sum = .false., &
        verbose = .true.)
    rewind (unit)
    beam_data%md5sum = md5sum (unit)
    close (unit)
end subroutine beam_data_compute_md5sum

```

16.2.4 Initializers: decays

This is the simplest one: decay in rest frame. We need just flavor and polarization. Color is inferred from flavor. Beam momentum and c.m. momentum coincide.

```

<Beams: beam data: TBP>+≡
    procedure :: init_decay => beam_data_init_decay
<Beams: sub interfaces>+≡
    module subroutine beam_data_init_decay &
        (beam_data, flv, smatrix, pol_f, rest_frame)
        class(beam_data_t), intent(out) :: beam_data
        type(flavor_t), dimension(1), intent(in) :: flv
        type(smatrix_t), dimension(1), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
        logical, intent(in), optional :: rest_frame
    end subroutine beam_data_init_decay
<Beams: procedures>+≡
    module subroutine beam_data_init_decay &
        (beam_data, flv, smatrix, pol_f, rest_frame)
        class(beam_data_t), intent(out) :: beam_data
        type(flavor_t), dimension(1), intent(in) :: flv
        type(smatrix_t), dimension(1), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
        logical, intent(in), optional :: rest_frame
        real(default), dimension(1) :: m
        m = flv%get_mass ()
        if (present (smatrix)) then
            call beam_data%init_sqrts (m(1), flv, smatrix, pol_f)
        else
            call beam_data%init_sqrts (m(1), flv, smatrix, pol_f)
        end if
        if (present (rest_frame)) beam_data%lab_is_cm = rest_frame
    end subroutine beam_data_init_decay

```

16.2.5 The beams type

Beam objects are interaction objects that contain the actual beam data including polarization and density matrix. For collisions, the beam object actually contains two beams.

```

(Beams: public)+≡
    public :: beam_t

(Beams: types)+≡
    type :: beam_t
    private
        type(interaction_t) :: int
    end type beam_t

```

The constructor contains code that converts beam data into the (entangled) particle-pair quantum state. First, we set the number of particles and polarization mask. (The polarization mask is handed over to all later interactions, so if helicity is diagonal or absent, this fact is used when constructing the hard-interaction events.) Then, we construct the entangled state that combines helicity, flavor and color of the two particles (where flavor and color are unique, while several helicity states are possible). Then, we transfer this state together with the associated values from the spin density matrix into the `interaction_t` object.

Calling the `add_state` method of the interaction object, we keep the entries of the helicity density matrix without adding them up. This ensures that for unpolarized states, we do not normalize but end up with an $1/N$ entry, where N is the initial-state multiplicity.

```

(Beams: public)+≡
    public :: beam_init

(Beams: sub interfaces)+≡
    module subroutine beam_init (beam, beam_data)
        type(beam_t), intent(out) :: beam
        type(beam_data_t), intent(in), target :: beam_data
    end subroutine beam_init

(Beams: procedures)+≡
    module subroutine beam_init (beam, beam_data)
        type(beam_t), intent(out) :: beam
        type(beam_data_t), intent(in), target :: beam_data
        logical, dimension(beam_data%n) :: polarized, diagonal
        type(quantum_numbers_mask_t), dimension(beam_data%n) :: mask, mask_d
        type(state_matrix_t), target :: state_hel, state_fc, state_tmp
        type(state_iterator_t) :: it_hel, it_tmp
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        complex(default) :: value
        real(default), parameter :: tolerance = 100 * epsilon (1._default)
        polarized = beam_data%pmatrix%is_polarized ()
        diagonal = beam_data%pmatrix%is_diagonal ()
        mask = quantum_numbers_mask (.false., .false., &
            mask_h = .not. polarized, &
            mask_hd = diagonal)
        mask_d = quantum_numbers_mask (.false., .false., .false., &
            mask_hd = polarized .and. diagonal)
    end subroutine beam_init

```

```

call beam%int%basic_init &
  (0, 0, beam_data%n, mask = mask, store_values = .true.)
state_hel = beam_data%get_helicity_state_matrix ()
allocate (qn (beam_data%n))
call qn%init (beam_data%flv, color_from_flavor (beam_data%flv, 1))
call state_fc%init ()
call state_fc%add_state (qn)
call merge_state_matrices (state_hel, state_fc, state_tmp)
call it_hel%init (state_hel)
call it_tmp%init (state_tmp)
do while (it_hel%is_valid ())
  qn = it_tmp%get_quantum_numbers ()
  value = it_hel%get_matrix_element ()
  if (any (qn%are_redundant (mask_d))) then
    ! skip off-diagonal elements for diagonal polarization
  else if (abs (value) <= tolerance) then
    ! skip zero entries
  else
    call beam%int%add_state (qn, value = value)
  end if
  call it_hel%advance ()
  call it_tmp%advance ()
end do
call beam%int%freeze ()
call beam%int%set_momenta (beam_data%p, outgoing = .true.)
call state_hel%final ()
call state_fc%final ()
call state_tmp%final ()
end subroutine beam_init

```

Finalizer:

```

(Beams: public)+≡
  public :: beam_final

(Beams: sub interfaces)+≡
  module subroutine beam_final (beam)
    type(beam_t), intent(inout) :: beam
  end subroutine beam_final

(Beams: procedures)+≡
  module subroutine beam_final (beam)
    type(beam_t), intent(inout) :: beam
    call beam%int%final ()
  end subroutine beam_final

```

I/O:

```

(Beams: public)+≡
  public :: beam_write

(Beams: sub interfaces)+≡
  module subroutine beam_write &
    (beam, unit, verbose, show_momentum_sum, show_mass, col_verbose)
    type(beam_t), intent(in) :: beam
    integer, intent(in), optional :: unit

```

```

        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: col_verbose
    end subroutine beam_write
<Beams: procedures>+≡
    module subroutine beam_write &
        (beam, unit, verbose, show_momentum_sum, show_mass, col_verbose)
        type(beam_t), intent(in) :: beam
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: col_verbose
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        select case (beam%int%get_n_out ())
        case (1); write (u, *) "Decaying particle:"
        case (2); write (u, *) "Colliding beams:"
        end select
        call beam%int%basic_write &
            (unit, verbose = verbose, show_momentum_sum = &
                show_momentum_sum, show_mass = show_mass, &
                col_verbose = col_verbose)
    end subroutine beam_write

```

Defined assignment: deep copy

```

<Beams: public>+≡
    public :: assignment(=)
<Beams: interfaces>≡
    interface assignment(=)
        module procedure beam_assign
    end interface
<Beams: sub interfaces>+≡
    module subroutine beam_assign (beam_out, beam_in)
        type(beam_t), intent(out) :: beam_out
        type(beam_t), intent(in) :: beam_in
    end subroutine beam_assign
<Beams: procedures>+≡
    module subroutine beam_assign (beam_out, beam_in)
        type(beam_t), intent(out) :: beam_out
        type(beam_t), intent(in) :: beam_in
        beam_out%int = beam_in%int
    end subroutine beam_assign

```

16.2.6 Inherited procedures

```

<Beams: public>+≡
    public :: interaction_set_source_link_beam
<Beams: sub interfaces>+≡
    module subroutine interaction_set_source_link_beam (int, i, beam1, i1)
        type(interaction_t), intent(inout) :: int
        type(beam_t), intent(in), target :: beam1
    end subroutine interaction_set_source_link_beam

```

```

        integer, intent(in) :: i, i1
    end subroutine interaction_set_source_link_beam

<Beams: procedures>+≡
    module subroutine interaction_set_source_link_beam (int, i, beam1, i1)
        type(interaction_t), intent(inout) :: int
        type(beam_t), intent(in), target :: beam1
        integer, intent(in) :: i, i1
        call int%set_source_link (i, beam1%int, i1)
    end subroutine interaction_set_source_link_beam

```

16.2.7 Accessing contents

Return the interaction component – as a pointer, to avoid any copying.

```

<Beams: public>+≡
    public :: beam_get_int_ptr

<Beams: sub interfaces>+≡
    module function beam_get_int_ptr (beam) result (int)
        type(interaction_t), pointer :: int
        type(beam_t), intent(in), target :: beam
    end function beam_get_int_ptr

<Beams: procedures>+≡
    module function beam_get_int_ptr (beam) result (int)
        type(interaction_t), pointer :: int
        type(beam_t), intent(in), target :: beam
        int => beam%int
    end function beam_get_int_ptr

```

Set beam momenta directly. (Used for cascade decays.)

```

<Beams: public>+≡
    public :: beam_set_momenta

<Beams: sub interfaces>+≡
    module subroutine beam_set_momenta (beam, p)
        type(beam_t), intent(inout) :: beam
        type(vector4_t), dimension(:), intent(in) :: p
    end subroutine beam_set_momenta

<Beams: procedures>+≡
    module subroutine beam_set_momenta (beam, p)
        type(beam_t), intent(inout) :: beam
        type(vector4_t), dimension(:), intent(in) :: p
        call beam%int%set_momenta (p)
    end subroutine beam_set_momenta

```

16.2.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<beams_ut.f90>≡
    <File header>

```

```

module beams_ut
  use unit_tests
  use beams_uti

  <Standard module head>

  <Beams: public test>

  contains

  <Beams: test driver>

end module beams_ut

<beams_uti.f90>≡
<File header>

module beams_uti

  <Use kinds>
  use lorentz
  use flavors
  use interactions, only: reset_interaction_counter
  use polarizations, only: smatrix_t
  use model_data
  use beam_structures

  use beams

  <Standard module head>

  <Beams: test declarations>

  contains

  <Beams: tests>

end module beams_uti

```

API: driver for the unit tests below.

```

<Beams: public test>≡
  public :: beams_test

<Beams: test driver>≡
  subroutine beams_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Beams: execute tests>
  end subroutine beams_test

```

Test the basic beam setup.

```

<Beams: execute tests>≡
  call test (beam_1, "beam_1", &
    "check basic beam setup", &

```



```

        u, results)
<Beams: test declarations>≡
    public :: beam_1
<Beams: tests>≡
    subroutine beam_1 (u)
        integer, intent(in) :: u
        type(beam_data_t), target :: beam_data
        type(beam_t) :: beam
        real(default) :: sqrts
        type(flavor_t), dimension(2) :: flv
        type(smatrix_t), dimension(2) :: smatrix
        real(default), dimension(2) :: pol_f
        type(model_data_t), target :: model

        write (u, "(A)")  "* Test output: beam_1"
        write (u, "(A)")  "* Purpose: test basic beam setup"
        write (u, "(A)")

        write (u, "(A)")  "* Reading model file"
        write (u, "(A)")

        call reset_interaction_counter ()

        call model%init_sm_test ()

        write (u, "(A)")  "* Unpolarized scattering, massless fermions"
        write (u, "(A)")

        call reset_interaction_counter ()
        sqrts = 500
        call flv%init ([1,-1], model)

        call beam_data%init_sqrts (sqrts, flv)
        call beam_data%write (u)
        write (u, "(A)")
        call beam_init (beam, beam_data)
        call beam_write (beam, u)
        call beam_final (beam)
        call beam_data%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Unpolarized scattering, massless bosons"
        write (u, "(A)")

        call reset_interaction_counter ()
        sqrts = 500
        call flv%init ([22,22], model)

        call beam_data%init_sqrts (sqrts, flv)
        call beam_data%write (u)
        write (u, "(A)")
        call beam_init (beam, beam_data)
        call beam_write (beam, u)

```

```

call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_data%init_sqrts (sqrts, flv)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Polarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)

call smatrix(1)%init (2, 1)
call smatrix(1)%set_entry (1, [1,1], (1._default, 0._default))
pol_f(1) = 0.5_default

call smatrix(2)%init (2, 3)
call smatrix(2)%set_entry (1, [1,1], (1._default, 0._default))
call smatrix(2)%set_entry (2, [-1,-1], (1._default, 0._default))
call smatrix(2)%set_entry (3, [-1,1], (1._default, 0._default))
pol_f(2) = 1._default

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call smatrix(1)%init (2, 0)

```

```

pol_f(1) = 0._default

call smatrix(2)%init (2, 1)
call smatrix(2)%set_entry (1, [1,1], (1._default, 0._default))
pol_f(2) = 1._default

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call smatrix(1)%init (2, 0)
pol_f(1) = 0._default

call smatrix(2)%init (2, 1)
call smatrix(2)%set_entry (1, [0,0], (1._default, 0._default))
pol_f(2) = 1._default

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)

call beam_data%init_decay (flv(1:1))
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Polarized decay, massive boson"
write (u, "(A)")

```

```

call reset_interaction_counter ()
call flv(1)%init (23, model)
call smatrix(1)%init (2, 1)
call smatrix(1)%set_entry (1, [0,0], (1._default, 0._default))
pol_f(1) = 0.4_default

call beam_data%init_decay (flv(1:1), smatrix(1:1), pol_f(1:1))
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call beam_final (beam)
call beam_data%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_1"

end subroutine beam_1

```

Test advanced beam setup.

```

<Beams: execute tests>+≡
  call test (beam_2, "beam_2", &
    "beam initialization", &
    u, results)

<Beams: test declarations>+≡
  public :: beam_2

<Beams: tests>+≡
  subroutine beam_2 (u)
    integer, intent(in) :: u
    type(beam_data_t), target :: beam_data
    type(beam_t) :: beam
    real(default) :: sqrts
    type(flavor_t), dimension(2) :: flv
    integer, dimension(0) :: no_records
    type(beam_structure_t) :: beam_structure
    type(model_data_t), target :: model

    write (u, "(A)")  "* Test output: beam_2"
    write (u, "(A)")  "* Purpose: transfer beam polarization using &
      &beam structure"
    write (u, "(A)")

    write (u, "(A)")  "* Reading model file"
    write (u, "(A)")

    call model%init_sm_test ()

```

```

write (u, "(A)")  "* Unpolarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)
call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

```

```

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Polarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)
call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 1)
call beam_structure%set_sentry (1, 1, [1,1], (1._default, 0._default))

call beam_structure%init_smatrix (2, 3)
call beam_structure%set_sentry (2, 1, [1,1], (1._default, 0._default))
call beam_structure%set_sentry (2, 2, [-1,-1], (1._default, 0._default))
call beam_structure%set_sentry (2, 3, [-1,1], (1._default, 0._default))

call beam_structure%set_pol_f ([0.5_default, 1._default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)
write (u, *)

call beam_init (beam, beam_data)
call beam_write (beam, u)

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_pol ()
call beam_structure%final_sf ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

```

```

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 0)

call beam_structure%init_smatrix (2, 1)
call beam_structure%set_sentry (2, 1, [1,1], (1._default, 0._default))

call beam_structure%set_pol_f ([0._default, 1._default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 0)

call beam_structure%init_smatrix (2, 1)
call beam_structure%set_sentry (2, 1, [0,0], (1._default, 0._default))
call beam_structure%write (u)

write (u, "(A)")
call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()

```

```

call flv(1)%init (23, model)

call beam_structure%init_sf ([flv(1)%get_name ()], no_records)
call beam_structure%final_pol ()
call beam_structure%write (u)

write (u, "(A)")
call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Polarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)
call beam_structure%init_sf ([flv(1)%get_name ()], no_records)

call beam_structure%init_pol (1)

call beam_structure%init_smatrix (1, 1)
call beam_structure%set_sentry (1, 1, [0,0], (1._default, 0._default))
call beam_structure%set_pol_f ([0.4_default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call beam_final (beam)
call beam_data%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_2"

end subroutine beam_2

```

Test advanced beam setup, completely arbitrary momenta.

(Beams: execute tests)+≡

```

call test (beam_3, "beam_3", &
  "generic beam momenta", &

```



```

        u, results)
<Beams: test declarations>+≡
    public :: beam_3
<Beams: tests>+≡
    subroutine beam_3 (u)
        integer, intent(in) :: u
        type(beam_data_t), target :: beam_data
        type(beam_t) :: beam
        type(flavor_t), dimension(2) :: flv
        integer, dimension(0) :: no_records
        type(model_data_t), target :: model
        type(beam_structure_t) :: beam_structure
        type(vector3_t), dimension(2) :: p3
        type(vector4_t), dimension(2) :: p

        write (u, "(A)")  "* Test output: beam_3"
        write (u, "(A)")  "* Purpose: set up beams with generic momenta"
        write (u, "(A)")

        write (u, "(A)")  "* Reading model file"
        write (u, "(A)")

        call reset_interaction_counter ()

        call model%init_sm_test ()

        write (u, "(A)")  "* 1: Scattering process"
        write (u, "(A)")

        call flv%init ([2212,2212], model)

        p3(1) = vector3_moving ([5._default, 0._default, 10._default])
        p3(2) = -vector3_moving ([1._default, 1._default, -10._default])

        call beam_structure%init_sf (flv%get_name (), no_records)
        call beam_structure%set_momentum (p3 ** 1)
        call beam_structure%set_theta (polar_angle (p3))
        call beam_structure%set_phi (azimuthal_angle (p3))
        call beam_structure%write (u)
        write (u, *)

        call beam_data%init_structure (beam_structure, 0._default, model)
        call pacify (beam_data%l_cm_to_lab, 1e-20_default)
        call beam_data%compute_md5sum ()
        call beam_data%write (u, verbose = .true.)
        write (u, *)

        write (u, "(1x,A)")  "Beam momenta reconstructed from LT:"
        p = beam_data%L_cm_to_lab * beam_data%p_cm
        call pacify (p, 1e-12_default)
        call vector4_write (p(1), u)
        call vector4_write (p(2), u)
        write (u, "(A)")

```

```

call beam_init (beam, beam_data)
call beam_write (beam, u)

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_sf ()
call beam_structure%final_mom ()

write (u, "(A)")
write (u, "(A)")  "* 2: Decay"
write (u, "(A)")

call flv(1)%init (23, model)
p3(1) = vector3_moving ([10._default, 5._default, 50._default])

call beam_structure%init_sf ([flv(1)%get_name ()], no_records)
call beam_structure%set_momentum ([p3(1) ** 1])
call beam_structure%set_theta ([polar_angle (p3(1))])
call beam_structure%set_phi ([azimuthal_angle (p3(1))])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, 0._default, model)
call beam_data%write (u, verbose = .true.)
write (u, "(A)")

write (u, "(1x,A)")  "Beam momentum reconstructed from LT:"
p(1) = beam_data%L_cm_to_lab * beam_data%p_cm(1)
call pacify (p(1), 1e-12_default)
call vector4_write (p(1), u)
write (u, "(A)")

call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_sf ()
call beam_structure%final_mom ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_3"

end subroutine beam_3

```

16.3 Tools

This module contains auxiliary procedures that can be accessed by the structure function code.

```
<sf_aux.f90>≡  
<File header>  
  
module sf_aux  
  
  <Use kinds>  
  use constants, only: twopi  
  use lorentz  
  
  <Standard module head>  
  
  <SF aux: public>  
  
  <SF aux: parameters>  
  
  <SF aux: types>  
  
  interface  
  <SF aux: sub interfaces>  
  end interface  
  
end module sf_aux  
  
<sf_aux_sub.f90>≡  
<File header>  
  
submodule (sf_aux) sf_aux_s  
  
  use io_units  
  use numeric_utils  
  
  implicit none  
  
contains  
  
  <SF aux: procedures>  
  
end submodule sf_aux_s
```

16.3.1 Momentum splitting

Let us consider first an incoming parton with momentum k and invariant mass squared $s = k^2$ that splits into two partons with momenta q, p and invariant masses $t = q^2$ and $u = p^2$. (This is an abuse of the Mandelstam notation. t is actually the momentum transfer, assuming that p is radiated and q initiates the hard process.) The energy is split among the partons such that if $E = k^0$, we have $q^0 = xE$ and $p^0 = \bar{x}E$, where $\bar{x} \equiv 1 - x$.

We define the angle θ as the polar angle of p w.r.t. the momentum axis of the incoming momentum k . Ignoring azimuthal angle, we can write the four-momenta in the basis (E, p_T, p_L) as

$$k = \begin{pmatrix} E \\ 0 \\ p \end{pmatrix}, \quad p = \begin{pmatrix} \bar{x}E \\ \bar{x}\bar{p}\sin\theta \\ \bar{x}\bar{p}\cos\theta \end{pmatrix}, \quad q = \begin{pmatrix} xE \\ -\bar{x}\bar{p}\sin\theta \\ p - \bar{x}\bar{p}\cos\theta \end{pmatrix}, \quad (16.1)$$

where the first two mass-shell conditions are

$$p^2 = E^2 - s, \quad \bar{p}^2 = E^2 - \frac{u}{\bar{x}^2}. \quad (16.2)$$

The second condition implies that, for positive u , $\bar{x}^2 > u/E^2$, or equivalently

$$x < 1 - \sqrt{u}/E. \quad (16.3)$$

We are interested in the third mass-shell conditions: s and u are fixed, so we need t as a function of $\cos\theta$:

$$t = -2\bar{x}(E^2 - p\bar{p}\cos\theta) + s + u. \quad (16.4)$$

Solving for $\cos\theta$, we get

$$\cos\theta = \frac{2\bar{x}E^2 + t - s - u}{2\bar{x}p\bar{p}}. \quad (16.5)$$

We can compute $\sin\theta$ numerically as $\sin^2\theta = 1 - \cos^2\theta$, but it is important to reexpress this in view of numerical stability. To this end, we first determine the bounds for t . The cosine must be between -1 and 1 , so the bounds are

$$t_0 = -2\bar{x}(E^2 + p\bar{p}) + s + u, \quad (16.6)$$

$$t_1 = -2\bar{x}(E^2 - p\bar{p}) + s + u. \quad (16.7)$$

Computing $\sin^2\theta$ from $\cos\theta$ above, we observe that the numerator is a quadratic polynomial in t which has the zeros t_0 and t_1 , while the common denominator is given by $(2\bar{x}p\bar{p})^2$. Hence, we can write

$$\sin^2\theta = -\frac{(t-t_0)(t-t_1)}{(2\bar{x}p\bar{p})^2} \quad \text{and} \quad \cos\theta = \frac{(t-t_0) + (t-t_1)}{4\bar{x}p\bar{p}}, \quad (16.8)$$

which is free of large cancellations near $t = t_0$ or $t = t_1$.

If all is massless, i.e., $s = u = 0$, this simplifies to

$$t_0 = -4\bar{x}E^2, \quad t_1 = 0, \quad (16.9)$$

$$\sin^2\theta = -\frac{t}{\bar{x}E^2} \left(1 + \frac{t}{4\bar{x}E^2}\right), \quad \cos\theta = 1 + \frac{t}{2\bar{x}E^2}. \quad (16.10)$$

Here is the implementation. First, we define a container for the kinematical integration limits and some further data.

Note: contents are public only for easy access in unit test.

```
<SF aux: public>≡
  public :: splitting_data_t
```

```

<SF aux: types>≡
  type :: splitting_data_t
  !      private
        logical :: collinear = .false.
        real(default) :: x0 = 0
        real(default) :: x1
        real(default) :: t0
        real(default) :: t1
        real(default) :: phi0 = 0
        real(default) :: phi1 = twopi
        real(default) :: E, p, s, u, m2
        real(default) :: x, xb, pb
        real(default) :: t = 0
        real(default) :: phi = 0
  contains
    <SF aux: splitting data: TBP>
  end type splitting_data_t

```

I/O for debugging:

```

<SF aux: splitting data: TBP>≡
  procedure :: write => splitting_data_write

<SF aux: sub interfaces>≡
  module subroutine splitting_data_write (d, unit)
    class(splitting_data_t), intent(in) :: d
    integer, intent(in), optional :: unit
  end subroutine splitting_data_write

<SF aux: procedures>≡
  module subroutine splitting_data_write (d, unit)
    class(splitting_data_t), intent(in) :: d
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A)") "Splitting data:"
    write (u, "(2x,A,L1)") "collinear = ", d%collinear
1   format (2x,A,1x,ES15.8)
    write (u, 1) "x0  =", d%x0
    write (u, 1) "x   =", d%x
    write (u, 1) "xb  =", d%xb
    write (u, 1) "x1  =", d%x1
    write (u, 1) "t0  =", d%t0
    write (u, 1) "t   =", d%t
    write (u, 1) "t1  =", d%t1
    write (u, 1) "phi0 =", d%phi0
    write (u, 1) "phi  =", d%phi
    write (u, 1) "phi1 =", d%phi1
    write (u, 1) "E   =", d%E
    write (u, 1) "p   =", d%p
    write (u, 1) "pb  =", d%pb
    write (u, 1) "s   =", d%s
    write (u, 1) "u   =", d%u
    write (u, 1) "m2  =", d%m2
  end subroutine splitting_data_write

```

16.3.2 Constant data

This is the initializer for the data. The input consists of the incoming momentum, its invariant mass squared, and the invariant mass squared of the radiated particle. m_2 is the *physical* mass squared of the outgoing particle. The t bounds depend on the chosen x value and cannot be determined yet.

```

<SF aux: splitting data: TBP>+≡
  procedure :: init => splitting_data_init

<SF aux: sub interfaces>+≡
  module subroutine splitting_data_init (d, k, mk2, mr2, mo2, collinear)
    class(splitting_data_t), intent(out) :: d
    type(vector4_t), intent(in) :: k
    real(default), intent(in) :: mk2, mr2, mo2
    logical, intent(in), optional :: collinear
  end subroutine splitting_data_init

<SF aux: procedures>+≡
  module subroutine splitting_data_init (d, k, mk2, mr2, mo2, collinear)
    class(splitting_data_t), intent(out) :: d
    type(vector4_t), intent(in) :: k
    real(default), intent(in) :: mk2, mr2, mo2
    logical, intent(in), optional :: collinear
    if (present (collinear)) d%collinear = collinear
    d%E = energy (k)
    d%x1 = 1 - sqrt (max (mr2, 0._default)) / d%E
    d%p = sqrt (d%E**2 - mk2)
    d%s = mk2
    d%u = mr2
    d%m2 = mo2
  end subroutine splitting_data_init

```

Retrieve the x bounds, if needed for x sampling. Generating an x value is done by the caller, since this is the part that depends on the nature of the structure function.

```

<SF aux: splitting data: TBP>+≡
  procedure :: get_x_bounds => splitting_get_x_bounds

<SF aux: sub interfaces>+≡
  module function splitting_get_x_bounds (d) result (x)
    class(splitting_data_t), intent(in) :: d
    real(default), dimension(2) :: x
  end function splitting_get_x_bounds

<SF aux: procedures>+≡
  module function splitting_get_x_bounds (d) result (x)
    class(splitting_data_t), intent(in) :: d
    real(default), dimension(2) :: x
    x = [ d%x0, d%x1 ]
  end function splitting_get_x_bounds

```

Now set the momentum fraction and compute t_0 and t_1 .

[The calculation of t_1 is subject to numerical problems. The exact formula is ($s = m_i^2$, $u = m_r^2$)

$$t_1 = -2\bar{x}E^2 + m_i^2 + m_r^2 + 2\bar{x}\sqrt{E^2 - m_i^2}\sqrt{E^2 - m_r^2/\bar{x}^2}. \quad (16.11)$$

The structure-function paradigm is useful only if $E \gg m_i, m_r$. In a Taylor expansion for large E , the leading term cancels. The expansion of the square roots (to subleading order) yields

$$t_1 = xm_i^2 - \frac{x}{\bar{x}}m_r^2. \quad (16.12)$$

There are two cases of interest: $m_i = m_o$ and $m_r = 0$,

$$t_1 = xm_o^2 \quad (16.13)$$

and $m_i = m_r$ and $m_o = 0$,

$$t_1 = -\frac{x^2}{\bar{x}}m_i^2. \quad (16.14)$$

In both cases, $t_1 \leq m_o^2$.]

That said, it turns out that taking the t_1 evaluation at face value leads to less problems than the approximation. We express the angles in terms of $t - t_0$ and $t - t_1$. Numerical noise in t_1 can then be tolerated.

```

<SF aux: splitting data: TBP>+≡
  procedure :: set_t_bounds => splitting_set_t_bounds

<SF aux: sub interfaces>+≡
  elemental module subroutine splitting_set_t_bounds (d, x, xb)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in), optional :: x, xb
  end subroutine splitting_set_t_bounds

<SF aux: procedures>+≡
  elemental module subroutine splitting_set_t_bounds (d, x, xb)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in), optional :: x, xb
    real(default) :: tp, tm
    if (present (x)) d%x = x
    if (present (xb)) d%xb = xb
    if (vanishes (d%u)) then
      d%pb = d%E
    else
      if (.not. vanishes (d%xb)) then
        d%pb = sqrt (max (d%E**2 - d%u / d%xb**2, 0._default))
      else
        d%pb = 0
      end if
    end if
    tp = -2 * d%xb * d%E**2 + d%s + d%u
    tm = -2 * d%xb * d%p * d%pb
    d%t0 = tp + tm
    d%t1 = tp - tm
    d%t = d%t1
  end subroutine splitting_set_t_bounds

```

16.3.3 Sampling recoil

Compute a value for the momentum transfer t , using a random number r . We assume a logarithmic distribution for $t - m^2$, corresponding to the propagator $1/(t - m^2)$ with the physical mass m for the outgoing particle. Optionally, we can narrow the kinematical bounds.

If all three masses in the splitting vanish, the upper limit for t is zero. In that case, the t value is set to zero and the splitting will be collinear.

```

<SF aux: splitting data: TBP>+≡
  procedure :: sample_t => splitting_sample_t

<SF aux: sub interfaces>+≡
  module subroutine splitting_sample_t (d, r, t0, t1)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
    real(default), intent(in), optional :: t0, t1
  end subroutine splitting_sample_t

<SF aux: procedures>+≡
  module subroutine splitting_sample_t (d, r, t0, t1)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
    real(default), intent(in), optional :: t0, t1
    real(default) :: tt0, tt1, tt0m, tt1m
    if (d%collinear) then
      d%t = d%t1
    else
      tt0 = d%t0; if (present (t0)) tt0 = max (t0, tt0)
      tt1 = d%t1; if (present (t1)) tt1 = min (t1, tt1)
      tt0m = tt0 - d%m2
      tt1m = tt1 - d%m2
      if (tt0m < 0 .and. tt1m < 0 .and. abs(tt0m) > &
          epsilon(tt0m) .and. abs(tt1m) > epsilon(tt0m)) then
        d%t = d%m2 + tt0m * exp (r * log (tt1m / tt0m))
      else
        d%t = tt1
      end if
    end if
  end subroutine splitting_sample_t

```

The inverse operation: Given t , we recover the value of r that would have produced this value.

```

<SF aux: splitting data: TBP>+≡
  procedure :: inverse_t => splitting_inverse_t

<SF aux: sub interfaces>+≡
  module subroutine splitting_inverse_t (d, r, t0, t1)
    class(splitting_data_t), intent(in) :: d
    real(default), intent(out) :: r
    real(default), intent(in), optional :: t0, t1
  end subroutine splitting_inverse_t

<SF aux: procedures>+≡
  module subroutine splitting_inverse_t (d, r, t0, t1)
    class(splitting_data_t), intent(in) :: d

```



```

real(default), intent(out) :: r
real(default), intent(in), optional :: t0, t1
real(default) :: tt0, tt1, tt0m, tt1m
if (d%collinear) then
  r = 0
else
  tt0 = d%t0; if (present (t0)) tt0 = max (t0, tt0)
  tt1 = d%t1; if (present (t1)) tt1 = min (t1, tt1)
  tt0m = tt0 - d%m2
  tt1m = tt1 - d%m2
  if (tt0m < 0 .and. tt1m < 0) then
    r = log ((d%t - d%m2) / tt0m) / log (tt1m / tt0m)
  else
    r = 0
  end if
end if
end subroutine splitting_inverse_t

```

This is trivial, but provided for convenience:

```

<SF aux: splitting data: TBP>+≡
  procedure :: sample_phi => splitting_sample_phi

<SF aux: sub interfaces>+≡
  module subroutine splitting_sample_phi (d, r)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
  end subroutine splitting_sample_phi

<SF aux: procedures>+≡
  module subroutine splitting_sample_phi (d, r)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
    if (d%collinear) then
      d%phi = 0
    else
      d%phi = (1-r) * d%phi0 + r * d%phi1
    end if
  end subroutine splitting_sample_phi

```

Inverse:

```

<SF aux: splitting data: TBP>+≡
  procedure :: inverse_phi => splitting_inverse_phi

<SF aux: sub interfaces>+≡
  module subroutine splitting_inverse_phi (d, r)
    class(splitting_data_t), intent(in) :: d
    real(default), intent(out) :: r
  end subroutine splitting_inverse_phi

<SF aux: procedures>+≡
  module subroutine splitting_inverse_phi (d, r)
    class(splitting_data_t), intent(in) :: d
    real(default), intent(out) :: r
    if (d%collinear) then
      r = 0
    end if
  end subroutine splitting_inverse_phi

```

```

else
  r = (d%phi - d%phi0) / (d%phi1 - d%phi0)
end if
end subroutine splitting_inverse_phi

```

16.3.4 Splitting

In this function, we actually perform the splitting. The incoming momentum k is split into (if no recoil) $q_1 = (1 - x)k$ and $q_2 = xk$.

Apart from the splitting data, we need the incoming momentum k , the momentum transfer t , and the azimuthal angle ϕ . The momentum fraction x is already known here.

Alternatively, we can split without recoil. The azimuthal angle is irrelevant, and the momentum transfer is always equal to the upper limit t_1 , so the polar angle is zero. Obviously, if there are nonzero masses it is not possible to keep both energy-momentum conservation and at the same time all particles on shell. We choose for dropping the on-shell condition here.

```

<SF aux: splitting data: TBP>+=
  procedure :: split_momentum => splitting_split_momentum

<SF aux: sub interfaces>+=
  module function splitting_split_momentum (d, k) result (q)
    class(splitting_data_t), intent(in) :: d
    type(vector4_t), dimension(2) :: q
    type(vector4_t), intent(in) :: k
  end function splitting_split_momentum

<SF aux: procedures>+=
  module function splitting_split_momentum (d, k) result (q)
    class(splitting_data_t), intent(in) :: d
    type(vector4_t), dimension(2) :: q
    type(vector4_t), intent(in) :: k
    real(default) :: st2, ct2, st, ct, cp, sp
    type(lorentz_transformation_t) :: rot
    real(default) :: tt0, tt1, den
    type(vector3_t) :: kk, q1, q2
    if (d%collinear) then
      if (vanishes(d%s) .and. vanishes(d%u)) then
        q(1) = d%xb * k
        q(2) = d%x * k
      else
        kk = space_part (k)
        q1 = d%xb * (d%pb / d%p) * kk
        q2 = kk - q1
        q(1) = vector4_moving (d%xb * d%E, q1)
        q(2) = vector4_moving (d%x * d%E, q2)
      end if
    else
      den = 2 * d%xb * d%p * d%pb
      tt0 = max (d%t - d%t0, 0._default)
      tt1 = min (d%t - d%t1, 0._default)
      if (den**2 <= epsilon(den)) then
        st2 = 0

```

```

else
    st2 = - (tt0 * tt1) / den ** 2
end if
if (st2 > 1) then
    st2 = 1
end if
ct2 = 1 - st2
st = sqrt (max (st2, 0._default))
ct = sqrt (max (ct2, 0._default))
if ((d%t - d%t0 + d%t - d%t1) < 0) then
    ct = - ct
end if
sp = sin (d%phi)
cp = cos (d%phi)
rot = rotation_to_2nd (3, space_part (k))
q1 = vector3_moving (d%xb * d%pb * [st * cp, st * sp, ct])
q2 = vector3_moving (d%p, 3) - q1
q(1) = rot * vector4_moving (d%xb * d%E, q1)
q(2) = rot * vector4_moving (d%x * d%E, q2)
end if
end function splitting_split_momentum

```

Momenta generated by splitting will in general be off-shell. They are on-shell only if they are collinear and massless. This subroutine puts them on shell by brute force, violating either momentum or energy conservation. The direction of three-momentum is always retained.

If the energy is below mass shell, we return a zero momentum.

```

<SF aux: parameters>≡
    integer, parameter, public :: KEEP_ENERGY = 0, KEEP_MOMENTUM = 1

<SF aux: public>+≡
    public :: on_shell

<SF aux: sub interfaces>+≡
    elemental module subroutine on_shell (p, m2, keep)
        type(vector4_t), intent(inout) :: p
        real(default), intent(in) :: m2
        integer, intent(in) :: keep
    end subroutine on_shell

<SF aux: procedures>+≡
    elemental module subroutine on_shell (p, m2, keep)
        type(vector4_t), intent(inout) :: p
        real(default), intent(in) :: m2
        integer, intent(in) :: keep
        real(default) :: E, E2, pn
        select case (keep)
        case (KEEP_ENERGY)
            E = energy (p)
            E2 = E ** 2
            if (E2 >= m2) then
                pn = sqrt (E2 - m2)
                p = vector4_moving (E, pn * direction (space_part (p)))
            else
                p = vector4_null
            end if
        case default
            p = vector4_null
        end select
    end subroutine on_shell

```

```

        end if
    case (KEEP_MOMENTUM)
        E = sqrt (space_part (p) ** 2 + m2)
        p = vector4_moving (E, space_part (p))
    end select
end subroutine on_shell

```

16.3.5 Recovering the splitting

This is the inverse problem. We have on-shell momenta and want to deduce the splitting parameters x , t , and ϕ .

Update 2018-08-22: As a true inverse to `splitting_split_momentum`, we now use not just a single momentum `q2` as before, but the momentum pair `q1`, `q2` for recovering x and \bar{x} separately. If x happens to be close to 1, we would completely lose the tiny \bar{x} value, otherwise, and thus get a meaningless result.

```

<SF aux: splitting data: TBP>+≡
    procedure :: recover => splitting_recover

<SF aux: sub interfaces>+≡
    module subroutine splitting_recover (d, k, q, keep)
        class(splitting_data_t), intent(inout) :: d
        type(vector4_t), intent(in) :: k
        type(vector4_t), dimension(2), intent(in) :: q
        integer, intent(in) :: keep
    end subroutine splitting_recover

<SF aux: procedures>+≡
    module subroutine splitting_recover (d, k, q, keep)
        class(splitting_data_t), intent(inout) :: d
        type(vector4_t), intent(in) :: k
        type(vector4_t), dimension(2), intent(in) :: q
        integer, intent(in) :: keep
        type(lorentz_transformation_t) :: rot
        type(vector4_t) :: k0
        type(vector4_t), dimension(2) :: q0
        real(default) :: p1, p2, p3, pt2, pp2, p1
        real(default) :: aux, den, norm
        real(default) :: st2, ct2, ct
        rot = inverse (rotation_to_2nd (3, space_part (k)))
        q0 = rot * q
        p1 = vector4_get_component (q0(2), 1)
        p2 = vector4_get_component (q0(2), 2)
        p3 = vector4_get_component (q0(2), 3)
        pt2 = p1 ** 2 + p2 ** 2
        pp2 = p1 ** 2 + p2 ** 2 + p3 ** 2
        p1 = abs (p3)
        k0 = vector4_moving (d%E, d%p, 3)
        select case (keep)
        case (KEEP_ENERGY)
            d%x = energy (q0(2)) / d%E
            d%xb = energy (q0(1)) / d%E
            call d%set_t_bounds ()
            if (.not. d%collinear) then

```

```

        aux = (d%xb * d%pb) ** 2 * pp2 - d%p ** 2 * pt2
        den = d%p ** 2 - (d%xb * d%pb) ** 2
        if (aux >= 0 .and. den > 0) then
            norm = (d%p * p1 + sqrt (aux)) / den
        else
            norm = 1
        end if
    end if
end if
case (KEEP_MOMENTUM)
    d%xb = sqrt (space_part (q0(1)) ** 2 + d%u) / d%E
    d%x = 1 - d%xb
    call d%set_t_bounds ()
    norm = 1
end select
if (d%collinear) then
    d%t = d%t1
    d%phi = 0
else
    if ((d%xb * d%pb * norm)**2 < epsilon(d%xb)) then
        st2 = 1
    else
        st2 = pt2 / (d%xb * d%pb * norm) ** 2
    end if
    if (st2 > 1) then
        st2 = 1
    end if
    ct2 = 1 - st2
    ct = sqrt (max (ct2, 0._default))
    if (.not. vanishes (1 + ct)) then
        d%t = d%t1 - 2 * d%xb * d%p * d%pb * st2 / (1 + ct)
    else
        d%t = d%t0
    end if
    if (.not. vanishes (p1) .or. .not. vanishes (p2)) then
        d%phi = atan2 (-p2, -p1)
    else
        d%phi = 0
    end if
end if
end if
end subroutine splitting_recover

```

16.3.6 Extract data

```

<SF aux: splitting data: TBP>+≡
    procedure :: get_x => splitting_get_x
    procedure :: get_xb => splitting_get_xb

<SF aux: sub interfaces>+≡
    module function splitting_get_x (sd) result (x)
        class(splitting_data_t), intent(in) :: sd
        real(default) :: x
    end function splitting_get_x
    module function splitting_get_xb (sd) result (xb)

```

```

        class(splitting_data_t), intent(in) :: sd
        real(default) :: xb
    end function splitting_get_xb

<SF aux: procedures>+≡
module function splitting_get_x (sd) result (x)
    class(splitting_data_t), intent(in) :: sd
    real(default) :: x
    x = sd%x
end function splitting_get_x

module function splitting_get_xb (sd) result (xb)
    class(splitting_data_t), intent(in) :: sd
    real(default) :: xb
    xb = sd%xb
end function splitting_get_xb

```

16.3.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_aux_ut.f90>≡
<File header>

module sf_aux_ut
    use unit_tests
    use sf_aux_uti

<Standard module head>

<SF aux: public test>

contains

<SF aux: test driver>

end module sf_aux_ut

<sf_aux_uti.f90>≡
<File header>

module sf_aux_uti

<Use kinds>
    use numeric_utils, only: pacify
    use lorentz

    use sf_aux

<Standard module head>

<SF aux: test declarations>

contains

```

<SF aux: tests>

end module sf_aux_util

API: driver for the unit tests below.

<SF aux: public test>≡

public :: sf_aux_test

<SF aux: test driver>≡

subroutine sf_aux_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SF aux: execute tests>

end subroutine sf_aux_test

Momentum splitting: massless radiation

Compute momentum splitting for generic kinematics. It turns out that for $x = 0.5$, where $t - m^2$ is the geometric mean between its upper and lower bounds (this can be directly seen from the logarithmic distribution in the function `sample_t` for $r \equiv x = 1 - x = 0.5$), we arrive at an exact number $t = -0.15$ for the given input values.

<SF aux: execute tests>≡

call test (sf_aux_1, "sf_aux_1", &
"massless radiation", &
u, results)

<SF aux: test declarations>≡

public :: sf_aux_1

<SF aux: tests>≡

subroutine sf_aux_1 (u)

integer, intent(in) :: u

type(splitting_data_t) :: sd

type(vector4_t) :: k

type(vector4_t), dimension(2) :: q, q0

real(default) :: E, mk, mp, mq

real(default) :: x, r1, r2, r1o, r2o

real(default) :: k2, q0_2, q1_2, q2_2

write (u, "(A)") "* Test output: sf_aux_1"

write (u, "(A)") "* Purpose: compute momentum splitting"

write (u, "(A)") " (massless radiated particle)"

write (u, "(A)")

E = 1

mk = 0.3_default

mp = 0

mq = mk

k = vector4_moving (E, sqrt (E**2 - mk**2), 3)

k2 = k ** 2; call pacify (k2, 1e-10_default)

```

x = 0.6_default
r1 = 0.5_default
r2 = 0.125_default

write (u, "(A)")  "* (1) Non-collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%sample_t (r1)
call sd%sample_phi (r2)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2;  call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2;  call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: s"
write (u, "(2(1x,F11.8))")  sd%s, k2

write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  sd%t, q2_2

write (u, "(A)")  "Compare: u"
write (u, "(2(1x,F11.8))")  sd%u, q1_2

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  sd%x, energy (q(2)) / energy (k)

write (u, "(A)")  "Compare: 1-x"
write (u, "(2(1x,F11.8))")  sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)")  "Extract: x, 1-x"
write (u, "(2(1x,F11.8))")  sd%get_x (), sd%get_xb ()

write (u, "(A)")
write (u, "(A)")  "* Project on-shell (keep energy)"

```



```

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")

```

```

write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (2) Collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

```

```

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

```

```

write (u, "(A)")  "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))")  sd%m2, q0_2
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  q2_2, sd%t

write (u, "(A)")
call sd%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_aux_1"

end subroutine sf_aux_1

```

Momentum splitting: massless parton

Compute momentum splitting for generic kinematics. It turns out that for $x = 0.5$, where $t - m^2$ is the geometric mean between its upper and lower bounds, we arrive at an exact number $t = -0.36$ for the given input values.

```

<SF aux: execute tests>+≡
  call test (sf_aux_2, "sf_aux_2", &
    "massless parton", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_2

<SF aux: tests>+≡
  subroutine sf_aux_2 (u)
    integer, intent(in) :: u
    type(splitting_data_t) :: sd
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q, q0
    real(default) :: E, mk, mp, mq
    real(default) :: x, r1, r2, r1o, r2o
    real(default) :: k2, q02_2, q1_2, q2_2

    write (u, "(A)")  "* Test output: sf_aux_2"
    write (u, "(A)")  "* Purpose: compute momentum splitting"
    write (u, "(A)")  "          (massless outgoing particle)"
    write (u, "(A)")

    E = 1
    mk = 0.3_default
    mp = mk
    mq = 0

    k = vector4_moving (E, sqrt (E**2 - mk**2), 3)
    k2 = k ** 2; call pacify (k2, 1e-10_default)

    x = 0.6_default
    r1 = 0.5_default
    r2 = 0.125_default

    write (u, "(A)")  "* (1) Non-collinear setup"
    write (u, "(A)")

    call sd%init (k, mk**2, mp**2, mq**2)
    call sd%set_t_bounds (x, 1 - x)
    call sd%sample_t (r1)
    call sd%sample_phi (r2)

```

```

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

```

```

write (u, "(A)") "Compare: mo~2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write(k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo~2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)

```

```

write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)")  "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)")  "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "* (2) Collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2;  call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2;  call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

```



```

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")

```

```

call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "** Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)")  "** Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_aux_2"

end subroutine sf_aux_2

```

Momentum splitting: all massless

Compute momentum splitting for massless kinematics. In the non-collinear case, we need a lower cutoff for $|t|$, otherwise a logarithmic distribution is not possible.

```

<SF aux: execute tests>+≡
  call test (sf_aux_3, "sf_aux_3", &
    "massless parton", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_3

<SF aux: tests>+≡
  subroutine sf_aux_3 (u)
    integer, intent(in) :: u
    type(splitting_data_t) :: sd
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q, q0
    real(default) :: E, mk, mp, mq, qmin, qmax
    real(default) :: x, r1, r2, r1o, r2o
    real(default) :: k2, q02_2, q1_2, q2_2

    write (u, "(A)")  "* Test output: sf_aux_3"
    write (u, "(A)")  "* Purpose: compute momentum splitting"
    write (u, "(A)")  "      (all massless, q cuts)"
    write (u, "(A)")

    E = 1
    mk = 0
    mp = 0
    mq = 0
    qmin = 1e-2_default
    qmax = 1e0_default

    k = vector4_moving (E, sqrt (E**2 - mk**2), 3)
    k2 = k ** 2; call pacify (k2, 1e-10_default)

    x = 0.6_default
    r1 = 0.5_default
    r2 = 0.125_default

    write (u, "(A)")  "* (1) Non-collinear setup"
    write (u, "(A)")

    call sd%init (k, mk**2, mp**2, mq**2)
    call sd%set_t_bounds (x, 1 - x)
    call sd%sample_t (r1, t1 = - qmin ** 2, t0 = - qmax **2)
    call sd%sample_phi (r2)

    call sd%write (u)

    q = sd%split_momentum (k)
    q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
    q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

    write (u, "(A)")
    write (u, "(A)")  "Incoming momentum k ="
    call vector4_write (k, u)
    write (u, "(A)")

```

```

write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)

```

```

call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o, t1 = - qmin ** 2, t0 = - qmax **2)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

```

```

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o, t1 = - qmin ** 2, t0 = - qmax **2)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (2) Collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

```

```

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="

```

```

call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_aux_3"

end subroutine sf_aux_3

```

Endpoint stability

Compute momentum splitting for collinear kinematics close to both endpoints. In particular, check both directions $x \rightarrow$ momenta and momenta $\rightarrow x$.

For purely massless collinear splitting, the KEEP_XXX flag is irrelevant. We choose KEEP_ENERGY here.

```

<SF aux: execute tests>+≡
  call test (sf_aux_4, "sf_aux_4", &
    "endpoint numerics", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_4

<SF aux: tests>+≡
  subroutine sf_aux_4 (u)

```



```

integer, intent(in) :: u
type(splitting_data_t) :: sd
type(vector4_t) :: k
type(vector4_t), dimension(2) :: q
real(default) :: E, mk, mp, mq, qmin, qmax
real(default) :: x, xb

write (u, "(A)")  "* Test output: sf_aux_4"
write (u, "(A)")  "* Purpose: compute massless collinear splitting near endpoint"

E = 1
mk = 0
mp = 0
mq = 0
qmin = 1e-2_default
qmax = 1e0_default

k = vector4_moving (E, sqrt (E**2 - mk**2), 3)

x = 0.1_default
xb = 1 - x

write (u, "(A)")
write (u, "(A)")  "* (1) Collinear setup, moderate kinematics"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

```

```

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (2) Close to x=0"
write (u, "(A)")

x = 1e-9_default
xb = 1 - x

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")

```

```

write (u, "(A)")  "* (3) Close to x=1"
write (u, "(A)")

xb = 1e-9_default
x = 1 - xb

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x

write (u, "(A)")  "Compare: 1-x"
write (u, "(2(1x,F11.8))")  xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_aux_4"

end subroutine sf_aux_4

```

16.4 Mappings for structure functions

In this module, we provide a wrapper for useful mappings of the unit (hyper-)square that we can apply to a set of structure functions.

In some cases it is useful, or even mandatory, to map the MC input parameters nontrivially onto a set of structure functions for the two beams. In all cases considered here, instead of x_1, x_2, \dots as parameters for the beams, we generate one parameter that is equal, or related to, the product $x_1 x_2 \dots$ (so it directly corresponds to \sqrt{s}). The other parameters describe the distribution of energy (loss) between beams and radiations.

```

<sf_mappings.f90>≡
  <File header>

  module sf_mappings

    <Use kinds>
    use kinds, only: double

    <Standard module head>

    <SF mappings: public>

    <SF mappings: parameters>

    <SF mappings: types>

    <SF mappings: interfaces>

    interface
    <SF mappings: sub interfaces>
    end interface

    contains

    <SF mappings: main procedures>

  end module sf_mappings

<sf_mappings_sub.f90>≡
  <File header>

  submodule (sf_mappings) sf_mappings_s

    use io_units
    use constants, only: pi, zero, one
    use numeric_utils
    use diagnostics

    implicit none

    contains

    <SF mappings: procedures>

  end submodule sf_mappings_s

```

16.4.1 Base type

First, we define an abstract base type for the mapping. In all cases we need to store the indices of the parameters on which the mapping applies. Additional parameters can be stored in the extensions of this type.

```
<SF mappings: public>≡  
  public :: sf_mapping_t  
<SF mappings: types>≡  
  type, abstract :: sf_mapping_t  
    integer, dimension(:), allocatable :: i  
    contains  
    <SF mappings: sf mapping: TBP>  
  end type sf_mapping_t
```

The output routine is deferred:

```
<SF mappings: sf mapping: TBP>≡  
  procedure (sf_mapping_write), deferred :: write  
<SF mappings: interfaces>≡  
  abstract interface  
    subroutine sf_mapping_write (object, unit)  
      import  
      class(sf_mapping_t), intent(in) :: object  
      integer, intent(in), optional :: unit  
    end subroutine sf_mapping_write  
  end interface
```

Initializer for the base type. The array of parameter indices is allocated but initialized to zero.

```
<SF mappings: sf mapping: TBP>+≡  
  procedure :: base_init => sf_mapping_base_init  
<SF mappings: sub interfaces>≡  
  module subroutine sf_mapping_base_init (mapping, n_par)  
    class(sf_mapping_t), intent(out) :: mapping  
    integer, intent(in) :: n_par  
  end subroutine sf_mapping_base_init  
<SF mappings: procedures>≡  
  module subroutine sf_mapping_base_init (mapping, n_par)  
    class(sf_mapping_t), intent(out) :: mapping  
    integer, intent(in) :: n_par  
    allocate (mapping%i (n_par))  
    mapping%i = 0  
  end subroutine sf_mapping_base_init
```

Set an index value.

```
<SF mappings: sf mapping: TBP>+≡  
  procedure :: set_index => sf_mapping_set_index  
<SF mappings: sub interfaces>+≡  
  module subroutine sf_mapping_set_index (mapping, j, i)  
    class(sf_mapping_t), intent(inout) :: mapping  
    integer, intent(in) :: j, i  
  end subroutine sf_mapping_set_index
```

```

⟨SF mappings: procedures⟩+≡
  module subroutine sf_mapping_set_index (mapping, j, i)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
  end subroutine sf_mapping_set_index

```

Retrieve an index value.

```

⟨SF mappings: sf mapping: TBP⟩+≡
  procedure :: get_index => sf_mapping_get_index

⟨SF mappings: sub interfaces⟩+≡
  module function sf_mapping_get_index (mapping, j) result (i)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j
    integer :: i
  end function sf_mapping_get_index

⟨SF mappings: procedures⟩+≡
  module function sf_mapping_get_index (mapping, j) result (i)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j
    integer :: i
    i = mapping%i(j)
  end function sf_mapping_get_index

```

Return the dimensionality, i.e., the number of parameters.

```

⟨SF mappings: sf mapping: TBP⟩+≡
  procedure :: get_n_dim => sf_mapping_get_n_dim

⟨SF mappings: sub interfaces⟩+≡
  module function sf_mapping_get_n_dim (mapping) result (n)
    class(sf_mapping_t), intent(in) :: mapping
    integer :: n
  end function sf_mapping_get_n_dim

⟨SF mappings: procedures⟩+≡
  module function sf_mapping_get_n_dim (mapping) result (n)
    class(sf_mapping_t), intent(in) :: mapping
    integer :: n
    n = size (mapping%i)
  end function sf_mapping_get_n_dim

```

Computation: the values **p** are the input parameters, the values **r** are the output parameters. The values **rb** are defined as $\bar{r} = 1 - r$, but provided explicitly. They allow us to avoid numerical problems near $r = 1$.

The extra parameter **x_free** indicates that the total energy has already been renormalized by this factor. We have to take such a factor into account in a resonance or on-shell mapping.

The Jacobian is **f**. We modify only the two parameters indicated by the indices **i**.

```

⟨SF mappings: sf mapping: TBP⟩+≡
  procedure (sf_mapping_compute), deferred :: compute

```

```

<SF mappings: interfaces>+≡
  abstract interface
    subroutine sf_mapping_compute (mapping, r, rb, f, p, pb, x_free)
      import
      class(sf_mapping_t), intent(inout) :: mapping
      real(default), dimension(:), intent(out) :: r, rb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(in) :: p, pb
      real(default), intent(inout), optional :: x_free
    end subroutine sf_mapping_compute
  end interface

```

The inverse mapping. Use *r* and/or *rb* to reconstruct *p* and also compute *f*.

```

<SF mappings: sf mapping: TBP>+≡
  procedure (sf_mapping_inverse), deferred :: inverse

<SF mappings: interfaces>+≡
  abstract interface
    subroutine sf_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
      import
      class(sf_mapping_t), intent(inout) :: mapping
      real(default), dimension(:), intent(in) :: r, rb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(out) :: p, pb
      real(default), intent(inout), optional :: x_free
    end subroutine sf_mapping_inverse
  end interface

```

16.4.2 Methods for self-tests

This is a shorthand for: inject parameters, compute the mapping, display results, compute the inverse, display again. We provide an output format for the parameters and, optionally, a different output format for the Jacobians.

```

<SF mappings: sf mapping: TBP>+≡
  procedure :: check => sf_mapping_check

<SF mappings: sub interfaces>+≡
  module subroutine sf_mapping_check (mapping, u, p_in, pb_in, fmt_p, fmt_f)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: u
    real(default), dimension(:), intent(in) :: p_in, pb_in
    character(*), intent(in) :: fmt_p
    character(*), intent(in), optional :: fmt_f
  end subroutine sf_mapping_check

<SF mappings: procedures>+≡
  module subroutine sf_mapping_check (mapping, u, p_in, pb_in, fmt_p, fmt_f)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: u
    real(default), dimension(:), intent(in) :: p_in, pb_in
    character(*), intent(in) :: fmt_p
    character(*), intent(in), optional :: fmt_f
    real(default), dimension(size(p_in)) :: p, pb, r, rb

```

```

real(default), dimension(size(p_in)) :: p_orig, pb_orig, r_orig, rb_orig
real(default) :: f, tolerance
tolerance = 1.5E-17_default
p = p_in
pb= pb_in
call mapping%compute (r, rb, f, p, pb)
p_orig = p
pb_orig = pb
r_orig = r
rb_orig = rb
call pacify (p, tolerance)
call pacify (pb, tolerance)
call pacify (r, tolerance)
call pacify (rb, tolerance)
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "p =", p
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "pb=", pb
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "r =", r
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "rb=", rb
if (present (fmt_f)) then
  write (u, "(3x,A,9(1x," // fmt_f // "))" ) "f =", f
else
  write (u, "(3x,A,9(1x," // fmt_p // "))" ) "f =", f
end if
write (u, *)
call mapping%inverse (r_orig, rb_orig, f, p_orig, pb_orig)
p = p_orig
pb = pb_orig
r = r_orig
rb = rb_orig
call pacify (p, tolerance)
call pacify (pb, tolerance)
call pacify (r, tolerance)
call pacify (rb, tolerance)
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "p =", p
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "pb=", pb
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "r =", r
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "rb=", rb
if (present (fmt_f)) then
  write (u, "(3x,A,9(1x," // fmt_f // "))" ) "f =", f
else
  write (u, "(3x,A,9(1x," // fmt_p // "))" ) "f =", f
end if
write (u, *)
write (u, "(3x,A,9(1x," // fmt_p // "))" ) "*r=", product (r)
end subroutine sf_mapping_check

```

This is a consistency check for the self-tests: the integral over the unit square should be unity. We estimate this by a simple binning and adding up the values; this should be sufficient for a self-test.

The argument is the requested number of sampling points. We take the square root for binning in both dimensions, so the precise number might be different.

$\langle SF \text{ mappings: } sf \text{ mapping: } TBP \rangle + \equiv$


```

    procedure :: integral => sf_mapping_integral
  (SF mappings: sub interfaces)+≡
    module function sf_mapping_integral (mapping, n_calls) result (integral)
      class(sf_mapping_t), intent(inout) :: mapping
      integer, intent(in) :: n_calls
      real(default) :: integral
    end function sf_mapping_integral
  (SF mappings: procedures)+≡
    module function sf_mapping_integral (mapping, n_calls) result (integral)
      class(sf_mapping_t), intent(inout) :: mapping
      integer, intent(in) :: n_calls
      real(default) :: integral
      integer :: n_dim, n_bin, k
      real(default), dimension(:), allocatable :: p, pb, r, rb
      integer, dimension(:), allocatable :: ii
      real(default) :: dx, f, s

      n_dim = mapping%get_n_dim ()
      allocate (p (n_dim))
      allocate (pb(n_dim))
      allocate (r (n_dim))
      allocate (rb(n_dim))
      allocate (ii(n_dim))
      n_bin = nint (real (n_calls, default) ** (1._default / n_dim))
      dx = 1._default / n_bin
      s = 0
      ii = 1

      SAMPLE: do
        do k = 1, n_dim
          p(k) = ii(k) * dx - dx/2
          pb(k) = (n_bin - ii(k)) * dx + dx/2
        end do
        call mapping%compute (r, rb, f, p, pb)
        s = s + f
      INCR: do k = 1, n_dim
        ii(k) = ii(k) + 1
        if (ii(k) <= n_bin) then
          exit INCR
        else if (k < n_dim) then
          ii(k) = 1
        else
          exit SAMPLE
        end if
      end do INCR
    end do SAMPLE

    integral = s / real (n_bin, default) ** n_dim

  end function sf_mapping_integral

```

16.4.3 Implementation: standard mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio.

```

<SF mappings: public>+≡
    public :: sf_s_mapping_t

<SF mappings: types>+≡
    type, extends (sf_mapping_t) :: sf_s_mapping_t
        logical :: power_set = .false.
        real(default) :: power = 1
    contains
        <SF mappings: sf standard mapping: TBP>
    end type sf_s_mapping_t

```

Output.

```

<SF mappings: sf standard mapping: TBP>≡
    procedure :: write => sf_s_mapping_write

<SF mappings: sub interfaces>+≡
    module subroutine sf_s_mapping_write (object, unit)
        class(sf_s_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_s_mapping_write

<SF mappings: procedures>+≡
    module subroutine sf_s_mapping_write (object, unit)
        class(sf_s_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',I0,',',',I0,')')", advance="no") object%i
        end if
        write (u, "(A,F7.5,A)" " : standard (" , object%power, ")")
    end subroutine sf_s_mapping_write

```

Initialize: index pair and power parameter.

```

<SF mappings: sf standard mapping: TBP>+≡
    procedure :: init => sf_s_mapping_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_s_mapping_init (mapping, power)
        class(sf_s_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: power
    end subroutine sf_s_mapping_init

<SF mappings: procedures>+≡
    module subroutine sf_s_mapping_init (mapping, power)
        class(sf_s_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: power
        call mapping%base_init (2)
        if (present (power)) then
            mapping%power_set = .true.

```

```

        mapping%power = power
    end if
end subroutine sf_s_mapping_init

```

Apply mapping.

```

<SF mappings: sf standard mapping: TBP>+≡
    procedure :: compute => sf_s_mapping_compute

<SF mappings: sub interfaces>+≡
    module subroutine sf_s_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_s_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_s_mapping_compute

<SF mappings: procedures>+≡
    module subroutine sf_s_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_s_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(2) :: r2
        integer :: j
        if (mapping%power_set) then
            call map_unit_square (r2, f, p(mapping%i), mapping%power)
        else
            call map_unit_square (r2, f, p(mapping%i))
        end if
        r = p
        rb = pb
        do j = 1, 2
            r (mapping%i(j)) = r2(j)
            rb(mapping%i(j)) = 1 - r2(j)
        end do
    end subroutine sf_s_mapping_compute

```

Apply inverse.

```

<SF mappings: sf standard mapping: TBP>+≡
    procedure :: inverse => sf_s_mapping_inverse

<SF mappings: sub interfaces>+≡
    module subroutine sf_s_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
        class(sf_s_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_s_mapping_inverse

<SF mappings: procedures>+≡
    module subroutine sf_s_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
        class(sf_s_mapping_t), intent(inout) :: mapping

```

```

real(default), dimension(:), intent(in) :: r, rb
real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: p, pb
real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: p2
integer :: j
if (mapping%power_set) then
  call map_unit_square_inverse (r(mapping%i), f, p2, mapping%power)
else
  call map_unit_square_inverse (r(mapping%i), f, p2)
end if
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = 1 - p2(j)
end do
end subroutine sf_s_mapping_inverse

```

16.4.4 Implementation: resonance pair mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio, then it maps p_1 to itself according to a Breit-Wigner shape, i.e., a flat prior distribution in p_1 results in a Breit-Wigner distribution. Mass and width of the BW are rescaled by the energy, thus dimensionless fractions.

```

<SF mappings: public>+≡
  public :: sf_res_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_res_mapping_t
    real(default) :: m = 0
    real(default) :: w = 0
  contains
    <SF mappings: sf resonance mapping: TBP>
  end type sf_res_mapping_t

```

Output.

```

<SF mappings: sf resonance mapping: TBP>≡
  procedure :: write => sf_res_mapping_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_write (object, unit)
    class(sf_res_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_res_mapping_write

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_write (object, unit)
    class(sf_res_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"

```

```

    if (any (object%i /= 0)) then
        write (u, "('(',I0,',',I0,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,', ',F7.5,A)") ": resonance (" , object%m, object%w, ")"
end subroutine sf_res_mapping_write

```

Initialize: index pair and dimensionless mass and width parameters.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: init => sf_res_mapping_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_init (mapping, m, w)
    class(sf_res_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: m, w
  end subroutine sf_res_mapping_init

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_init (mapping, m, w)
    class(sf_res_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: m, w
    call mapping%base_init (2)
    mapping%m = m
    mapping%w = w
  end subroutine sf_res_mapping_init

```

Apply mapping.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: compute => sf_res_mapping_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_res_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_res_mapping_compute

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_res_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, p2
    real(default) :: fbw, f2, p1m
    integer :: j
    p2 = p(mapping%i)
    call map_breit_wigner &
      (p1m, fbw, p2(1), mapping%m, mapping%w, x_free)
    call map_unit_square (r2, f2, [p1m, p2(2)])
    f = fbw * f2
    r = p
    rb = pb
  end subroutine sf_res_mapping_compute

```

```

do j = 1, 2
  r(mapping%i(j)) = r2(j)
  rb(mapping%i(j)) = 1 - r2(j)
end do
end subroutine sf_res_mapping_compute

```

Apply inverse.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: inverse => sf_res_mapping_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_res_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_res_mapping_inverse

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_res_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: p2
    real(default) :: fbw, f2, p1m
    call map_unit_square_inverse (r(mapping%i), f2, p2)
    call map_breit_wigner_inverse &
      (p2(1), fbw, p1m, mapping%m, mapping%w, x_free)
    p = r
    pb = rb
    p(mapping%i(1)) = p1m
    pb(mapping%i(1)) = 1 - p1m
    p(mapping%i(2)) = p2(2)
    pb(mapping%i(2)) = 1 - p2(2)
    f = fbw * f2
  end subroutine sf_res_mapping_inverse

```

16.4.5 Implementation: resonance single mapping

While simpler, this is needed for structure-function setups only in exceptional cases.

This maps the unit interval (r_1) to itself according to a Breit-Wigner shape, i.e., a flat prior distribution in r_1 results in a Breit-Wigner distribution. Mass and width of the BW are rescaled by the energy, thus dimensionless fractions.

```

<SF mappings: public>+≡
  public :: sf_res_mapping_single_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_res_mapping_single_t
    real(default) :: m = 0

```

```

        real(default) :: w = 0
contains
  <SF mappings: sf resonance single mapping: TBP>
end type sf_res_mapping_single_t

```

Output.

```

<SF mappings: sf resonance single mapping: TBP>≡
  procedure :: write => sf_res_mapping_single_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_single_write (object, unit)
    class(sf_res_mapping_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_res_mapping_single_write

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_single_write (object, unit)
    class(sf_res_mapping_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,', ',F7.5,A)" ": resonance (" , object%m, object%w, ")")
  end subroutine sf_res_mapping_single_write

```

Initialize: single index (!) and dimensionless mass and width parameters.

```

<SF mappings: sf resonance single mapping: TBP>+≡
  procedure :: init => sf_res_mapping_single_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_single_init (mapping, m, w)
    class(sf_res_mapping_single_t), intent(out) :: mapping
    real(default), intent(in) :: m, w
  end subroutine sf_res_mapping_single_init

<SF mappings: procedures>+≡
  module subroutine sf_res_mapping_single_init (mapping, m, w)
    class(sf_res_mapping_single_t), intent(out) :: mapping
    real(default), intent(in) :: m, w
    call mapping%base_init (1)
    mapping%m = m
    mapping%w = w
  end subroutine sf_res_mapping_single_init

```

Apply mapping.

```

<SF mappings: sf resonance single mapping: TBP>+≡
  procedure :: compute => sf_res_mapping_single_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_res_mapping_single_compute &
    (mapping, r, rb, f, p, pb, x_free)
    class(sf_res_mapping_single_t), intent(inout) :: mapping

```

```

        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_res_mapping_single_compute
<SF mappings: procedures>+≡
    module subroutine sf_res_mapping_single_compute &
        (mapping, r, rb, f, p, pb, x_free)
        class(sf_res_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(1) :: r2, p2
        real(default) :: fbw
        integer :: j
        p2 = p(mapping%i)
        call map_breit_wigner &
            (r2(1), fbw, p2(1), mapping%m, mapping%w, x_free)
        f = fbw
        r = p
        rb= pb
        r (mapping%i(1)) = r2(1)
        rb(mapping%i(1)) = 1 - r2(1)
    end subroutine sf_res_mapping_single_compute

Apply inverse.
<SF mappings: sf resonance single mapping: TBP>+≡
    procedure :: inverse => sf_res_mapping_single_inverse
<SF mappings: sub interfaces>+≡
    module subroutine sf_res_mapping_single_inverse &
        (mapping, r, rb, f, p, pb, x_free)
        class(sf_res_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_res_mapping_single_inverse
<SF mappings: procedures>+≡
    module subroutine sf_res_mapping_single_inverse &
        (mapping, r, rb, f, p, pb, x_free)
        class(sf_res_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(1) :: p2
        real(default) :: fbw
        call map_breit_wigner_inverse &
            (r(mapping%i(1)), fbw, p2(1), mapping%m, mapping%w, x_free)
        p = r
        pb= rb

```



```

    p(mapping%i(1)) = p2(1)
    pb(mapping%i(1)) = 1 - p2(1)
    f = fbw
end subroutine sf_res_mapping_single_inverse

```

16.4.6 Implementation: on-shell mapping

This is a degenerate version of the unit-square mapping where the product $r_1 r_2$ is constant. This product is given by the rescaled squared mass. We introduce an artificial first parameter p_1 to keep the counting, but nothing depends on it. The second parameter is the same p_2 as for the standard unit-square mapping for $\alpha = 1$, it parameterizes the ratio of r_1 and r_2 .

```

<SF mappings: public>+≡
    public :: sf_os_mapping_t

<SF mappings: types>+≡
    type, extends (sf_mapping_t) :: sf_os_mapping_t
        real(default) :: m = 0
        real(default) :: lm2 = 0
    contains
        <SF mappings: sf on-shell mapping: TBP>
    end type sf_os_mapping_t

```

Output.

```

<SF mappings: sf on-shell mapping: TBP>≡
    procedure :: write => sf_os_mapping_write

<SF mappings: sub interfaces>+≡
    module subroutine sf_os_mapping_write (object, unit)
        class(sf_os_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_os_mapping_write

<SF mappings: procedures>+≡
    module subroutine sf_os_mapping_write (object, unit)
        class(sf_os_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',I0,',',',I0,')')", advance="no") object%i
        end if
        write (u, "(A,F7.5,A)" " ": on-shell (" , object%m, ")")
    end subroutine sf_os_mapping_write

```

Initialize: index pair and dimensionless mass parameter.

```

<SF mappings: sf on-shell mapping: TBP>+≡
    procedure :: init => sf_os_mapping_init

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_os_mapping_init (mapping, m)
    class(sf_os_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: m
  end subroutine sf_os_mapping_init

```

```

<SF mappings: procedures>+≡
  module subroutine sf_os_mapping_init (mapping, m)
    class(sf_os_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: m
    call mapping%base_init (2)
    mapping%m = m
    mapping%lm2 = abs (2 * log (mapping%m))
  end subroutine sf_os_mapping_init

```

Apply mapping. The `x_free` parameter rescales the total energy, which must be accounted for in the enclosed mapping.

```

<SF mappings: sf on-shell mapping: TBP>+≡
  procedure :: compute => sf_os_mapping_compute

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_os_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_os_mapping_compute

```

```

<SF mappings: procedures>+≡
  module subroutine sf_os_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, p2
    integer :: j
    p2 = p(mapping%i)
    call map_on_shell (r2, f, p2, mapping%lm2, x_free)
    r = p
    rb = pb
    do j = 1, 2
      r (mapping%i(j)) = r2(j)
      rb(mapping%i(j)) = 1 - r2(j)
    end do
  end subroutine sf_os_mapping_compute

```

Apply inverse. The irrelevant parameter p_1 is always set zero.

```

<SF mappings: sf on-shell mapping: TBP>+≡
  procedure :: inverse => sf_os_mapping_inverse

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_os_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_t), intent(inout) :: mapping

```

```

        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_os_mapping_inverse
<SF mappings: procedures>+≡
module subroutine sf_os_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: p2, r2
    r2 = r(mapping%i)
    call map_on_shell_inverse (r2, f, p2, mapping%lm2, x_free)
    p = r
    pb= rb
    p (mapping%i(1)) = p2(1)
    pb(mapping%i(1)) = 1 - p2(1)
    p (mapping%i(2)) = p2(2)
    pb(mapping%i(2)) = 1 - p2(2)
end subroutine sf_os_mapping_inverse

```

16.4.7 Implementation: on-shell single mapping

This is a degenerate version of the unit-interval mapping where the result r is constant. The value is given by the rescaled squared mass. The input parameter p_1 is actually ignored, nothing depends on it.

```

<SF mappings: public>+≡
    public :: sf_os_mapping_single_t
<SF mappings: types>+≡
type, extends (sf_mapping_t) :: sf_os_mapping_single_t
    real(default) :: m = 0
    real(default) :: lm2 = 0
contains
    <SF mappings: sf on-shell mapping single: TBP>
end type sf_os_mapping_single_t

```

Output.

```

<SF mappings: sf on-shell mapping single: TBP>≡
    procedure :: write => sf_os_mapping_single_write
<SF mappings: sub interfaces>+≡
    module subroutine sf_os_mapping_single_write (object, unit)
        class(sf_os_mapping_single_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_os_mapping_single_write
<SF mappings: procedures>+≡
module subroutine sf_os_mapping_single_write (object, unit)
    class(sf_os_mapping_single_t), intent(in) :: object
    integer, intent(in), optional :: unit

```

```

integer :: u
u = given_output_unit (unit)
write (u, "(1x,A)", advance="no") "map"
if (any (object%i /= 0)) then
    write (u, "('(',I0,')')", advance="no") object%i
end if
write (u, "(A,F7.5,A)" ": on-shell (" , object%m, ")")
end subroutine sf_os_mapping_single_write

```

Initialize: index pair and dimensionless mass parameter.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
    procedure :: init => sf_os_mapping_single_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_os_mapping_single_init (mapping, m)
        class(sf_os_mapping_single_t), intent(out) :: mapping
        real(default), intent(in) :: m
    end subroutine sf_os_mapping_single_init

<SF mappings: procedures>+≡
    module subroutine sf_os_mapping_single_init (mapping, m)
        class(sf_os_mapping_single_t), intent(out) :: mapping
        real(default), intent(in) :: m
        call mapping%base_init (1)
        mapping%m = m
        mapping%lm2 = abs (2 * log (mapping%m))
    end subroutine sf_os_mapping_single_init

```

Apply mapping. The `x_free` parameter rescales the total energy, which must be accounted for in the enclosed mapping.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
    procedure :: compute => sf_os_mapping_single_compute

<SF mappings: sub interfaces>+≡
    module subroutine sf_os_mapping_single_compute &
        (mapping, r, rb, f, p, pb, x_free)
        class(sf_os_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_os_mapping_single_compute

<SF mappings: procedures>+≡
    module subroutine sf_os_mapping_single_compute &
        (mapping, r, rb, f, p, pb, x_free)
        class(sf_os_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(1) :: r2, p2
        integer :: j
        p2 = p(mapping%i)
        call map_on_shell_single (r2, f, p2, mapping%lm2, x_free)

```

```

r = p
rb= pb
r (mapping%i(1)) = r2(1)
rb(mapping%i(1)) = 1 - r2(1)
end subroutine sf_os_mapping_single_compute

```

Apply inverse. The irrelevant parameter p_1 is always set zero.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
  procedure :: inverse => sf_os_mapping_single_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_os_mapping_single_inverse &
    (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_single_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_os_mapping_single_inverse

<SF mappings: procedures>+≡
  module subroutine sf_os_mapping_single_inverse &
    (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_single_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(1) :: p2, r2
    r2 = r(mapping%i)
    call map_on_shell_single_inverse (r2, f, p2, mapping%lm2, x_free)
    p = r
    pb= rb
    p (mapping%i(1)) = p2(1)
    pb(mapping%i(1)) = 1 - p2(1)
  end subroutine sf_os_mapping_single_inverse

```

16.4.8 Implementation: endpoint mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$. The enhancement is such that any power-like singularity is caught. This is useful for beamstrahlung spectra.

In addition, we allow for a delta-function singularity in r_1 and/or r_2 . The singularity is smeared to an interval of width ϵ . If nonzero, we distinguish the kinematical momentum fractions r_i from effective values x_i , which should go into the structure-function evaluation. A bin of width ϵ in r is mapped to $x = 1$ exactly, while the interval $(0, 1 - \epsilon)$ is mapped to $(0, 1)$ in x . The Jacobian reflects this distinction, and the logical `in_peak` allows for an unambiguous distinction.

The delta-peak fraction is used only for the integration self-test.

```

<SF mappings: public>+≡
  public :: sf_ep_mapping_t

```

```

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ep_mapping_t
    real(default) :: a = 1
  contains
    <SF mappings: sf endpoint mapping: TBP>
  end type sf_ep_mapping_t

```

Output.

```

<SF mappings: sf endpoint mapping: TBP>≡
  procedure :: write => sf_ep_mapping_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_ep_mapping_write (object, unit)
    class(sf_ep_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_ep_mapping_write

<SF mappings: procedures>+≡
  module subroutine sf_ep_mapping_write (object, unit)
    class(sf_ep_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,',',IO,')')", advance="no") object%i
    end if
    write (u, "(A,ES12.5,A)") ": endpoint (a =", object%a, ")"
  end subroutine sf_ep_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: init => sf_ep_mapping_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_ep_mapping_init (mapping, a)
    class(sf_ep_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a
  end subroutine sf_ep_mapping_init

<SF mappings: procedures>+≡
  module subroutine sf_ep_mapping_init (mapping, a)
    class(sf_ep_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a
    call mapping%base_init (2)
    if (present (a)) mapping%a = a
  end subroutine sf_ep_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: compute => sf_ep_mapping_compute

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_ep_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_ep_mapping_compute

<SF mappings: procedures>+≡
  module subroutine sf_ep_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, r2
    real(default) :: f1, f2
    integer :: j
    call map_endpoint_1 (px(1), f1, p(mapping%i(1)), mapping%a)
    call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)
    call map_unit_square (r2, f, px)
    f = f * f1 * f2
    r = p
    rb = pb
    do j = 1, 2
      r (mapping%i(j)) = r2(j)
      rb(mapping%i(j)) = 1 - r2(j)
    end do
  end subroutine sf_ep_mapping_compute

```

Apply inverse.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: inverse => sf_ep_mapping_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_ep_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_ep_mapping_inverse

<SF mappings: procedures>+≡
  module subroutine sf_ep_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, px, p2
    real(default) :: f1, f2
    integer :: j
    do j = 1, 2

```

```

        r2(j) = r(mapping%i(j))
    end do
    call map_unit_square_inverse (r2, f, px)
    call map_endpoint_inverse_1 (px(1), f1, p2(1), mapping%a)
    call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
    f = f * f1 * f2
    p = r
    pb= rb
    do j = 1, 2
        p (mapping%i(j)) = p2(j)
        pb(mapping%i(j)) = 1 - p2(j)
    end do
end subroutine sf_ep_mapping_inverse

```

16.4.9 Implementation: endpoint mapping with resonance

Like the endpoint mapping for p_2 , but replace the endpoint mapping by a Breit-Wigner mapping for p_1 . This covers resonance production in the presence of beamstrahlung.

If the flag `resonance` is unset, we skip the resonance mapping, so the parameter p_1 remains equal to $r_1 r_2$, as in the standard s-channel mapping.

```

<SF mappings: public>+≡
    public :: sf_epr_mapping_t

<SF mappings: types>+≡
    type, extends (sf_mapping_t) :: sf_epr_mapping_t
        real(default) :: a = 1
        real(default) :: m = 0
        real(default) :: w = 0
        logical :: resonance = .true.
    contains
        <SF mappings: sf endpoint/res mapping: TBP>
    end type sf_epr_mapping_t

```

Output.

```

<SF mappings: sf endpoint/res mapping: TBP>≡
    procedure :: write => sf_epr_mapping_write

<SF mappings: sub interfaces>+≡
    module subroutine sf_epr_mapping_write (object, unit)
        class(sf_epr_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_epr_mapping_write

<SF mappings: procedures>+≡
    module subroutine sf_epr_mapping_write (object, unit)
        class(sf_epr_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',IO,',',',IO,')')", advance="no") object%i

```



```

end if
if (object%resonance) then
  write (u, "(A,F7.5,A,F7.5,', ',F7.5,A)") ": ep/res (a = ", object%a, &
    " | ", object%m, object%w, ") "
else
  write (u, "(A,F7.5,A)") ": ep/nores (a = ", object%a, ") "
end if
end subroutine sf_epr_mapping_write

```

Initialize: if mass and width are not given, we initialize a non-resonant version of the mapping.

```

<SF mappings: sf endpoint/res mapping: TBP>+≡
  procedure :: init => sf_epr_mapping_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_epr_mapping_init (mapping, a, m, w)
    class(sf_epr_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a
    real(default), intent(in), optional :: m, w
  end subroutine sf_epr_mapping_init

<SF mappings: procedures>+≡
  module subroutine sf_epr_mapping_init (mapping, a, m, w)
    class(sf_epr_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a
    real(default), intent(in), optional :: m, w
    call mapping%base_init (2)
    mapping%a = a
    if (present (m) .and. present (w)) then
      mapping%m = m
      mapping%w = w
    else
      mapping%resonance = .false.
    end if
  end subroutine sf_epr_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint/res mapping: TBP>+≡
  procedure :: compute => sf_epr_mapping_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_epr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_epr_mapping_compute

<SF mappings: procedures>+≡
  module subroutine sf_epr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb

```

```

real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: px, r2
real(default) :: f1, f2
integer :: j
if (mapping%resonance) then
    call map_breit_wigner &
        (px(1), f1, p(mapping%i(1)), mapping%m, mapping%w, x_free)
else
    px(1) = p(mapping%i(1))
    f1 = 1
end if
call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)
call map_unit_square (r2, f, px)
f = f * f1 * f2
r = p
rb= pb
do j = 1, 2
    r (mapping%i(j)) = r2(j)
    rb(mapping%i(j)) = 1 - r2(j)
end do
end subroutine sf_epr_mapping_compute

```

Apply inverse.

<SF mappings: sf endpoint/res mapping: TBP>+≡

```

procedure :: inverse => sf_epr_mapping_inverse

```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_epr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
end subroutine sf_epr_mapping_inverse

```

<SF mappings: procedures>+≡

```

module subroutine sf_epr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, p2
    real(default) :: f1, f2
    integer :: j
    call map_unit_square_inverse (r(mapping%i), f, px)
    if (mapping%resonance) then
        call map_breit_wigner_inverse &
            (px(1), f1, p2(1), mapping%m, mapping%w, x_free)
    else
        p2(1) = px(1)
        f1 = 1
    end if
    call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
    f = f * f1 * f2

```

```

p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = 1 - p2(j)
end do
end subroutine sf_epr_mapping_inverse

```

16.4.10 Implementation: endpoint mapping for on-shell particle

Analogous to the resonance mapping, but the p_1 input is ignored altogether. This covers on-shell particle production in the presence of beamstrahlung.

```

<SF mappings: public>+≡
  public :: sf_epo_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_epo_mapping_t
    real(default) :: a = 1
    real(default) :: m = 0
    real(default) :: lm2 = 0
  contains
    <SF mappings: sf endpoint/os mapping: TBP>
  end type sf_epo_mapping_t

```

Output.

```

<SF mappings: sf endpoint/os mapping: TBP>≡
  procedure :: write => sf_epo_mapping_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_epo_mapping_write (object, unit)
    class(sf_epo_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_epo_mapping_write

<SF mappings: procedures>+≡
  module subroutine sf_epo_mapping_write (object, unit)
    class(sf_epo_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,',',I0,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A,F7.5,A)") ": ep/on-shell (a = ", object%a, &
      " | ", object%m, ") "
  end subroutine sf_epo_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf endpoint/os mapping: TBP>+≡
  procedure :: init => sf_epo_mapping_init

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_epo_mapping_init (mapping, a, m)
    class(sf_epo_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, m
  end subroutine sf_epo_mapping_init

```

```

<SF mappings: procedures>+≡
  module subroutine sf_epo_mapping_init (mapping, a, m)
    class(sf_epo_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, m
    call mapping%base_init (2)
    mapping%a = a
    mapping%m = m
    mapping%lm2 = abs (2 * log (mapping%m))
  end subroutine sf_epo_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint/os mapping: TBP>+≡
  procedure :: compute => sf_epo_mapping_compute

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_epo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_epo_mapping_compute

```

```

<SF mappings: procedures>+≡
  module subroutine sf_epo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, r2
    real(default) :: f2
    integer :: j
    px(1) = 0
    call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)
    call map_on_shell (r2, f, px, mapping%lm2)
    f = f * f2
    r = p
    rb= pb
    do j = 1, 2
      r (mapping%i(j)) = r2(j)
      rb(mapping%i(j)) = 1 - r2(j)
    end do
  end subroutine sf_epo_mapping_compute

```

Apply inverse.

```

<SF mappings: sf endpoint/os mapping: TBP>+≡
  procedure :: inverse => sf_epo_mapping_inverse

```

```

<SF mappings: sub interfaces>+≡
  module subroutine sf_epo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_epo_mapping_inverse

<SF mappings: procedures>+≡
  module subroutine sf_epo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, p2
    real(default) :: f2
    integer :: j
    call map_on_shell_inverse (r(mapping%i), f, px, mapping%lm2)
    p2(1) = 0
    call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
    f = f * f2
    p = r
    pb = rb
    do j = 1, 2
      p (mapping%i(j)) = p2(j)
      pb(mapping%i(j)) = 1 - p2(j)
    end do
  end subroutine sf_epo_mapping_inverse

```

16.4.11 Implementation: ISR endpoint mapping

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

```

<SF mappings: public>+≡
  public :: sf_ip_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ip_mapping_t
    real(default) :: eps = 0
  contains
    <SF mappings: sf power mapping: TBP>
  end type sf_ip_mapping_t

```

Output.

```

<SF mappings: sf power mapping: TBP>≡
  procedure :: write => sf_ip_mapping_write

```

```

<SF mappings: sub interfaces>+≡
    module subroutine sf_ip_mapping_write (object, unit)
        class(sf_ip_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_ip_mapping_write

<SF mappings: procedures>+≡
    module subroutine sf_ip_mapping_write (object, unit)
        class(sf_ip_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',I0,',',I0,')')", advance="no") object%i
        end if
        write (u, "(A,ES12.5,A)" " : isr (eps =", object%eps, ")")
    end subroutine sf_ip_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf power mapping: TBP>+≡
    procedure :: init => sf_ip_mapping_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_ip_mapping_init (mapping, eps)
        class(sf_ip_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: eps
    end subroutine sf_ip_mapping_init

<SF mappings: procedures>+≡
    module subroutine sf_ip_mapping_init (mapping, eps)
        class(sf_ip_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: eps
        call mapping%base_init (2)
        if (present (eps)) mapping%eps = eps
        if (mapping%eps <= 0) &
            call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
    end subroutine sf_ip_mapping_init

```

Apply mapping.

```

<SF mappings: sf power mapping: TBP>+≡
    procedure :: compute => sf_ip_mapping_compute

<SF mappings: sub interfaces>+≡
    module subroutine sf_ip_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_ip_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_ip_mapping_compute

<SF mappings: procedures>+≡
    module subroutine sf_ip_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_ip_mapping_t), intent(inout) :: mapping

```

```

real(default), dimension(:), intent(out) :: r, rb
real(default), intent(out) :: f
real(default), dimension(:), intent(in) :: p, pb
real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: px, pxb, r2, r2b
real(default) :: f1, f2, xb, y, yb
integer :: j
call map_power_1 (xb, f1, pb(mapping%i(1)), 2 * mapping%eps)
call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
px(1) = 1 - xb
pxb(1) = xb
px(2) = y
pxb(2) = yb
call map_unit_square_prec (r2, r2b, f, px, pxb)
f = f * f1 * f2
r = p
rb= pb
do j = 1, 2
    r (mapping%i(j)) = r2 (j)
    rb(mapping%i(j)) = r2b(j)
end do
end subroutine sf_ip_mapping_compute

```

Apply inverse.

<SF mappings: sf power mapping: TBP>+≡

```
procedure :: inverse => sf_ip_mapping_inverse
```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_ip_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ip_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
end subroutine sf_ip_mapping_inverse

```

<SF mappings: procedures>+≡

```

module subroutine sf_ip_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ip_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
    real(default) :: f1, f2, xb, y, yb
    integer :: j
    do j = 1, 2
        r2 (j) = r (mapping%i(j))
        r2b(j) = rb(mapping%i(j))
    end do
    call map_unit_square_inverse_prec (r2, r2b, f, px, pxb)
    xb = pxb(1)
    if (px(1) > 0) then
        y = px(2)
        yb = pxb(2)
    end if

```

```

else
  y = 0.5_default
  yb = 0.5_default
end if
call map_power_inverse_1 (xb, f1, p2b(1), 2 * mapping%eps)
call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
p2 = 1 - p2b
f = f * f1 * f2
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = p2b(j)
end do
end subroutine sf_ip_mapping_inverse

```

16.4.12 Implementation: ISR endpoint mapping, resonant

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

The resonance can be turned off by the flag **resonance**.

```

<SF mappings: public>+≡
  public :: sf_ipr_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ipr_mapping_t
    real(default) :: eps = 0
    real(default) :: m = 0
    real(default) :: w = 0
    logical :: resonance = .true.
  contains
    <SF mappings: sf power/res mapping: TBP>
  end type sf_ipr_mapping_t

```

Output.

```

<SF mappings: sf power/res mapping: TBP>≡
  procedure :: write => sf_ipr_mapping_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_ipr_mapping_write (object, unit)
    class(sf_ipr_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_ipr_mapping_write

<SF mappings: procedures>+≡
  module subroutine sf_ipr_mapping_write (object, unit)
    class(sf_ipr_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u

```



```

u = given_output_unit (unit)
write (u, "(1x,A)", advance="no") "map"
if (any (object%i /= 0)) then
    write (u, "('(',I0,',',',I0,')')", advance="no") object%i
end if
if (object%resonance) then
    write (u, "(A,F7.5,A,F7.5,', ',F7.5,A)") ": isr/res (eps = ", &
        object%eps, " | ", object%m, object%w, ")"
else
    write (u, "(A,F7.5,A)") ": isr/res (eps = ", object%eps, ")"
end if
end subroutine sf_ipr_mapping_write

```

Initialize:

```

<SF mappings: sf power/res mapping: TBP>+≡
    procedure :: init => sf_ipr_mapping_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_ipr_mapping_init (mapping, eps, m, w)
        class(sf_ipr_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: eps, m, w
    end subroutine sf_ipr_mapping_init

<SF mappings: procedures>+≡
    module subroutine sf_ipr_mapping_init (mapping, eps, m, w)
        class(sf_ipr_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: eps, m, w
        call mapping%base_init (2)
        if (present (eps)) mapping%eps = eps
        if (mapping%eps <= 0) &
            call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
        if (present (m) .and. present (w)) then
            mapping%m = m
            mapping%w = w
        else
            mapping%resonance = .false.
        end if
    end subroutine sf_ipr_mapping_init

```

Apply mapping.

```

<SF mappings: sf power/res mapping: TBP>+≡
    procedure :: compute => sf_ipr_mapping_compute

<SF mappings: sub interfaces>+≡
    module subroutine sf_ipr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_ipr_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_ipr_mapping_compute

<SF mappings: procedures>+≡
    module subroutine sf_ipr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_ipr_mapping_t), intent(inout) :: mapping

```

```

real(default), dimension(:), intent(out) :: r, rb
real(default), intent(out) :: f
real(default), dimension(:), intent(in) :: p, pb
real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: px, pxb, r2, r2b
real(default) :: f1, f2, y, yb
integer :: j
if (mapping%resonance) then
    call map_breit_wigner &
        (px(1), f1, p(mapping%i(1)), mapping%m, mapping%w, x_free)
else
    px(1) = p(mapping%i(1))
    f1 = 1
end if
call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
pxb(1) = 1 - px(1)
px(2) = y
pxb(2) = yb
call map_unit_square_prec (r2, r2b, f, px, pxb)
f = f * f1 * f2
r = p
rb= pb
do j = 1, 2
    r (mapping%i(j)) = r2 (j)
    rb(mapping%i(j)) = r2b(j)
end do
end subroutine sf_ipr_mapping_compute

```

Apply inverse.

```

<SF mappings: sf power/res mapping: TBP>+≡
    procedure :: inverse => sf_ipr_mapping_inverse

<SF mappings: sub interfaces>+≡
    module subroutine sf_ipr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
        class(sf_ipr_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_ipr_mapping_inverse

<SF mappings: procedures>+≡
    module subroutine sf_ipr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
        class(sf_ipr_mapping_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
        real(default) :: f1, f2, y, yb
        integer :: j
        do j = 1, 2
            r2 (j) = r (mapping%i(j))
            r2b(j) = rb(mapping%i(j))
        end do
    end subroutine sf_ipr_mapping_inverse

```

```

call map_unit_square_inverse_prec (r2, r2b, f, px, pxb)
if (px(1) > 0) then
  y = px(2)
  yb = pxb(2)
else
  y = 0.5_default
  yb = 0.5_default
end if
if (mapping%resonance) then
  call map_breit_wigner_inverse &
    (px(1), f1, p2(1), mapping%m, mapping%w, x_free)
else
  p2(1) = px(1)
  f1 = 1
end if
call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
p2b(1) = 1 - p2(1)
p2 (2) = 1 - p2b(2)
f = f * f1 * f2
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = p2b(j)
end do
end subroutine sf_ipr_mapping_inverse

```

16.4.13 Implementation: ISR on-shell mapping

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is ignored while the product $r_1 r_2$ is constant. p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

```

<SF mappings: public>+≡
  public :: sf_ipo_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ipo_mapping_t
    real(default) :: eps = 0
    real(default) :: m = 0
  contains
    <SF mappings: sf power/os mapping: TBP>
  end type sf_ipo_mapping_t

```

Output.

```

<SF mappings: sf power/os mapping: TBP>≡
  procedure :: write => sf_ipo_mapping_write

```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_ipo_mapping_write (object, unit)
  class(sf_ipo_mapping_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine sf_ipo_mapping_write

```

<SF mappings: procedures>+≡

```

module subroutine sf_ipo_mapping_write (object, unit)
  class(sf_ipo_mapping_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)", advance="no") "map"
  if (any (object%i /= 0)) then
    write (u, "('(',IO,',',IO,')')", advance="no") object%i
  end if
  write (u, "(A,F7.5,A,F7.5,A)") ": isr/os (eps = ", object%eps, &
    " | ", object%m, ")"
end subroutine sf_ipo_mapping_write

```

Initialize: no extra parameters.

<SF mappings: sf power/os mapping: TBP>+≡

```

procedure :: init => sf_ipo_mapping_init

```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_ipo_mapping_init (mapping, eps, m)
  class(sf_ipo_mapping_t), intent(out) :: mapping
  real(default), intent(in), optional :: eps, m
end subroutine sf_ipo_mapping_init

```

<SF mappings: procedures>+≡

```

module subroutine sf_ipo_mapping_init (mapping, eps, m)
  class(sf_ipo_mapping_t), intent(out) :: mapping
  real(default), intent(in), optional :: eps, m
  call mapping%base_init (2)
  if (present (eps)) mapping%eps = eps
  if (mapping%eps <= 0) &
    call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
  mapping%m = m
end subroutine sf_ipo_mapping_init

```

Apply mapping.

<SF mappings: sf power/os mapping: TBP>+≡

```

procedure :: compute => sf_ipo_mapping_compute

```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_ipo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
  class(sf_ipo_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(out) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(in) :: p, pb
  real(default), intent(inout), optional :: x_free
end subroutine sf_ipo_mapping_compute

```

<SF mappings: procedures>+≡

```

module subroutine sf_ipo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
  class(sf_ipo_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(out) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(in) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: px, pxb, r2, r2b
  real(default) :: f1, f2, y, yb
  integer :: j
  call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
  px(1) = mapping%m ** 2
  if (present (x_free)) px(1) = px(1) / x_free
  pxb(1) = 1 - px(1)
  px(2) = y
  pxb(2) = yb
  call map_unit_square_prec (r2, r2b, f1, px, pxb)
  f = f1 * f2
  r = p
  rb = pb
  do j = 1, 2
    r (mapping%i(j)) = r2 (j)
    rb(mapping%i(j)) = r2b(j)
  end do
end subroutine sf_ipo_mapping_compute

```

Apply inverse.

<SF mappings: sf power/os mapping: TBP>+≡

```

procedure :: inverse => sf_ipo_mapping_inverse

```

<SF mappings: sub interfaces>+≡

```

module subroutine sf_ipo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_ipo_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
end subroutine sf_ipo_mapping_inverse

```

<SF mappings: procedures>+≡

```

module subroutine sf_ipo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_ipo_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
  real(default) :: f1, f2, y, yb
  integer :: j
  do j = 1, 2
    r2 (j) = r (mapping%i(j))
    r2b(j) = rb(mapping%i(j))
  end do
  call map_unit_square_inverse_prec (r2, r2b, f1, px, pxb)
  y = px(2)

```

```

yb = pxb(2)
call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
p2(1) = 0
p2b(1)= 1
p2(2) = 1 - p2b(2)
f = f1 * f2
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = p2b(j)
end do
end subroutine sf_ipo_mapping_inverse

```

16.4.14 Implementation: Endpoint + ISR power mapping

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping. The first two parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively.

```

<SF mappings: public>+≡
  public :: sf_ei_mapping_t
<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ei_mapping_t
    type(sf_ep_mapping_t) :: ep
    type(sf_ip_mapping_t) :: ip
  contains
    <SF mappings: sf ep-ip mapping: TBP>
  end type sf_ei_mapping_t

```

Output.

```

<SF mappings: sf ep-ip mapping: TBP>≡
  procedure :: write => sf_ei_mapping_write
<SF mappings: sub interfaces>+≡
  module subroutine sf_ei_mapping_write (object, unit)
    class(sf_ei_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_ei_mapping_write
<SF mappings: procedures>+≡
  module subroutine sf_ei_mapping_write (object, unit)
    class(sf_ei_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
    end if
    write (u, "(A,ES12.5,A,ES12.5,A)") ": ep/isr (a =", object%ep%a, &
      ", eps =", object%ip%eps, ")"
  end subroutine sf_ei_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: init => sf_ei_mapping_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_ei_mapping_init (mapping, a, eps)
    class(sf_ei_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a, eps
  end subroutine sf_ei_mapping_init

<SF mappings: procedures>+≡
  module subroutine sf_ei_mapping_init (mapping, a, eps)
    class(sf_ei_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a, eps
    call mapping%base_init (4)
    call mapping%ep%init (a)
    call mapping%ip%init (eps)
  end subroutine sf_ei_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: set_index => sf_ei_mapping_set_index

<SF mappings: sub interfaces>+≡
  module subroutine sf_ei_mapping_set_index (mapping, j, i)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
  end subroutine sf_ei_mapping_set_index

<SF mappings: procedures>+≡
  module subroutine sf_ei_mapping_set_index (mapping, j, i)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
    select case (j)
    case (1:2); call mapping%ep%set_index (j, i)
    case (3:4); call mapping%ip%set_index (j-2, i)
    end select
  end subroutine sf_ei_mapping_set_index

```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: compute => sf_ei_mapping_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_ei_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_ei_mapping_compute

```

```

<SF mappings: procedures>+≡
module subroutine sf_ei_mapping_compute (mapping, r, rb, f, p, pb, x_free)
  class(sf_ei_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(out) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(in) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(size(p)) :: q, qb
  real(default) :: f1, f2
  call mapping%ep%compute (q, qb, f1, p, pb, x_free)
  call mapping%ip%compute (r, rb, f2, q, qb, x_free)
  f = f1 * f2
end subroutine sf_ei_mapping_compute

```

Apply inverse.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: inverse => sf_ei_mapping_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_ei_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_ei_mapping_inverse

<SF mappings: procedures>+≡
module subroutine sf_ei_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_ei_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(size(p)) :: q, qb
  real(default) :: f1, f2
  call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
  call mapping%ep%inverse (q, qb, f1, p, pb, x_free)
  f = f1 * f2
end subroutine sf_ei_mapping_inverse

```

16.4.15 Implementation: Endpoint + ISR + resonance

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping, adapted for an s-channel resonance. The first two internal parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively. The first and third parameters are the result of an overall resonance mapping, so on the outside, the first parameter is the total momentum fraction, the third one describes the distribution between beamstrahlung and ISR.

```

<SF mappings: public>+≡
  public :: sf_eir_mapping_t

```



```

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_eir_mapping_t
    type(sf_res_mapping_t) :: res
    type(sf_epr_mapping_t) :: ep
    type(sf_ipr_mapping_t) :: ip
  contains
    <SF mappings: sf ep-ip-res mapping: TBP>
  end type sf_eir_mapping_t

```

Output.

```

<SF mappings: sf ep-ip-res mapping: TBP>≡
  procedure :: write => sf_eir_mapping_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_eir_mapping_write (object, unit)
    class(sf_eir_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_eir_mapping_write

<SF mappings: procedures>+≡
  module subroutine sf_eir_mapping_write (object, unit)
    class(sf_eir_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A,F7.5,A,F7.5,', ',F7.5,A)") &
      ": ep/isr/res (a =", object%ep%a, &
      ", eps =", object%ip%eps, " | ", object%res%m, object%res%w, ") "
  end subroutine sf_eir_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: init => sf_eir_mapping_init

<SF mappings: sub interfaces>+≡
  module subroutine sf_eir_mapping_init (mapping, a, eps, m, w)
    class(sf_eir_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, eps, m, w
  end subroutine sf_eir_mapping_init

<SF mappings: procedures>+≡
  module subroutine sf_eir_mapping_init (mapping, a, eps, m, w)
    class(sf_eir_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, eps, m, w
    call mapping%base_init (4)
    call mapping%res%init (m, w)
    call mapping%ep%init (a)
    call mapping%ip%init (eps)
  end subroutine sf_eir_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: set_index => sf_eir_mapping_set_index

<SF mappings: sub interfaces>+≡
  module subroutine sf_eir_mapping_set_index (mapping, j, i)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
  end subroutine sf_eir_mapping_set_index

<SF mappings: procedures>+≡
  module subroutine sf_eir_mapping_set_index (mapping, j, i)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
    select case (j)
    case (1); call mapping%res%set_index (1, i)
    case (3); call mapping%res%set_index (2, i)
    end select
    select case (j)
    case (1:2); call mapping%ep%set_index (j, i)
    case (3:4); call mapping%ip%set_index (j-2, i)
    end select
  end subroutine sf_eir_mapping_set_index

```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: compute => sf_eir_mapping_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_eir_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_eir_mapping_compute

<SF mappings: procedures>+≡
  module subroutine sf_eir_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%res%compute (px, pxb, f0, p, pb, x_free)
    call mapping%ep%compute (q, qb, f1, px, pxb, x_free)
    call mapping%ip%compute (r, rb, f2, q, qb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eir_mapping_compute

```

Apply inverse.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: inverse => sf_eir_mapping_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_eir_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_eir_mapping_inverse

<SF mappings: procedures>+≡
  module subroutine sf_eir_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
    call mapping%ep%inverse (q, qb, f1, px, pxb, x_free)
    call mapping%res%inverse (px, pxb, f0, p, pb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eir_mapping_inverse

```

16.4.16 Implementation: Endpoint + ISR power mapping, on-shell

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping. The first two parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively. On top of that, we map the first and third parameter such that the product is constant. From the outside, the first parameter is irrelevant while the third parameter describes the distribution of energy (loss) among beamstrahlung and ISR.

```

<SF mappings: public>+≡
  public :: sf_eio_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_eio_mapping_t
    type(sf_os_mapping_t) :: os
    type(sf_epr_mapping_t) :: ep
    type(sf_ipr_mapping_t) :: ip
  contains
    <SF mappings: sf ep-ip-os mapping: TBP>
  end type sf_eio_mapping_t

```

Output.

```

<SF mappings: sf ep-ip-os mapping: TBP>≡
  procedure :: write => sf_eio_mapping_write

```

```

<SF mappings: sub interfaces>+≡
    module subroutine sf_eio_mapping_write (object, unit)
        class(sf_eio_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_eio_mapping_write

<SF mappings: procedures>+≡
    module subroutine sf_eio_mapping_write (object, unit)
        class(sf_eio_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
        end if
        write (u, "(A,F7.5,A,F7.5,A,F7.5,A)") ": ep/isr/os (a =", object%ep%a, &
            ", eps =", object%ip%eps, " | ", object%os%m, ")"
    end subroutine sf_eio_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
    procedure :: init => sf_eio_mapping_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_eio_mapping_init (mapping, a, eps, m)
        class(sf_eio_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: a, eps, m
    end subroutine sf_eio_mapping_init

<SF mappings: procedures>+≡
    module subroutine sf_eio_mapping_init (mapping, a, eps, m)
        class(sf_eio_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: a, eps, m
        call mapping%base_init (4)
        call mapping%os%init (m)
        call mapping%ep%init (a)
        call mapping%ip%init (eps)
    end subroutine sf_eio_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
    procedure :: set_index => sf_eio_mapping_set_index

<SF mappings: sub interfaces>+≡
    module subroutine sf_eio_mapping_set_index (mapping, j, i)
        class(sf_eio_mapping_t), intent(inout) :: mapping
        integer, intent(in) :: j, i
    end subroutine sf_eio_mapping_set_index

<SF mappings: procedures>+≡
    module subroutine sf_eio_mapping_set_index (mapping, j, i)
        class(sf_eio_mapping_t), intent(inout) :: mapping
        integer, intent(in) :: j, i
    end subroutine sf_eio_mapping_set_index

```

```

mapping%i(j) = i
select case (j)
case (1); call mapping%os%set_index (1, i)
case (3); call mapping%os%set_index (2, i)
end select
select case (j)
case (1:2); call mapping%ep%set_index (j, i)
case (3:4); call mapping%ip%set_index (j-2, i)
end select
end subroutine sf_eio_mapping_set_index

```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
  procedure :: compute => sf_eio_mapping_compute

<SF mappings: sub interfaces>+≡
  module subroutine sf_eio_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_eio_mapping_compute

<SF mappings: procedures>+≡
  module subroutine sf_eio_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%os%compute (px, pxb, f0, p, pb, x_free)
    call mapping%ep%compute (q, qb, f1, px, pxb, x_free)
    call mapping%ip%compute (r, rb, f2, q, qb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eio_mapping_compute

```

Apply inverse.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
  procedure :: inverse => sf_eio_mapping_inverse

<SF mappings: sub interfaces>+≡
  module subroutine sf_eio_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_eio_mapping_inverse

```

<SF mappings: procedures>+≡

```

module subroutine sf_eio_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_eio_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(size(p)) :: px, pxb, q, qb
  real(default) :: f0, f1, f2
  call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
  call mapping%ep%inverse (q, qb, f1, px, pxb, x_free)
  call mapping%os%inverse (px, pxb, f0, p, pb, x_free)
  f = f0 * f1 * f2
end subroutine sf_eio_mapping_inverse

```

16.4.17 Basic formulas

Standard mapping of the unit square

This mapping of the unit square is appropriate in particular for structure functions which are concentrated at the lower end. Instead of a rectangular grid, one set of grid lines corresponds to constant parton c.m. energy. The other set is chosen such that the jacobian is only mildly singular ($\ln x$ which is zero at $x = 1$), corresponding to an initial concentration of sampling points at the maximum energy. If **power** is greater than one (the default), points are also concentrated at the lower end.

The formula is (**power**= α):

$$r_1 = (p_1^{p_2})^\alpha \quad (16.15)$$

$$r_2 = (p_1^{1-p_2})^\alpha \quad (16.16)$$

$$f = \alpha^2 p_1^{\alpha-1} |\log p_1| \quad (16.17)$$

and for the default case $\alpha = 1$:

$$r_1 = p_1^{p_2} \quad (16.18)$$

$$r_2 = p_1^{1-p_2} \quad (16.19)$$

$$f = |\log p_1| \quad (16.20)$$

<SF mappings: procedures>+≡

```

subroutine map_unit_square (r, factor, p, power)
  real(default), dimension(2), intent(out) :: r
  real(default), intent(out) :: factor
  real(default), dimension(2), intent(in) :: p
  real(default), intent(in), optional :: power
  real(default) :: xx, yy
  factor = 1
  xx = p(1)
  yy = p(2)
  if (present(power)) then
    if (p(1) > 0 .and. power > 1) then
      xx = p(1)**power
    end if
  end if

```

```

        factor = factor * power * xx / p(1)
    end if
end if
if (.not. vanishes (xx)) then
    r(1) = xx ** yy
    r(2) = xx / r(1)
    factor = factor * abs (log (xx))
else
    r = 0
end if
end subroutine map_unit_square

```

This is the inverse mapping.

(SF mappings: procedures)+≡

```

subroutine map_unit_square_inverse (r, factor, p, power)
    real(kind=default), dimension(2), intent(in) :: r
    real(kind=default), intent(out) :: factor
    real(kind=default), dimension(2), intent(out) :: p
    real(kind=default), intent(in), optional :: power
    real(kind=default) :: lg, xx, yy
    factor = 1
    xx = r(1) * r(2)
    if (.not. vanishes (xx)) then
        lg = log (xx)
        if (.not. vanishes (lg)) then
            yy = log (r(1)) / lg
        else
            yy = 0
        end if
        p(2) = yy
        factor = factor * abs (lg)
        if (present(power)) then
            p(1) = xx**(1._default/power)
            factor = factor * power * xx / p(1)
        else
            p(1) = xx
        end if
    else
        p = 0
    end if
end subroutine map_unit_square_inverse

```

Precise mapping of the unit square

A more precise version (with unit power parameter). This version should be numerically stable near $x = 1$ and $y = 0, 1$. The formulas are again

$$r_1 = p_1^{p_2}, \quad r_2 = p_1^{\bar{p}_2}, \quad f = -\log p_1 \quad (16.21)$$

but we compute both r_i and \bar{r}_i simultaneously and make direct use of both p_i and \bar{p}_i as appropriate.

(SF mappings: procedures)+≡

```

subroutine map_unit_square_prec (r, rb, factor, p, pb)
  real(default), dimension(2), intent(out) :: r
  real(default), dimension(2), intent(out) :: rb
  real(default), intent(out) :: factor
  real(default), dimension(2), intent(in) :: p
  real(default), dimension(2), intent(in) :: pb
  if (p(1) > 0.5_default) then
    call compute_prec_xy_1 (r(1), rb(1), p(1), pb(1), p (2))
    call compute_prec_xy_1 (r(2), rb(2), p(1), pb(1), pb(2))
    factor = - log_prec (p(1), pb(1))
  else if (.not. vanishes (p(1))) then
    call compute_prec_xy_0 (r(1), rb(1), p(1), pb(1), p (2))
    call compute_prec_xy_0 (r(2), rb(2), p(1), pb(1), pb(2))
    factor = - log_prec (p(1), pb(1))
  else
    r  = 0
    rb = 1
    factor = 0
  end if
end subroutine map_unit_square_prec

```

This is the inverse mapping.

(SF mappings: procedures)+≡

```

subroutine map_unit_square_inverse_prec (r, rb, factor, p, pb)
  real(default), dimension(2), intent(in) :: r
  real(default), dimension(2), intent(in) :: rb
  real(default), intent(out) :: factor
  real(default), dimension(2), intent(out) :: p
  real(default), dimension(2), intent(out) :: pb
  call inverse_prec_x (r, rb, p(1), pb(1))
  if (all (r > 0)) then
    if (rb(1) < rb(2)) then
      call inverse_prec_y (r, rb, p(2), pb(2))
    else
      call inverse_prec_y ([r(2),r(1)], [rb(2),rb(1)], pb(2), p(2))
    end if
    factor = - log_prec (p(1), pb(1))
  else
    p(1) = 0
    pb(1) = 1
    p(2) = 0.5_default
    pb(2) = 0.5_default
    factor = 0
  end if
end subroutine map_unit_square_inverse_prec

```

This is an auxiliary function: evaluate the expression $\bar{z} = 1 - x^y$ in a numerically stable way. Instabilities occur for $y = 0$ and $x = 1$. The idea is to replace the bracket by the first terms of its Taylor expansion around $x = 1$ (read $\bar{x} \equiv 1 - x$)

$$1 - x^y = y\bar{x} \left(1 + \frac{1}{2}(1-y)\bar{x} + \frac{1}{6}(2-y)(1-y)\bar{x}^2 \right) \quad (16.22)$$

whenever this is the better approximation. Actually, the relative numerical

error of the exact formula is about $\eta/(y\bar{x})$ where η is given by `epsilon(KIND)` in Fortran. The relative error of the approximation is better than the last included term divided by $(y\bar{x})$.

The first subroutine computes z and \bar{z} near $x = 1$ where $\log x$ should be expanded, the second one near $x = 0$ where $\log x$ can be kept.

```

(SF mappings: procedures)+≡
subroutine compute_prec_xy_1 (z, zb, x, xb, y)
  real(default), intent(out) :: z, zb
  real(default), intent(in) :: x, xb, y
  real(default) :: a1, a2, a3
  a1 = y * xb
  a2 = a1 * (1 - y) * xb / 2
  a3 = a2 * (2 - y) * xb / 3
  if (abs (a3) < epsilon (a3)) then
    zb = a1 + a2 + a3
    z = 1 - zb
  else
    z = x ** y
    zb = 1 - z
  end if
end subroutine compute_prec_xy_1

subroutine compute_prec_xy_0 (z, zb, x, xb, y)
  real(default), intent(out) :: z, zb
  real(default), intent(in) :: x, xb, y
  real(default) :: a1, a2, a3, lx
  lx = -log (x)
  a1 = y * lx
  a2 = a1 * y * lx / 2
  a3 = a2 * y * lx / 3
  if (abs (a3) < epsilon (a3)) then
    zb = a1 + a2 + a3
    z = 1 - zb
  else
    z = x ** y
    zb = 1 - z
  end if
end subroutine compute_prec_xy_0

```

For the inverse calculation, we evaluate $x = r_1 r_2$ in a stable way. Since it is just a polynomial, the expansion near $x = 1$ is analytically exact, and we don't need to choose based on precision.

Fixed WK 2023-02-21: case selection (a0 check) was flipped. Note that the first case applies to small rb , i.e., to x near 1.

```

(SF mappings: procedures)+≡
subroutine inverse_prec_x (r, rb, x, xb)
  real(default), dimension(2), intent(in) :: r, rb
  real(default), intent(out) :: x, xb
  real(default) :: a0, a1
  a0 = rb(1) + rb(2)
  a1 = rb(1) * rb(2)
  if (a0 < 0.5_default) then
    xb = a0 - a1

```

```

      x = 1 - xb
    else
      x = r(1) * r(2)
      xb = 1 - x
    end if
  end subroutine inverse_prec_x

```

The inverse calculation for the relative momentum fraction

$$y = \frac{1}{1 + \frac{\log r_2}{\log r_1}} \quad (16.23)$$

is slightly more complicated. We should take the precise form of the logarithm, so we are safe near $r_i = 1$. A series expansion is required if $r_1 \ll r_2$, since then y becomes small. (We assume $r_1 < r_2$ here; for the opposite case, the arguments can be exchanged.)

Fixed WK 2023-02-21: removed special casing for either log near zero within the first branch. (y or yb was set to zero.) In some application (ISR peak mapping with resonance nearby) that apparent safeguard turned out to be fatal.

(SF mappings: procedures)+≡

```

subroutine inverse_prec_y (r, rb, y, yb)
  real(default), dimension(2), intent(in) :: r, rb
  real(default), intent(out) :: y, yb
  real(default) :: log1, log2, a1, a2, a3
  log1 = log_prec (r(1), rb(1))
  log2 = log_prec (r(2), rb(2))
  if (abs (log2**3) < epsilon (one)) then
    y = one / (one + log2 / log1)
    yb = one / (one + log1 / log2)
  else
    a1 = - rb(1) / log2
    a2 = - rb(1) ** 2 * (one / log2**2 + one / (2 * log2))
    a3 = - rb(1) ** 3 * (one / log2**3 + one / log2**2 + one/(3 * log2))
    if (abs (a3) < epsilon (a3)) then
      y = a1 + a2 + a3
      yb = one - y
    else
      y = one / (one + log2 / log1)
      yb = one / (one + log1 / log2)
    end if
  end if
end subroutine inverse_prec_y

```

Mapping for on-shell s-channel

The limiting case, if the product $r_1 r_2$ is fixed for on-shell production. The parameter p_1 is ignored. In the inverse mapping, it is returned zero.

The parameter `x_free`, if present, rescales the total energy. If it is less than one, the rescaled mass parameter m^2 should be increased accordingly.

Public for access in unit test.

(SF mappings: public)+≡

```

public :: map_on_shell
public :: map_on_shell_inverse

<SF mappings: sub interfaces>+=
  module subroutine map_on_shell (r, factor, p, lm2, x_free)
    real(default), dimension(2), intent(out) :: r
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(in) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
  end subroutine map_on_shell
  module subroutine map_on_shell_inverse (r, factor, p, lm2, x_free)
    real(default), dimension(2), intent(in) :: r
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(out) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
  end subroutine map_on_shell_inverse

<SF mappings: procedures>+=
  module subroutine map_on_shell (r, factor, p, lm2, x_free)
    real(default), dimension(2), intent(out) :: r
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(in) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
    real(default) :: lx
    lx = lm2; if (present (x_free)) lx = lx + log (x_free)
    r(1) = exp (- p(2) * lx)
    r(2) = exp (- (1 - p(2)) * lx)
    factor = lx
  end subroutine map_on_shell

  module subroutine map_on_shell_inverse (r, factor, p, lm2, x_free)
    real(default), dimension(2), intent(in) :: r
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(out) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
    real(default) :: lx
    lx = lm2; if (present (x_free)) lx = lx + log (x_free)
    p(1) = 0
    p(2) = abs (log (r(1))) / lx
    factor = lx
  end subroutine map_on_shell_inverse

```

Mapping for on-shell s-channel, single parameter

This is a pseudo-mapping which applies if there is actually just one parameter p . The output parameter r is fixed for on-shell production. The lone parameter p_1 is ignored. In the inverse mapping, it is returned zero.

The parameter x_free , if present, rescales the total energy. If it is less than one, the rescaled mass parameter m^2 should be increased accordingly.

Public for access in unit test.

```

<SF mappings: public>+≡
  public :: map_on_shell_single
  public :: map_on_shell_single_inverse

<SF mappings: sub interfaces>+≡
  module subroutine map_on_shell_single (r, factor, p, lm2, x_free)
    real(default), dimension(1), intent(out) :: r
    real(default), intent(out) :: factor
    real(default), dimension(1), intent(in) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
  end subroutine map_on_shell_single
  module subroutine map_on_shell_single_inverse (r, factor, p, lm2, x_free)
    real(default), dimension(1), intent(in) :: r
    real(default), intent(out) :: factor
    real(default), dimension(1), intent(out) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
  end subroutine map_on_shell_single_inverse

<SF mappings: procedures>+≡
  module subroutine map_on_shell_single (r, factor, p, lm2, x_free)
    real(default), dimension(1), intent(out) :: r
    real(default), intent(out) :: factor
    real(default), dimension(1), intent(in) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
    real(default) :: lx
    lx = lm2; if (present (x_free)) lx = lx + log (x_free)
    r(1) = exp (- lx)
    factor = 1
  end subroutine map_on_shell_single

  module subroutine map_on_shell_single_inverse (r, factor, p, lm2, x_free)
    real(default), dimension(1), intent(in) :: r
    real(default), intent(out) :: factor
    real(default), dimension(1), intent(out) :: p
    real(default), intent(in) :: lm2
    real(default), intent(in), optional :: x_free
    real(default) :: lx
    lx = lm2; if (present (x_free)) lx = lx + log (x_free)
    p(1) = 0
    factor = 1
  end subroutine map_on_shell_single_inverse

```

Mapping for a Breit-Wigner resonance

This is the standard Breit-Wigner mapping. We apply it to a single variable, independently of or in addition to a unit-square mapping. We assume here that the limits for the variable are 0 and 1, and that the mass m and width w are rescaled appropriately, so they are dimensionless and usually between 0 and 1.

If `x_free` is set, it rescales the total energy and thus mass and width, since these are defined with respect to the total energy.

(SF mappings: procedures) +≡

```

subroutine map_breit_wigner (r, factor, p, m, w, x_free)
  real(default), intent(out) :: r
  real(default), intent(out) :: factor
  real(default), intent(in)  :: p
  real(default), intent(in)  :: m
  real(default), intent(in)  :: w
  real(default), intent(in), optional :: x_free
  real(default) :: m2, mw, a1, a2, a3, z, tmp
  m2 = m ** 2
  mw = m * w
  if (present (x_free)) then
    m2 = m2 / x_free
    mw = mw / x_free
  end if
  a1 = atan (- m2 / mw)
  a2 = atan ((1 - m2) / mw)
  a3 = (a2 - a1) * mw
  z = (1-p) * a1 + p * a2
  if (-pi/2 < z .and. z < pi/2) then
    tmp = tan (z)
    r = max (m2 + mw * tmp, 0._default)
    factor = a3 * (1 + tmp ** 2)
  else
    r = 0
    factor = 0
  end if
end subroutine map_breit_wigner

subroutine map_breit_wigner_inverse (r, factor, p, m, w, x_free)
  real(default), intent(in)  :: r
  real(default), intent(out) :: factor
  real(default), intent(out) :: p
  real(default), intent(in)  :: m
  real(default), intent(in)  :: w
  real(default) :: m2, mw, a1, a2, a3, tmp
  real(default), intent(in), optional :: x_free
  m2 = m ** 2
  mw = m * w
  if (present (x_free)) then
    m2 = m2 / x_free
    mw = mw / x_free
  end if
  a1 = atan (- m2 / mw)
  a2 = atan ((1 - m2) / mw)
  a3 = (a2 - a1) * mw
  tmp = (r - m2) / mw
  p = (atan (tmp) - a1) / (a2 - a1)
  factor = a3 * (1 + tmp ** 2)
end subroutine map_breit_wigner_inverse

```

Mapping with endpoint enhancement

This is a mapping which is close to the unit mapping, except that at the endpoint(s), the output values are exponentially enhanced.

$$y = \tanh(a \tan(\frac{\pi}{2}x)) \quad (16.24)$$

We have two variants: one covers endpoints at 0 and 1 symmetrically, while the other one (which essentially maps one-half of the range), covers only the endpoint at 1.

(SF mappings: procedures)+≡

```
subroutine map_endpoint_1 (x3, factor, x1, a)
  real(default), intent(out) :: x3, factor
  real(default), intent(in) :: x1
  real(default), intent(in) :: a
  real(default) :: x2
  if (abs (x1) < 1) then
    x2 = tan (x1 * pi / 2)
    x3 = tanh (a * x2)
    factor = a * pi/2 * (1 + x2 ** 2) * (1 - x3 ** 2)
  else
    x3 = x1
    factor = 0
  end if
end subroutine map_endpoint_1

subroutine map_endpoint_inverse_1 (x3, factor, x1, a)
  real(default), intent(in) :: x3
  real(default), intent(out) :: x1, factor
  real(default), intent(in) :: a
  real(default) :: x2
  if (abs (x3) < 1) then
    x2 = atanh (x3) / a
    x1 = 2 / pi * atan (x2)
    factor = a * pi/2 * (1 + x2 ** 2) * (1 - x3 ** 2)
  else
    x1 = x3
    factor = 0
  end if
end subroutine map_endpoint_inverse_1

subroutine map_endpoint_01 (x4, factor, x0, a)
  real(default), intent(out) :: x4, factor
  real(default), intent(in) :: x0
  real(default), intent(in) :: a
  real(default) :: x1, x3
  x1 = 2 * x0 - 1
  call map_endpoint_1 (x3, factor, x1, a)
  x4 = (x3 + 1) / 2
end subroutine map_endpoint_01

subroutine map_endpoint_inverse_01 (x4, factor, x0, a)
  real(default), intent(in) :: x4
  real(default), intent(out) :: x0, factor
```

```

real(default), intent(in) :: a
real(default) :: x1, x3
x3 = 2 * x4 - 1
call map_endpoint_inverse_1 (x3, factor, x1, a)
x0 = (x1 + 1) / 2
end subroutine map_endpoint_inverse_01

```

Mapping with endpoint enhancement (ISR)

This is another endpoint mapping. It is designed to flatten the ISR singularity which is of power type at $x = 1$, i.e., if

$$\sigma = \int_0^1 dx f(x) G(x) = \int_0^1 dx \epsilon (1-x)^{-1+\epsilon} G(x), \quad (16.25)$$

we replace this by

$$r = x^\epsilon \implies \sigma = \int_0^1 dr G(1 - (1-r)^{1/\epsilon}). \quad (16.26)$$

We expect that ϵ is small.

The actual mapping is $r \rightarrow x$ (so x emerges closer to 1). The Jacobian that we return is thus $1/f(x)$. We compute the mapping in terms of $\bar{x} \equiv 1 - x$, so we can achieve the required precision. Because some compilers show quite wild numeric fluctuations, we internally convert numeric types to explicit `double` precision.

```

<SF mappings: public>+≡
  public :: map_power_1
  public :: map_power_inverse_1

<SF mappings: sub interfaces>+≡
  module subroutine map_power_1 (xb, factor, rb, eps)
    real(default), intent(out) :: xb, factor
    real(default), intent(in) :: rb
    real(default), intent(in) :: eps
  end subroutine map_power_1
  module subroutine map_power_inverse_1 (xb, factor, rb, eps)
    real(default), intent(in) :: xb
    real(default), intent(out) :: rb, factor
    real(default), intent(in) :: eps
  end subroutine map_power_inverse_1

<SF mappings: procedures>+≡
  module subroutine map_power_1 (xb, factor, rb, eps)
    real(default), intent(out) :: xb, factor
    real(default), intent(in) :: rb
    real(double) :: rb_db, factor_db, eps_db, xb_db
    real(default), intent(in) :: eps
    rb_db = real (rb, kind=double)
    eps_db = real (eps, kind=double)
    xb_db = rb_db ** (1 / eps_db)
    if (rb_db > 0) then
      factor_db = xb_db / rb_db / eps_db
    end if
  end subroutine map_power_1

```

```

        factor = real (factor_db, kind=default)
    else
        factor = 0
    end if
    xb = real (xb_db, kind=default)
end subroutine map_power_1

module subroutine map_power_inverse_1 (xb, factor, rb, eps)
    real(default), intent(in) :: xb
    real(default), intent(out) :: rb, factor
    real(double) :: xb_db, factor_db, eps_db, rb_db
    real(default), intent(in) :: eps
    xb_db = real (xb, kind=double)
    eps_db = real (eps, kind=double)
    rb_db = xb_db ** eps_db
    if (xb_db > 0) then
        factor_db = xb_db / rb_db / eps_db
        factor = real (factor_db, kind=default)
    else
        factor = 0
    end if
    rb = real (rb_db, kind=default)
end subroutine map_power_inverse_1

```

Here we apply a power mapping to both endpoints. We divide the interval in two equal halves and apply the power mapping for the nearest endpoint, either 0 or 1.

(SF mappings: procedures)+≡

```

subroutine map_power_01 (y, yb, factor, r, eps)
    real(default), intent(out) :: y, yb, factor
    real(default), intent(in) :: r
    real(default), intent(in) :: eps
    real(default) :: u, ub, zp, zm
    u = 2 * r - 1
    if (u > 0) then
        ub = 2 * (1 - r)
        call map_power_1 (zm, factor, ub, eps)
        zp = 2 - zm
    else if (u < 0) then
        ub = 2 * r
        call map_power_1 (zp, factor, ub, eps)
        zm = 2 - zp
    else
        factor = 1 / eps
        zp = 1
        zm = 1
    end if
    y = zp / 2
    yb = zm / 2
end subroutine map_power_01

subroutine map_power_inverse_01 (y, yb, factor, r, eps)
    real(default), intent(in) :: y, yb

```



```

real(default), intent(out) :: r, factor
real(default), intent(in) :: eps
real(default) :: ub, zp, zm
zp = 2 * y
zm = 2 * yb
if (zm < zp) then
    call map_power_inverse_1 (zm, factor, ub, eps)
    r = 1 - ub / 2
else if (zp < zm) then
    call map_power_inverse_1 (zp, factor, ub, eps)
    r = ub / 2
else
    factor = 1 / eps
    ub = 1
    r = ub / 2
end if
end subroutine map_power_inverse_01

```

Structure-function channels

A structure-function chain parameterization (channel) may contain a mapping that applies to multiple structure functions. This is described by an extension of the `sf_mapping_t` type. In addition, it may contain mappings that apply to (other) individual structure functions. The details of these mappings are implementation-specific.

The `sf_channel_t` type combines this information. It contains an array of map codes, one for each structure-function entry. The code values are:

none MC input parameters r directly become energy fractions x

single default mapping for a single structure-function entry

multi/s map $r \rightarrow x$ such that one MC input parameter is \hat{s}/s

multi/resonance as before, adapted to s-channel resonance

multi/on-shell as before, adapted to an on-shell particle in the s channel

multi/endpoint like multi/s, but enhance the region near $r_i = 1$

multi/endpoint/res endpoint mapping with resonance

multi/endpoint/os endpoint mapping for on-shell

multi/power/os like multi/endpoint, regulating a power singularity

$\langle SF \text{ mappings: parameters} \rangle \equiv$

```

integer, parameter :: SFMAP_NONE = 0
integer, parameter :: SFMAP_SINGLE = 1
integer, parameter :: SFMAP_MULTI_S = 2
integer, parameter :: SFMAP_MULTI_RES = 3
integer, parameter :: SFMAP_MULTI_ONS = 4
integer, parameter :: SFMAP_MULTI_EP = 5
integer, parameter :: SFMAP_MULTI_EPR = 6

```

```

integer, parameter :: SFMAP_MULTI_EPO = 7
integer, parameter :: SFMAP_MULTI_IP = 8
integer, parameter :: SFMAP_MULTI_IPR = 9
integer, parameter :: SFMAP_MULTI_IPO = 10
integer, parameter :: SFMAP_MULTI_EI = 11
integer, parameter :: SFMAP_MULTI_SRS = 13
integer, parameter :: SFMAP_MULTI_SON = 14

```

Then, it contains an allocatable entry for the multi mapping. This entry holds the MC-parameter indices on which the mapping applies (there may be more than one MC parameter per structure-function entry) and any parameters associated with the mapping.

There can be only one multi-mapping per channel.

```

<SF mappings: public>+≡
  public :: sf_channel_t

<SF mappings: types>+≡
  type :: sf_channel_t
    integer, dimension(:), allocatable :: map_code
    class(sf_mapping_t), allocatable :: multi_mapping
    contains
    <SF mappings: sf channel: TBP>
  end type sf_channel_t

```

The output format prints a single character for each structure-function entry and, if applicable, an account of the mapping parameters.

```

<SF mappings: sf channel: TBP>≡
  procedure :: write => sf_channel_write

<SF mappings: sub interfaces>+≡
  module subroutine sf_channel_write (object, unit)
    class(sf_channel_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine sf_channel_write

<SF mappings: procedures>+≡
  module subroutine sf_channel_write (object, unit)
    class(sf_channel_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    if (allocated (object%map_code)) then
      do i = 1, size (object%map_code)
        select case (object%map_code (i))
          case (SFMAP_NONE)
            write (u, "(1x,A)", advance="no") "-"
          case (SFMAP_SINGLE)
            write (u, "(1x,A)", advance="no") "+"
          case (SFMAP_MULTI_S)
            write (u, "(1x,A)", advance="no") "s"
          case (SFMAP_MULTI_RES, SFMAP_MULTI_SRS)
            write (u, "(1x,A)", advance="no") "r"
          case (SFMAP_MULTI_ONS, SFMAP_MULTI_SON)
            write (u, "(1x,A)", advance="no") "o"

```

```

        case (SFMAP_MULTI_EP)
            write (u, "(1x,A)", advance="no") "e"
        case (SFMAP_MULTI_EPR)
            write (u, "(1x,A)", advance="no") "p"
        case (SFMAP_MULTI_EPO)
            write (u, "(1x,A)", advance="no") "q"
        case (SFMAP_MULTI_IP)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_IPR)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_IPO)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_EI)
            write (u, "(1x,A)", advance="no") "i"
        case default
            write (u, "(1x,A)", advance="no") "?"
        end select
    end do
else
    write (u, "(1x,A)", advance="no") "-"
end if
if (allocated (object%multi_mapping)) then
    write (u, "(1x,'/')" , advance="no")
    call object%multi_mapping%write (u)
else
    write (u, *)
end if
end if
end subroutine sf_channel_write

```

Initializer for a single `sf_channel` object.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: init => sf_channel_init

<SF mappings: sub interfaces>+≡
    module subroutine sf_channel_init (channel, n_strfun)
        class(sf_channel_t), intent(out) :: channel
        integer, intent(in) :: n_strfun
    end subroutine sf_channel_init

<SF mappings: procedures>+≡
    module subroutine sf_channel_init (channel, n_strfun)
        class(sf_channel_t), intent(out) :: channel
        integer, intent(in) :: n_strfun
        allocate (channel%map_code (n_strfun))
        channel%map_code = SFMAP_NONE
    end subroutine sf_channel_init

```

Assignment. This merely copies intrinsic assignment.

```

<SF mappings: sf channel: TBP>+≡
    generic :: assignment (=) => sf_channel_assign
    procedure :: sf_channel_assign

<SF mappings: sub interfaces>+≡
    module subroutine sf_channel_assign (copy, original)

```

```

        class(sf_channel_t), intent(out) :: copy
        type(sf_channel_t), intent(in) :: original
    end subroutine sf_channel_assign
<SF mappings: procedures>+≡
module subroutine sf_channel_assign (copy, original)
    class(sf_channel_t), intent(out) :: copy
    type(sf_channel_t), intent(in) :: original
    allocate (copy%map_code (size (original%map_code)))
    copy%map_code = original%map_code
    if (allocated (original%multi_mapping)) then
        allocate (copy%multi_mapping, source = original%multi_mapping)
    end if
end subroutine sf_channel_assign

```

This initializer allocates an array of channels with common number of structure-function entries, therefore it is not a type-bound procedure.

```

<SF mappings: public>+≡
    public :: allocate_sf_channels
<SF mappings: sub interfaces>+≡
    module subroutine allocate_sf_channels (channel, n_channel, n_strfun)
        type(sf_channel_t), dimension(:), intent(out), allocatable :: channel
        integer, intent(in) :: n_channel
        integer, intent(in) :: n_strfun
    end subroutine allocate_sf_channels
<SF mappings: procedures>+≡
module subroutine allocate_sf_channels (channel, n_channel, n_strfun)
    type(sf_channel_t), dimension(:), intent(out), allocatable :: channel
    integer, intent(in) :: n_channel
    integer, intent(in) :: n_strfun
    integer :: c
    allocate (channel (n_channel))
    do c = 1, n_channel
        call channel(c)%init (n_strfun)
    end do
end subroutine allocate_sf_channels

```

This marks a given subset of indices as single-mapping.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: activate_mapping => sf_channel_activate_mapping
<SF mappings: sub interfaces>+≡
    module subroutine sf_channel_activate_mapping (channel, i_sf)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
    end subroutine sf_channel_activate_mapping
<SF mappings: procedures>+≡
module subroutine sf_channel_activate_mapping (channel, i_sf)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    channel%map_code(i_sf) = SFMAP_SINGLE
end subroutine sf_channel_activate_mapping

```

This sets an s-channel multichannel mapping. The parameter indices are not yet set. Gfortran 7/8/9 bug, has to remain in module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_s_mapping => sf_channel_set_s_mapping

<SF mappings: main procedures>≡
  subroutine sf_channel_set_s_mapping (channel, i_sf, power)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in), optional :: power
    channel%map_code(i_sf) = SFMAP_MULTI_S
    allocate (sf_s_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
      type is (sf_s_mapping_t)
        call mapping%init (power)
      end select
  end subroutine sf_channel_set_s_mapping

```

This sets an s-channel resonance multichannel mapping. Gfortran 7/8/9 bug, has to remain in module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_res_mapping => sf_channel_set_res_mapping

<SF mappings: main procedures>+≡
  subroutine sf_channel_set_res_mapping (channel, i_sf, m, w, single)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in) :: m, w
    logical, intent(in) :: single
    if (single) then
      channel%map_code(i_sf) = SFMAP_MULTI_SRS
      allocate (sf_res_mapping_single_t :: channel%multi_mapping)
      select type (mapping => channel%multi_mapping)
        type is (sf_res_mapping_single_t)
          call mapping%init (m, w)
        end select
    else
      channel%map_code(i_sf) = SFMAP_MULTI_RES
      allocate (sf_res_mapping_t :: channel%multi_mapping)
      select type (mapping => channel%multi_mapping)
        type is (sf_res_mapping_t)
          call mapping%init (m, w)
        end select
    end if
  end subroutine sf_channel_set_res_mapping

```

This sets an s-channel on-shell multichannel mapping. The length of the i_sf array must be 2. (The first parameter actually becomes an irrelevant dummy.) Gfortran 7/8/9 bug, has to remain in module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_os_mapping => sf_channel_set_os_mapping

```

```

<SF mappings: main procedures>+≡
subroutine sf_channel_set_os_mapping (channel, i_sf, m, single)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in) :: m
  logical, intent(in) :: single
  if (single) then
    channel%map_code(i_sf) = SFMAP_MULTI_SON
    allocate (sf_os_mapping_single_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_os_mapping_single_t)
      call mapping%init (m)
    end select
  else
    channel%map_code(i_sf) = SFMAP_MULTI_ONS
    allocate (sf_os_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_os_mapping_t)
      call mapping%init (m)
    end select
  end if
end subroutine sf_channel_set_os_mapping

```

This sets an s-channel endpoint mapping. The parameter a is the slope parameter (default 1); increasing it moves the endpoint region (at $x = 1$ to lower values in the input parameter) even more. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_ep_mapping => sf_channel_set_ep_mapping

<SF mappings: main procedures>+≡
subroutine sf_channel_set_ep_mapping (channel, i_sf, a)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in), optional :: a
  channel%map_code(i_sf) = SFMAP_MULTI_EP
  allocate (sf_ep_mapping_t :: channel%multi_mapping)
  select type (mapping => channel%multi_mapping)
  type is (sf_ep_mapping_t)
    call mapping%init (a = a)
  end select
end subroutine sf_channel_set_ep_mapping

```

This sets a resonant endpoint mapping. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_epr_mapping => sf_channel_set_epr_mapping

<SF mappings: main procedures>+≡
subroutine sf_channel_set_epr_mapping (channel, i_sf, a, m, w)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in) :: a, m, w

```

```

channel%map_code(i_sf) = SFMAP_MULTI_EPR
allocate (sf_epr_mapping_t :: channel%multi_mapping)
select type (mapping => channel%multi_mapping)
type is (sf_epr_mapping_t)
    call mapping%init (a, m, w)
end select
end subroutine sf_channel_set_epr_mapping

```

This sets an on-shell endpoint mapping. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_epo_mapping => sf_channel_set_epo_mapping

<SF mappings: main procedures>+≡
    subroutine sf_channel_set_epo_mapping (channel, i_sf, a, m)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        real(default), intent(in) :: a, m
        channel%map_code(i_sf) = SFMAP_MULTI_EPO
        allocate (sf_epo_mapping_t :: channel%multi_mapping)
        select type (mapping => channel%multi_mapping)
        type is (sf_epo_mapping_t)
            call mapping%init (a, m)
        end select
    end subroutine sf_channel_set_epo_mapping

```

This sets an s-channel power mapping, regulating a singularity of type $(1 - x)^{-1+\epsilon}$. The parameter ϵ depends on the structure function. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_ip_mapping => sf_channel_set_ip_mapping

<SF mappings: main procedures>+≡
    subroutine sf_channel_set_ip_mapping (channel, i_sf, eps)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        real(default), intent(in), optional :: eps
        channel%map_code(i_sf) = SFMAP_MULTI_IP
        allocate (sf_ip_mapping_t :: channel%multi_mapping)
        select type (mapping => channel%multi_mapping)
        type is (sf_ip_mapping_t)
            call mapping%init (eps)
        end select
    end subroutine sf_channel_set_ip_mapping

```

This sets an s-channel resonant power mapping, regulating a singularity of type $(1 - x)^{-1+\epsilon}$ in the presence of an s-channel resonance. The parameter ϵ depends on the structure function. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_ipr_mapping => sf_channel_set_ipr_mapping

```

```

<SF mappings: main procedures>+≡
subroutine sf_channel_set_ipr_mapping (channel, i_sf, eps, m, w)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in), optional :: eps, m, w
  channel%map_code(i_sf) = SFMAP_MULTI_IPR
  allocate (sf_ipr_mapping_t :: channel%multi_mapping)
  select type (mapping => channel%multi_mapping)
    type is (sf_ipr_mapping_t)
      call mapping%init (eps, m, w)
  end select
end subroutine sf_channel_set_ipr_mapping

```

This sets an on-shell power mapping, regulating a singularity of type $(1-x)^{-1+\epsilon}$ for the production of a single on-shell particle.. The parameter ϵ depends on the structure function. Gfortran 7/8/9 bug: has to remain in module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_ipo_mapping => sf_channel_set_ipo_mapping
<SF mappings: main procedures>+≡
subroutine sf_channel_set_ipo_mapping (channel, i_sf, eps, m)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in), optional :: eps, m
  channel%map_code(i_sf) = SFMAP_MULTI_IPO
  allocate (sf_ipo_mapping_t :: channel%multi_mapping)
  select type (mapping => channel%multi_mapping)
    type is (sf_ipo_mapping_t)
      call mapping%init (eps, m)
  end select
end subroutine sf_channel_set_ipo_mapping

```

This sets a combined endpoint/ISR mapping. Gfortran 7/8/9 bug, remains in module.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_ei_mapping => sf_channel_set_ei_mapping
<SF mappings: main procedures>+≡
subroutine sf_channel_set_ei_mapping (channel, i_sf, a, eps)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in), optional :: a, eps
  channel%map_code(i_sf) = SFMAP_MULTI_EI
  allocate (sf_ei_mapping_t :: channel%multi_mapping)
  select type (mapping => channel%multi_mapping)
    type is (sf_ei_mapping_t)
      call mapping%init (a, eps)
  end select
end subroutine sf_channel_set_ei_mapping

```

This sets a combined endpoint/ISR mapping with resonance. Gfortran 7/8/9 bug, remains in module.

```

<SF mappings: sf channel: TBP>+≡

```



```

        procedure :: set_eir_mapping => sf_channel_set_eir_mapping
<SF mappings: main procedures>+≡
    subroutine sf_channel_set_eir_mapping (channel, i_sf, a, eps, m, w)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        real(default), intent(in), optional :: a, eps, m, w
        channel%map_code(i_sf) = SFMAP_MULTI_EI
        allocate (sf_eir_mapping_t :: channel%multi_mapping)
        select type (mapping => channel%multi_mapping)
            type is (sf_eir_mapping_t)
                call mapping%init (a, eps, m, w)
            end select
        end subroutine sf_channel_set_eir_mapping

```

This sets a combined endpoint/ISR mapping, on-shell. Gfortran 7/8/9 bug, remains in module.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_eio_mapping => sf_channel_set_eio_mapping
<SF mappings: main procedures>+≡
    subroutine sf_channel_set_eio_mapping (channel, i_sf, a, eps, m)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        real(default), intent(in), optional :: a, eps, m
        channel%map_code(i_sf) = SFMAP_MULTI_EI
        allocate (sf_eio_mapping_t :: channel%multi_mapping)
        select type (mapping => channel%multi_mapping)
            type is (sf_eio_mapping_t)
                call mapping%init (a, eps, m)
            end select
        end subroutine sf_channel_set_eio_mapping

```

Return true if the mapping code at position i_sf is SFMAP_SINGLE.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: is_single_mapping => sf_channel_is_single_mapping
<SF mappings: sub interfaces>+≡
    module function sf_channel_is_single_mapping (channel, i_sf) result (flag)
        class(sf_channel_t), intent(in) :: channel
        integer, intent(in) :: i_sf
        logical :: flag
    end function sf_channel_is_single_mapping
<SF mappings: procedures>+≡
    module function sf_channel_is_single_mapping (channel, i_sf) result (flag)
        class(sf_channel_t), intent(in) :: channel
        integer, intent(in) :: i_sf
        logical :: flag
        flag = channel%map_code(i_sf) == SFMAP_SINGLE
    end function sf_channel_is_single_mapping

```

Return true if the mapping code at position `i_sf` is any of the `SFMAP_MULTI` mappings.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: is_multi_mapping => sf_channel_is_multi_mapping

<SF mappings: sub interfaces>+≡
    module function sf_channel_is_multi_mapping (channel, i_sf) result (flag)
        class(sf_channel_t), intent(in) :: channel
        integer, intent(in) :: i_sf
        logical :: flag
    end function sf_channel_is_multi_mapping

<SF mappings: procedures>+≡
    module function sf_channel_is_multi_mapping (channel, i_sf) result (flag)
        class(sf_channel_t), intent(in) :: channel
        integer, intent(in) :: i_sf
        logical :: flag
        select case (channel%map_code(i_sf))
        case (SFMAP_NONE, SFMAP_SINGLE)
            flag = .false.
        case default
            flag = .true.
        end select
    end function sf_channel_is_multi_mapping

```

Return the number of parameters that the multi-mapping requires. The mapping object must be allocated.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: get_multi_mapping_n_par => sf_channel_get_multi_mapping_n_par

<SF mappings: sub interfaces>+≡
    module function sf_channel_get_multi_mapping_n_par (channel) result (n_par)
        class(sf_channel_t), intent(in) :: channel
        integer :: n_par
    end function sf_channel_get_multi_mapping_n_par

<SF mappings: procedures>+≡
    module function sf_channel_get_multi_mapping_n_par (channel) result (n_par)
        class(sf_channel_t), intent(in) :: channel
        integer :: n_par
        if (allocated (channel%multi_mapping)) then
            n_par = channel%multi_mapping%get_n_dim ()
        else
            n_par = 0
        end if
    end function sf_channel_get_multi_mapping_n_par

```

Return true if there is any nontrivial mapping in any of the channels.

```

<SF mappings: public>+≡
    public :: any_sf_channel_has_mapping

<SF mappings: sub interfaces>+≡
    module function any_sf_channel_has_mapping (channel) result (flag)
        type(sf_channel_t), dimension(:), intent(in) :: channel
        logical :: flag
    end function any_sf_channel_has_mapping

```

```

<SF mappings: procedures>+≡
module function any_sf_channel_has_mapping (channel) result (flag)
  type(sf_channel_t), dimension(:), intent(in) :: channel
  logical :: flag
  integer :: c
  flag = .false.
  do c = 1, size (channel)
    flag = flag .or. any (channel(c)%map_code /= SFMAP_NONE)
  end do
end function any_sf_channel_has_mapping

```

Set a parameter index for an active multi mapping. We assume that the index array is allocated properly.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_par_index => sf_channel_set_par_index

<SF mappings: sub interfaces>+≡
  module subroutine sf_channel_set_par_index (channel, j, i_par)
    class(sf_channel_t), intent(inout) :: channel
    integer, intent(in) :: j
    integer, intent(in) :: i_par
  end subroutine sf_channel_set_par_index

<SF mappings: procedures>+≡
module subroutine sf_channel_set_par_index (channel, j, i_par)
  class(sf_channel_t), intent(inout) :: channel
  integer, intent(in) :: j
  integer, intent(in) :: i_par
  associate (mapping => channel%multi_mapping)
    if (j >= 1 .and. j <= mapping%get_n_dim ()) then
      if (mapping%get_index (j) == 0) then
        call channel%multi_mapping%set_index (j, i_par)
      else
        call msg_bug ("Structure-function setup: mapping index set twice")
      end if
    else
      call msg_bug ("Structure-function setup: mapping index out of range")
    end if
  end associate
end subroutine sf_channel_set_par_index

```

16.4.18 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_mappings_ut.f90>≡
  <File header>

  module sf_mappings_ut
    use unit_tests
    use sf_mappings_uti

    <Standard module head>

```

```

    <SF mappings: public test>

contains

    <SF mappings: test driver>

    end module sf_mappings_ut
<sf_mappings_uti.f90>≡
    <File header>

    module sf_mappings_uti

    <Use kinds>
        use format_defs, only: FMT_11, FMT_12, FMT_13, FMT_14, FMT_15, FMT_16

        use sf_mappings

    <Standard module head>

    <SF mappings: test declarations>

contains

    <SF mappings: tests>

    end module sf_mappings_uti
API: driver for the unit tests below.
<SF mappings: public test>≡
    public :: sf_mappings_test
<SF mappings: test driver>≡
    subroutine sf_mappings_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF mappings: execute tests>
    end subroutine sf_mappings_test

```

Check standard mapping

Probe the standard mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>≡
    call test (sf_mappings_1, "sf_mappings_1", &
        "standard pair mapping", &
        u, results)

<SF mappings: test declarations>≡
    public :: sf_mappings_1

```

```

<SF mappings: tests>≡
subroutine sf_mappings_1 (u)
  integer, intent(in) :: u
  class(sf_mapping_t), allocatable :: mapping
  real(default), dimension(2) :: p

  write (u, "(A)")  "* Test output: sf_mappings_1"
  write (u, "(A)")  "* Purpose: probe standard mapping"
  write (u, "(A)")

  allocate (sf_s_mapping_t :: mapping)
  select type (mapping)
  type is (sf_s_mapping_t)
    call mapping%init ()
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
  end select

  call mapping%write (u)

  write (u, *)
  write (u, "(A)")  "Probe at (0,0):"
  p = [0._default, 0._default]
  call mapping%check (u, p, 1-p, "F7.5")

  write (u, *)
  write (u, "(A)")  "Probe at (0.5,0.5):"
  p = [0.5_default, 0.5_default]
  call mapping%check (u, p, 1-p, "F7.5")

  write (u, *)
  write (u, "(A)")  "Probe at (0.1,0.5):"
  p = [0.1_default, 0.5_default]
  call mapping%check (u, p, 1-p, "F7.5")

  write (u, *)
  write (u, "(A)")  "Probe at (0.1,0.1):"
  p = [0.1_default, 0.1_default]
  call mapping%check (u, p, 1-p, "F7.5")

  write (u, *)
  write (u, "(A)")  "Compute integral:"
  write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

  deallocate (mapping)
  allocate (sf_s_mapping_t :: mapping)
  select type (mapping)
  type is (sf_s_mapping_t)
    call mapping%init (power=2._default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
  end select

  write (u, *)

```

```

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.1):"
p = [0.1_default, 0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_1"

end subroutine sf_mappings_1

```

Channel entries

Construct channel entries and print them.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_2, "sf_mappings_2", &
    "structure-function mapping channels", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_2

<SF mappings: tests>+≡
  subroutine sf_mappings_2 (u)
    integer, intent(in) :: u
    type(sf_channel_t), dimension(:), allocatable :: channel
    integer :: c

    write (u, "(A)") "* Test output: sf_mappings_2"
    write (u, "(A)") "* Purpose: construct and display &
      &mapping-channel objects"
    write (u, "(A)")

    call allocate_sf_channels (channel, n_channel = 8, n_strfun = 2)

```

```

call channel(2)%activate_mapping ([1])
call channel(3)%set_s_mapping ([1,2])
call channel(4)%set_s_mapping ([1,2], power=2._default)
call channel(5)%set_res_mapping ([1,2], m = 0.5_default, w = 0.1_default, single = .false.)
call channel(6)%set_os_mapping ([1,2], m = 0.5_default, single = .false.)
call channel(7)%set_res_mapping ([1], m = 0.5_default, w = 0.1_default, single = .true.)
call channel(8)%set_os_mapping ([1], m = 0.5_default, single = .true.)

call channel(3)%set_par_index (1, 1)
call channel(3)%set_par_index (2, 4)

call channel(4)%set_par_index (1, 1)
call channel(4)%set_par_index (2, 4)

call channel(5)%set_par_index (1, 1)
call channel(5)%set_par_index (2, 3)

call channel(6)%set_par_index (1, 1)
call channel(6)%set_par_index (2, 2)

call channel(7)%set_par_index (1, 1)

call channel(8)%set_par_index (1, 1)

do c = 1, size (channel)
  write (u, "(I0,':')", advance="no") c
  call channel(c)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_2"

end subroutine sf_mappings_2

```

Check resonance mapping

Probe the resonance mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

The resonance mass is at $1/2$ the energy, the width is $1/10$.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_3, "sf_mappings_3", &
    "resonant pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_3

<SF mappings: tests>+≡
  subroutine sf_mappings_3 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

```

```

write (u, "(A)")  "* Test output: sf_mappings_3"
write (u, "(A)")  "* Purpose: probe resonance pair mapping"
write (u, "(A)")

allocate (sf_res_mapping_t :: mapping)
select type (mapping)
type is (sf_res_mapping_t)
  call mapping%init (0.5_default, 0.1_default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.1,0.1):"
p = [0.1_default, 0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_3"

end subroutine sf_mappings_3

```

Check on-shell mapping

Probe the on-shell mapping of the unit square for different parameter values. Also calculates integrals. In this case, the Jacobian is constant and given by $|\log m^2|$, so this is also the value of the integral. The factor results from the variable change in the δ function $\delta(m^2 - x_1 x_2)$ which multiplies the cross section

for the case at hand.

For the test, the (rescaled) resonance mass is set at 1/2 the energy.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_4, "sf_mappings_4", &
    "on-shell pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_4

<SF mappings: tests>+≡
  subroutine sf_mappings_4 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)")  "* Test output: sf_mappings_4"
    write (u, "(A)")  "* Purpose: probe on-shell pair mapping"
    write (u, "(A)")

    allocate (sf_os_mapping_t :: mapping)
    select type (mapping)
    type is (sf_os_mapping_t)
      call mapping%init (0.5_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)")  "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0,0.1):"
    p = [0._default, 0.1_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0,1.0):"
    p = [0._default, 1.0_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Compute integral:"
    write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

    deallocate (mapping)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_4"

end subroutine sf_mappings_4

```

Check endpoint mapping

Probe the endpoint mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_5, "sf_mappings_5", &
    "endpoint pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_5

<SF mappings: tests>+≡
  subroutine sf_mappings_5 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)")  "* Test output: sf_mappings_5"
    write (u, "(A)")  "* Purpose: probe endpoint pair mapping"
    write (u, "(A)")

    allocate (sf_ep_mapping_t :: mapping)
    select type (mapping)
    type is (sf_ep_mapping_t)
      call mapping%init ()
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)")  "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.1,0.5):"
    p = [0.1_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

```

```

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_5"

end subroutine sf_mappings_5

```

Check endpoint resonant mapping

Probe the endpoint mapping with resonance. Also calculates integrals.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_6, "sf_mappings_6", &
    "endpoint resonant mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_6

<SF mappings: tests>+≡
  subroutine sf_mappings_6 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)") "* Test output: sf_mappings_6"
    write (u, "(A)") "* Purpose: probe endpoint resonant mapping"
    write (u, "(A)")

    allocate (sf_epr_mapping_t :: mapping)
    select type (mapping)
    type is (sf_epr_mapping_t)
      call mapping%init (a = 1._default, m = 0.5_default, w = 0.1_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)") "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)

```

```

write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Same mapping without resonance:"
write (u, "(A)")

allocate (sf_epr_mapping_t :: mapping)
select type (mapping)
type is (sf_epr_mapping_t)
  call mapping%init (a = 1._default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
call mapping%check (u, p, 1-p, "F7.5")

```

```

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_6"

end subroutine sf_mappings_6

```

Check endpoint on-shell mapping

Probe the endpoint mapping with an on-shell particle. Also calculates integrals.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_7, "sf_mappings_7", &
    "endpoint on-shell mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_7

<SF mappings: tests>+≡
  subroutine sf_mappings_7 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)")  "* Test output: sf_mappings_7"
    write (u, "(A)")  "* Purpose: probe endpoint on-shell mapping"
    write (u, "(A)")

    allocate (sf_epo_mapping_t :: mapping)
    select type (mapping)
    type is (sf_epo_mapping_t)
      call mapping%init (a = 1._default, m = 0.5_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)") "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.1,0.5):"

```

```

p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_7"

end subroutine sf_mappings_7

```

Check power mapping

Probe the power mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_8, "sf_mappings_8", &
    "power pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_8

<SF mappings: tests>+≡
  subroutine sf_mappings_8 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p, pb

    write (u, "(A)")  "* Test output: sf_mappings_8"
    write (u, "(A)")  "* Purpose: probe power pair mapping"
    write (u, "(A)")

    allocate (sf_ip_mapping_t :: mapping)
    select type (mapping)
    type is (sf_ip_mapping_t)
      call mapping%init (eps = 0.1_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)

```

```

write (u, "(A)") "Probe at (0,0.5):"
p = [0._default, 0.5_default]
pb= [1._default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.9,0.5):"
p = [0.9_default, 0.5_default]
pb= [0.1_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.99,0.02):"
p = [0.99_default, 0.02_default]
pb= [0.01_default, 0.98_default]
call mapping%check (u, p, pb, FMT_14, FMT_12)

write (u, *)
write (u, "(A)") "Probe at (0.99,0.98):"
p = [0.99_default, 0.98_default]
pb= [0.01_default, 0.02_default]
call mapping%check (u, p, pb, FMT_14, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "** Test output end: sf_mappings_8"

end subroutine sf_mappings_8

```

Check resonant power mapping

Probe the power mapping of the unit square, adapted for an s-channel resonance, for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```
<SF mappings: execute tests>+≡
  call test (sf_mappings_9, "sf_mappings_9", &
    "power resonance mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_9

<SF mappings: tests>+≡
  subroutine sf_mappings_9 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p, pb

    write (u, "(A)")  "* Test output: sf_mappings_9"
    write (u, "(A)")  "* Purpose: probe power resonant pair mapping"
    write (u, "(A)")

    allocate (sf_ipr_mapping_t :: mapping)
    select type (mapping)
    type is (sf_ipr_mapping_t)
      call mapping%init (eps = 0.1_default, m = 0.5_default, w = 0.1_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)")  "Probe at (0,0.5):"
    p = [0._default, 0.5_default]
    pb= [1._default, 0.5_default]
    call mapping%check (u, p, pb, FMT_16)

    write (u, *)
    write (u, "(A)")  "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    pb= [0.5_default, 0.5_default]
    call mapping%check (u, p, pb, FMT_16)

    write (u, *)
    write (u, "(A)")  "Probe at (0.9,0.5):"
    p = [0.9_default, 0.5_default]
    pb= [0.1_default, 0.5_default]
    call mapping%check (u, p, pb, FMT_16)

    write (u, *)
    write (u, "(A)")  "Probe at (0.7,0.2):"
    p = [0.7_default, 0.2_default]
```



```

pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.9999,0.02):"
p = [0.9999_default, 0.02_default]
pb= [0.0001_default, 0.98_default]
call mapping%check (u, p, pb, FMT_11, FMT_12)

write (u, *)
write (u, "(A)") "Probe at (0.9999,0.98):"
p = [0.9999_default, 0.98_default]
pb= [0.0001_default, 0.02_default]
call mapping%check (u, p, pb, FMT_11, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Same mapping without resonance:"
write (u, "(A)")

allocate (sf_ipr_mapping_t :: mapping)
select type (mapping)
type is (sf_ipr_mapping_t)
    call mapping%init (eps = 0.1_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0.5):"
p = [0._default, 0.5_default]
pb= [1._default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)

```

```

write (u, "(A)") "Probe at (0.9,0.5):"
p = [0.9_default, 0.5_default]
pb= [0.1_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_9"

end subroutine sf_mappings_9

```

Check on-shell power mapping

Probe the power mapping of the unit square, adapted for single-particle production, for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_10, "sf_mappings_10", &
    "power on-shell mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_10

<SF mappings: tests>+≡
  subroutine sf_mappings_10 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p, pb

    write (u, "(A)") "* Test output: sf_mappings_10"
    write (u, "(A)") "* Purpose: probe power on-shell mapping"
    write (u, "(A)")

    allocate (sf_ipo_mapping_t :: mapping)

```

```

select type (mapping)
type is (sf_ipo_mapping_t)
    call mapping%init (eps = 0.1_default, m = 0.5_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0.5):"
p = [0._default, 0.5_default]
pb= [1._default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0,0.02):"
p = [0._default, 0.02_default]
pb= [1._default, 0.98_default]
call mapping%check (u, p, pb, FMT_15, FMT_12)

write (u, *)
write (u, "(A)") "Probe at (0,0.98):"
p = [0._default, 0.98_default]
pb= [1._default, 0.02_default]
call mapping%check (u, p, pb, FMT_15, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_10"

end subroutine sf_mappings_10

```

Check combined endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

```

<SF mappings: execute tests>+≡
    call test (sf_mappings_11, "sf_mappings_11", &
        "endpoint/power combined mapping", &
        u, results)

<SF mappings: test declarations>+≡
    public :: sf_mappings_11

<SF mappings: tests>+≡
    subroutine sf_mappings_11 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(4) :: p, pb

```

```

write (u, "(A)")  "* Test output: sf_mappings_11"
write (u, "(A)")  "* Purpose: probe power pair mapping"
write (u, "(A)")

allocate (sf_ei_mapping_t :: mapping)
select type (mapping)
type is (sf_ei_mapping_t)
  call mapping%init (eps = 0.1_default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
  call mapping%set_index (3, 3)
  call mapping%set_index (4, 4)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0.5, 0.5, 0.5, 0.5):"
p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.7, 0.2, 0.4, 0.8):"
p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.9, 0.06, 0.95, 0.1):"
p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
call mapping%check (u, p, pb, FMT_13, FMT_12)

write (u, *)
write (u, "(A)")  "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_11"

end subroutine sf_mappings_11

```

Check resonant endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

(SF mappings: execute tests)+=

```

call test (sf_mappings_12, "sf_mappings_12", &
  "endpoint/power resonant combined mapping", &
  u, results)

```

```

<SF mappings: test declarations>+≡
    public :: sf_mappings_12

<SF mappings: tests>+≡
    subroutine sf_mappings_12 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(4) :: p, pb

        write (u, "(A)")  "* Test output: sf_mappings_12"
        write (u, "(A)")  "*   Purpose: probe resonant combined mapping"
        write (u, "(A)")

        allocate (sf_eir_mapping_t :: mapping)
        select type (mapping)
        type is (sf_eir_mapping_t)
            call mapping%init (a = 1._default, &
                               eps = 0.1_default, m = 0.5_default, w = 0.1_default)
            call mapping%set_index (1, 1)
            call mapping%set_index (2, 2)
            call mapping%set_index (3, 3)
            call mapping%set_index (4, 4)
        end select

        call mapping%write (u)

        write (u, *)
        write (u, "(A)")  "Probe at (0.5, 0.5, 0.5, 0.5):"
        p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
        pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.7, 0.2, 0.4, 0.8):"
        p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
        pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.9, 0.06, 0.95, 0.1):"
        p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
        pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
        call mapping%check (u, p, pb, FMT_15, FMT_12)

        write (u, *)
        write (u, "(A)")  "Compute integral:"
        write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

        deallocate (mapping)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: sf_mappings_12"

    end subroutine sf_mappings_12

```

Check on-shell endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

```
<SF mappings: execute tests>+≡
    call test (sf_mappings_13, "sf_mappings_13", &
        "endpoint/power on-shell combined mapping", &
        u, results)

<SF mappings: test declarations>+≡
    public :: sf_mappings_13

<SF mappings: tests>+≡
    subroutine sf_mappings_13 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(4) :: p, pb

        write (u, "(A)")  "* Test output: sf_mappings_13"
        write (u, "(A)")  "* Purpose: probe on-shell combined mapping"
        write (u, "(A)")

        allocate (sf_eio_mapping_t :: mapping)
        select type (mapping)
        type is (sf_eio_mapping_t)
            call mapping%init (a = 1._default, eps = 0.1_default, m = 0.5_default)
            call mapping%set_index (1, 1)
            call mapping%set_index (2, 2)
            call mapping%set_index (3, 3)
            call mapping%set_index (4, 4)
        end select

        call mapping%write (u)

        write (u, *)
        write (u, "(A)")  "Probe at (0.5, 0.5, 0.5, 0.5):"
        p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
        pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.7, 0.2, 0.4, 0.8):"
        p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
        pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.9, 0.06, 0.95, 0.1):"
        p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
        pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
        call mapping%check (u, p, pb, FMT_14, FMT_12)

        write (u, *)
        write (u, "(A)")  "Compute integral:"
        write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)
```

```

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_mappings_13"

end subroutine sf_mappings_13

```

Check rescaling

Check the rescaling factor in on-shell basic mapping.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_14, "sf_mappings_14", &
    "rescaled on-shell mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_14

<SF mappings: tests>+≡
  subroutine sf_mappings_14 (u)
    integer, intent(in) :: u
    real(default), dimension(2) :: p2, r2
    real(default), dimension(1) :: p1, r1
    real(default) :: f, x_free, m2

    write (u, "(A)")  "** Test output: sf_mappings_14"
    write (u, "(A)")  "** Purpose: probe rescaling in os mapping"
    write (u, "(A)")

    x_free = 0.9_default
    m2 = 0.5_default

    write (u, "(A)")  "** Two parameters"
    write (u, "(A)")

    p2 = [0.1_default, 0.2_default]

    call map_on_shell (r2, f, p2, -log (m2), x_free)

    write (u, "(A,9(1x," // FMT_14 // ")")")  "p =", p2
    write (u, "(A,9(1x," // FMT_14 // ")")")  "r =", r2
    write (u, "(A,9(1x," // FMT_14 // ")")")  "f =", f
    write (u, "(A,9(1x," // FMT_14 // ")")")  "**r=", x_free * product (r2)

    write (u, *)

    call map_on_shell_inverse (r2, f, p2, -log (m2), x_free)

    write (u, "(A,9(1x," // FMT_14 // ")")")  "p =", p2
    write (u, "(A,9(1x," // FMT_14 // ")")")  "r =", r2
    write (u, "(A,9(1x," // FMT_14 // ")")")  "f =", f
    write (u, "(A,9(1x," // FMT_14 // ")")")  "**r=", x_free * product (r2)

    write (u, "(A)")

```

```

write (u, "(A)")  "* One parameter"
write (u, "(A)")

p1 = [0.1_default]

call map_on_shell_single (r1, f, p1, -log (m2), x_free)

write (u, "(A,9(1x," // FMT_14 // "))") "p =", p1
write (u, "(A,9(1x," // FMT_14 // "))") "r =", r1
write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r1)

write (u, *)

call map_on_shell_single_inverse (r1, f, p1, -log (m2), x_free)

write (u, "(A,9(1x," // FMT_14 // "))") "p =", p1
write (u, "(A,9(1x," // FMT_14 // "))") "r =", r1
write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_14"

end subroutine sf_mappings_14

```

Check single parameter resonance mapping

Probe the resonance mapping of the unit interval for different parameter values.
Also calculates integrals.

The resonance mass is at $1/2$ the energy, the width is $1/10$.

```

<SF mappings: execute tests>+≡
call test (sf_mappings_15, "sf_mappings_15", &
  "resonant single mapping", &
  u, results)

<SF mappings: test declarations>+≡
public :: sf_mappings_15

<SF mappings: tests>+≡
subroutine sf_mappings_15 (u)
  integer, intent(in) :: u
  class(sf_mapping_t), allocatable :: mapping
  real(default), dimension(1) :: p

  write (u, "(A)")  "* Test output: sf_mappings_15"
  write (u, "(A)")  "* Purpose: probe resonance single mapping"
  write (u, "(A)")

  allocate (sf_res_mapping_single_t :: mapping)
  select type (mapping)
  type is (sf_res_mapping_single_t)
    call mapping%init (0.5_default, 0.1_default)

```



```

        call mapping%set_index (1, 1)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0):"
p = [0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.5):"
p = [0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.1):"
p = [0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_15"

end subroutine sf_mappings_15

```

Check single parameter on-shell mapping

Probe the on-shell (pseudo) mapping of the unit interval for different parameter values. Also calculates integrals.

The resonance mass is at $1/2$ the energy.

```

<SF mappings: execute tests>+≡
    call test (sf_mappings_16, "sf_mappings_16", &
        "on-shell single mapping", &
        u, results)

<SF mappings: test declarations>+≡
    public :: sf_mappings_16

<SF mappings: tests>+≡
    subroutine sf_mappings_16 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(1) :: p

        write (u, "(A)")  "* Test output: sf_mappings_16"
        write (u, "(A)")  "* Purpose: probe on-shell single mapping"
        write (u, "(A)")

```

```

allocate (sf_os_mapping_single_t :: mapping)
select type (mapping)
type is (sf_os_mapping_single_t)
    call mapping%init (0.5_default)
    call mapping%set_index (1, 1)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0):"
p = [0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5):"
p = [0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_16"

end subroutine sf_mappings_16

```

16.5 Structure function base

$\langle sf_base.f90 \rangle \equiv$
 $\langle File\ header \rangle$

module sf_base

$\langle Use\ kinds \rangle$

$\langle Use\ strings \rangle$

```

use numeric_utils, only: pacify
use lorentz
use quantum_numbers
use pdg_arrays
use interactions
use evaluators
use beams
use sf_aux
use sf_mappings

```

$\langle Standard\ module\ head \rangle$

```

    <SF base: public>

    <SF base: parameters>

    <SF base: types>

    <SF base: interfaces>

    interface
    <SF base: sub interfaces>
    end interface

end module sf_base

<sf_base_sub.f90>≡
<File header>

submodule (sf_base) sf_base_s

    use io_units
    use format_utils, only: write_separator
    use format_defs, only: FMT_17, FMT_19
    use constants, only: one, two
    use diagnostics
    use physics_defs, only: n_beams_rescaled

    implicit none

contains

    <SF base: procedures>

end submodule sf_base_s

```

16.5.1 Abstract rescale data-type

NLO calculations require the treatment of initial state parton radiation. The radiation of a parton rescales the energy fraction which enters the hard process. We allow for different rescale settings by extending the abstract. `sf_rescale_t` data type.

```

<SF base: public>≡
    public :: sf_rescale_t

<SF base: types>≡
    type, abstract :: sf_rescale_t
        integer :: i_beam = 0
    contains
    <SF base: rescaling function: TBP>
    end type sf_rescale_t

<SF base: rescaling function: TBP>≡
    procedure (sf_rescale_apply), deferred :: apply

```

```

⟨SF base: interfaces⟩≡
  abstract interface
    subroutine sf_rescale_apply (func, x)
      import
      class(sf_rescale_t), intent(in) :: func
      real(default), intent(inout) :: x
    end subroutine sf_rescale_apply
  end interface

⟨SF base: rescaling function: TBP⟩+≡
  procedure :: set_i_beam => sf_rescale_set_i_beam

⟨SF base: sub interfaces⟩≡
  module subroutine sf_rescale_set_i_beam (func, i_beam)
    class(sf_rescale_t), intent(inout) :: func
    integer, intent(in) :: i_beam
  end subroutine sf_rescale_set_i_beam

⟨SF base: procedures⟩≡
  module subroutine sf_rescale_set_i_beam (func, i_beam)
    class(sf_rescale_t), intent(inout) :: func
    integer, intent(in) :: i_beam
    func%i_beam = i_beam
  end subroutine sf_rescale_set_i_beam

⟨SF base: public⟩+≡
  public :: sf_rescale_collinear_t

⟨SF base: types⟩+≡
  type, extends (sf_rescale_t) :: sf_rescale_collinear_t
    real(default) :: xi_tilde
  contains
    ⟨SF base: rescale collinear: TBP⟩
  end type sf_rescale_collinear_t

```

For the subtraction terms we need to rescale the Born x of both beams in the collinear limit. This leaves one beam unaffected and rescales the other according to

$$x = \frac{\bar{x}}{1 - \xi} \quad (16.27)$$

which is the collinear limit of `sf_rescale_real_apply`.

```

⟨SF base: rescale collinear: TBP⟩≡
  procedure :: apply => sf_rescale_collinear_apply

⟨SF base: sub interfaces⟩+≡
  module subroutine sf_rescale_collinear_apply (func, x)
    class(sf_rescale_collinear_t), intent(in) :: func
    real(default), intent(inout) :: x
  end subroutine sf_rescale_collinear_apply

⟨SF base: procedures⟩+≡
  module subroutine sf_rescale_collinear_apply (func, x)
    class(sf_rescale_collinear_t), intent(in) :: func
    real(default), intent(inout) :: x

```

```

real(default) :: xi
if (debug2_active (D_BEAMS)) then
  print *, 'Rescaling function - Collinear: '
  print *, 'Input, unscaled x: ', x
  print *, 'xi_tilde: ', func%xi_tilde
end if
xi = func%xi_tilde * (one - x)
x = x / (one - xi)
if (debug2_active (D_BEAMS)) print *, 'rescaled x: ', x
end subroutine sf_rescale_collinear_apply

```

<SF base: rescale collinear: TBP>+≡

```

procedure :: set => sf_rescale_collinear_set

```

<SF base: sub interfaces>+≡

```

module subroutine sf_rescale_collinear_set (func, xi_tilde)
  class(sf_rescale_collinear_t), intent(inout) :: func
  real(default), intent(in) :: xi_tilde
end subroutine sf_rescale_collinear_set

```

<SF base: procedures>+≡

```

module subroutine sf_rescale_collinear_set (func, xi_tilde)
  class(sf_rescale_collinear_t), intent(inout) :: func
  real(default), intent(in) :: xi_tilde
  func%xi_tilde = xi_tilde
end subroutine sf_rescale_collinear_set

```

<SF base: public>+≡

```

public :: sf_rescale_real_t

```

<SF base: types>+≡

```

type, extends (sf_rescale_t) :: sf_rescale_real_t
  real(default) :: xi, y
contains
  <SF base: rescale real: TBP>
end type sf_rescale_real_t

```

In case of IS Splittings, the beam x changes from Born to real and thus needs to be rescaled according to

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}} \quad (16.28)$$

Refs:

- [0709.2092] Eq. (5.7).
- [0907.4076] Eq. (2.21).
- Christian Weiss' PhD Thesis (DESY-THESIS-2017-025), Eq. (A.2.3).

<SF base: rescale real: TBP>≡

```

procedure :: apply => sf_rescale_real_apply

```

```

<SF base: sub interfaces>+≡
    module subroutine sf_rescale_real_apply (func, x)
        class(sf_rescale_real_t), intent(in) :: func
        real(default), intent(inout) :: x
    end subroutine sf_rescale_real_apply

<SF base: procedures>+≡
    module subroutine sf_rescale_real_apply (func, x)
        class(sf_rescale_real_t), intent(in) :: func
        real(default), intent(inout) :: x
        real(default) :: onepy, onemy
        if (debug2_active (D_BEAMS)) then
            print *, 'Rescaling function - Real: '
            print *, 'Input, unscaled: ', x
            print *, 'Beam index: ', func%i_beam
            print *, 'xi: ', func%xi, 'y: ', func%y
        end if
        x = x / sqrt (one - func%xi)
        onepy = one + func%y; onemy = one - func%y
        if (func%i_beam == 1) then
            x = x * sqrt ((two - func%xi * onemy) / (two - func%xi * onepy))
        else if (func%i_beam == 2) then
            x = x * sqrt ((two - func%xi * onepy) / (two - func%xi * onemy))
        else
            call msg_fatal ("sf_rescale_real_apply - invalid beam index")
        end if
        if (debug2_active (D_BEAMS)) print *, 'rescaled x: ', x
    end subroutine sf_rescale_real_apply

<SF base: rescale real: TBP>+≡
    procedure :: set => sf_rescale_real_set

<SF base: sub interfaces>+≡
    module subroutine sf_rescale_real_set (func, xi, y)
        class(sf_rescale_real_t), intent(inout) :: func
        real(default), intent(in) :: xi, y
    end subroutine sf_rescale_real_set

<SF base: procedures>+≡
    module subroutine sf_rescale_real_set (func, xi, y)
        class(sf_rescale_real_t), intent(inout) :: func
        real(default), intent(in) :: xi, y
        func%xi = xi; func%y = y
    end subroutine sf_rescale_real_set

<SF base: public>+≡
    public :: sf_rescale_dglap_t

<SF base: types>+≡
    type, extends(sf_rescale_t) :: sf_rescale_dglap_t
        real(default), dimension(:), allocatable :: z
        contains
        <SF base: rescale dglap: TBP>
    end type sf_rescale_dglap_t

```

```

<SF base: rescale dglap: TBP>≡
  procedure :: apply => sf_rescale_dglap_apply
<SF base: sub interfaces>+≡
  module subroutine sf_rescale_dglap_apply (func, x)
    class(sf_rescale_dglap_t), intent(in) :: func
    real(default), intent(inout) :: x
  end subroutine sf_rescale_dglap_apply
<SF base: procedures>+≡
  module subroutine sf_rescale_dglap_apply (func, x)
    class(sf_rescale_dglap_t), intent(in) :: func
    real(default), intent(inout) :: x
    if (debug2_active (D_BEAMS)) then
      print *, "Rescaling function - DGLAP:"
      print *, "Input: ", x
      print *, "Beam index: ", func%i_beam
      print *, "z: ", func%z
    end if
    x = x / func%z(func%i_beam)
    if (debug2_active (D_BEAMS)) print *, "scaled x: ", x
  end subroutine sf_rescale_dglap_apply

<SF base: rescale dglap: TBP>+≡
  procedure :: set => sf_rescale_dglap_set
<SF base: sub interfaces>+≡
  module subroutine sf_rescale_dglap_set (func, z)
    class(sf_rescale_dglap_t), intent(inout) :: func
    real(default), dimension(:), intent(in) :: z
  end subroutine sf_rescale_dglap_set
<SF base: procedures>+≡
  module subroutine sf_rescale_dglap_set (func, z)
    class(sf_rescale_dglap_t), intent(inout) :: func
    real(default), dimension(:), intent(in) :: z
    func%z = z
  end subroutine sf_rescale_dglap_set

```

16.5.2 Abstract structure-function data type

This type should hold all configuration data for a specific type of structure function. The base object is empty; the implementations will fill it.

```

<SF base: public>+≡
  public :: sf_data_t
<SF base: types>+≡
  type, abstract :: sf_data_t
    contains
    <SF base: sf data: TBP>
  end type sf_data_t

```

Output.

```

<SF base: sf data: TBP>≡
  procedure (sf_data_write), deferred :: write

```

```

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_data_write (data, unit, verbose)
      import
      class(sf_data_t), intent(in) :: data
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: verbose
    end subroutine sf_data_write
  end interface

```

Return true if this structure function is in generator mode. In that case, all parameters are free, otherwise bound. (We do not support mixed cases.) Default is: no generator.

```

<SF base: sf data: TBP>+≡
  procedure :: is_generator => sf_data_is_generator

<SF base: sub interfaces>+≡
  module function sf_data_is_generator (data) result (flag)
    class(sf_data_t), intent(in) :: data
    logical :: flag
  end function sf_data_is_generator

<SF base: procedures>+≡
  module function sf_data_is_generator (data) result (flag)
    class(sf_data_t), intent(in) :: data
    logical :: flag
    flag = .false.
  end function sf_data_is_generator

```

Return the number of input parameters that determine the structure function.

```

<SF base: sf data: TBP>+≡
  procedure (sf_data_get_int), deferred :: get_n_par

<SF base: interfaces>+≡
  abstract interface
    function sf_data_get_int (data) result (n)
      import
      class(sf_data_t), intent(in) :: data
      integer :: n
    end function sf_data_get_int
  end interface

```

Return the outgoing particle PDG codes for the current setup. The codes can be an array of particles, for each beam.

```

<SF base: sf data: TBP>+≡
  procedure (sf_data_get_pdg_out), deferred :: get_pdg_out

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_data_get_pdg_out (data, pdg_out)
      import
      class(sf_data_t), intent(in) :: data
      type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine sf_data_get_pdg_out
  end interface

```



```
end interface
```

Allocate a matching structure function interaction object and properly initialize it.

```
<SF base: sf data: TBP>+≡
  procedure (sf_data_allocate_sf_int), deferred :: allocate_sf_int

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_data_allocate_sf_int (data, sf_int)
      import
      class(sf_data_t), intent(in) :: data
      class(sf_int_t), intent(inout), allocatable :: sf_int
    end subroutine sf_data_allocate_sf_int
  end interface
```

Return the PDF set index, if applicable. We implement a default method which returns zero. The PDF (builtin and LHA) implementations will override this.

```
<SF base: sf data: TBP>+≡
  procedure :: get_pdf_set => sf_data_get_pdf_set

<SF base: sub interfaces>+≡
  elemental module function sf_data_get_pdf_set (data) result (pdf_set)
    class(sf_data_t), intent(in) :: data
    integer :: pdf_set
  end function sf_data_get_pdf_set

<SF base: procedures>+≡
  elemental module function sf_data_get_pdf_set (data) result (pdf_set)
    class(sf_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = 0
  end function sf_data_get_pdf_set
```

Return the spectrum file, if applicable. We implement a default method which returns zero. CIRCE1, CIRCE2 and the beam spectrum will override this.

```
<SF base: sf data: TBP>+≡
  procedure :: get_beam_file => sf_data_get_beam_file

<SF base: sub interfaces>+≡
  module function sf_data_get_beam_file (data) result (file)
    class(sf_data_t), intent(in) :: data
    type(string_t) :: file
  end function sf_data_get_beam_file

<SF base: procedures>+≡
  module function sf_data_get_beam_file (data) result (file)
    class(sf_data_t), intent(in) :: data
    type(string_t) :: file
    file = ""
  end function sf_data_get_beam_file
```

16.5.3 Structure-function chain configuration

This is the data type that the `process` module uses for setting up its structure-function chain. For each structure function described by the beam data, there is an entry. The `i` array indicates the beam(s) to which this structure function applies, and the `data` object contains the actual configuration data.

```
<SF base: public>+≡
    public :: sf_config_t
```

```
<SF base: types>+≡
    type :: sf_config_t
        integer, dimension(:), allocatable :: i
        class(sf_data_t), allocatable :: data
    contains
        <SF base: sf config: TBP>
    end type sf_config_t
```

Output:

```
<SF base: sf config: TBP>≡
    procedure :: write => sf_config_write

<SF base: sub interfaces>+≡
    module subroutine sf_config_write (object, unit, verbose)
        class(sf_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine sf_config_write

<SF base: procedures>+≡
    module subroutine sf_config_write (object, unit, verbose)
        class(sf_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        u = given_output_unit (unit)
        if (allocated (object%i)) then
            write (u, "(1x,A,2(1x,I0))") "Structure-function configuration: &
                &beam(s)", object%i
            if (allocated (object%data)) &
                call object%data%write (u, verbose = verbose)
        else
            write (u, "(1x,A)") "Structure-function configuration: [undefined]"
        end if
    end subroutine sf_config_write
```

Initialize.

```
<SF base: sf config: TBP>+≡
    procedure :: init => sf_config_init

<SF base: sub interfaces>+≡
    module subroutine sf_config_init (sf_config, i_beam, sf_data)
        class(sf_config_t), intent(out) :: sf_config
        integer, dimension(:), intent(in) :: i_beam
        class(sf_data_t), intent(in) :: sf_data
    end subroutine sf_config_init
```

```

<SF base: procedures>+=
  module subroutine sf_config_init (sf_config, i_beam, sf_data)
    class(sf_config_t), intent(out) :: sf_config
    integer, dimension(:), intent(in) :: i_beam
    class(sf_data_t), intent(in) :: sf_data
    allocate (sf_config%i (size (i_beam)), source = i_beam)
    allocate (sf_config%data, source = sf_data)
  end subroutine sf_config_init

```

Return the PDF set, if any.

```

<SF base: sf config: TBP>+=
  procedure :: get_pdf_set => sf_config_get_pdf_set

<SF base: sub interfaces>+=
  elemental module function sf_config_get_pdf_set (sf_config) result (pdf_set)
    class(sf_config_t), intent(in) :: sf_config
    integer :: pdf_set
  end function sf_config_get_pdf_set

<SF base: procedures>+=
  elemental module function sf_config_get_pdf_set (sf_config) result (pdf_set)
    class(sf_config_t), intent(in) :: sf_config
    integer :: pdf_set
    pdf_set = sf_config%data%get_pdf_set ()
  end function sf_config_get_pdf_set

```

Return the beam spectrum file, if any.

```

<SF base: sf config: TBP>+=
  procedure :: get_beam_file => sf_config_get_beam_file

<SF base: sub interfaces>+=
  module function sf_config_get_beam_file (sf_config) result (file)
    class(sf_config_t), intent(in) :: sf_config
    type(string_t) :: file
  end function sf_config_get_beam_file

<SF base: procedures>+=
  module function sf_config_get_beam_file (sf_config) result (file)
    class(sf_config_t), intent(in) :: sf_config
    type(string_t) :: file
    file = sf_config%data%get_beam_file ()
  end function sf_config_get_beam_file

```

16.5.4 Structure-function instance

The `sf_int_t` data type contains an `interaction_t` object (it is an extension of this type) and a pointer to the `sf_data_t` configuration data. This interaction, or copies of it, is used to implement structure-function kinematics and dynamics in the context of process evaluation.

The status code `status` tells whether the interaction is undefined, has defined kinematics (but matrix elements invalid), or is completely defined. There is also a status code for failure. The implementation is responsible for updating the status.

The entries `mi2`, `mr2`, and `mo2` hold the squared invariant masses of the incoming, radiated, and outgoing particle, respectively. They are supposed to be set upon initialization, but could also be varied event by event.

If the radiated or outgoing mass is nonzero, we may need to apply an on-shell projection. The projection mode is stored as `on_shell_mode`.

The array `beam_index` is the list of beams on which this structure function applies (1, 2, or both). The arrays `incoming`, `radiated`, and `outgoing` contain the indices of the respective particle sets within the interaction, for convenient lookup. The array `par_index` indicates the MC input parameters that this entry will use up in the structure-function chain. The first parameter (or the first two, for a spectrum) in this array determines the momentum fraction and is thus subject to global mappings.

In the abstract base type, we do not implement the data pointer. This allows us to restrict its type in the implementations.

```

<SF base: public>+≡
  public :: sf_int_t

<SF base: types>+≡
  type, abstract, extends (interaction_t) :: sf_int_t
    integer :: status = SF_UNDEFINED
    real(default), dimension(:), allocatable :: mi2
    real(default), dimension(:), allocatable :: mr2
    real(default), dimension(:), allocatable :: mo2
    integer :: on_shell_mode = KEEP_ENERGY
    logical :: qmin_defined = .false.
    logical :: qmax_defined = .false.
    real(default), dimension(:), allocatable :: qmin
    real(default), dimension(:), allocatable :: qmax
    integer, dimension(:), allocatable :: beam_index
    integer, dimension(:), allocatable :: incoming
    integer, dimension(:), allocatable :: radiated
    integer, dimension(:), allocatable :: outgoing
    integer, dimension(:), allocatable :: par_index
    integer, dimension(:), allocatable :: par_primary
  contains
    <SF base: sf_int: TBP>
  end type sf_int_t

```

Status codes. The codes that refer to links, masks, and connections, apply to structure-function chains only.

The status codes are public.

```

<SF base: parameters>≡
  integer, parameter, public :: SF_UNDEFINED = 0
  integer, parameter, public :: SF_INITIAL = 1
  integer, parameter, public :: SF_DONE_LINKS = 2
  integer, parameter, public :: SF_FAILED_MASK = 3
  integer, parameter, public :: SF_DONE_MASK = 4
  integer, parameter, public :: SF_FAILED_CONNECTIONS = 5
  integer, parameter, public :: SF_DONE_CONNECTIONS = 6
  integer, parameter, public :: SF_SEED_KINEMATICS = 10
  integer, parameter, public :: SF_FAILED_KINEMATICS = 11
  integer, parameter, public :: SF_DONE_KINEMATICS = 12

```

```
integer, parameter, public :: SF_FAILED_EVALUATION = 13
integer, parameter, public :: SF_EVALUATED = 20
```

Write a string version of the status code:

```
<SF base: procedures>+=
subroutine write_sf_status (status, u)
  integer, intent(in) :: status
  integer, intent(in) :: u
  select case (status)
  case (SF_UNDEFINED)
    write (u, "(1x,'[',A,']')") "undefined"
  case (SF_INITIAL)
    write (u, "(1x,'[',A,']')") "initialized"
  case (SF_DONE_LINKS)
    write (u, "(1x,'[',A,']')") "links set"
  case (SF_FAILED_MASK)
    write (u, "(1x,'[',A,']')") "mask mismatch"
  case (SF_DONE_MASK)
    write (u, "(1x,'[',A,']')") "mask set"
  case (SF_FAILED_CONNECTIONS)
    write (u, "(1x,'[',A,']')") "connections failed"
  case (SF_DONE_CONNECTIONS)
    write (u, "(1x,'[',A,']')") "connections set"
  case (SF_SEED_KINEMATICS)
    write (u, "(1x,'[',A,']')") "incoming momenta set"
  case (SF_FAILED_KINEMATICS)
    write (u, "(1x,'[',A,']')") "kinematics failed"
  case (SF_DONE_KINEMATICS)
    write (u, "(1x,'[',A,']')") "kinematics set"
  case (SF_FAILED_EVALUATION)
    write (u, "(1x,'[',A,']')") "evaluation failed"
  case (SF_EVALUATED)
    write (u, "(1x,'[',A,']')") "evaluated"
  end select
end subroutine write_sf_status
```

This is the basic output routine. Display status and interaction.

```
<SF base: sf int: TBP>=
procedure :: base_write => sf_int_base_write

<SF base: sub interfaces>+=
module subroutine sf_int_base_write (object, unit, testflag)
  class(sf_int_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
end subroutine sf_int_base_write

<SF base: procedures>+=
module subroutine sf_int_base_write (object, unit, testflag)
  class(sf_int_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
```

```

write (u, "(1x,A)", advance="no") "SF instance:"
call write_sf_status (object%status, u)
if (allocated (object%beam_index)) &
    write (u, "(3x,A,2(1x,I0))") "beam      =", object%beam_index
if (allocated (object%incoming)) &
    write (u, "(3x,A,2(1x,I0))") "incoming =", object%incoming
if (allocated (object%radiated)) &
    write (u, "(3x,A,2(1x,I0))") "radiated  =", object%radiated
if (allocated (object%outgoing)) &
    write (u, "(3x,A,2(1x,I0))") "outgoing  =", object%outgoing
if (allocated (object%par_index)) &
    write (u, "(3x,A,2(1x,I0))") "parameter =", object%par_index
if (object%qmin_defined) &
    write (u, "(3x,A,1x," // FMT_19 // ")") "q_min      =", object%qmin
if (object%qmax_defined) &
    write (u, "(3x,A,1x," // FMT_19 // ")") "q_max      =", object%qmax
call object%interaction_t%basic_write (u, testflag = testflag)
end subroutine sf_int_base_write

```

The type string identifies the structure function class, and possibly more details about the structure function.

```

<SF base: sf_int: TBP>+≡
    procedure (sf_int_type_string), deferred :: type_string

<SF base: interfaces>+≡
    abstract interface
        function sf_int_type_string (object) result (string)
            import
            class(sf_int_t), intent(in) :: object
            type(string_t) :: string
        end function sf_int_type_string
    end interface

```

Output of the concrete object. We should not forget to call the output routine for the base type.

```

<SF base: sf_int: TBP>+≡
    procedure (sf_int_write), deferred :: write

<SF base: interfaces>+≡
    abstract interface
        subroutine sf_int_write (object, unit, testflag)
            import
            class(sf_int_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: testflag
        end subroutine sf_int_write
    end interface

```

Basic initialization: set the invariant masses for the particles and initialize the interaction. The caller should then add states to the interaction and freeze it.

The dimension of the mask should be equal to the sum of the dimensions of the mass-squared arrays, which determine incoming, radiated, and outgoing particles, respectively.

Optionally, we can define minimum and maximum values for the momentum transfer to the outgoing particle(s). If all masses are zero, this is actually required for non-collinear splitting.

```

<SF base: sf_int: TBP>+≡
  procedure :: base_init => sf_int_base_init

<SF base: sub interfaces>+≡
  module subroutine sf_int_base_init &
    (sf_int, mask, mi2, mr2, mo2, qmin, qmax, hel_lock)
    class(sf_int_t), intent(out) :: sf_int
    type (quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    real(default), dimension(:), intent(in) :: mi2, mr2, mo2
    real(default), dimension(:), intent(in), optional :: qmin, qmax
    integer, dimension(:), intent(in), optional :: hel_lock
  end subroutine sf_int_base_init

<SF base: procedures>+≡
  module subroutine sf_int_base_init &
    (sf_int, mask, mi2, mr2, mo2, qmin, qmax, hel_lock)
    class(sf_int_t), intent(out) :: sf_int
    type (quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    real(default), dimension(:), intent(in) :: mi2, mr2, mo2
    real(default), dimension(:), intent(in), optional :: qmin, qmax
    integer, dimension(:), intent(in), optional :: hel_lock
    allocate (sf_int%mi2 (size (mi2)))
    sf_int%mi2 = mi2
    allocate (sf_int%mr2 (size (mr2)))
    sf_int%mr2 = mr2
    allocate (sf_int%mo2 (size (mo2)))
    sf_int%mo2 = mo2
    if (present (qmin)) then
      sf_int%qmin_defined = .true.
      allocate (sf_int%qmin (size (qmin)))
      sf_int%qmin = qmin
    end if
    if (present (qmax)) then
      sf_int%qmax_defined = .true.
      allocate (sf_int%qmax (size (qmax)))
      sf_int%qmax = qmax
    end if
    call sf_int%interaction_t%basic_init &
      (size (mi2), 0, size (mr2) + size (mo2), &
       mask = mask, hel_lock = hel_lock, set_relations = .true.)
  end subroutine sf_int_base_init

```

Set the indices of the incoming, radiated, and outgoing particles, respectively.

```

<SF base: sf_int: TBP>+≡
  procedure :: set_incoming => sf_int_set_incoming
  procedure :: set_radiated => sf_int_set_radiated
  procedure :: set_outgoing => sf_int_set_outgoing

<SF base: sub interfaces>+≡
  module subroutine sf_int_set_incoming (sf_int, incoming)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: incoming

```

```

end subroutine sf_int_set_incoming
module subroutine sf_int_set_radiated (sf_int, radiated)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: radiated
end subroutine sf_int_set_radiated
module subroutine sf_int_set_outgoing (sf_int, outgoing)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: outgoing
end subroutine sf_int_set_outgoing

<SF base: procedures>+=
module subroutine sf_int_set_incoming (sf_int, incoming)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: incoming
  allocate (sf_int%incoming (size (incoming)))
  sf_int%incoming = incoming
end subroutine sf_int_set_incoming

module subroutine sf_int_set_radiated (sf_int, radiated)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: radiated
  allocate (sf_int%radiated (size (radiated)))
  sf_int%radiated = radiated
end subroutine sf_int_set_radiated

module subroutine sf_int_set_outgoing (sf_int, outgoing)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: outgoing
  allocate (sf_int%outgoing (size (outgoing)))
  sf_int%outgoing = outgoing
end subroutine sf_int_set_outgoing

```

Initialization. This proceeds via an abstract data object, which for the actual implementation should have the matching concrete type. Since all implementations have the same signature, we can prepare a deferred procedure. The data object will become the target of a corresponding pointer within the `sf_int_t` implementation.

This should call the previous procedure.

```

<SF base: sf_int: TBP>+=
  procedure (sf_int_init), deferred :: init

<SF base: interfaces>+=
  abstract interface
    subroutine sf_int_init (sf_int, data)
      import
      class(sf_int_t), intent(out) :: sf_int
      class(sf_data_t), intent(in), target :: data
    end subroutine sf_int_init
  end interface

```

Complete initialization. This routine contains initializations that can only be performed after the interaction object got its final shape, i.e., redundant helicities have been eliminated by matching with beams and process.

The default implementation does nothing.

The **target** attribute is formally required since some overriding implementations use a temporary pointer (iterator) to the state-matrix component. It doesn't appear to make a real difference, though.

```

<SF base: sf_int: TBP>+≡
  procedure :: setup_constants => sf_int_setup_constants

<SF base: sub interfaces>+≡
  module subroutine sf_int_setup_constants (sf_int)
    class(sf_int_t), intent(inout), target :: sf_int
  end subroutine sf_int_setup_constants

<SF base: procedures>+≡
  module subroutine sf_int_setup_constants (sf_int)
    class(sf_int_t), intent(inout), target :: sf_int
  end subroutine sf_int_setup_constants

```

Set beam indices, i.e., the beam(s) on which this structure function applies.

```

<SF base: sf_int: TBP>+≡
  procedure :: set_beam_index => sf_int_set_beam_index

<SF base: sub interfaces>+≡
  module subroutine sf_int_set_beam_index (sf_int, beam_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: beam_index
  end subroutine sf_int_set_beam_index

<SF base: procedures>+≡
  module subroutine sf_int_set_beam_index (sf_int, beam_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: beam_index
    allocate (sf_int%beam_index (size (beam_index)))
    sf_int%beam_index = beam_index
  end subroutine sf_int_set_beam_index

```

Set parameter indices, indicating which MC input parameters are to be used for evaluating this structure function.

```

<SF base: sf_int: TBP>+≡
  procedure :: set_par_index => sf_int_set_par_index

<SF base: sub interfaces>+≡
  module subroutine sf_int_set_par_index (sf_int, par_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: par_index
  end subroutine sf_int_set_par_index

<SF base: procedures>+≡
  module subroutine sf_int_set_par_index (sf_int, par_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: par_index
    allocate (sf_int%par_index (size (par_index)))
    sf_int%par_index = par_index
  end subroutine sf_int_set_par_index

```

Initialize the structure-function kinematics, setting incoming momenta. We assume that array shapes match.

Three versions. The first version relies on the momenta being linked to another interaction. The second version sets the momenta explicitly. In the third version, we first compute momenta for the specified energies and store those.

```
(SF base: sf_int: TBP)+≡
  generic :: seed_kinematics => sf_int_receive_momenta
  generic :: seed_kinematics => sf_int_seed_momenta
  generic :: seed_kinematics => sf_int_seed_energies
  procedure :: sf_int_receive_momenta
  procedure :: sf_int_seed_momenta
  procedure :: sf_int_seed_energies
```

```
(SF base: sub interfaces)+≡
  module subroutine sf_int_receive_momenta (sf_int)
    class(sf_int_t), intent(inout) :: sf_int
  end subroutine sf_int_receive_momenta
  module subroutine sf_int_seed_momenta (sf_int, k)
    class(sf_int_t), intent(inout) :: sf_int
    type(vector4_t), dimension(:), intent(in) :: k
  end subroutine sf_int_seed_momenta
  module subroutine sf_int_seed_energies (sf_int, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: E
    type(vector4_t), dimension(:), allocatable :: k
  end subroutine sf_int_seed_energies
```

```
(SF base: procedures)+≡
  module subroutine sf_int_receive_momenta (sf_int)
    class(sf_int_t), intent(inout) :: sf_int
    if (sf_int%status >= SF_INITIAL) then
      call sf_int%receive_momenta ()
      sf_int%status = SF_SEED_KINEMATICS
    end if
  end subroutine sf_int_receive_momenta

  module subroutine sf_int_seed_momenta (sf_int, k)
    class(sf_int_t), intent(inout) :: sf_int
    type(vector4_t), dimension(:), intent(in) :: k
    if (sf_int%status >= SF_INITIAL) then
      call sf_int%set_momenta (k, outgoing=.false.)
      sf_int%status = SF_SEED_KINEMATICS
    end if
  end subroutine sf_int_seed_momenta

  module subroutine sf_int_seed_energies (sf_int, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: E
    type(vector4_t), dimension(:), allocatable :: k
    integer :: j
    if (sf_int%status >= SF_INITIAL) then
      allocate (k (size (E)))
      if (all (E**2 >= sf_int%mi2)) then
        do j = 1, size (E)
```

```

        k(j) = vector4_moving (E(j), &
            (3-2*j) * sqrt (E(j)**2 - sf_int%mi2(j)), 3)
    end do
    call sf_int%seed_kinematics (k)
end if
end if
end subroutine sf_int_seed_energies

```

Tell if in generator mode. By default, this is false. To be overridden where appropriate; we may refer to the `is_generator` method of the `data` component in the concrete type.

```

<SF base: sf_int: TBP>+≡
    procedure :: is_generator => sf_int_is_generator

<SF base: sub interfaces>+≡
    module function sf_int_is_generator (sf_int) result (flag)
        class(sf_int_t), intent(in) :: sf_int
        logical :: flag
    end function sf_int_is_generator

<SF base: procedures>+≡
    module function sf_int_is_generator (sf_int) result (flag)
        class(sf_int_t), intent(in) :: sf_int
        logical :: flag
        flag = .false.
    end function sf_int_is_generator

```

Generate free parameters `r`. Parameters are free if they do not correspond to integration parameters (i.e., are bound), but are generated by the structure function object itself. By default, all parameters are bound, and the output values of this procedure will be discarded. With free parameters, we have to override this procedure.

The value `x_free` is the renormalization factor of the total energy that corresponds to the free parameters. If there are no free parameters, the procedure will not change its value, which starts as unity. Otherwise, the fraction is typically decreased, but may also be increased in some cases.

```

<SF base: sf_int: TBP>+≡
    procedure :: generate_free => sf_int_generate_free

<SF base: sub interfaces>+≡
    module subroutine sf_int_generate_free (sf_int, r, rb, x_free)
        class(sf_int_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
    end subroutine sf_int_generate_free

<SF base: procedures>+≡
    module subroutine sf_int_generate_free (sf_int, r, rb, x_free)
        class(sf_int_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        r = 0
        rb = 1
    end subroutine sf_int_generate_free

```

Complete the structure-function kinematics, derived from an input parameter (array) r between 0 and 1. The interaction momenta are calculated, and we return x (the momentum fraction), and f (the Jacobian factor for the map $r \rightarrow x$), if `map` is set.

If the `map` flag is unset, r and x values will coincide, and f will become unity. If it is set, the structure-function implementation chooses a convenient mapping from r to x with Jacobian f .

In the `inverse_kinematics` variant, we exchange the intent of `x` and `r`. The momenta are calculated only if the optional flag `set_momenta` is present and set. Internal parameters of `sf_int` are calculated only if the optional flag `set_x` is present and set.

Update 2018-08-22: Throughout this algorithm, we now carry $xb=1-x$ together with x values, as we did for `r` before. This allows us to handle unstable endpoint numerics wherever necessary. The only place where the changes actually did matter was for inverse kinematics in the ISR setup, with a very soft photon, but it might be most sensible to apply the extension with `xb` everywhere.

```

(SF base: sf_int: TBP)+≡
  procedure (sf_int_complete_kinematics), deferred :: complete_kinematics
  procedure (sf_int_inverse_kinematics), deferred :: inverse_kinematics

(SF base: interfaces)+≡
  abstract interface
    subroutine sf_int_complete_kinematics (sf_int, x, xb, f, r, rb, map)
      import
      class(sf_int_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(out) :: x
      real(default), dimension(:), intent(out) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(in) :: r
      real(default), dimension(:), intent(in) :: rb
      logical, intent(in) :: map
    end subroutine sf_int_complete_kinematics
  end interface

  abstract interface
    subroutine sf_int_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
      import
      class(sf_int_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(in) :: x
      real(default), dimension(:), intent(in) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(out) :: r
      real(default), dimension(:), intent(out) :: rb
      logical, intent(in) :: map
      logical, intent(in), optional :: set_momenta
    end subroutine sf_int_inverse_kinematics
  end interface

```

Single splitting: compute momenta, given x input parameters. We assume that the incoming momentum is set. The status code is set to `SF_FAILED_KINEMATICS` if the x array does not correspond to a valid momentum configuration. Otherwise, it is updated to `SF_DONE_KINEMATICS`.

We force the outgoing particle on-shell. The on-shell projection is determined by the `on_shell_mode`. The radiated particle should already be on shell.

```

(SF base: sf_int: TBP)+≡
  procedure :: split_momentum => sf_int_split_momentum

(SF base: sub interfaces)+≡
  module subroutine sf_int_split_momentum (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
  end subroutine sf_int_split_momentum

(SF base: procedures)+≡
  module subroutine sf_int_split_momentum (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    type(splitting_data_t) :: sd
    real(default) :: E1, E2
    logical :: fail
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      k = sf_int%get_momentum (1)
      call sd%init (k, &
        sf_int%mi2(1), sf_int%mr2(1), sf_int%mo2(1), &
        collinear = size (x) == 1)
      call sd%set_t_bounds (x(1), xb(1))
      select case (size (x))
      case (1)
      case (3)
        if (sf_int%qmax_defined) then
          if (sf_int%qmin_defined) then
            call sd%sample_t (x(2), &
              t0 = - sf_int%qmax(1) ** 2, t1 = - sf_int%qmin(1) ** 2)
          else
            call sd%sample_t (x(2), &
              t0 = - sf_int%qmax(1) ** 2)
          end if
        else
          if (sf_int%qmin_defined) then
            call sd%sample_t (x(2), t1 = - sf_int%qmin(1) ** 2)
          else
            call sd%sample_t (x(2))
          end if
        end if
        call sd%sample_phi (x(3))
      case default
        call msg_bug ("Structure function: impossible number of parameters")
      end select
      q = sd%split_momentum (k)
      call on_shell (q, [sf_int%mr2, sf_int%mo2], &
        sf_int%on_shell_mode)
      call sf_int%set_momenta (q, outgoing=.true.)
      E1 = energy (q(1))
    end if
  end subroutine

```

```

      E2 = energy (q(2))
      fail = E1 < 0 .or. E2 < 0 &
        .or. E1 ** 2 < sf_int%mr2(1) &
        .or. E2 ** 2 < sf_int%mo2(1)
      if (fail) then
        sf_int%status = SF_FAILED_KINEMATICS
      else
        sf_int%status = SF_DONE_KINEMATICS
      end if
    end if
  end if
end subroutine sf_int_split_momentum

```

Pair splitting: two incoming momenta, two radiated, two outgoing. This is simple because we insist on all momenta being collinear.

(SF base: sf_int: TBP)+≡

```

  procedure :: split_momenta => sf_int_split_momenta

```

(SF base: sub interfaces)+≡

```

  module subroutine sf_int_split_momenta (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
  end subroutine sf_int_split_momenta

```

(SF base: procedures)+≡

```

  module subroutine sf_int_split_momenta (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(4) :: q
    real(default), dimension(4) :: E
    logical :: fail
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      select case (size (x))
      case (2)
      case default
        call msg_bug ("Pair structure function: recoil requested &
          &but not implemented yet")
      end select
      k(1) = sf_int%get_momentum (1)
      k(2) = sf_int%get_momentum (2)
      q(1:2) = xb * k
      q(3:4) = x * k
      select case (size (sf_int%mr2))
      case (2)
        call on_shell (q, &
          [sf_int%mr2(1), sf_int%mr2(2), &
          sf_int%mo2(1), sf_int%mo2(2)], &
          sf_int%on_shell_mode)
        call sf_int%set_momenta (q, outgoing=.true.)
        E = energy (q)
        fail = any (E < 0) &
          .or. any (E(1:2) ** 2 < sf_int%mr2) &
          .or. any (E(3:4) ** 2 < sf_int%mo2)
      end case
    end if
  end subroutine sf_int_split_momenta

```

```

        case default; call msg_bug ("split momenta: incorrect use")
    end select
    if (fail) then
        sf_int%status = SF_FAILED_KINEMATICS
    else
        sf_int%status = SF_DONE_KINEMATICS
    end if
end if
end if
end subroutine sf_int_split_momenta

```

Pair spectrum: the reduced version of the previous splitting, without radiated momenta.

<SF base: sf_int: TBP>+≡

```

    procedure :: reduce_momenta => sf_int_reduce_momenta

```

<SF base: sub interfaces>+≡

```

    module subroutine sf_int_reduce_momenta (sf_int, x)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    end subroutine sf_int_reduce_momenta

```

<SF base: procedures>+≡

```

    module subroutine sf_int_reduce_momenta (sf_int, x)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(2) :: q
    real(default), dimension(2) :: E
    logical :: fail
    if (sf_int%status >= SF_SEED_KINEMATICS) then
        select case (size(x))
        case (2)
        case default
            call msg_bug ("Pair spectrum: recoil requested &
                &but not implemented yet")
        end select
        k(1) = sf_int%get_momentum (1)
        k(2) = sf_int%get_momentum (2)
        q = x * k
        call on_shell (q, &
            [sf_int%mo2(1), sf_int%mo2(2)], &
            sf_int%on_shell_mode)
        call sf_int%set_momenta (q, outgoing=.true.)
        E = energy (q)
        fail = any (E < 0) &
            .or. any (E ** 2 < sf_int%mo2)
        if (fail) then
            sf_int%status = SF_FAILED_KINEMATICS
        else
            sf_int%status = SF_DONE_KINEMATICS
        end if
    end if
end if
end subroutine sf_int_reduce_momenta

```

The inverse procedure: we compute the x array from the momentum configuration. In an overriding TBP, we may also set internal data that depend on this, for convenience.

NOTE: Here and above, the single-particle case is treated in detail, allowing for non-collinearity and non-vanishing masses and nontrivial momentum-transfer bounds. For the pair case, we currently implement only collinear splitting and assume massless particles. This should be improved.

Update 2017-08-22: recover also xb , using the updated `recover` method of the splitting-data object. Th

```

(SF base: sf_int: TBP)+≡
  procedure :: recover_x => sf_int_recover_x
  procedure :: base_recover_x => sf_int_recover_x

(SF base: sub interfaces)+≡
  module subroutine sf_int_recover_x (sf_int, x, xb, x_free)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_int_recover_x

(SF base: procedures)+≡
  module subroutine sf_int_recover_x (sf_int, x, xb, x_free)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    type(vector4_t), dimension(:), allocatable :: k
    type(vector4_t), dimension(:), allocatable :: q
    type(splitting_data_t) :: sd
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      allocate (k (sf_int%interaction_t%get_n_in ()))
      allocate (q (sf_int%interaction_t%get_n_out ()))
      k = sf_int%get_momenta (outgoing=.false.)
      q = sf_int%get_momenta (outgoing=.true.)
      select case (size (k))
      case (1)
        call sd%init (k(1), &
                     sf_int%mi2(1), sf_int%mr2(1), sf_int%mo2(1), &
                     collinear = size (x) == 1)
        call sd%recover (k(1), q, sf_int%on_shell_mode)
        x(1) = sd%get_x ()
        xb(1) = sd%get_xb ()
        select case (size (x))
        case (1)
        case (3)
          if (sf_int%qmax_defined) then
            if (sf_int%qmin_defined) then
              call sd%inverse_t (x(2), &
                                t0 = - sf_int%qmax(1) ** 2, t1 = - sf_int%qmin(1) ** 2)
            else
              call sd%inverse_t (x(2), &
                                t0 = - sf_int%qmax(1) ** 2)
            end if
          end if
        end select
      end select
    end if
  end subroutine sf_int_recover_x

```



```

else
  if (sf_int%qmin_defined) then
    call sd%inverse_t (x(2), t1 = - sf_int%qmin(1) ** 2)
  else
    call sd%inverse_t (x(2))
  end if
end if
call sd%inverse_phi (x(3))
xb(2:3) = 1 - x(2:3)
case default
  call msg_bug ("Structure function: impossible number &
    &of parameters")
end select
case (2)
  select case (size (x))
  case (2)
  case default
    call msg_bug ("Pair structure function: recoil requested &
      &but not implemented yet")
  end select
  select case (sf_int%on_shell_mode)
  case (KEEP_ENERGY)
    select case (size (q))
    case (4)
      x = energy (q(3:4)) / energy (k)
      xb= energy (q(1:2)) / energy (k)
    case (2)
      x = energy (q) / energy (k)
      xb= 1 - x
    end select
  case (KEEP_MOMENTUM)
    select case (size (q))
    case (4)
      x = longitudinal_part (q(3:4)) / longitudinal_part (k)
      xb= longitudinal_part (q(1:2)) / longitudinal_part (k)
    case (2)
      x = longitudinal_part (q) / longitudinal_part (k)
      xb= 1 - x
    end select
  end select
end select
end if
end subroutine sf_int_recover_x

```

Apply the structure function, i.e., evaluate the interaction. For the calculation, we may use the stored momenta, any further information stored inside the `sf_int` implementation during kinematics setup, and the given energy scale. It may happen that for the given kinematics the value is not defined. This should be indicated by the status code.

```

⟨SF base: sf_int: TBP⟩+≡
  procedure (sf_int_apply), deferred :: apply
⟨SF base: interfaces⟩+≡
  abstract interface

```

```

subroutine sf_int_apply (sf_int, scale, negative_sf, rescale, i_sub)
  import
  class(sf_int_t), intent(inout) :: sf_int
  real(default), intent(in) :: scale
  logical, intent(in), optional :: negative_sf
  class(sf_rescale_t), intent(in), optional :: rescale
  integer, intent(in), optional :: i_sub
end subroutine sf_int_apply
end interface

```

16.5.5 Accessing the structure function

Return metadata. Once `interaction_t` is rewritten in OO, some of this will be inherited.

The number of outgoing particles is equal to the number of incoming particles. The radiated particles are the difference.

(SF base: sf_int: TBP)+≡

```

procedure :: get_n_in => sf_int_get_n_in
procedure :: get_n_rad => sf_int_get_n_rad
procedure :: get_n_out => sf_int_get_n_out

```

(SF base: sub interfaces)+≡

```

pure module function sf_int_get_n_in (object) result (n_in)
  class(sf_int_t), intent(in) :: object
  integer :: n_in
end function sf_int_get_n_in
pure module function sf_int_get_n_rad (object) result (n_rad)
  class(sf_int_t), intent(in) :: object
  integer :: n_rad
end function sf_int_get_n_rad
pure module function sf_int_get_n_out (object) result (n_out)
  class(sf_int_t), intent(in) :: object
  integer :: n_out
end function sf_int_get_n_out

```

(SF base: procedures)+≡

```

pure module function sf_int_get_n_in (object) result (n_in)
  class(sf_int_t), intent(in) :: object
  integer :: n_in
  n_in = object%interaction_t%get_n_in ()
end function sf_int_get_n_in

pure module function sf_int_get_n_rad (object) result (n_rad)
  class(sf_int_t), intent(in) :: object
  integer :: n_rad
  n_rad = object%interaction_t%get_n_out () &
    - object%interaction_t%get_n_in ()
end function sf_int_get_n_rad

pure module function sf_int_get_n_out (object) result (n_out)
  class(sf_int_t), intent(in) :: object
  integer :: n_out
  n_out = object%interaction_t%get_n_in ()

```

```
end function sf_int_get_n_out
```

Number of matrix element entries in the interaction:

```
<SF base: sf_int: TBP>+≡
  procedure :: get_n_states => sf_int_get_n_states

<SF base: sub interfaces>+≡
  module function sf_int_get_n_states (sf_int) result (n_states)
    class(sf_int_t), intent(in) :: sf_int
    integer :: n_states
  end function sf_int_get_n_states

<SF base: procedures>+≡
  module function sf_int_get_n_states (sf_int) result (n_states)
    class(sf_int_t), intent(in) :: sf_int
    integer :: n_states
    n_states = sf_int%get_n_matrix_elements ()
  end function sf_int_get_n_states
```

Return a specific state as a quantum-number array.

```
<SF base: sf_int: TBP>+≡
  procedure :: get_state => sf_int_get_state

<SF base: sub interfaces>+≡
  module function sf_int_get_state (sf_int, i) result (qn)
    class(sf_int_t), intent(in) :: sf_int
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer, intent(in) :: i
  end function sf_int_get_state

<SF base: procedures>+≡
  module function sf_int_get_state (sf_int, i) result (qn)
    class(sf_int_t), intent(in) :: sf_int
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer, intent(in) :: i
    allocate (qn (sf_int%get_n_tot ()))
    qn = sf_int%get_quantum_numbers (i)
  end function sf_int_get_state
```

Return the matrix-element values for all states. We can assume that the matrix elements are real, so we take the real part.

```
<SF base: sf_int: TBP>+≡
  procedure :: get_values => sf_int_get_values

<SF base: sub interfaces>+≡
  module subroutine sf_int_get_values (sf_int, value)
    class(sf_int_t), intent(in) :: sf_int
    real(default), dimension(:), intent(out) :: value
  end subroutine sf_int_get_values

<SF base: procedures>+≡
  module subroutine sf_int_get_values (sf_int, value)
    class(sf_int_t), intent(in) :: sf_int
    real(default), dimension(:), intent(out) :: value
    integer :: i
```

```

if (sf_int%status >= SF_EVALUATED) then
  do i = 1, size (value)
    value(i) = real (sf_int%get_matrix_element (i))
  end do
else
  value = 0
end if
end subroutine sf_int_get_values

```

16.5.6 Direct calculations

Compute a structure function value (array) directly, given an array of x values and a scale. If the energy is also given, we initialize the kinematics for that energy, otherwise take it from a previous run.

We assume that the E array has dimension n_in , and the x array has n_par .

Note: the output x values (xx and xxb) are unused in this use case.

```

<SF base: sf_int: TBP>+≡
  procedure :: compute_values => sf_int_compute_values

<SF base: sub interfaces>+≡
  module subroutine sf_int_compute_values (sf_int, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
  end subroutine sf_int_compute_values

<SF base: procedures>+≡
  module subroutine sf_int_compute_values (sf_int, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
    real(default), dimension(size (x)) :: xx, xxb
    real(default) :: f
    if (present (E)) call sf_int%seed_kinematics (E)
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      call sf_int%complete_kinematics (xx, xxb, f, x, xb, map=.false.)
      call sf_int%apply (scale)
      call sf_int%get_values (value)
      value = value * f
    else
      value = 0
    end if
  end subroutine sf_int_compute_values

```

Compute just a single value for one of the states, i.e., throw the others away.

```

<SF base: sf_int: TBP>+≡
  procedure :: compute_value => sf_int_compute_value

```

```

<SF base: sub interfaces>+≡
  module subroutine sf_int_compute_value &
    (sf_int, i_state, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    integer, intent(in) :: i_state
    real(default), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
  end subroutine sf_int_compute_value

<SF base: procedures>+≡
  module subroutine sf_int_compute_value &
    (sf_int, i_state, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    integer, intent(in) :: i_state
    real(default), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
    real(default), dimension(:), allocatable :: value_array
    if (sf_int%status >= SF_INITIAL) then
      allocate (value_array (sf_int%get_n_states ()))
      call sf_int%compute_values (value_array, x, xb, scale, E)
      value = value_array(i_state)
    else
      value = 0
    end if
  end subroutine sf_int_compute_value

```

16.5.7 Structure-function instance

This is a wrapper for `sf_int_t` objects, such that we can build an array with different structure-function types. The structure-function contains an array (a sequence) of `sf_int_t` objects.

The object, it holds the evaluator that connects the preceding part of the structure-function chain to the current interaction.

It also stores the input and output parameter values for the contained structure function. The `r` array has a second dimension, corresponding to the mapping channels in a multi-channel configuration. There is a Jacobian entry `f` for each channel. The corresponding logical array `mapping` tells whether we apply the mapping appropriate for the current structure function in this channel. The `x` parameter values (energy fractions) are common to all channels.

```

<SF base: types>+≡
  type :: sf_instance_t
    class(sf_int_t), allocatable :: int
    type(evaluator_t) :: eval
    real(default), dimension(:, :), allocatable :: r
    real(default), dimension(:, :), allocatable :: rb
    real(default), dimension(:), allocatable :: f

```

```

    logical, dimension(:), allocatable :: m
    real(default), dimension(:), allocatable :: x
    real(default), dimension(:), allocatable :: xb
end type sf_instance_t

```

16.5.8 Structure-function chain

A chain is an array of structure functions `sf`, initiated by a beam setup. We do not use this directly for evaluation, but create instances with copies of the contained interactions.

`n_par` is the total number of parameters that is necessary for completely determining the structure-function chain. `n_bound` is the number of MC input parameters that are requested from the integrator. The difference of `n_par` and `n_bound` is the number of free parameters, which are generated by a structure-function object in generator mode.

```

<SF base: public>+≡
    public :: sf_chain_t

<SF base: types>+≡
    type, extends (beam_t) :: sf_chain_t
        type(beam_data_t), pointer :: beam_data => null ()
        integer :: n_in = 0
        integer :: n_strfun = 0
        integer :: n_par = 0
        integer :: n_bound = 0
        type(sf_instance_t), dimension(:), allocatable :: sf
        logical :: trace_enable = .false.
        integer :: trace_unit = 0
    contains
        <SF base: sf chain: TBP>
    end type sf_chain_t

```

Finalizer.

```

<SF base: sf chain: TBP>≡
    procedure :: final => sf_chain_final

<SF base: sub interfaces>+≡
    module subroutine sf_chain_final (object)
        class(sf_chain_t), intent(inout) :: object
    end subroutine sf_chain_final

<SF base: procedures>+≡
    module subroutine sf_chain_final (object)
        class(sf_chain_t), intent(inout) :: object
        integer :: i
        call object%final_tracing ()
        if (allocated (object%sf)) then
            do i = 1, size (object%sf, 1)
                associate (sf => object%sf(i))
                    if (allocated (sf%int)) then
                        call sf%int%final ()
                    end if
                end associate
            end do
        end if
    end subroutine sf_chain_final

```

```

        end do
    end if
    call beam_final (object%beam_t)
end subroutine sf_chain_final

```

Output.

```

⟨SF base: sf chain: TBP⟩+≡
    procedure :: write => sf_chain_write

⟨SF base: sub interfaces⟩+≡
    module subroutine sf_chain_write (object, unit)
        class(sf_chain_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine sf_chain_write

⟨SF base: procedures⟩+≡
    module subroutine sf_chain_write (object, unit)
        class(sf_chain_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Incoming particles / structure-function chain:"
        if (associated (object%beam_data)) then
            write (u, "(3x,A,I0)") "n_in      = ", object%n_in
            write (u, "(3x,A,I0)") "n_strfun  = ", object%n_strfun
            write (u, "(3x,A,I0)") "n_par     = ", object%n_par
            if (object%n_par /= object%n_bound) then
                write (u, "(3x,A,I0)") "n_bound  = ", object%n_bound
            end if
            call object%beam_data%write (u)
            call write_separator (u)
            call beam_write (object%beam_t, u)
            if (allocated (object%sf)) then
                do i = 1, object%n_strfun
                    associate (sf => object%sf(i))
                        call write_separator (u)
                        if (allocated (sf%int)) then
                            call sf%int%write (u)
                        else
                            write (u, "(1x,A)") "SF instance: [undefined]"
                        end if
                    end associate
                end do
            end if
        else
            write (u, "(3x,A)") "[undefined]"
        end if
    end subroutine sf_chain_write

```

Initialize: setup beams. The `beam_data` target must remain valid for the lifetime of the chain, since we just establish a pointer. The structure-function configuration array is used to initialize the individual structure-function entries. The target attribute is needed because the `sf_int` entries establish pointers to the

configuration data.

```

<SF base: sf chain: TBP>+≡
  procedure :: init => sf_chain_init

<SF base: sub interfaces>+≡
  module subroutine sf_chain_init (sf_chain, beam_data, sf_config)
    class(sf_chain_t), intent(out) :: sf_chain
    type(beam_data_t), intent(in), target :: beam_data
    type(sf_config_t), dimension(:), intent(in), optional, target :: sf_config
  end subroutine sf_chain_init

<SF base: procedures>+≡
  module subroutine sf_chain_init (sf_chain, beam_data, sf_config)
    class(sf_chain_t), intent(out) :: sf_chain
    type(beam_data_t), intent(in), target :: beam_data
    type(sf_config_t), dimension(:), intent(in), optional, target :: sf_config
    integer :: i
    sf_chain%beam_data => beam_data
    sf_chain%n_in = beam_data%get_n_in ()
    call beam_init (sf_chain%beam_t, beam_data)
    if (present (sf_config)) then
      sf_chain%n_strfun = size (sf_config)
      allocate (sf_chain%sf (sf_chain%n_strfun))
      do i = 1, sf_chain%n_strfun
        call sf_chain%set_strfun (i, sf_config(i)%i, sf_config(i)%data)
      end do
    end if
  end subroutine sf_chain_init

```

Receive the beam momenta from a source to which the beam interaction is linked.

```

<SF base: sf chain: TBP>+≡
  procedure :: receive_beam_momenta => sf_chain_receive_beam_momenta

<SF base: sub interfaces>+≡
  module subroutine sf_chain_receive_beam_momenta (sf_chain)
    class(sf_chain_t), intent(inout), target :: sf_chain
    type(interaction_t), pointer :: beam_int
  end subroutine sf_chain_receive_beam_momenta

<SF base: procedures>+≡
  module subroutine sf_chain_receive_beam_momenta (sf_chain)
    class(sf_chain_t), intent(inout), target :: sf_chain
    type(interaction_t), pointer :: beam_int
    beam_int => sf_chain%get_beam_int_ptr ()
    call beam_int%receive_momenta ()
  end subroutine sf_chain_receive_beam_momenta

```

Explicitly set the beam momenta.

```

<SF base: sf chain: TBP>+≡
  procedure :: set_beam_momenta => sf_chain_set_beam_momenta

<SF base: sub interfaces>+≡
  module subroutine sf_chain_set_beam_momenta (sf_chain, p)
    class(sf_chain_t), intent(inout) :: sf_chain

```



```

        type(vector4_t), dimension(:), intent(in) :: p
    end subroutine sf_chain_set_beam_momenta

<SF base: procedures>+=
    module subroutine sf_chain_set_beam_momenta (sf_chain, p)
        class(sf_chain_t), intent(inout) :: sf_chain
        type(vector4_t), dimension(:), intent(in) :: p
        call beam_set_momenta (sf_chain%beam_t, p)
    end subroutine sf_chain_set_beam_momenta

```

Set a structure-function entry. We use the data input to allocate the int structure-function instance with appropriate type, then initialize the entry. The entry establishes a pointer to data.

The index i is the structure-function index in the chain.

```

<SF base: sf chain: TBP>+=
    procedure :: set_strfun => sf_chain_set_strfun

<SF base: sub interfaces>+=
    module subroutine sf_chain_set_strfun (sf_chain, i, beam_index, data)
        class(sf_chain_t), intent(inout) :: sf_chain
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: beam_index
        class(sf_data_t), intent(in), target :: data
    end subroutine sf_chain_set_strfun

<SF base: procedures>+=
    module subroutine sf_chain_set_strfun (sf_chain, i, beam_index, data)
        class(sf_chain_t), intent(inout) :: sf_chain
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: beam_index
        class(sf_data_t), intent(in), target :: data
        integer :: n_par, j
        n_par = data%get_n_par ()
        call data%allocate_sf_int (sf_chain%sf(i)%int)
        associate (sf_int => sf_chain%sf(i)%int)
            call sf_int%init (data)
            call sf_int%set_beam_index (beam_index)
            call sf_int%set_par_index &
                ([ (j, j = sf_chain%n_par + 1, sf_chain%n_par + n_par)])
            sf_chain%n_par = sf_chain%n_par + n_par
            if (.not. data%is_generator ()) then
                sf_chain%n_bound = sf_chain%n_bound + n_par
            end if
        end associate
    end subroutine sf_chain_set_strfun

```

Return the number of structure-function parameters.

```

<SF base: sf chain: TBP>+=
    procedure :: get_n_par => sf_chain_get_n_par
    procedure :: get_n_bound => sf_chain_get_n_bound

<SF base: sub interfaces>+=
    module function sf_chain_get_n_par (sf_chain) result (n)
        class(sf_chain_t), intent(in) :: sf_chain
        integer :: n
    end function sf_chain_get_n_par

```

```

end function sf_chain_get_n_par
module function sf_chain_get_n_bound (sf_chain) result (n)
  class(sf_chain_t), intent(in) :: sf_chain
  integer :: n
end function sf_chain_get_n_bound

<SF base: procedures>+≡
module function sf_chain_get_n_par (sf_chain) result (n)
  class(sf_chain_t), intent(in) :: sf_chain
  integer :: n
  n = sf_chain%n_par
end function sf_chain_get_n_par

module function sf_chain_get_n_bound (sf_chain) result (n)
  class(sf_chain_t), intent(in) :: sf_chain
  integer :: n
  n = sf_chain%n_bound
end function sf_chain_get_n_bound

```

Return a pointer to the beam interaction.

```

<SF base: sf chain: TBP>+≡
  procedure :: get_beam_int_ptr => sf_chain_get_beam_int_ptr

<SF base: sub interfaces>+≡
  module function sf_chain_get_beam_int_ptr (sf_chain) result (int)
    type(interaction_t), pointer :: int
    class(sf_chain_t), intent(in), target :: sf_chain
  end function sf_chain_get_beam_int_ptr

<SF base: procedures>+≡
  module function sf_chain_get_beam_int_ptr (sf_chain) result (int)
    type(interaction_t), pointer :: int
    class(sf_chain_t), intent(in), target :: sf_chain
    int => beam_get_int_ptr (sf_chain%beam_t)
  end function sf_chain_get_beam_int_ptr

```

Enable the trace feature: record structure function data (input parameters, x values, evaluation result) to an external file.

```

<SF base: sf chain: TBP>+≡
  procedure :: setup_tracing => sf_chain_setup_tracing
  procedure :: final_tracing => sf_chain_final_tracing

<SF base: sub interfaces>+≡
  module subroutine sf_chain_setup_tracing (sf_chain, file)
    class(sf_chain_t), intent(inout) :: sf_chain
    type(string_t), intent(in) :: file
  end subroutine sf_chain_setup_tracing
  module subroutine sf_chain_final_tracing (sf_chain)
    class(sf_chain_t), intent(inout) :: sf_chain
  end subroutine sf_chain_final_tracing

<SF base: procedures>+≡
  module subroutine sf_chain_setup_tracing (sf_chain, file)
    class(sf_chain_t), intent(inout) :: sf_chain
    type(string_t), intent(in) :: file

```

```

    if (sf_chain%n_strfun > 0) then
        sf_chain%trace_enable = .true.
        sf_chain%trace_unit = free_unit ()
        open (sf_chain%trace_unit, file = char (file), action = "write", &
            status = "replace")
        call sf_chain%write_trace_header ()
    else
        call msg_error ("Beam structure: no structure functions, tracing &
            &disabled")
    end if
end subroutine sf_chain_setup_tracing

module subroutine sf_chain_final_tracing (sf_chain)
    class(sf_chain_t), intent(inout) :: sf_chain
    if (sf_chain%trace_enable) then
        close (sf_chain%trace_unit)
        sf_chain%trace_enable = .false.
    end if
end subroutine sf_chain_final_tracing

```

Write the header for the tracing file.

```

<SF base: sf chain: TBP>+≡
    procedure :: write_trace_header => sf_chain_write_trace_header

<SF base: sub interfaces>+≡
    module subroutine sf_chain_write_trace_header (sf_chain)
        class(sf_chain_t), intent(in) :: sf_chain
        end subroutine sf_chain_write_trace_header

<SF base: procedures>+≡
    module subroutine sf_chain_write_trace_header (sf_chain)
        class(sf_chain_t), intent(in) :: sf_chain
        integer :: u
        if (sf_chain%trace_enable) then
            u = sf_chain%trace_unit
            write (u, "('# ',A)") "WHIZARD output: &
                &structure-function sampling data"
            write (u, "('# ',A,1x,I0)") "Number of sf records:", sf_chain%n_strfun
            write (u, "('# ',A,1x,I0)") "Number of parameters:", sf_chain%n_par
            write (u, "('# ',A)") "Columns: channel, p(n_par), x(n_par), f, Jac * f"
        end if
    end subroutine sf_chain_write_trace_header

```

Write a record which collects the structure function data for the current data point. For the selected channel, we print first the input integration parameters, then the x values, then the structure-function value summed over all quantum numbers, then the structure function value times the mapping Jacobian.

```

<SF base: sf chain: TBP>+≡
    procedure :: trace => sf_chain_trace

<SF base: sub interfaces>+≡
    module subroutine sf_chain_trace (sf_chain, c_sel, p, x, f, sf_sum)
        class(sf_chain_t), intent(in) :: sf_chain
        integer, intent(in) :: c_sel
    end subroutine sf_chain_trace

```

```

        real(default), dimension(:,:), intent(in) :: p
        real(default), dimension(:), intent(in) :: x
        real(default), dimension(:), intent(in) :: f
        real(default), intent(in) :: sf_sum
    end subroutine sf_chain_trace
<SF base: procedures>+≡
module subroutine sf_chain_trace (sf_chain, c_sel, p, x, f, sf_sum)
    class(sf_chain_t), intent(in) :: sf_chain
    integer, intent(in) :: c_sel
    real(default), dimension(:,:), intent(in) :: p
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: f
    real(default), intent(in) :: sf_sum
    real(default) :: sf_sum_pac, f_sf_sum_pac
    integer :: u, i
    if (sf_chain%trace_enable) then
        u = sf_chain%trace_unit
        write (u, "(1x,I0)", advance="no") c_sel
        write (u, "(2x)", advance="no")
        do i = 1, sf_chain%n_par
            write (u, "(1x," // FMT_17 // ")", advance="no") p(i,c_sel)
        end do
        write (u, "(2x)", advance="no")
        do i = 1, sf_chain%n_par
            write (u, "(1x," // FMT_17 // ")", advance="no") x(i)
        end do
        write (u, "(2x)", advance="no")
        sf_sum_pac = sf_sum
        f_sf_sum_pac = f(c_sel) * sf_sum
        call pacify (sf_sum_pac, 1.E-28_default)
        call pacify (f_sf_sum_pac, 1.E-28_default)
        write (u, "(2(1x," // FMT_17 // "))" sf_sum_pac, f_sf_sum_pac
    end if
end subroutine sf_chain_trace

```

16.5.9 Chain instances

A structure-function chain instance contains copies of the interactions in the configuration chain, suitably linked to each other and connected by evaluators.

After initialization, `out_sf` should point, for each beam, to the last structure function that affects this beam. `out_sf_i` should indicate the index of the corresponding outgoing particle within that structure-function interaction.

Analogously, `out_eval` is the last evaluator in the structure-function chain, which contains the complete set of outgoing particles. `out_eval_i` should indicate the index of the outgoing particles, within that evaluator, which will initiate the collision.

When calculating actual kinematics, we fill the `p`, `r`, and `x` arrays and the `f` factor. The `p` array denotes the MC input parameters as they come from the random-number generator. The `r` array results from applying global mappings. The `x` array results from applying structure-function local mappings. The `x` values can be interpreted directly as momentum fractions (or angle fractions,

where recoil is involved). The **f** factor is the Jacobian that results from applying all mappings.

Update 2017-08-22: carry and output all complements (**pb**, **rb**, **xb**). Previously, **xb** was not included in the record, and the output did not contain either. It does become more verbose, however.

The **mapping** entry may store a global mapping that is applied to a combination of *x* values and structure functions, as opposed to mappings that affect only a single structure function. It is applied before the latter mappings, in the transformation from the **p** array to the **r** array. For parameters affected by this mapping, we should ensure that they are not involved in a local mapping.

```

<SF base: public>+≡
    public :: sf_chain_instance_t

<SF base: types>+≡
    type, extends (beam_t) :: sf_chain_instance_t
        type(sf_chain_t), pointer :: config => null ()
        integer :: status = SF_UNDEFINED
        type(sf_instance_t), dimension(:), allocatable :: sf
        integer, dimension(:), allocatable :: out_sf
        integer, dimension(:), allocatable :: out_sf_i
        integer :: out_eval = 0
        integer, dimension(:), allocatable :: out_eval_i
        integer :: selected_channel = 0
        real(default), dimension(:, :), allocatable :: p, pb
        real(default), dimension(:, :), allocatable :: r, rb
        real(default), dimension(:), allocatable :: f
        real(default), dimension(:), allocatable :: x, xb
        logical, dimension(:), allocatable :: bound
        real(default) :: x_free = 1
        type(sf_channel_t), dimension(:), allocatable :: channel
    contains
        <SF base: sf chain instance: TBP>
    end type sf_chain_instance_t

```

Finalizer.

```

<SF base: sf chain instance: TBP>≡
    procedure :: final => sf_chain_instance_final

<SF base: sub interfaces>+≡
    module subroutine sf_chain_instance_final (object)
        class(sf_chain_instance_t), intent(inout) :: object
    end subroutine sf_chain_instance_final

<SF base: procedures>+≡
    module subroutine sf_chain_instance_final (object)
        class(sf_chain_instance_t), intent(inout) :: object
        integer :: i
        if (allocated (object%sf)) then
            do i = 1, size (object%sf, 1)
                associate (sf => object%sf(i))
                    if (allocated (sf%int)) then
                        call sf%eval%final ()
                        call sf%int%final ()
                    end if
                end associate
            end do
        end if
    end subroutine sf_chain_instance_final

```

```

        end associate
    end do
end if
call beam_final (object%beam_t)
end subroutine sf_chain_instance_final

```

Output.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: write => sf_chain_instance_write

<SF base: sub interfaces>+≡
    module subroutine sf_chain_instance_write (object, unit, col_verbose)
        class(sf_chain_instance_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: col_verbose
    end subroutine sf_chain_instance_write

<SF base: procedures>+≡
    module subroutine sf_chain_instance_write (object, unit, col_verbose)
        class(sf_chain_instance_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: col_verbose
        integer :: u, i, c
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "Structure-function chain instance:"
        call write_sf_status (object%status, u)
        if (allocated (object%out_sf)) then
            write (u, "(3x,A)", advance="no") "outgoing (interactions) ="
            do i = 1, size (object%out_sf)
                write (u, "(1x,I0,':',I0)", advance="no") &
                    object%out_sf(i), object%out_sf_i(i)
            end do
            write (u, *)
        end if
        if (object%out_eval /= 0) then
            write (u, "(3x,A)", advance="no") "outgoing (evaluators) ="
            do i = 1, size (object%out_sf)
                write (u, "(1x,I0,':',I0)", advance="no") &
                    object%out_eval, object%out_eval_i(i)
            end do
            write (u, *)
        end if
        if (allocated (object%sf)) then
            if (size (object%sf) /= 0) then
                write (u, "(1x,A)") "Structure-function parameters:"
                do c = 1, size (object%f)
                    write (u, "(1x,A,I0,A)", advance="no") "Channel #", c, ":"
                    if (c == object%selected_channel) then
                        write (u, "(1x,A)") "[selected]"
                    else
                        write (u, *)
                    end if
                    write (u, "(3x,A,9(1x,F9.7))") "p =", object%p(:,c)
                    write (u, "(3x,A,9(1x,F9.7))") "pb=", object%pb(:,c)
                    write (u, "(3x,A,9(1x,F9.7))") "r =", object%r(:,c)
                end do
            end if
        end if
    end subroutine sf_chain_instance_write

```

```

        write (u, "(3x,A,9(1x,F9.7))") "rb=", object%rb(:,c)
        write (u, "(3x,A,9(1x,ES13.7))") "f=", object%f(c)
        write (u, "(3x,A)", advance="no") "m ="
        call object%channel(c)%write (u)
    end do
    write (u, "(3x,A,9(1x,F9.7))") "x =", object%x
    write (u, "(3x,A,9(1x,F9.7))") "xb=", object%xb
    if (.not. all (object%bound)) then
        write (u, "(3x,A,9(1x,L1))") "bound =", object%bound
    end if
end if
end if
call write_separator (u)
call beam_write (object%beam_t, u, col_verbose = col_verbose)
if (allocated (object%sf)) then
    do i = 1, size (object%sf)
        associate (sf => object%sf(i))
            call write_separator (u)
            if (allocated (sf%int)) then
                if (allocated (sf%r)) then
                    write (u, "(1x,A)") "Structure-function parameters:"
                    do c = 1, size (sf%f)
                        write (u, "(1x,A,I0,A)", advance="no") "Channel #", c, ":"
                        if (c == object%selected_channel) then
                            write (u, "(1x,A)") "[selected]"
                        else
                            write (u, *)
                        end if
                        write (u, "(3x,A,9(1x,F9.7))") "r =", sf%r(:,c)
                        write (u, "(3x,A,9(1x,F9.7))") "rb=", sf%rb(:,c)
                        write (u, "(3x,A,9(1x,ES13.7))") "f =", sf%f(c)
                        write (u, "(3x,A,9(1x,L1,7x))") "m =", sf%m(c)
                    end do
                    write (u, "(3x,A,9(1x,F9.7))") "x =", sf%x
                    write (u, "(3x,A,9(1x,F9.7))") "xb=", sf%xb
                end if
                call sf%int%write(u)
                if (.not. sf%eval%is_empty ()) then
                    call sf%eval%write (u, col_verbose = col_verbose)
                end if
            end if
        end associate
    end do
end if
end subroutine sf_chain_instance_write

```

Initialize. This creates a copy of the interactions in the configuration chain, assumed to be properly initialized. In the copy, we allocate the `p` etc. arrays.

The brute-force assignment of the `sf` component would be straightforward, but we provide a more fine-grained copy. In any case, the copy is deep as far as allocatables are concerned, but for the contained `interaction_t` objects the copy is shallow, as long as we do not bind defined assignment to the type. Therefore, we have to re-assign the `interaction_t` components explicitly, this time

calling the proper defined assignment. Furthermore, we allocate the parameter arrays for each structure function.

(SF base: sf chain instance: TBP)+≡

```
procedure :: init => sf_chain_instance_init
```

(SF base: sub interfaces)+≡

```
module subroutine sf_chain_instance_init (chain, config, n_channel)
  class(sf_chain_instance_t), intent(out), target :: chain
  type(sf_chain_t), intent(in), target :: config
  integer, intent(in) :: n_channel
end subroutine sf_chain_instance_init
```

(SF base: procedures)+≡

```
module subroutine sf_chain_instance_init (chain, config, n_channel)
  class(sf_chain_instance_t), intent(out), target :: chain
  type(sf_chain_t), intent(in), target :: config
  integer, intent(in) :: n_channel
  integer :: i, j
  integer :: n_par_tot, n_par, n_strfun
  chain%config => config
  n_strfun = config%n_strfun
  chain%beam_t = config%beam_t
  allocate (chain%out_sf (config%n_in), chain%out_sf_i (config%n_in))
  allocate (chain%out_eval_i (config%n_in))
  chain%out_sf = 0
  chain%out_sf_i = [(i, i = 1, config%n_in)]
  chain%out_eval_i = chain%out_sf_i
  n_par_tot = 0
  if (n_strfun /= 0) then
    allocate (chain%sf (n_strfun))
    do i = 1, n_strfun
      associate (sf => chain%sf(i))
        allocate (sf%int, source=config%sf(i)%int)
        sf%int%interaction_t = config%sf(i)%int%interaction_t
        n_par = size (sf%int%par_index)
        allocate (sf%r (n_par, n_channel)); sf%r = 0
        allocate (sf%rb(n_par, n_channel)); sf%rb= 0
        allocate (sf%f (n_channel)); sf%f = 0
        allocate (sf%m (n_channel)); sf%m = .false.
        allocate (sf%x (n_par)); sf%x = 0
        allocate (sf%xb(n_par)); sf%xb= 0
        n_par_tot = n_par_tot + n_par
      end associate
    end do
    allocate (chain%p (n_par_tot, n_channel)); chain%p = 0
    allocate (chain%pb(n_par_tot, n_channel)); chain%pb= 0
    allocate (chain%r (n_par_tot, n_channel)); chain%r = 0
    allocate (chain%rb(n_par_tot, n_channel)); chain%rb= 0
    allocate (chain%f (n_channel)); chain%f = 0
    allocate (chain%x (n_par_tot)); chain%x = 0
    allocate (chain%xb(n_par_tot)); chain%xb= 0
    call allocate_sf_channels &
      (chain%channel, n_channel=n_channel, n_strfun=n_strfun)
  end if
  allocate (chain%bound (n_par_tot), source = .true.)
```



```

do i = 1, n_strfun
  associate (sf => chain%sf(i))
    if (sf%int%is_generator ()) then
      do j = 1, size (sf%int%par_index)
        chain%bound(sf%int%par_index(j)) = .false.
      end do
    end if
  end associate
end do
chain%status = SF_INITIAL
end subroutine sf_chain_instance_init

```

Manually select a channel.

```

<SF base: sf chain instance: TBP>+≡
  procedure :: select_channel => sf_chain_instance_select_channel

<SF base: sub interfaces>+≡
  module subroutine sf_chain_instance_select_channel (chain, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in), optional :: channel
  end subroutine sf_chain_instance_select_channel

<SF base: procedures>+≡
  module subroutine sf_chain_instance_select_channel (chain, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in), optional :: channel
    if (present (channel)) then
      chain%selected_channel = channel
    else
      chain%selected_channel = 0
    end if
  end subroutine sf_chain_instance_select_channel

```

Copy a channel-mapping object to the structure-function chain instance. We assume that assignment is sufficient, i.e., any non-static components of the **channel** object are allocatable and thus recursively copied.

After the copy, we extract the single-entry mappings and activate them for the individual structure functions. If there is a multi-entry mapping, we obtain the corresponding MC parameter indices and set them in the copy of the channel object.

```

<SF base: sf chain instance: TBP>+≡
  procedure :: set_channel => sf_chain_instance_set_channel

<SF base: sub interfaces>+≡
  module subroutine sf_chain_instance_set_channel (chain, c, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in) :: c
    type(sf_channel_t), intent(in) :: channel
  end subroutine sf_chain_instance_set_channel

<SF base: procedures>+≡
  module subroutine sf_chain_instance_set_channel (chain, c, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in) :: c

```

```

type(sf_channel_t), intent(in) :: channel
integer :: i, j, k
if (chain%status >= SF_INITIAL) then
  chain%channel(c) = channel
  j = 0
  do i = 1, chain%config%n_strfun
    associate (sf => chain%sf(i))
      sf%m(c) = channel%is_single_mapping (i)
      if (channel%is_multi_mapping (i)) then
        do k = 1, size (sf%int%beam_index)
          j = j + 1
          call chain%channel(c)%set_par_index &
            (j, sf%int%par_index(k))
        end do
      end if
    end associate
  end do
  if (j /= chain%channel(c)%get_multi_mapping_n_par ()) then
    print *, "index last filled   = ", j
    print *, "number of parameters = ", &
      chain%channel(c)%get_multi_mapping_n_par ()
    call msg_bug ("Structure-function setup: mapping index mismatch")
  end if
  chain%status = SF_INITIAL
end if
end subroutine sf_chain_instance_set_channel

```

Link the interactions in the chain. First, link the beam instance to its template in the configuration chain, which should have the appropriate momenta fixed.

Then, we follow the chain via the arrays `out_sf` and `out_sf_i`. The arrays are (up to) two-dimensional, the entries correspond to the beam particle(s). For each beam, the entry `out_sf` points to the last interaction that affected this beam, and `out_sf_i` is the out-particle index within that interaction. For the initial beam, `out_sf` is zero by definition.

For each entry in the chain, we scan the affected beams (one or two). We look for `out_sf` and link the out-particle there to the corresponding in-particle in the current interaction. Then, we update the entry in `out_sf` and `out_sf_i` to point to the current interaction.

<SF base: sf chain instance: TBP>+≡

```

procedure :: link_interactions => sf_chain_instance_link_interactions

```

<SF base: sub interfaces>+≡

```

module subroutine sf_chain_instance_link_interactions (chain)
  class(sf_chain_instance_t), intent(inout), target :: chain
end subroutine sf_chain_instance_link_interactions

```

<SF base: procedures>+≡

```

module subroutine sf_chain_instance_link_interactions (chain)
  class(sf_chain_instance_t), intent(inout), target :: chain
  type(interaction_t), pointer :: int
  integer :: i, j, b
  if (chain%status >= SF_INITIAL) then
    do b = 1, chain%config%n_in
      int => beam_get_int_ptr (chain%beam_t)

```

```

        call interaction_set_source_link_beam (int, b, &
            chain%config%beam_t, b)
    end do
    if (allocated (chain%sf)) then
        do i = 1, size (chain%sf)
            associate (sf_int => chain%sf(i)%int)
                do j = 1, size (sf_int%beam_index)
                    b = sf_int%beam_index(j)
                    call link (sf_int%interaction_t, b, sf_int%incoming(j))
                    chain%out_sf(b) = i
                    chain%out_sf_i(b) = sf_int%outgoing(j)
                end do
            end associate
        end do
    end if
    chain%status = SF_DONE_LINKS
end if
contains
subroutine link (int, b, in_index)
    type(interaction_t), intent(inout) :: int
    integer, intent(in) :: b, in_index
    integer :: i
    i = chain%out_sf(b)
    select case (i)
        case (0)
            call interaction_set_source_link_beam (int, in_index, &
                chain%beam_t, chain%out_sf_i(b))
        case default
            call int%set_source_link (in_index, &
                chain%sf(i)%int, chain%out_sf_i(b))
    end select
end subroutine link
end subroutine sf_chain_instance_link_interactions

```

Exchange the quantum-number masks between the interactions in the chain, so we can combine redundant entries and detect any obvious mismatch.

We proceed first in the forward direction and then backwards again.

After this is finished, we finalize initialization by calling the `setup_constants` method, which prepares constant data that depend on the matrix element structure.

(SF base: sf chain instance: TBP)+≡

```

    procedure :: exchange_mask => sf_chain_exchange_mask

```

(SF base: sub interfaces)+≡

```

    module subroutine sf_chain_exchange_mask (chain)
        class(sf_chain_instance_t), intent(inout), target :: chain
    end subroutine sf_chain_exchange_mask

```

(SF base: procedures)+≡

```

    module subroutine sf_chain_exchange_mask (chain)
        class(sf_chain_instance_t), intent(inout), target :: chain
        type(interaction_t), pointer :: int
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        integer :: i

```

```

if (chain%status >= SF_DONE_LINKS) then
  if (allocated (chain%sf)) then
    int => beam_get_int_ptr (chain%beam_t)
    allocate (mask (int%get_n_out ()))
    mask = int%get_mask ()
    if (size (chain%sf) /= 0) then
      do i = 1, size (chain%sf) - 1
        call chain%sf(i)%int%exchange_mask ()
      end do
      do i = size (chain%sf), 1, -1
        call chain%sf(i)%int%exchange_mask ()
      end do
      if (any (mask .neqv. int%get_mask ())) then
        chain%status = SF_FAILED_MASK
        return
      end if
      do i = 1, size (chain%sf)
        call chain%sf(i)%int%setup_constants ()
      end do
    end if
  end if
  chain%status = SF_DONE_MASK
end if
end subroutine sf_chain_exchange_mask

```

Initialize the evaluators that connect the interactions in the chain.

(SF base: sf chain instance: TBP)+≡

```

procedure :: init_evaluators => sf_chain_instance_init_evaluators

```

(SF base: sub interfaces)+≡

```

module subroutine sf_chain_instance_init_evaluators (chain, extended_sf)
  class(sf_chain_instance_t), intent(inout), target :: chain
  logical, intent(in), optional :: extended_sf
end subroutine sf_chain_instance_init_evaluators

```

(SF base: procedures)+≡

```

module subroutine sf_chain_instance_init_evaluators (chain, extended_sf)
  class(sf_chain_instance_t), intent(inout), target :: chain
  logical, intent(in), optional :: extended_sf
  type(interaction_t), pointer :: int
  type(quantum_numbers_mask_t) :: mask
  integer :: i
  logical :: yorn
  yorn = .false.; if (present (extended_sf)) yorn = extended_sf
  if (chain%status >= SF_DONE_MASK) then
    if (allocated (chain%sf)) then
      if (size (chain%sf) /= 0) then
        mask = quantum_numbers_mask (.false., .false., .true.)
        int => beam_get_int_ptr (chain%beam_t)
        do i = 1, size (chain%sf)
          associate (sf => chain%sf(i))
            if (yorn) then
              if (int%get_n_sub () == 0) then
                call int%declare_subtraction (n_beams_rescaled)
              end if
            end if
          end associate
        end do
      end if
    end if
  end if

```

```

        if (sf%int%interaction_t%get_n_sub () == 0) then
            call sf%int%interaction_t%declare_subtraction (n_beams_rescaled)
        end if
    end if
    call sf%eval%init_product (int, sf%int%interaction_t, mask,&
        & ignore_sub_for_qn = .true.)
    if (sf%eval%is_empty ()) then
        chain%status = SF_FAILED_CONNECTIONS
        return
    end if
    int => sf%eval%interaction_t
end associate
end do
call find_outgoing_particles ()
end if
else if (chain%out_eval == 0) then
    int => beam_get_int_ptr (chain%beam_t)
    call int%tag_hard_process ()
end if
chain%status = SF_DONE_CONNECTIONS
end if
contains
<SF base: init evaluators: find outgoing particles>
end subroutine sf_chain_instance_init_evaluators

```

For debug purposes

```

<SF base: sf chain instance: TBP>+≡
    procedure :: write_interaction => sf_chain_instance_write_interaction

<SF base: sub interfaces>+≡
    module subroutine sf_chain_instance_write_interaction &
        (chain, i_sf, i_int, unit)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: i_sf, i_int
        integer, intent(in) :: unit
    end subroutine sf_chain_instance_write_interaction

<SF base: procedures>+≡
    module subroutine sf_chain_instance_write_interaction &
        (chain, i_sf, i_int, unit)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: i_sf, i_int
        integer, intent(in) :: unit
        class(interaction_t), pointer :: int_in1 => null ()
        class(interaction_t), pointer :: int_in2 => null ()
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (chain%status >= SF_DONE_MASK) then
            if (allocated (chain%sf)) then
                int_in1 => evaluator_get_int_in_ptr (chain%sf(i_sf)%eval, 1)
                int_in2 => evaluator_get_int_in_ptr (chain%sf(i_sf)%eval, 2)
                if (int_in1%get_tag () == i_int) then
                    call int_in1%basic_write (u)
                else if (int_in2%get_tag () == i_int) then
                    call int_in2%basic_write (u)
                end if
            end if
        end if
    end subroutine sf_chain_instance_write_interaction

```

```

        else
            write (u, "(A,1x,I0,1x,A,1x,I0)") 'No tag of sf', i_sf, 'matches' , i_int
        end if
    else
        write (u, "(A)") 'No sf_chain allocated!'
    end if
else
    write (u, "(A)") 'sf_chain not ready!'
end if
end subroutine sf_chain_instance_write_interaction

```

This is an internal subroutine of the previous one: After evaluators are set, trace the outgoing particles to the last evaluator. We only need the first channel, all channels are equivalent for this purpose.

For each beam, the outgoing particle is located by `out_sf` (the structure-function object where it originates) and `out_sf_i` (the index within that object). This particle is referenced by the corresponding evaluator, which in turn is referenced by the next evaluator, until we are at the end of the chain. We can trace back references by `interaction_find_link`. Knowing that `out_eval` is the index of the last evaluator, we thus determine `out_eval_i`, the index of the outgoing particle within that evaluator.

(SF base: init evaluators: find outgoing particles)≡

```

subroutine find_outgoing_particles ()
    type(interaction_t), pointer :: int, int_next
    integer :: i, j, out_sf, out_i
    chain%out_eval = size (chain%sf)
    do j = 1, size (chain%out_eval_i)
        out_sf = chain%out_sf(j)
        out_i = chain%out_sf_i(j)
        if (out_sf == 0) then
            int => beam_get_int_ptr (chain%beam_t)
            out_sf = 1
        else
            int => chain%sf(out_sf)%int%interaction_t
        end if
        do i = out_sf, chain%out_eval
            int_next => chain%sf(i)%eval%interaction_t
            out_i = interaction_find_link (int_next, int, out_i)
            int => int_next
        end do
        chain%out_eval_i(j) = out_i
    end do
    call int%tag_hard_process (chain%out_eval_i)
end subroutine find_outgoing_particles

```

Compute the kinematics in the chain instance. We can assume that the seed momenta are set in the configuration beams. Scanning the chain, we first transfer the incoming momenta. Then, the use up the MC input parameter array `p` to compute the radiated and outgoing momenta.

In the multi-channel case, `c_sel` is the channel which we use for computing the kinematics and the `x` values. In the other channels, we invert the kinematics in order to recover the corresponding rows in the `r` array, and the Jacobian `f`.

We first apply any global mapping to transform the input \mathbf{p} into the array \mathbf{r} . This is then given to the structure functions which compute the final array \mathbf{x} and Jacobian factors \mathbf{f} , which we multiply to obtain the overall Jacobian.

```

(SF base: sf chain instance: TBP)+≡
  procedure :: compute_kinematics => sf_chain_instance_compute_kinematics

(SF base: sub interfaces)+≡
  module subroutine sf_chain_instance_compute_kinematics (chain, c_sel, p_in)
    class(sf_chain_instance_t), intent(inout), target :: chain
    integer, intent(in) :: c_sel
    real(default), dimension(:), intent(in) :: p_in
  end subroutine sf_chain_instance_compute_kinematics

(SF base: procedures)+≡
  module subroutine sf_chain_instance_compute_kinematics (chain, c_sel, p_in)
    class(sf_chain_instance_t), intent(inout), target :: chain
    integer, intent(in) :: c_sel
    real(default), dimension(:), intent(in) :: p_in
    type(interaction_t), pointer :: int
    real(default) :: f_mapping
    integer :: i, j, c
    if (chain%status >= SF_DONE_CONNECTIONS) then
      call chain%select_channel (c_sel)
      int => beam_get_int_ptr (chain%beam_t)
      call int%receive_momenta ()
      if (allocated (chain%sf)) then
        if (size (chain%sf) /= 0) then
          forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
          chain%p (:,c_sel) = unpack (p_in, chain%bound, 0._default)
          chain%pb(:,c_sel) = 1 - chain%p(:,c_sel)
          chain%f = 1
          chain%x_free = 1
          do i = 1, size (chain%sf)
            associate (sf => chain%sf(i))
              call sf%int%generate_free (sf%r(:,c_sel), sf%rb(:,c_sel), &
                chain%x_free)
              do j = 1, size (sf%x)
                if (.not. chain%bound(sf%int%par_index(j))) then
                  chain%p (sf%int%par_index(j),c_sel) = sf%r (j,c_sel)
                  chain%pb(sf%int%par_index(j),c_sel) = sf%rb(j,c_sel)
                end if
              end do
            end associate
          end do
          if (allocated (chain%channel(c_sel)%multi_mapping)) then
            call chain%channel(c_sel)%multi_mapping%compute &
              (chain%r(:,c_sel), chain%rb(:,c_sel), &
                f_mapping, &
                chain%p(:,c_sel), chain%pb(:,c_sel), &
                chain%x_free)
            chain%f(c_sel) = f_mapping
          else
            chain%r (:,c_sel) = chain%p (:,c_sel)
            chain%rb(:,c_sel) = chain%pb(:,c_sel)
            chain%f(c_sel) = 1
          end if
        end if
      end if
    end if
  end subroutine sf_chain_instance_compute_kinematics

```

```

end if
do i = 1, size (chain%sf)
  associate (sf => chain%sf(i))
    call sf%int%seed_kinematics ()
    do j = 1, size (sf%x)
      sf%r (j,c_sel) = chain%r (sf%int%par_index(j),c_sel)
      sf%rb(j,c_sel) = chain%rb(sf%int%par_index(j),c_sel)
    end do
    call sf%int%complete_kinematics &
      (sf%x, sf%xb, sf%f(c_sel), sf%r(:,c_sel), sf%rb(:,c_sel), &
        sf%m(c_sel))
    do j = 1, size (sf%x)
      chain%x(sf%int%par_index(j)) = sf%x(j)
      chain%xb(sf%int%par_index(j)) = sf%xb(j)
    end do
    if (sf%int%status <= SF_FAILED_KINEMATICS) then
      chain%status = SF_FAILED_KINEMATICS
      return
    end if
    do c = 1, size (sf%f)
      if (c /= c_sel) then
        call sf%int%inverse_kinematics &
          (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c))
        do j = 1, size (sf%x)
          chain%r (sf%int%par_index(j),c) = sf%r (j,c)
          chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
        end do
        end if
        chain%f(c) = chain%f(c) * sf%f(c)
      end do
      if (.not. sf%eval%is_empty ()) then
        call sf%eval%receive_momenta ()
      end if
    end associate
  end do
  do c = 1, size (chain%f)
    if (c /= c_sel) then
      if (allocated (chain%channel(c)%multi_mapping)) then
        call chain%channel(c)%multi_mapping%inverse &
          (chain%r(:,c), chain%rb(:,c), &
            f_mapping, &
            chain%p(:,c), chain%pb(:,c), &
            chain%x_free)
        chain%f(c) = chain%f(c) * f_mapping
      else
        chain%p (:,c) = chain%r (:,c)
        chain%pb(:,c) = chain%rb(:,c)
      end if
    end if
  end do
end if
end if
chain%status = SF_DONE_KINEMATICS
end if

```



```
end subroutine sf_chain_instance_compute_kinematics
```

This is a variant of the previous procedure. We know the x parameters and reconstruct the momenta and the MC input parameters p . We do not need to select a channel.

Note: this is probably redundant, since the method we actually want starts from the momenta, recovers all x parameters, and then inverts mappings. See below `recover_kinematics`.

(SF base: sf chain instance: TBP)+≡

```
procedure :: inverse_kinematics => sf_chain_instance_inverse_kinematics
```

(SF base: sub interfaces)+≡

```
module subroutine sf_chain_instance_inverse_kinematics (chain, x, xb)
  class(sf_chain_instance_t), intent(inout), target :: chain
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
end subroutine sf_chain_instance_inverse_kinematics
```

(SF base: procedures)+≡

```
module subroutine sf_chain_instance_inverse_kinematics (chain, x, xb)
  class(sf_chain_instance_t), intent(inout), target :: chain
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
  type(interaction_t), pointer :: int
  real(default) :: f_mapping
  integer :: i, j, c
  if (chain%status >= SF_DONE_CONNECTIONS) then
    call chain%select_channel ()
    int => beam_get_int_ptr (chain%beam_t)
    call int%receive_momenta ()
    if (allocated (chain%sf)) then
      chain%f = 1
      if (size (chain%sf) /= 0) then
        forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
        chain%x = x
        chain%xb = xb
        do i = 1, size (chain%sf)
          associate (sf => chain%sf(i))
            call sf%int%seed_kinematics ()
            do j = 1, size (sf%x)
              sf%x(j) = chain%x(sf%int%par_index(j))
              sf%xb(j) = chain%xb(sf%int%par_index(j))
            end do
            do c = 1, size (sf%f)
              call sf%int%inverse_kinematics &
                (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c), &
                  set_momenta = c==1)
              chain%f(c) = chain%f(c) * sf%f(c)
            end do
            do j = 1, size (sf%x)
              chain%r (sf%int%par_index(j),c) = sf%r (j,c)
              chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
            end do
          end do
        end do
        if (.not. sf%eval%is_empty ()) then
```

```

        call sf%eval%receive_momenta ()
    end if
    end associate
end do
do c = 1, size (chain%f)
    if (allocated (chain%channel(c)%multi_mapping)) then
        call chain%channel(c)%multi_mapping%inverse &
            (chain%r(:,c), chain%rb(:,c), &
             f_mapping, &
             chain%p(:,c), chain%pb(:,c), &
             chain%x_free)
        chain%f(c) = chain%f(c) * f_mapping
    else
        chain%p(:,c) = chain%r(:,c)
        chain%pb(:,c) = chain%rb(:,c)
    end if
end do
end if
end if
chain%status = SF_DONE_KINEMATICS
end if
end subroutine sf_chain_instance_inverse_kinematics

```

Recover the kinematics: assuming that the last evaluator has been filled with a valid set of momenta, we travel the momentum links backwards and fill the preceding evaluators and, as a side effect, interactions. We stop at the beam interaction.

After all momenta are set, apply the `inverse_kinematics` procedure above, suitably modified, to recover the x and p parameters and the Jacobian factors.

The `c_sel` (channel) argument is just used to mark a selected channel for the records, otherwise the recovery procedure is independent of this.

(SF base: sf chain instance: TBP)+≡

```

    procedure :: recover_kinematics => sf_chain_instance_recover_kinematics

```

(SF base: sub interfaces)+≡

```

    module subroutine sf_chain_instance_recover_kinematics (chain, c_sel)
        class(sf_chain_instance_t), intent(inout), target :: chain
        integer, intent(in) :: c_sel
    end subroutine sf_chain_instance_recover_kinematics

```

(SF base: procedures)+≡

```

    module subroutine sf_chain_instance_recover_kinematics (chain, c_sel)
        class(sf_chain_instance_t), intent(inout), target :: chain
        integer, intent(in) :: c_sel
        real(default) :: f_mapping
        integer :: i, j, c
        if (chain%status >= SF_DONE_CONNECTIONS) then
            call chain%select_channel (c_sel)
            if (allocated (chain%sf)) then
                do i = size (chain%sf), 1, -1
                    associate (sf => chain%sf(i))
                        if (.not. sf%eval%is_empty ()) then
                            call sf%eval%send_momenta ()
                        end if
                    end associate
                end do
            end if
        end if
    end subroutine sf_chain_instance_recover_kinematics

```

```

        end associate
    end do
    chain%f = 1
    if (size (chain%sf) /= 0) then
        forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
        chain%x_free = 1
        do i = 1, size (chain%sf)
            associate (sf => chain%sf(i))
                call sf%int%seed_kinematics ()
                call sf%int%recover_x (sf%x, sf%xb, chain%x_free)
                do j = 1, size (sf%x)
                    chain%x(sf%int%par_index(j)) = sf%x(j)
                    chain%xb(sf%int%par_index(j)) = sf%xb(j)
                end do
            end do
            do c = 1, size (sf%f)
                call sf%int%inverse_kinematics &
                    (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c), &
                    set_momenta = .false.)
                chain%f(c) = chain%f(c) * sf%f(c)
                do j = 1, size (sf%x)
                    chain%r (sf%int%par_index(j),c) = sf%r (j,c)
                    chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
                end do
            end do
        end do
    end associate
end do
do c = 1, size (chain%f)
    if (allocated (chain%channel(c)%multi_mapping)) then
        call chain%channel(c)%multi_mapping%inverse &
            (chain%r(:,c), chain%rb(:,c), &
            f_mapping, &
            chain%p(:,c), chain%pb(:,c), &
            chain%x_free)
        chain%f(c) = chain%f(c) * f_mapping
    else
        chain%p(:,c) = chain%r(:,c)
        chain%pb(:,c) = chain%rb(:,c)
    end if
end do
end if
chain%status = SF_DONE_KINEMATICS
end if
end subroutine sf_chain_instance_recover_kinematics

```

Return the initial beam momenta to their source, thus completing kinematics recovery. Obviously, this works as a side effect.

(SF base: sf chain instance: TBP)+≡

```

    procedure :: return_beam_momenta => sf_chain_instance_return_beam_momenta

```

(SF base: sub interfaces)+≡

```

    module subroutine sf_chain_instance_return_beam_momenta (chain)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(interaction_t), pointer :: int

```

```

end subroutine sf_chain_instance_return_beam_momenta
<SF base: procedures>+=
module subroutine sf_chain_instance_return_beam_momenta (chain)
  class(sf_chain_instance_t), intent(in), target :: chain
  type(interaction_t), pointer :: int
  if (chain%status >= SF_DONE_KINEMATICS) then
    int => beam_get_int_ptr (chain%beam_t)
    call int%send_momenta ()
  end if
end subroutine sf_chain_instance_return_beam_momenta

```

Evaluate all interactions in the chain and the product evaluators. We provide a `scale` argument that is given to all structure functions in the chain.

Hadronic NLO calculations involve rescaled fractions of the original beam momentum. In particular, we have to handle the following cases:

- normal evaluation (where $i_{\text{sub}} = 0$) for all terms except the real non-subtracted,
- rescaled momentum fraction for both beams in the case of the real non-subtracted term ($i_{\text{sub}} = 0$),
- and rescaled momentum fraction for one of both beams in the case of the subtraction and DGLAP component ($i_{\text{sub}} = 1, 2$).

For the collinear final or initial state counter terms, we apply a rescaling to one beam, and keep the other beam as is. We redo it then vice versa having now two subtractions.

```

<SF base: sf chain instance: TBP>+=
procedure :: evaluate => sf_chain_instance_evaluate
<SF base: sub interfaces>+=
module subroutine sf_chain_instance_evaluate &
  (chain, scale, negative_sf, sf_rescale)
  class(sf_chain_instance_t), intent(inout), target :: chain
  real(default), intent(in) :: scale
  logical, intent(in), optional :: negative_sf
  class(sf_rescale_t), intent(inout), optional :: sf_rescale
end subroutine sf_chain_instance_evaluate
<SF base: procedures>+=
module subroutine sf_chain_instance_evaluate &
  (chain, scale, negative_sf, sf_rescale)
  class(sf_chain_instance_t), intent(inout), target :: chain
  real(default), intent(in) :: scale
  logical, intent(in), optional :: negative_sf
  class(sf_rescale_t), intent(inout), optional :: sf_rescale
  type(interaction_t), pointer :: out_int
  real(default) :: sf_sum
  integer :: i_beam, i_sub, n_sub
  logical :: rescale
  n_sub = 0
  rescale = .false.; if (present (sf_rescale)) rescale = .true.
  if (rescale) then

```

```

        n_sub = chain%get_n_sub ()
    end if
    if (chain%status >= SF_DONE_KINEMATICS) then
        if (allocated (chain%sf)) then
            if (size (chain%sf) /= 0) then
                do i_beam = 1, size (chain%sf)
                    associate (sf => chain%sf(i_beam))
                        if (rescale) then
                            call sf_rescale%set_i_beam (i_beam)
                            do i_sub = 0, n_sub
                                select case (i_sub)
                                    case (0)
                                        if (n_sub == 0) then
                                            call sf%int%apply (scale, negative_sf, sf_rescale, i_sub = i_sub)
                                        else
                                            call sf%int%apply (scale, negative_sf, i_sub = i_sub)
                                        end if
                                    case default
                                        if (i_beam == i_sub) then
                                            call sf%int%apply (scale, negative_sf, sf_rescale, i_sub = i_sub)
                                        else
                                            call sf%int%apply (scale, negative_sf, i_sub = i_sub)
                                        end if
                                end select
                            end do
                        else
                            call sf%int%apply (scale, negative_sf, i_sub = n_sub)
                        end if
                    end if
                    if (sf%int%status <= SF_FAILED_EVALUATION) then
                        chain%status = SF_FAILED_EVALUATION
                        return
                    end if
                    if (.not. sf%eval%is_empty ()) call sf%eval%evaluate ()
                end associate
            end do
            out_int => chain%get_out_int_ptr ()
            sf_sum = real (out_int%sum ())
            call chain%config%trace &
                (chain%selected_channel, chain%p, chain%x, chain%f, sf_sum)
        end if
    end if
    chain%status = SF_EVALUATED
end if
end subroutine sf_chain_instance_evaluate

```

16.5.10 Access to the chain instance

Transfer the outgoing momenta to the array p. We assume that array sizes match.

(SF base: sf chain instance: TBP)+≡

```
procedure :: get_out_momenta => sf_chain_instance_get_out_momenta
```

```

<SF base: sub interfaces>+≡
    module subroutine sf_chain_instance_get_out_momenta (chain, p)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(vector4_t), dimension(:), intent(out) :: p
    end subroutine sf_chain_instance_get_out_momenta

```

```

<SF base: procedures>+≡
    module subroutine sf_chain_instance_get_out_momenta (chain, p)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(vector4_t), dimension(:), intent(out) :: p
        type(interaction_t), pointer :: int
        integer :: i, j
        if (chain%status >= SF_DONE_KINEMATICS) then
            do j = 1, size (chain%out_sf)
                i = chain%out_sf(j)
                select case (i)
                    case (0)
                        int => beam_get_int_ptr (chain%beam_t)
                    case default
                        int => chain%sf(i)%int%interaction_t
                end select
                p(j) = int%get_momentum (chain%out_sf_i(j))
            end do
        end if
    end subroutine sf_chain_instance_get_out_momenta

```

Return a pointer to the last evaluator in the chain (to the interaction).

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_out_int_ptr => sf_chain_instance_get_out_int_ptr

```

```

<SF base: sub interfaces>+≡
    module function sf_chain_instance_get_out_int_ptr (chain) result (int)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(interaction_t), pointer :: int
    end function sf_chain_instance_get_out_int_ptr

```

```

<SF base: procedures>+≡
    module function sf_chain_instance_get_out_int_ptr (chain) result (int)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(interaction_t), pointer :: int
        if (chain%out_eval == 0) then
            int => beam_get_int_ptr (chain%beam_t)
        else
            int => chain%sf(chain%out_eval)%eval%interaction_t
        end if
    end function sf_chain_instance_get_out_int_ptr

```

Return the index of the j-th outgoing particle, within the last evaluator.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_out_i => sf_chain_instance_get_out_i

```

```

<SF base: sub interfaces>+≡
    module function sf_chain_instance_get_out_i (chain, j) result (i)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: j

```

```

        integer :: i
    end function sf_chain_instance_get_out_i
<SF base: procedures>+≡
module function sf_chain_instance_get_out_i (chain, j) result (i)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: j
    integer :: i
    i = chain%out_eval_i(j)
end function sf_chain_instance_get_out_i

```

Return the mask for the outgoing particle(s), within the last evaluator.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_out_mask => sf_chain_instance_get_out_mask
<SF base: sub interfaces>+≡
    module function sf_chain_instance_get_out_mask (chain) result (mask)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
    end function sf_chain_instance_get_out_mask
<SF base: procedures>+≡
    module function sf_chain_instance_get_out_mask (chain) result (mask)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        type(interaction_t), pointer :: int
        allocate (mask (chain%config%n_in))
        int => chain%get_out_int_ptr ()
        mask = int%get_mask (chain%out_eval_i)
    end function sf_chain_instance_get_out_mask

```

Return the array of MC input parameters that corresponds to channel c. This is the p array, the parameters before all mappings.

The p array may be deallocated. This should correspond to a zero-size r argument, so nothing to do then.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_mcpair => sf_chain_instance_get_mcpair
<SF base: sub interfaces>+≡
    module subroutine sf_chain_instance_get_mcpair (chain, c, r)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
    end subroutine sf_chain_instance_get_mcpair
<SF base: procedures>+≡
    module subroutine sf_chain_instance_get_mcpair (chain, c, r)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
        if (allocated (chain%p)) r = pack (chain%p(:,c), chain%bound)
    end subroutine sf_chain_instance_get_mcpair

```

Return the Jacobian factor that corresponds to channel c.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_f => sf_chain_instance_get_f

```

```

<SF base: sub interfaces>+≡
  module function sf_chain_instance_get_f (chain, c) result (f)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: c
    real(default) :: f
  end function sf_chain_instance_get_f

```

```

<SF base: procedures>+≡
  module function sf_chain_instance_get_f (chain, c) result (f)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: c
    real(default) :: f
    if (allocated (chain%f)) then
      f = chain%f(c)
    else
      f = 1
    end if
  end function sf_chain_instance_get_f

```

Return the evaluation status.

```

<SF base: sf chain instance: TBP>+≡
  procedure :: get_status => sf_chain_instance_get_status

```

```

<SF base: sub interfaces>+≡
  module function sf_chain_instance_get_status (chain) result (status)
    class(sf_chain_instance_t), intent(in) :: chain
    integer :: status
  end function sf_chain_instance_get_status

```

```

<SF base: procedures>+≡
  module function sf_chain_instance_get_status (chain) result (status)
    class(sf_chain_instance_t), intent(in) :: chain
    integer :: status
    status = chain%status
  end function sf_chain_instance_get_status

```

```

<SF base: sf chain instance: TBP>+≡
  procedure :: get_matrix_elements => sf_chain_instance_get_matrix_elements

```

```

<SF base: sub interfaces>+≡
  module subroutine sf_chain_instance_get_matrix_elements (chain, i, ff)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: i
    real(default), intent(out), dimension(:), allocatable :: ff
  end subroutine sf_chain_instance_get_matrix_elements

```

```

<SF base: procedures>+≡
  module subroutine sf_chain_instance_get_matrix_elements (chain, i, ff)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: i
    real(default), intent(out), dimension(:), allocatable :: ff

    associate (sf => chain%sf(i))
      ff = real (sf%int%get_matrix_element ())
    end associate
  end subroutine sf_chain_instance_get_matrix_elements

```



```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_beam_int_ptr => sf_chain_instance_get_beam_int_ptr

<SF base: sub interfaces>+≡
    module function sf_chain_instance_get_beam_int_ptr (chain) result (int)
        type(interaction_t), pointer :: int
        class(sf_chain_instance_t), intent(in), target :: chain
    end function sf_chain_instance_get_beam_int_ptr

<SF base: procedures>+≡
    module function sf_chain_instance_get_beam_int_ptr (chain) result (int)
        type(interaction_t), pointer :: int
        class(sf_chain_instance_t), intent(in), target :: chain
        int => beam_get_int_ptr (chain%beam_t)
    end function sf_chain_instance_get_beam_int_ptr

<SF base: sf chain instance: TBP>+≡
    procedure :: get_n_sub => sf_chain_instance_get_n_sub

<SF base: sub interfaces>+≡
    module function sf_chain_instance_get_n_sub (chain) result (n_sub)
        type(interaction_t), pointer :: int
        class(sf_chain_instance_t), intent(in), target :: chain
        integer :: n_sub
    end function sf_chain_instance_get_n_sub

<SF base: procedures>+≡
    module function sf_chain_instance_get_n_sub (chain) result (n_sub)
        type(interaction_t), pointer :: int
        class(sf_chain_instance_t), intent(in), target :: chain
        integer :: n_sub
        int => beam_get_int_ptr (chain%beam_t)
        n_sub = int%get_n_sub ()
    end function sf_chain_instance_get_n_sub

```

16.5.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_base_ut.f90>≡
    <File header>

    module sf_base_ut
        use unit_tests
        use sf_base_uti

    <Standard module head>

    <SF base: public test auxiliary>

    <SF base: public test>

    contains

    <SF base: test driver>

```

```

    end module sf_base_ut

<sf_base_uti.f90>≡
  <File header>

  module sf_base_uti

    <Use kinds>
    <Use strings>
    use io_units
    use format_defs, only: FMT_19
    use format_utils, only: write_separator
    use diagnostics
    use lorentz
    use pdg_arrays
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions
    use particles
    use model_data
    use beams
    use sf_aux
    use sf_mappings

    use sf_base

    <Standard module head>

    <SF base: test declarations>

    <SF base: public test auxiliary>

    <SF base: test types>

    contains

    <SF base: tests>

    <SF base: test auxiliary>

    end module sf_base_uti
API: driver for the unit tests below.
<SF base: public test>≡
  public :: sf_base_test
<SF base: test driver>≡
  subroutine sf_base_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SF base: execute tests>
  end subroutine sf_base_test

```

16.5.12 Test implementation: structure function

This is a template for the actual structure-function implementation which will be defined in separate modules.

Configuration data

The test structure function uses the `Test` model. It describes a scalar within an arbitrary initial particle, which is given in the initialization. The radiated particle is also a scalar, the same one, but we set its mass artificially to zero.

```
<SF base: public test auxiliary>≡
  public :: sf_test_data_t

<SF base: test types>≡
  type, extends (sf_data_t) :: sf_test_data_t
    class(model_data_t), pointer :: model => null ()
    integer :: mode = 0
    type(flavor_t) :: flv_in
    type(flavor_t) :: flv_out
    type(flavor_t) :: flv_rad
    real(default) :: m = 0
    logical :: collinear = .true.
    real(default), dimension(:), allocatable :: qbounds
  contains
    <SF base: sf test data: TBP>
  end type sf_test_data_t
```

Output.

```
<SF base: sf test data: TBP>≡
  procedure :: write => sf_test_data_write

<SF base: test auxiliary>≡
  subroutine sf_test_data_write (data, unit, verbose)
    class(sf_test_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "SF test data:"
    write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
    write (u, "(3x,A)", advance="no") "incoming  = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "outgoing  = "
    call data%flv_out%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "radiated  = "
    call data%flv_rad%write (u); write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") "mass      = ", data%m
    write (u, "(3x,A,L1)") "collinear = ", data%collinear
    if (.not. data%collinear .and. allocated (data%qbounds)) then
      write (u, "(3x,A," // FMT_19 // ")") "qmin      = ", data%qbounds(1)
      write (u, "(3x,A," // FMT_19 // ")") "qmax      = ", data%qbounds(2)
```

```

        end if
    end subroutine sf_test_data_write

```

Initialization.

```

<SF base: sf test data: TBP>+≡
    procedure :: init => sf_test_data_init

<SF base: test auxiliary>+≡
    subroutine sf_test_data_init (data, model, pdg_in, collinear, qbounds, mode)
        class(sf_test_data_t), intent(out) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), intent(in) :: pdg_in
        logical, intent(in), optional :: collinear
        real(default), dimension(2), intent(in), optional :: qbounds
        integer, intent(in), optional :: mode
        data%model => model
        if (present (mode)) data%mode = mode
        if (pdg_in%get (1) /= 25) then
            call msg_fatal ("Test spectrum function: input flavor must be 's'")
        end if
        call data%flv_in%init (25, model)
        data%m = data%flv_in%get_mass ()
        if (present (collinear)) data%collinear = collinear
        call data%flv_out%init (25, model)
        call data%flv_rad%init (25, model)
        if (present (qbounds)) then
            allocate (data%qbounds (2))
            data%qbounds = qbounds
        end if
    end subroutine sf_test_data_init

```

Return the number of parameters: 1 if only consider collinear splitting, 3 otherwise.

```

<SF base: sf test data: TBP>+≡
    procedure :: get_n_par => sf_test_data_get_n_par

<SF base: test auxiliary>+≡
    function sf_test_data_get_n_par (data) result (n)
        class(sf_test_data_t), intent(in) :: data
        integer :: n
        if (data%collinear) then
            n = 1
        else
            n = 3
        end if
    end function sf_test_data_get_n_par

```

Return the outgoing particle PDG code: 25

```

<SF base: sf test data: TBP>+≡
    procedure :: get_pdg_out => sf_test_data_get_pdg_out

<SF base: test auxiliary>+≡
    subroutine sf_test_data_get_pdg_out (data, pdg_out)

```

```

class(sf_test_data_t), intent(in) :: data
type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
pdg_out(1) = 25
end subroutine sf_test_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test data: TBP>+≡
  procedure :: allocate_sf_int => sf_test_data_allocate_sf_int

<SF base: test auxiliary>+≡
  subroutine sf_test_data_allocate_sf_int (data, sf_int)
    class(sf_test_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    if (allocated (sf_int)) deallocate (sf_int)
    allocate (sf_test_t :: sf_int)
  end subroutine sf_test_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+≡
  type, extends (sf_int_t) :: sf_test_t
    type(sf_test_data_t), pointer :: data => null ()
    real(default) :: x = 0
  contains
    <SF base: sf test int: TBP>
  end type sf_test_t

```

Type string: constant

```

<SF base: sf test int: TBP>≡
  procedure :: type_string => sf_test_type_string

<SF base: test auxiliary>+≡
  function sf_test_type_string (object) result (string)
    class(sf_test_t), intent(in) :: object
    type(string_t) :: string
    string = "Test"
  end function sf_test_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF base: sf test int: TBP>+≡
  procedure :: write => sf_test_write

<SF base: test auxiliary>+≡
  subroutine sf_test_write (object, unit, testflag)
    class(sf_test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    end if
  end subroutine sf_test_write

```

```

else
  write (u, "(1x,A)") "SF test data: [undefined]"
end if
end subroutine sf_test_write

```

Initialize. We know that `data` will be of concrete type `sf_test_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

⟨SF base: sf test int: TBP⟩+=
  procedure :: init => sf_test_init

⟨SF base: test auxiliary⟩+=
  subroutine sf_test_init (sf_int, data)
    class(sf_test_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    type(helicity_t) :: hel0
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(3) :: qn
    mask = quantum_numbers_mask (.false., .false., .false.)
    select type (data)
    type is (sf_test_data_t)
      if (allocated (data%qbounds)) then
        call sf_int%base_init (mask, &
          [data%m**2], [0._default], [data%m**2], &
          [data%qbounds(1)], [data%qbounds(2)])
      else
        call sf_int%base_init (mask, &
          [data%m**2], [0._default], [data%m**2])
      end if
      sf_int%data => data
      call hel0%init (0)
      call col0%init ()
      call qn(1)%init (data%flv_in, col0, hel0)
      call qn(2)%init (data%flv_rad, col0, hel0)
      call qn(3)%init (data%flv_out, col0, hel0)
      call sf_int%add_state (qn)
      call sf_int%freeze ()
      call sf_int%set_incoming ([1])
      call sf_int%set_radiated ([2])
      call sf_int%set_outgoing ([3])
    end select
    sf_int%status = SF_INITIAL
  end subroutine sf_test_init

```

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

```

⟨SF base: sf test int: TBP⟩+=

```

```

    procedure :: complete_kinematics => sf_test_complete_kinematics
  (SF base: test auxiliary)+≡
    subroutine sf_test_complete_kinematics (sf_int, x, xb, f, r, rb, map)
      class(sf_test_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(out) :: x
      real(default), dimension(:), intent(out) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(in) :: r
      real(default), dimension(:), intent(in) :: rb
      logical, intent(in) :: map
      if (map) then
        x(1) = r(1)**2
        f = 2 * r(1)
      else
        x(1) = r(1)
        f = 1
      end if
      xb(1) = 1 - x(1)
      if (size (x) == 3) then
        x(2:3) = r(2:3)
        xb(2:3) = rb(2:3)
      end if
      call sf_int%split_momentum (x, xb)
      sf_int%x = x(1)
      select case (sf_int%status)
        case (SF_FAILED_KINEMATICS); f = 0
      end select
    end subroutine sf_test_complete_kinematics

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

  (SF base: sf test int: TBP)+≡
    procedure :: inverse_kinematics => sf_test_inverse_kinematics
  (SF base: test auxiliary)+≡
    subroutine sf_test_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
      class(sf_test_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(in) :: x
      real(default), dimension(:), intent(in) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(out) :: r
      real(default), dimension(:), intent(out) :: rb
      logical, intent(in) :: map
      logical, intent(in), optional :: set_momenta
      logical :: set_mom
      set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
      if (map) then
        r(1) = sqrt (x(1))
        f = 2 * r(1)
      else
        r(1) = x(1)
        f = 1
      end if
    end subroutine sf_test_inverse_kinematics

```

```

end if
if (size (x) == 3)  r(2:3) = x(2:3)
rb = 1 - r
sf_int%x = x(1)
if (set_mom) then
  call sf_int%split_momentum (x, xb)
  select case (sf_int%status)
  case (SF_FAILED_KINEMATICS);  f = 0
  end select
end if
end subroutine sf_test_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

If the mode indicator is one, the matrix element is equal to the parameter x .

(SF base: sf test int: TBP)+≡

```

procedure :: apply => sf_test_apply

```

(SF base: test auxiliary)+≡

```

subroutine sf_test_apply (sf_int, scale, negative_sf, rescale, i_sub)
  class(sf_test_t), intent(inout) :: sf_int
  real(default), intent(in) :: scale
  logical, intent(in), optional :: negative_sf
  class(sf_rescale_t), intent(in), optional :: rescale
  integer, intent(in), optional :: i_sub
  select case (sf_int%data%mode)
  case (0)
    call sf_int%set_matrix_element &
      (cmplx (1._default, kind=default))
  case (1)
    call sf_int%set_matrix_element &
      (cmplx (sf_int%x, kind=default))
  end select
  sf_int%status = SF_EVALUATED
end subroutine sf_test_apply

```

16.5.13 Test implementation: pair spectrum

Another template, this time for a incoming particle pair, splitting into two radiated and two outgoing particles.

Configuration data

For simplicity, the spectrum contains two mirror images of the previous structure-function configuration: the incoming and all outgoing particles are test scalars.

We have two versions, one with radiated particles, one without.

(SF base: test types)+≡

```

type, extends (sf_data_t) :: sf_test_spectrum_data_t
  class(model_data_t), pointer :: model => null ()
  type(flavor_t) :: flv_in
  type(flavor_t) :: flv_out

```



```

        type(flavor_t) :: flv_rad
        logical :: with_radiation = .true.
        real(default) :: m = 0
contains
  <SF base: sf test spectrum data: TBP>
end type sf_test_spectrum_data_t

```

Output.

```

<SF base: sf test spectrum data: TBP>≡
  procedure :: write => sf_test_spectrum_data_write

<SF base: test auxiliary>+≡
  subroutine sf_test_spectrum_data_write (data, unit, verbose)
    class(sf_test_spectrum_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "SF test spectrum data:"
    write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
    write (u, "(3x,A)", advance="no") "incoming  = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "outgoing   = "
    call data%flv_out%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "radiated   = "
    call data%flv_rad%write (u); write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") "mass       = ", data%m
  end subroutine sf_test_spectrum_data_write

```

Initialization.

```

<SF base: sf test spectrum data: TBP>+≡
  procedure :: init => sf_test_spectrum_data_init

<SF base: test auxiliary>+≡
  subroutine sf_test_spectrum_data_init (data, model, pdg_in, with_radiation)
    class(sf_test_spectrum_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    logical, intent(in) :: with_radiation
    data%model => model
    data%with_radiation = with_radiation
    if (pdg_in%get (1) /= 25) then
      call msg_fatal ("Test structure function: input flavor must be 's'")
    end if
    call data%flv_in%init (25, model)
    data%m = data%flv_in%get_mass ()
    call data%flv_out%init (25, model)
    if (with_radiation) then
      call data%flv_rad%init (25, model)
    end if
  end subroutine sf_test_spectrum_data_init

```

Return the number of parameters: 2, since we have only collinear splitting here.

```

<SF base: sf test spectrum data: TBP>+≡
  procedure :: get_n_par => sf_test_spectrum_data_get_n_par

<SF base: test auxiliary>+≡
  function sf_test_spectrum_data_get_n_par (data) result (n)
    class(sf_test_spectrum_data_t), intent(in) :: data
    integer :: n
    n = 2
  end function sf_test_spectrum_data_get_n_par

```

Return the outgoing particle PDG codes: 25

```

<SF base: sf test spectrum data: TBP>+≡
  procedure :: get_pdg_out => sf_test_spectrum_data_get_pdg_out

<SF base: test auxiliary>+≡
  subroutine sf_test_spectrum_data_get_pdg_out (data, pdg_out)
    class(sf_test_spectrum_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    pdg_out(1) = 25
    pdg_out(2) = 25
  end subroutine sf_test_spectrum_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test spectrum data: TBP>+≡
  procedure :: allocate_sf_int => &
    sf_test_spectrum_data_allocate_sf_int

<SF base: test auxiliary>+≡
  subroutine sf_test_spectrum_data_allocate_sf_int (data, sf_int)
    class(sf_test_spectrum_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (sf_test_spectrum_t :: sf_int)
  end subroutine sf_test_spectrum_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+≡
  type, extends (sf_int_t) :: sf_test_spectrum_t
    type(sf_test_spectrum_data_t), pointer :: data => null ()
  contains
    <SF base: sf test spectrum: TBP>
  end type sf_test_spectrum_t

<SF base: sf test spectrum: TBP>≡
  procedure :: type_string => sf_test_spectrum_type_string

<SF base: test auxiliary>+≡
  function sf_test_spectrum_type_string (object) result (string)
    class(sf_test_spectrum_t), intent(in) :: object
    type(string_t) :: string
    string = "Test Spectrum"
  end function sf_test_spectrum_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

(SF base: sf test spectrum: TBP)+≡
  procedure :: write => sf_test_spectrum_write

(SF base: test auxiliary)+≡
  subroutine sf_test_spectrum_write (object, unit, testflag)
    class(sf_test_spectrum_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "SF test spectrum data: [undefined]"
    end if
  end subroutine sf_test_spectrum_write

```

Initialize. We know that data will be of concrete type `sf_test_spectrum_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

(SF base: sf test spectrum: TBP)+≡
  procedure :: init => sf_test_spectrum_init

(SF base: test auxiliary)+≡
  subroutine sf_test_spectrum_init (sf_int, data)
    class(sf_test_spectrum_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(6) :: mask
    type(helicity_t) :: hel0
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(6) :: qn
    mask = quantum_numbers_mask (.false., .false., .false.)
    select type (data)
    type is (sf_test_spectrum_data_t)
      if (data%with_radiation) then
        call sf_int%base_init (mask(1:6), &
          [data%m**2, data%m**2], &
          [0._default, 0._default], &
          [data%m**2, data%m**2])
        sf_int%data => data
        call hel0%init (0)
        call col0%init ()
        call qn(1)%init (data%flv_in, col0, hel0)
        call qn(2)%init (data%flv_in, col0, hel0)
        call qn(3)%init (data%flv_rad, col0, hel0)
        call qn(4)%init (data%flv_rad, col0, hel0)
        call qn(5)%init (data%flv_out, col0, hel0)
        call qn(6)%init (data%flv_out, col0, hel0)
        call sf_int%add_state (qn(1:6))
      end if
    end select
  end subroutine sf_test_spectrum_init

```

```

        call sf_int%set_incoming ([1,2])
        call sf_int%set_radiated ([3,4])
        call sf_int%set_outgoing ([5,6])
    else
        call sf_int%base_init (mask(1:4), &
            [data%m**2, data%m**2], &
            [real(default) :: ], &
            [data%m**2, data%m**2])
        sf_int%data => data
        call hel0%init (0)
        call col0%init ()
        call qn(1)%init (data%flv_in, col0, hel0)
        call qn(2)%init (data%flv_in, col0, hel0)
        call qn(3)%init (data%flv_out, col0, hel0)
        call qn(4)%init (data%flv_out, col0, hel0)
        call sf_int%add_state (qn(1:4))
        call sf_int%set_incoming ([1,2])
        call sf_int%set_outgoing ([3,4])
    end if
    call sf_int%freeze ()
end select
sf_int%status = SF_INITIAL
end subroutine sf_test_spectrum_init

```

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ (as above) for both x parameters and consequently $f(r) = 4r_1r_2$.

(SF base: sf test spectrum: TBP) +=

```

    procedure :: complete_kinematics => sf_test_spectrum_complete_kinematics

```

(SF base: test auxiliary) +=

```

subroutine sf_test_spectrum_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    real(default), dimension(2) :: xb1
    if (map) then
        x = r**2
        f = 4 * r(1) * r(2)
    else
        x = r
        f = 1
    end if
    xb = 1 - x
    if (sf_int%data%with_radiation) then
        call sf_int%split_momenta (x, xb)
    else
        call sf_int%reduce_momenta (x)
    end if
end if

```

```

    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS); f = 0
    end select
end subroutine sf_test_spectrum_complete_kinematics

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF base: sf test spectrum: TBP>+=
  procedure :: inverse_kinematics => sf_test_spectrum_inverse_kinematics

<SF base: test auxiliary>+=
  subroutine sf_test_spectrum_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default), dimension(2) :: xb1
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
      r = sqrt (x)
      f = 4 * r(1) * r(2)
    else
      r = x
      f = 1
    end if
    rb = 1 - r
    if (set_mom) then
      if (sf_int%data%with_radiation) then
        call sf_int%split_momenta (x, xb)
      else
        call sf_int%reduce_momenta (x)
      end if
      select case (sf_int%status)
      case (SF_FAILED_KINEMATICS); f = 0
      end select
    end if
  end subroutine sf_test_spectrum_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

```

<SF base: sf test spectrum: TBP>+=
  procedure :: apply => sf_test_spectrum_apply

<SF base: test auxiliary>+=
  subroutine sf_test_spectrum_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale

```

```

logical, intent(in), optional :: negative_sf
class(sf_rescale_t), intent(in), optional :: rescale
integer, intent(in), optional :: i_sub
call sf_int%set_matrix_element &
    (cmplx (1._default, kind=default))
sf_int%status = SF_EVALUATED
end subroutine sf_test_spectrum_apply

```

16.5.14 Test implementation: generator spectrum

A generator for two beams, no radiation (for simplicity).

Configuration data

For simplicity, the spectrum contains two mirror images of the previous structure-function configuration: the incoming and all outgoing particles are test scalars.

We have two versions, one with radiated particles, one without.

```

<SF base: test types>+≡
type, extends (sf_data_t) :: sf_test_generator_data_t
    class(model_data_t), pointer :: model => null ()
    type(flavor_t) :: flv_in
    type(flavor_t) :: flv_out
    type(flavor_t) :: flv_rad
    real(default) :: m = 0
contains
    <SF base: sf test generator data: TBP>
end type sf_test_generator_data_t

```

Output.

```

<SF base: sf test generator data: TBP>≡
procedure :: write => sf_test_generator_data_write

<SF base: test auxiliary>+≡
subroutine sf_test_generator_data_write (data, unit, verbose)
    class(sf_test_generator_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "SF test generator data:"
    write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
    write (u, "(3x,A)", advance="no") "incoming  = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "outgoing  = "
    call data%flv_out%write (u); write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") "mass      = ", data%m
end subroutine sf_test_generator_data_write

```

Initialization.

```

<SF base: sf test generator data: TBP>+≡
procedure :: init => sf_test_generator_data_init

```

```

<SF base: test auxiliary>+=
subroutine sf_test_generator_data_init (data, model, pdg_in)
  class(sf_test_generator_data_t), intent(out) :: data
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t), intent(in) :: pdg_in
  data%model => model
  if (pdg_in%get (1) /= 25) then
    call msg_fatal ("Test generator: input flavor must be 's'")
  end if
  call data%flv_in%init (25, model)
  data%m = data%flv_in%get_mass ()
  call data%flv_out%init (25, model)
end subroutine sf_test_generator_data_init

```

This structure function is a generator.

```

<SF base: sf test generator data: TBP>+=
procedure :: is_generator => sf_test_generator_data_is_generator

<SF base: test auxiliary>+=
function sf_test_generator_data_is_generator (data) result (flag)
  class(sf_test_generator_data_t), intent(in) :: data
  logical :: flag
  flag = .true.
end function sf_test_generator_data_is_generator

```

Return the number of parameters: 2, since we have only collinear splitting here.

```

<SF base: sf test generator data: TBP>+=
procedure :: get_n_par => sf_test_generator_data_get_n_par

<SF base: test auxiliary>+=
function sf_test_generator_data_get_n_par (data) result (n)
  class(sf_test_generator_data_t), intent(in) :: data
  integer :: n
  n = 2
end function sf_test_generator_data_get_n_par

```

Return the outgoing particle PDG codes: 25

```

<SF base: sf test generator data: TBP>+=
procedure :: get_pdg_out => sf_test_generator_data_get_pdg_out

<SF base: test auxiliary>+=
subroutine sf_test_generator_data_get_pdg_out (data, pdg_out)
  class(sf_test_generator_data_t), intent(in) :: data
  type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  pdg_out(1) = 25
  pdg_out(2) = 25
end subroutine sf_test_generator_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test generator data: TBP>+=
procedure :: allocate_sf_int => &
  sf_test_generator_data_allocate_sf_int

```

```

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_data_allocate_sf_int (data, sf_int)
    class(sf_test_generator_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (sf_test_generator_t :: sf_int)
  end subroutine sf_test_generator_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+≡
  type, extends (sf_int_t) :: sf_test_generator_t
    type(sf_test_generator_data_t), pointer :: data => null ()
    contains
    <SF base: sf test generator: TBP>
  end type sf_test_generator_t

<SF base: sf test generator: TBP>≡
  procedure :: type_string => sf_test_generator_type_string

<SF base: test auxiliary>+≡
  function sf_test_generator_type_string (object) result (string)
    class(sf_test_generator_t), intent(in) :: object
    type(string_t) :: string
    string = "Test Generator"
  end function sf_test_generator_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF base: sf test generator: TBP>+≡
  procedure :: write => sf_test_generator_write

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_write (object, unit, testflag)
    class(sf_test_generator_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "SF test generator data: [undefined]"
    end if
  end subroutine sf_test_generator_write

```

Initialize. We know that `data` will be of concrete type `sf_test_generator_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass. No radiation.

```

<SF base: sf test generator: TBP>+≡
  procedure :: init => sf_test_generator_init

```



```

<SF base: test auxiliary>+=
subroutine sf_test_generator_init (sf_int, data)
  class(sf_test_generator_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  type(quantum_numbers_mask_t), dimension(4) :: mask
  type(helicity_t) :: hel0
  type(color_t) :: col0
  type(quantum_numbers_t), dimension(4) :: qn
  mask = quantum_numbers_mask (.false., .false., .false.)
  select type (data)
  type is (sf_test_generator_data_t)
    call sf_int%base_init (mask(1:4), &
      [data%m**2, data%m**2], &
      [real(default) :: ], &
      [data%m**2, data%m**2])
    sf_int%data => data
    call hel0%init (0)
    call col0%init ()
    call qn(1)%init (data%flv_in, col0, hel0)
    call qn(2)%init (data%flv_in, col0, hel0)
    call qn(3)%init (data%flv_out, col0, hel0)
    call qn(4)%init (data%flv_out, col0, hel0)
    call sf_int%add_state (qn(1:4))
    call sf_int%set_incoming ([1,2])
    call sf_int%set_outgoing ([3,4])
    call sf_int%freeze ()
  end select
  sf_int%status = SF_INITIAL
end subroutine sf_test_generator_init

```

This structure function is a generator.

```

<SF base: sf test generator: TBP>+=
procedure :: is_generator => sf_test_generator_is_generator

<SF base: test auxiliary>+=
function sf_test_generator_is_generator (sf_int) result (flag)
  class(sf_test_generator_t), intent(in) :: sf_int
  logical :: flag
  flag = sf_int%data%is_generator ()
end function sf_test_generator_is_generator

```

Generate free parameters. This mock generator always produces the nubmers 0.8 and 0.5.

```

<SF base: sf test generator: TBP>+=
procedure :: generate_free => sf_test_generator_generate_free

<SF base: test auxiliary>+=
subroutine sf_test_generator_generate_free (sf_int, r, rb, x_free)
  class(sf_test_generator_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(out) :: r, rb
  real(default), intent(inout) :: x_free
  r = [0.8, 0.5]
  rb= 1 - r
  x_free = x_free * product (r)

```

```
end subroutine sf_test_generator_generate_free
```

Recover momentum fractions. Since the x values are free, we also set the x_{free} parameter.

```
<SF base: sf test generator: TBP>+≡
  procedure :: recover_x => sf_test_generator_recover_x

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_recover_x (sf_int, x, xb, x_free)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb)
    if (present (x_free)) x_free = x_free * product (x)
  end subroutine sf_test_generator_recover_x
```

Set kinematics. Since this is a generator, just transfer input to output.

```
<SF base: sf test generator: TBP>+≡
  procedure :: complete_kinematics => sf_test_generator_complete_kinematics

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    x = r
    xb = rb
    f = 1
    call sf_int%reduce_momenta (x)
  end subroutine sf_test_generator_complete_kinematics
```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```
<SF base: sf test generator: TBP>+≡
  procedure :: inverse_kinematics => sf_test_generator_inverse_kinematics

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
```

```

logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
r = x
rb= xb
f = 1
if (set_mom) call sf_int%reduce_momenta (x)
end subroutine sf_test_generator_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

```

<SF base: sf test generator: TBP>+≡
  procedure :: apply => sf_test_generator_apply

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    call sf_int%set_matrix_element &
      (cmplx (1._default, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine sf_test_generator_apply

```

Test structure function data

Construct and display a test structure function data object.

```

<SF base: execute tests>≡
  call test (sf_base_1, "sf_base_1", &
    "structure function configuration", &
    u, results)

<SF base: test declarations>≡
  public :: sf_base_1

<SF base: tests>≡
  subroutine sf_base_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_base_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test structure function data"
    write (u, "(A)")

    call model%init_test ()
    pdg_in = 25

```

```

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle code:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_base_1"

end subroutine sf_base_1

```

Test and probe structure function

Construct and display a structure function object based on the test structure function.

```

<SF base: execute tests>+≡
    call test (sf_base_2, "sf_base_2", &
        "structure function instance", &
        u, results)

<SF base: test declarations>+≡
    public :: sf_base_2

<SF base: tests>+≡
    subroutine sf_base_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        type(vector4_t), dimension(2) :: q
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f

        write (u, "(A)") "* Test output: sf_base_2"
        write (u, "(A)") "* Purpose: initialize and fill &
            &test structure function object"
        write (u, "(A)")
    end subroutine sf_base_2

```

```

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
pdg_in = 25
call flv%init (25, model)

call reset_interaction_counter ()

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=1"
write (u, "(A)")

```

```

r = 1
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics with mapping for r=0.8"
write (u, "(A)")

r = 0.8_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

```

```

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Compute inverse kinematics for x=0.64 and evaluate"
write (u, "(A)")

x = 0.64_default
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_2"

end subroutine sf_base_2

```

Collinear kinematics

Scan over the possibilities for mass assignment and on-shell projections, collinear case.

```

<SF base: execute tests>+≡
  call test (sf_base_3, "sf_base_3", &
    "alternatives for collinear kinematics", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_3

<SF base: tests>+≡
  subroutine sf_base_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

```

```

write (u, "(A)")  "* Test output: sf_base_3"
write (u, "(A)")  "* Purpose: check various kinematical setups"
write (u, "(A)")  "*           for collinear structure-function splitting."
write (u, "(A)")  "           (two masses equal, one zero)"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
pdg_in = 25
call flv%init (25, model)

call reset_interaction_counter ()

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%write (u)

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"

E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set radiated mass to zero"

sf_int%mr2 = 0
sf_int%mo2 = sf_int%mi2

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r

```



```

sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set outgoing mass to zero"

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"

```

```

write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set incoming mass to zero"

k = vector4_moving (E, E, 3)
call sf_int%seed_kinematics ([k])

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = sf_int%mi2
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

```

```

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set all masses to zero"

sf_int%mr2 = 0
sf_int%mo2 = 0
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r

```

```

write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_3"

end subroutine sf_base_3

```

Non-collinear kinematics

Scan over the possibilities for mass assignment and on-shell projections, non-collinear case.

```

<SF base: execute tests>+≡
  call test (sf_base_4, "sf_base_4", &
    "alternatives for non-collinear kinematics", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_4

<SF base: tests>+≡
  subroutine sf_base_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data

```

```

class(sf_int_t), allocatable :: sf_int
type(vector4_t) :: k
real(default) :: E
real(default), dimension(:), allocatable :: r, rb, x, xb
real(default) :: f

write (u, "(A)")  "* Test output: sf_base_4"
write (u, "(A)")  "* Purpose: check various kinematical setups"
write (u, "(A)")  "*           for free structure-function splitting."
write (u, "(A)")  "           (two masses equal, one zero)"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
pdg_in = 25
call flv%init (25, model)

call reset_interaction_counter ()

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in, collinear=.false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%write (u)

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"

E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set radiated mass to zero"

sf_int%mr2 = 0
sf_int%mo2 = sf_int%mi2

write (u, "(A)")

```

```

write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set outgoing mass to zero"

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY

```

```

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set incoming mass to zero"

k = vector4_moving (E, E, 3)
call sf_int%seed_kinematics ([k])

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = sf_int%mi2
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set all masses to zero"

sf_int%mr2 = 0
sf_int%mo2 = 0
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Re-Initialize structure-function object with Q bounds"

call reset_interaction_counter ()

select type (data)
type is (sf_test_data_t)
  call data%init (model, pdg_in, collinear=.false., &
    qbounds = [1._default, 100._default])
end select

call sf_int%init (data)
call sf_int%seed_kinematics ([k])

```



```

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_4"

end subroutine sf_base_4

```

Pair spectrum

Construct and display a structure function object for a pair spectrum (a structure function involving two particles simultaneously).

```
<SF base: execute tests>+≡
  call test (sf_base_5, "sf_base_5", &
    "pair spectrum with radiation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_5

<SF base: tests>+≡
  subroutine sf_base_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(2) :: pdg_out
    integer, dimension(:), allocatable :: pdg1, pdg2
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(4) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_base_5"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &a pair spectrum object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    allocate (sf_test_spectrum_data_t :: data)
    select type (data)
    type is (sf_test_spectrum_data_t)
      call data%init (model, pdg_in, with_radiation=.true.)
    end select

    write (u, "(1x,A)") "Outgoing particle codes:"
    call data%get_pdg_out (pdg_out)
    pdg1 = pdg_out(1)
    pdg2 = pdg_out(2)
    write (u, "(2x,99(1x,I0))") pdg1, pdg2

    write (u, "(A)")
```

```

write (u, "(A)")  "* Initialize spectrum object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics (k)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.4,0.8"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.4_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics with mapping for r=0.6,0.8"
write (u, "(A)")

r = [0.6_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)

```

```

call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()
call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Compute inverse kinematics for x=0.36,0.64 &
    &and evaluate"
write (u, "(A)")

x = [0.36_default, 0.64_default]
xb = 1 - x
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_5"

end subroutine sf_base_5

```

Pair spectrum without radiation

Construct and display a structure function object for a pair spectrum (a structure function involving two particles simultaneously).

```

<SF base: execute tests>+≡
  call test (sf_base_6, "sf_base_6", &
    "pair spectrum without radiation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_6

<SF base: tests>+≡

```

```

subroutine sf_base_6 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(pdg_array_t) :: pdg_in
  type(flavor_t) :: flv
  class(sf_data_t), allocatable, target :: data
  class(sf_int_t), allocatable :: sf_int
  type(vector4_t), dimension(2) :: k
  type(vector4_t), dimension(2) :: q
  real(default) :: E
  real(default), dimension(:), allocatable :: r, rb, x, xb
  real(default) :: f

  write (u, "(A)")  "* Test output: sf_base_6"
  write (u, "(A)")  "* Purpose: initialize and fill &
    &a pair spectrum object"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize configuration data"
  write (u, "(A)")

  call model%init_test ()
  call flv%init (25, model)
  pdg_in = 25

  call reset_interaction_counter ()

  allocate (sf_test_spectrum_data_t :: data)
  select type (data)
  type is (sf_test_spectrum_data_t)
    call data%init (model, pdg_in, with_radiation=.false.)
  end select

  write (u, "(A)")  "* Initialize spectrum object"
  write (u, "(A)")

  call data%allocate_sf_int (sf_int)
  call sf_int%init (data)

  write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

  E = 500
  k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
  k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
  call sf_int%seed_kinematics (k)

  write (u, "(A)")
  write (u, "(A)")  "* Set kinematics for x=0.4,0.8"
  write (u, "(A)")

  allocate (r (data%get_n_par ()))
  allocate (rb(size (r)))
  allocate (x (size (r)))
  allocate (xb(size (r)))

```

```

r = [0.4_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()
call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)") "* Compute inverse kinematics for x=0.4,0.8 &
&and evaluate"
write (u, "(A)")

x = [0.4_default, 0.8_default]
xb = 1 - x
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_base_6"

```

```
end subroutine sf_base_6
```

Direct access to structure function

Probe a structure function directly.

```
<SF base: execute tests>+≡
  call test (sf_base_7, "sf_base_7", &
    "direct access", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_7

<SF base: tests>+≡
  subroutine sf_base_7 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    real(default), dimension(:), allocatable :: value

    write (u, "(A)")  "* Test output: sf_base_7"
    write (u, "(A)")  "*   Purpose: check direct access method"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    allocate (sf_test_data_t :: data)
    select type (data)
    type is (sf_test_data_t)
      call data%init (model, pdg_in)
    end select

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)

    write (u, "(A)")  "* Probe structure function: states"
    write (u, "(A)")

    write (u, "(A,I0)") "n_states = ", sf_int%get_n_states ()
    write (u, "(A,I0)") "n_in      = ", sf_int%get_n_in ()
    write (u, "(A,I0)") "n_rad     = ", sf_int%get_n_rad ()
```

```

write (u, "(A,IO)") "n_out    = ", sf_int%get_n_out ()
write (u, "(A)")
write (u, "(A)", advance="no") "state(1) = "
call quantum_numbers_write (sf_int%get_state (1), u)
write (u, *)

allocate (value (sf_int%get_n_states ()))
call sf_int%compute_values (value, &
    E=[500._default], x=[0.5_default], xb=[0.5_default], scale=0._default)

write (u, "(A)")
write (u, "(A)", advance="no") "value (E=500, x=0.5) ="
write (u, "(9(1x," // FMT_19 // "))" value

call sf_int%compute_values (value, &
    x=[0.1_default], xb=[0.9_default], scale=0._default)

write (u, "(A)")
write (u, "(A)", advance="no") "value (E=500, x=0.1) ="
write (u, "(9(1x," // FMT_19 // "))" value

write (u, "(A)")
write (u, "(A)") "* Initialize spectrum object"
write (u, "(A)")

deallocate (value)
call sf_int%final ()
deallocate (sf_int)
deallocate (data)

allocate (sf_test_spectrum_data_t :: data)
select type (data)
type is (sf_test_spectrum_data_t)
    call data%init (model, pdg_in, with_radiation=.false.)
end select

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

write (u, "(A)") "* Probe spectrum: states"
write (u, "(A)")

write (u, "(A,IO)") "n_states = ", sf_int%get_n_states ()
write (u, "(A,IO)") "n_in    = ", sf_int%get_n_in ()
write (u, "(A,IO)") "n_rad   = ", sf_int%get_n_rad ()
write (u, "(A,IO)") "n_out   = ", sf_int%get_n_out ()
write (u, "(A)")
write (u, "(A)", advance="no") "state(1) = "
call quantum_numbers_write (sf_int%get_state (1), u)
write (u, *)

allocate (value (sf_int%get_n_states ()))
call sf_int%compute_value (1, value(1), &

```



```

      E = [500._default, 500._default], &
      x = [0.5_default, 0.6_default], &
      xb= [0.5_default, 0.4_default], &
      scale = 0._default)

write (u, "(A)")
write (u, "(A)", advance="no") "value (E=500,500, x=0.5,0.6) ="
write (u, "(9(1x," // FMT_19 // "))" value

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_7"

end subroutine sf_base_7

```

Structure function chain configuration

```

<SF base: execute tests>+≡
  call test (sf_base_8, "sf_base_8", &
    "structure function chain configuration", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_8

<SF base: tests>+≡
  subroutine sf_base_8 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    class(sf_data_t), allocatable, target :: data_spectrum
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_chain_t) :: sf_chain

    write (u, "(A)")  "* Test output: sf_base_8"
    write (u, "(A)")  "* Purpose: set up a structure-function chain"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

```

```

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_spectrum_data_t :: data_spectrum)
select type (data_spectrum)
type is (sf_test_spectrum_data_t)
    call data_spectrum%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(A)")  "* Set up chain with beams only"
write (u, "(A)")

call sf_chain%init (beam_data)
call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with structure function"
write (u, "(A)")

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_8"

end subroutine sf_base_8

```

Structure function instance configuration

We create a structure-function chain instance which implements a configured structure-function chain. We link the momentum entries in the interactions and compute kinematics.

We do not actually connect the interactions and create evaluators. We skip this step and manually advance the status of the chain instead.

```

<SF base: execute tests>+≡
  call test (sf_base_9, "sf_base_9", &
    "structure function chain instance", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_9

<SF base: tests>+≡
  subroutine sf_base_9 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    class(sf_data_t), allocatable, target :: data_spectrum
    type(sf_config_t), dimension(:), allocatable, target :: sf_config
    type(sf_chain_t), target :: sf_chain
    type(sf_chain_instance_t), target :: sf_chain_instance
    type(sf_channel_t), dimension(2) :: sf_channel
    type(vector4_t), dimension(2) :: p
    integer :: j

    write (u, "(A)")  "* Test output: sf_base_9"
    write (u, "(A)")  "* Purpose: set up a structure-function chain &
      &and create an instance"
    write (u, "(A)")  "* compute kinematics"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

```

```

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_spectrum_data_t :: data_spectrum)
select type (data_spectrum)
type is (sf_test_spectrum_data_t)
    call data_spectrum%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(A)")  "* Set up chain with beams only"
write (u, "(A)")

call sf_chain%init (beam_data)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [real(default) ::])

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
    write (u, "(A)")
    call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with structure function"
write (u, "(A)")

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

```

```

call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [0.8_default])

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
    write (u, "(A)")
    call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics &
    (1, [0.5_default, 0.6_default, 0.8_default])

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

```

```

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
  write (u, "(A)")
  call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_9"

end subroutine sf_base_9

```

Structure function chain mappings

Set up a structure function chain instance with a pair of single-particle structure functions. We test different global mappings for this setup.

Again, we skip evaluators.

```

<SF base: execute tests>+≡
call test (sf_base_10, "sf_base_10", &
  "structure function chain mapping", &
  u, results)

<SF base: test declarations>+≡
public :: sf_base_10

<SF base: tests>+≡
subroutine sf_base_10 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(pdg_array_t) :: pdg_in
  type(beam_data_t), target :: beam_data
  class(sf_data_t), allocatable, target :: data_strfun
  type(sf_config_t), dimension(:), allocatable, target :: sf_config
  type(sf_chain_t), target :: sf_chain
  type(sf_chain_instance_t), target :: sf_chain_instance
  type(sf_channel_t), dimension(2) :: sf_channel
  real(default), dimension(2) :: x_saved

  write (u, "(A)")  "* Test output: sf_base_10"
  write (u, "(A)")  "* Purpose: set up a structure-function chain"

```

```

write (u, "(A)")  "*"          and check mappings"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

write (u, "(A)")  "* Set up chain with structure function pair &
    &and standard mapping"
write (u, "(A)")

allocate (sf_config (2))
call sf_config(1)%init ([1], data_strfun)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(1)%init (2)
call sf_channel(1)%set_s_mapping ([1,2])
call sf_chain_instance%set_channel (1, sf_channel(1))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [0.8_default, 0.6_default])

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Invert the kinematics calculation"
write (u, "(A)")

x_saved = sf_chain_instance%x

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(2)%init (2)
call sf_channel(2)%set_s_mapping ([1, 2])
call sf_chain_instance%set_channel (1, sf_channel(2))

```

```

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%inverse_kinematics (x_saved, 1 - x_saved)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_10"

end subroutine sf_base_10

```

Structure function chain evaluation

Here, we test the complete workflow for structure-function chains. First, we create the template chain, then initialize an instance. We set up links, mask, and evaluators. Finally, we set kinematics and evaluate the matrix elements and their products.

```

<SF base: execute tests>+≡
call test (sf_base_11, "sf_base_11", &
  "structure function chain evaluation", &
  u, results)

<SF base: test declarations>+≡
public :: sf_base_11

<SF base: tests>+≡
subroutine sf_base_11 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(pdg_array_t) :: pdg_in
  type(beam_data_t), target :: beam_data
  class(sf_data_t), allocatable, target :: data_strfun
  class(sf_data_t), allocatable, target :: data_spectrum
  type(sf_config_t), dimension(:), allocatable, target :: sf_config
  type(sf_chain_t), target :: sf_chain
  type(sf_chain_instance_t), target :: sf_chain_instance
  type(sf_channel_t), dimension(2) :: sf_channel
  type(particle_set_t) :: pset
  type(interaction_t), pointer :: int
  logical :: ok

```



```

write (u, "(A)")  "* Test output: sf_base_11"
write (u, "(A)")  "* Purpose: set up a structure-function chain"
write (u, "(A)")  "*           create an instance and evaluate"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_spectrum_data_t :: data_spectrum)
select type (data_spectrum)
type is (sf_test_spectrum_data_t)
    call data_spectrum%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(A)")  "* Set up chain with beams only"
write (u, "(A)")

call sf_chain%init (beam_data)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics (1, [real(default) ::])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()
call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

```

```

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()
call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()
call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")
write (u, "(A)")
write (u, "(A)")  "* Set up chain with structure function"
write (u, "(A)")

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics (1, [0.8_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()

```

```

call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()
call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()
call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")
write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))

```

```

call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics &
    (1, [0.5_default, 0.6_default, 0.8_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()
call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()
call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()
call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_base_11"

end subroutine sf_base_11

```

Multichannel case

We set up a structure-function chain as before, but with three different parameterizations. The first instance is without mappings, the second one with single-particle mappings, and the third one with two-particle mappings.

```

<SF base: execute tests>+≡
  call test (sf_base_12, "sf_base_12", &
    "multi-channel structure function chain", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_12

<SF base: tests>+≡
  subroutine sf_base_12 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data
    type(sf_config_t), dimension(:), allocatable, target :: sf_config
    type(sf_chain_t), target :: sf_chain
    type(sf_chain_instance_t), target :: sf_chain_instance
    real(default), dimension(2) :: x_saved
    real(default), dimension(2,3) :: p_saved
    type(sf_channel_t), dimension(:), allocatable :: sf_channel

    write (u, "(A)")  "** Test output: sf_base_12"
    write (u, "(A)")  "** Purpose: set up and evaluate a multi-channel &
      &structure-function chain"
    write (u, "(A)")

    write (u, "(A)")  "** Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    call beam_data%init_sqrts (1000._default, [flv, flv])

    allocate (sf_test_data_t :: data)
    select type (data)

```

```

type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Set up chain with structure function pair &
                  &and three different mappings"
write (u, "(A)")

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 3)

call allocate_sf_channels (sf_channel, n_channel = 3, n_strfun = 2)

! channel 1: no mapping
call sf_chain_instance%set_channel (1, sf_channel(1))

! channel 2: single-particle mappings
call sf_channel(2)%activate_mapping ([1,2])
! call sf_chain_instance%activate_mapping (2, [1,2])
call sf_chain_instance%set_channel (2, sf_channel(2))

! channel 3: two-particle mapping
call sf_channel(3)%set_s_mapping ([1,2])
! call sf_chain_instance%set_s_mapping (3, [1, 2])
call sf_chain_instance%set_channel (3, sf_channel(3))

call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

write (u, "(A)")  "* Compute kinematics in channel 1 and evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (1, [0.8_default, 0.6_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Invert the kinematics calculation"
write (u, "(A)")

x_saved = sf_chain_instance%x

call sf_chain_instance%inverse_kinematics (x_saved, 1 - x_saved)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)

```

```

call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Compute kinematics in channel 2 and evaluate"
write (u, "(A)")

p_saved = sf_chain_instance%p

call sf_chain_instance%compute_kinematics (2, p_saved(:,2))
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Compute kinematics in channel 3 and evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (3, p_saved(:,3))
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_chain_instance%final ()
call sf_chain%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_12"

end subroutine sf_base_12

```

Generated spectrum

Construct and evaluate a structure function object for a pair spectrum which is evaluated as a beam-event generator.

```

<SF base: execute tests>+≡
  call test (sf_base_13, "sf_base_13", &
    "pair spectrum generator", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_13

<SF base: tests>+≡

```

```

subroutine sf_base_13 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(pdg_array_t) :: pdg_in
  class(sf_data_t), allocatable, target :: data
  class(sf_int_t), allocatable :: sf_int
  type(vector4_t), dimension(2) :: k
  type(vector4_t), dimension(2) :: q
  real(default) :: E
  real(default), dimension(:), allocatable :: r, rb, x, xb
  real(default) :: f, x_free

  write (u, "(A)")  "* Test output: sf_base_13"
  write (u, "(A)")  "* Purpose: initialize and fill &
    &a pair generator object"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize configuration data"
  write (u, "(A)")

  call model%init_test ()
  call flv%init (25, model)
  pdg_in = 25

  call reset_interaction_counter ()

  allocate (sf_test_generator_data_t :: data)
  select type (data)
  type is (sf_test_generator_data_t)
    call data%init (model, pdg_in)
  end select

  write (u, "(A)")  "* Initialize generator object"
  write (u, "(A)")

  call data%allocate_sf_int (sf_int)
  call sf_int%init (data)

  allocate (r (data%get_n_par ()))
  allocate (rb(size (r)))
  allocate (x (size (r)))
  allocate (xb(size (r)))

  write (u, "(A)")  "* Generate free r values"
  write (u, "(A)")

  x_free = 1
  call sf_int%generate_free (r, rb, x_free)

  write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

  E = 500
  k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)

```



```

k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics (k)

write (u, "(A)")
write (u, "(A)")  "* Complete kinematics"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()
call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
x_free = 1
call sf_int%recover_x (x, xb, x_free)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Compute inverse kinematics &
    &and evaluate"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_13"

end subroutine sf_base_13

```

Structure function chain evaluation

Here, we test the complete workflow for a structure-function chain with generator. First, we create the template chain, then initialize an instance. We set up links, mask, and evaluators. Finally, we set kinematics and evaluate the matrix elements and their products.

```

<SF base: execute tests>+≡
  call test (sf_base_14, "sf_base_14", &
    "structure function generator evaluation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_14

<SF base: tests>+≡
  subroutine sf_base_14 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    class(sf_data_t), allocatable, target :: data_generator
    type(sf_config_t), dimension(:), allocatable, target :: sf_config
    real(default), dimension(:), allocatable :: p_in
    type(sf_chain_t), target :: sf_chain
    type(sf_chain_instance_t), target :: sf_chain_instance

    write (u, "(A)")  "* Test output: sf_base_14"
    write (u, "(A)")  "* Purpose: set up a structure-function chain"
    write (u, "(A)")  "* create an instance and evaluate"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    call beam_data%init_sqrts (1000._default, [flv, flv])

    allocate (sf_test_data_t :: data_strfun)
    select type (data_strfun)

```

```

type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_generator_data_t :: data_generator)
select type (data_generator)
type is (sf_test_generator_data_t)
    call data_generator%init (model, pdg_in)
end select

write (u, "(A)")  "* Set up chain with generator and structure function"
write (u, "(A)")

allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_generator)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

write (u, "(A)")  "* Inject integration parameter"
write (u, "(A)")

allocate (p_in (sf_chain%get_n_bound ()), source = 0.9_default)
write (u, "(A,9(1x,F10.7))")  "p_in =", p_in

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (1, p_in)
call sf_chain_instance%evaluate (scale=0._default)

call sf_chain_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract integration parameter"
write (u, "(A)")

call sf_chain_instance%get_mcpair (1, p_in)
write (u, "(A,9(1x,F10.7))")  "p_in =", p_in

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: sf_base_14"

    end subroutine sf_base_14

```

16.6 Photon radiation: ISR

```

⟨sf_isr.f90⟩≡
  ⟨File header⟩

  module sf_isr

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use pdg_arrays
    use model_data
    use flavors
    use sf_aux
    use sf_mappings
    use sf_base
    use electron_pdfs

    ⟨Standard module head⟩

    ⟨SF_isr: public⟩

    ⟨SF_isr: parameters⟩

    ⟨SF_isr: types⟩

    interface
    ⟨SF_isr: sub interfaces⟩
    end interface

    contains

    ⟨SF_isr: main procedures⟩

  end module sf_isr

⟨sf_isr_sub.f90⟩≡
  ⟨File header⟩

  submodule (sf_isr) sf_isr_s

    use io_units
    use constants, only: pi
    use format_defs, only: FMT_15, FMT_19
    use numeric_utils
    use diagnostics
    use physics_defs, only: PHOTON
    use sm_physics, only: Li2
    use lorentz

```

```

use colors
use quantum_numbers
use polarizations

implicit none

contains

<SF_isr: procedures>

end submodule sf_isr_s

```

16.6.1 Physics

The ISR structure function is in the most crude approximation (LLA without α corrections, i.e. ϵ^0)

$$f_0(x) = \epsilon(1-x)^{-1+\epsilon} \quad \text{with} \quad \epsilon = \frac{\alpha}{\pi} q_e^2 \ln \frac{s}{m^2}, \quad (16.29)$$

where m is the mass of the incoming (and outgoing) particle, which is initially assumed on-shell.

In $f_0(x)$, there is an integrable singularity at $x = 1$ which does not spoil the integration, but would lead to an unbounded f_{\max} . Therefore, we map this singularity like

$$x = 1 - (1-x')^{1/\epsilon} \quad (16.30)$$

such that

$$\int dx f_0(x) = \int dx' \quad (16.31)$$

For the detailed form of the QED ISR structure function cf. Chap. 10.

16.6.2 Implementation

In the concrete implementation, the zeroth order mapping (16.30) is implemented, and the Jacobian is equal to $f_i(x)/f_0(x)$. This can be written as

$$\frac{f_0(x)}{f_0(x)} = 1 \quad (16.32)$$

$$\frac{f_1(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon - \frac{1-x^2}{2(1-x')} \quad (16.33)$$

$$\begin{aligned} \frac{f_2(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon + \frac{27-8\pi^2}{96}\epsilon^2 - \frac{1-x^2}{2(1-x')} \\ - \frac{(1+3x^2)\ln x + (1-x)(4(1+x)\ln(1-x) + 5+x)}{8(1-x')}\epsilon \end{aligned} \quad (16.34)$$

For $x = 1$ (i.e., numerically indistinguishable from 1), this reduces to

$$\frac{f_0(x)}{f_0(x)} = 1 \quad (16.35)$$

$$\frac{f_1(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon \quad (16.36)$$

$$\frac{f_2(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon + \frac{27 - 8\pi^2}{96}\epsilon^2 \quad (16.37)$$

The last line in (16.34) is zero for

$$x_{\min} = 0.00714053329734592839549879772019 \quad (16.38)$$

(Mathematica result), independent of ϵ . For x values less than this we ignore this correction because of the logarithmic singularity which should in principle be resummed.

16.6.3 The ISR data block

```

<SF isr: public>≡
  public :: isr_data_t

<SF isr: types>≡
  type, extends (sf_data_t) :: isr_data_t
  private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(:), allocatable :: flv_in
    type(qed_pdf_t) :: pdf
    real(default) :: alpha = 0
    real(default) :: q_max = 0
    real(default) :: real_mass = 0
    real(default) :: mass = 0
    real(default) :: eps = 0
    real(default) :: log = 0
    logical :: recoil = .false.
    logical :: keep_energy = .true.
    integer :: order = 3
    integer :: error = NONE
  contains
    <SF isr: isr data: TBP>
  end type isr_data_t

```

Error codes

```

<SF isr: parameters>≡
  integer, parameter :: NONE = 0
  integer, parameter :: ZERO_MASS = 1
  integer, parameter :: Q_MAX_TOO_SMALL = 2
  integer, parameter :: EPS_TOO_LARGE = 3
  integer, parameter :: INVALID_ORDER = 4
  integer, parameter :: CHARGE_MIX = 5
  integer, parameter :: CHARGE_ZERO = 6
  integer, parameter :: MASS_MIX = 7

```

Generate flavor-dependent ISR data:

$\langle SF \text{ isr: isr data: TBP} \rangle \equiv$

```
procedure :: init => isr_data_init
```

$\langle SF \text{ isr: sub interfaces} \rangle \equiv$

```
module subroutine isr_data_init (data, model, pdg_in, alpha, q_max, &
    mass, order, recoil, keep_energy)
    class(isr_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: alpha
    real(default), intent(in) :: q_max
    real(default), intent(in), optional :: mass
    integer, intent(in), optional :: order
    logical, intent(in), optional :: recoil
    logical, intent(in), optional :: keep_energy
end subroutine isr_data_init
```

$\langle SF \text{ isr: procedures} \rangle \equiv$

```
module subroutine isr_data_init (data, model, pdg_in, alpha, q_max, &
    mass, order, recoil, keep_energy)
    class(isr_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: alpha
    real(default), intent(in) :: q_max
    real(default), intent(in), optional :: mass
    integer, intent(in), optional :: order
    logical, intent(in), optional :: recoil
    logical, intent(in), optional :: keep_energy
    integer :: i, n_flv
    real(default) :: charge
    data%model => model
    n_flv = pdg_in%get_length ()
    allocate (data%flv_in (n_flv))
    do i = 1, n_flv
        call data%flv_in(i)%init (pdg_in%get (i), model)
    end do
    data%alpha = alpha
    data%q_max = q_max
    if (present (order)) then
        call data%set_order (order)
    end if
    if (present (recoil)) then
        data%recoil = recoil
    end if
    if (present (keep_energy)) then
        data%keep_energy = keep_energy
    end if
    data%real_mass = data%flv_in(1)%get_mass ()
    if (present (mass)) then
        if (mass > 0) then
            data%mass = mass
        else
            data%mass = data%real_mass
        end if
    end if
end subroutine isr_data_init
```

```

        if (any (data%flv_in%get_mass () /= data%mass)) then
            data%error = MASS_MIX; return
        end if
    end if
else
    data%mass = data%real_mass
    if (any (data%flv_in%get_mass () /= data%mass)) then
        data%error = MASS_MIX; return
    end if
end if
if (vanishes (data%mass)) then
    data%error = ZERO_MASS; return
else if (data%mass >= data%q_max) then
    data%error = Q_MAX_TOO_SMALL; return
end if
data%log = log (1 + (data%q_max / data%mass)**2)
charge = data%flv_in(1)%get_charge ()
if (any (abs (data%flv_in%get_charge ()) /= abs (charge))) then
    data%error = CHARGE_MIX; return
else if (charge == 0) then
    data%error = CHARGE_ZERO; return
end if
data%eps = data%alpha / pi * charge ** 2 &
    * (2 * log (data%q_max / data%mass) - 1)
if (data%eps > 1) then
    data%error = EPS_TOO_LARGE; return
end if
call data%pdf%init (data%mass, data%alpha, charge, data%q_max, data%order, &
    0, 1)
end subroutine isr_data_init

```

Explicitly set ISR order

```

<SF isr: data: TBP>+≡
    procedure :: set_order => isr_data_set_order

<SF isr: sub interfaces>+≡
    elemental module subroutine isr_data_set_order (data, order)
        class(isr_data_t), intent(inout) :: data
        integer, intent(in) :: order
    end subroutine isr_data_set_order

<SF isr: procedures>+≡
    elemental module subroutine isr_data_set_order (data, order)
        class(isr_data_t), intent(inout) :: data
        integer, intent(in) :: order
        if (order < 0 .or. order > 3) then
            data%error = INVALID_ORDER
        else
            data%order = order
        end if
    end subroutine isr_data_set_order

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.


```

<SF isr: isr data: TBP>+≡
  procedure :: check => isr_data_check

<SF isr: sub interfaces>+≡
  module subroutine isr_data_check (data)
    class(isr_data_t), intent(in) :: data
  end subroutine isr_data_check

<SF isr: procedures>+≡
  module subroutine isr_data_check (data)
    class(isr_data_t), intent(in) :: data
    select case (data%error)
    case (ZERO_MASS)
      call msg_fatal ("ISR: Particle mass is zero")
    case (Q_MAX_TOO_SMALL)
      call msg_fatal ("ISR: Particle mass exceeds Qmax")
    case (EPS_TOO_LARGE)
      call msg_fatal ("ISR: Expansion parameter too large, " // &
        "perturbative expansion breaks down")
    case (INVALID_ORDER)
      call msg_error ("ISR: LLA order invalid (valid values are 0,1,2,3)")
    case (MASS_MIX)
      call msg_fatal ("ISR: Incoming particle masses must be uniform")
    case (CHARGE_MIX)
      call msg_fatal ("ISR: Incoming particle charges must be uniform")
    case (CHARGE_ZERO)
      call msg_fatal ("ISR: Incoming particle must be charged")
    end select
  end subroutine isr_data_check

```

Output

```

<SF isr: isr data: TBP>+≡
  procedure :: write => isr_data_write

<SF isr: sub interfaces>+≡
  module subroutine isr_data_write (data, unit, verbose)
    class(isr_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine isr_data_write

<SF isr: procedures>+≡
  module subroutine isr_data_write (data, unit, verbose)
    class(isr_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "ISR data:"
    if (allocated (data%flv_in)) then
      write (u, "(3x,A)", advance="no") " flavor = "
      do i = 1, size (data%flv_in)
        if (i > 1) write (u, "(?,',1x)", advance="no")
        call data%flv_in(i)%write (u)
      end do
    end do
    write (u, *)

```

```

        write (u, "(3x,A," // FMT_19 // ")") " alpha      = ", data%alpha
        write (u, "(3x,A," // FMT_19 // ")") " q_max      = ", data%q_max
        write (u, "(3x,A," // FMT_19 // ")") " mass       = ", data%mass
        write (u, "(3x,A," // FMT_19 // ")") " eps        = ", data%eps
        write (u, "(3x,A," // FMT_19 // ")") " log        = ", data%log
        write (u, "(3x,A,I2)") " order      = ", data%order
        write (u, "(3x,A,L2)") " recoil    = ", data%recoil
        write (u, "(3x,A,L2)") " keep en. = ", data%keep_energy
    else
        write (u, "(3x,A)") "[undefined]"
    end if
end subroutine isr_data_write

```

For ISR, there is the option to generate transverse momentum is generated. Hence, there can be up to three parameters, x , and two angles.

```

<SF isr: isr data: TBP>+≡
    procedure :: get_n_par => isr_data_get_n_par

<SF isr: sub interfaces>+≡
    module function isr_data_get_n_par (data) result (n)
        class(isr_data_t), intent(in) :: data
        integer :: n
    end function isr_data_get_n_par

<SF isr: procedures>+≡
    module function isr_data_get_n_par (data) result (n)
        class(isr_data_t), intent(in) :: data
        integer :: n
        if (data%recoil) then
            n = 3
        else
            n = 1
        end if
    end function isr_data_get_n_par

```

Return the outgoing particles PDG codes. For ISR, these are identical to the incoming particles.

```

<SF isr: isr data: TBP>+≡
    procedure :: get_pdg_out => isr_data_get_pdg_out

<SF isr: sub interfaces>+≡
    module subroutine isr_data_get_pdg_out (data, pdg_out)
        class(isr_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine isr_data_get_pdg_out

<SF isr: procedures>+≡
    module subroutine isr_data_get_pdg_out (data, pdg_out)
        class(isr_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        pdg_out(1) = data%flv_in%get_pdg ()
    end subroutine isr_data_get_pdg_out

```

Return the `eps` value. We need it for an appropriate mapping of structure-function parameters.

```

<SF isr: isr data: TBP>+≡
  procedure :: get_eps => isr_data_get_eps
<SF isr: sub interfaces>+≡
  module function isr_data_get_eps (data) result (eps)
    class(isr_data_t), intent(in) :: data
    real(default) :: eps
  end function isr_data_get_eps
<SF isr: procedures>+≡
  module function isr_data_get_eps (data) result (eps)
    class(isr_data_t), intent(in) :: data
    real(default) :: eps
    eps = data%eps
  end function isr_data_get_eps

```

Allocate the interaction record. Gfortran 7/8/9 bug, has to remain in the module.

```

<SF isr: isr data: TBP>+≡
  procedure :: allocate_sf_int => isr_data_allocate_sf_int
<SF isr: main procedures>≡
  subroutine isr_data_allocate_sf_int (data, sf_int)
    class(isr_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (isr_t :: sf_int)
  end subroutine isr_data_allocate_sf_int

```

16.6.4 The ISR object

The `isr_t` data type is a $1 \rightarrow 2$ interaction, i.e., we allow for single-photon emission only (but use the multi-photon resummed radiator function). The particles are ordered as (incoming, photon, outgoing).

There is no need to handle several flavors (and data blocks) in parallel, since ISR is always applied immediately after beam collision. (ISR for partons is accounted for by the PDFs themselves.) Polarization is carried through, i.e., we retain the polarization of the incoming particle and treat the emitted photon as unpolarized. Color is trivially carried through. This implies that particles 1 and 3 should be locked together. For ISR we don't need the `q` variable.

```

<SF isr: public>+≡
  public :: isr_t
<SF isr: types>+≡
  type, extends (sf_int_t) :: isr_t
  private
  type(isr_data_t), pointer :: data => null ()
  real(default) :: x = 0
  real(default) :: xb= 0
  contains
  <SF isr: isr: TBP>
  end type isr_t

```

Type string: has to be here, but there is no string variable on which ISR depends.
Hence, a dummy routine.

```

<SF isr: isr: TBP>+=
  procedure :: type_string => isr_type_string
<SF isr: sub interfaces>+=
  module function isr_type_string (object) result (string)
    class(isr_t), intent(in) :: object
    type(string_t) :: string
  end function isr_type_string
<SF isr: procedures>+=
  module function isr_type_string (object) result (string)
    class(isr_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "ISR: e+ e- ISR spectrum"
    else
      string = "ISR: [undefined]"
    end if
  end function isr_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF isr: isr: TBP>+=
  procedure :: write => isr_write
<SF isr: sub interfaces>+=
  module subroutine isr_write (object, unit, testflag)
    class(isr_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine isr_write
<SF isr: procedures>+=
  module subroutine isr_write (object, unit, testflag)
    class(isr_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_15 // ")") "x =", object%x
        write (u, "(3x,A," // FMT_15 // ")") "xb=", object%xb
      end if
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "ISR data: [undefined]"
    end if
  end subroutine isr_write

```

Explicitly set ISR order (for unit test).

```

<SF isr: isr: TBP>+=
  procedure :: set_order => isr_set_order

```

```

<SF isr: sub interfaces>+≡
  module subroutine isr_set_order (object, order)
    class(isr_t), intent(inout) :: object
    integer, intent(in) :: order
  end subroutine isr_set_order

```

```

<SF isr: procedures>+≡
  module subroutine isr_set_order (object, order)
    class(isr_t), intent(inout) :: object
    integer, intent(in) :: order
    call object%data%set_order (order)
    call object%data%pdf%set_order (order)
  end subroutine isr_set_order

```

16.6.5 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ were trivial. The ISR structure function allows for a straightforward mapping of the unit interval. So, to leading order, the structure function value is unity, but the x value is transformed. Higher orders affect the function value.

The structure function implementation applies the above mapping to the input (random) number \mathbf{r} to generate the momentum fraction \mathbf{x} and the function value \mathbf{f} . For numerical stability reasons, we also output \mathbf{xb} , which is $\bar{x} = 1 - x$.

For the ISR structure function, the mapping Jacobian cancels the structure function (to order zero). We apply the cancellation explicitly, therefore both the Jacobian \mathbf{f} and the zeroth-order value (see the `apply` method) are unity if mapping is turned on. If mapping is turned off, the Jacobian \mathbf{f} includes the value of the (zeroth-order) structure function, and strongly peaked.

```

<SF isr: isr: TBP>+≡
  procedure :: complete_kinematics => isr_complete_kinematics

```

```

<SF isr: sub interfaces>+≡
  module subroutine isr_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
  end subroutine isr_complete_kinematics

```

```

<SF isr: procedures>+≡
  module subroutine isr_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    real(default) :: eps
    eps = sf_int%data%eps
  end subroutine isr_complete_kinematics

```

```

if (map) then
  call map_power_1 (sf_int%xb, f, rb(1), eps)
else
  sf_int%xb = rb(1)
  if (rb(1) > 0) then
    f = 1
  else
    f = 0
  end if
end if
sf_int%x = 1 - sf_int%xb
x(1) = sf_int%x
xb(1) = sf_int%xb
if (size (x) == 3) then
  x(2:3) = r(2:3)
  xb(2:3) = rb(2:3)
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  sf_int%xb = 0
  f = 0
end select
end subroutine isr_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum configuration. In the specific case of ISR, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

```

<SF isr: isr: TBP>+≡
  procedure :: recover_x => sf_isr_recover_x

<SF isr: sub interfaces>+≡
  module subroutine sf_isr_recover_x (sf_int, x, xb, x_free)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
  end subroutine sf_isr_recover_x

<SF isr: procedures>+≡
  module subroutine sf_isr_recover_x (sf_int, x, xb, x_free)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
    sf_int%xb = xb(1)
  end subroutine sf_isr_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

For extracting x , we rely on the stored \bar{x} value, since the x value in the argument is likely imprecise. This means that either `complete_kinematics` or `recover_x` must be called first, for the current sampling point (but maybe another channel).

```

<SF isr: isr: TBP>+≡
  procedure :: inverse_kinematics => isr_inverse_kinematics

<SF isr: sub interfaces>+≡
  module subroutine isr_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine isr_inverse_kinematics

<SF isr: procedures>+≡
  module subroutine isr_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default) :: eps
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    eps = sf_int%data%eps
    if (map) then
      call map_power_inverse_1 (xb(1), f, rb(1), eps)
    else
      rb(1) = xb(1)
      if (rb(1) > 0) then
        f = 1
      else
        f = 0
      end if
    end if
    r(1) = 1 - rb(1)
    if (size(r) == 3) then
      r(2:3) = x(2:3)
      rb(2:3) = xb(2:3)
    end if
    if (set_mom) then
      call sf_int%split_momentum (x, xb)
      select case (sf_int%status)
      case (SF_FAILED_KINEMATICS)
        r = 0

```

```

        rb= 0
        f = 0
    end select
end if
end subroutine isr_inverse_kinematics

<SF isr: isr: TBP>+≡
    procedure :: init => isr_init

<SF isr: sub interfaces>+≡
    module subroutine isr_init (sf_int, data)
        class(isr_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
    end subroutine isr_init

<SF isr: procedures>+≡
    module subroutine isr_init (sf_int, data)
        class(isr_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
        type(quantum_numbers_mask_t), dimension(3) :: mask
        integer, dimension(3) :: hel_lock
        type(polarization_t), target :: pol
        type(quantum_numbers_t), dimension(1) :: qn_fc
        type(flavor_t) :: flv_photon
        type(color_t) :: col_photon
        type(quantum_numbers_t) :: qn_hel, qn_photon, qn
        type(polarization_iterator_t) :: it_hel
        real(default) :: m2
        integer :: i
        mask = quantum_numbers_mask (.false., .false., &
            mask_h = [.false., .true., .false.])
        hel_lock = [3, 0, 1]
        select type (data)
        type is (isr_data_t)
            m2 = data%mass**2
            call sf_int%base_init (mask, [m2], [0._default], [m2], &
                hel_lock = hel_lock)
            sf_int%data => data
            call flv_photon%init (PHOTON, data%model)
            call col_photon%init ()
            call qn_photon%init (flv_photon, col_photon)
            call qn_photon%tag_radiated ()
            do i = 1, size (data%flv_in)
                call pol%init_generic (data%flv_in(i))
                call qn_fc(1)%init (&
                    flv = data%flv_in(i), &
                    col = color_from_flavor (data%flv_in(i), 1))
                call it_hel%init (pol)
            do while (it_hel%is_valid ())
                qn_hel = it_hel%get_quantum_numbers ()
                qn = qn_hel .merge. qn_fc(1)
                call sf_int%add_state ([qn, qn_photon, qn])
                call it_hel%advance ()
            end do
            ! call pol%final () !!! Obsolete
        end select
    end subroutine isr_init

```



```

end do
call sf_int%freeze ()
if (data%keep_energy) then
  sf_int%on_shell_mode = KEEP_ENERGY
else
  sf_int%on_shell_mode = KEEP_MOMENTUM
end if
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
sf_int%status = SF_INITIAL
end select
end subroutine isr_init

```

16.6.6 ISR application

For ISR, we could in principle compute kinematics and function value in a single step. In order to be able to reweight matrix elements including structure functions we split kinematics and structure function calculation. The structure function works on a single beam, assuming that the input momentum has been set.

For the structure-function evaluation, we rely on the fact that the power mapping, which we apply in the kinematics method (if the `map` flag is set), has a Jacobian which is just the inverse lowest-order structure function. With mapping active, the two should cancel exactly.

After splitting momenta, we set the outgoing momenta on-shell. We choose to conserve momentum, so energy conservation may be violated.

```

<SF isr: isr: TBP>+≡
  procedure :: apply => isr_apply

<SF isr: sub interfaces>+≡
  module subroutine isr_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(isr_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine isr_apply

<SF isr: procedures>+≡
  module subroutine isr_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(isr_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f, finv, x, xb, eps, rb
    real(default) :: log_x, log_xb, x_2
    associate (data => sf_int%data)
      eps = sf_int%data%eps
      x = sf_int%x
      xb = sf_int%xb
    end associate
  end subroutine isr_apply

```

```

    call map_power_inverse_1 (xb, finv, rb, eps)
    if (finv > 0) then
        f = 1 / finv
    else
        f = 0
    end if
    call data%pdf%evolve_qed_pdf (x, xb, rb, f)
end associate
call sf_int%set_matrix_element (cmplx (f, kind=default))
sf_int%status = SF_EVALUATED
end subroutine isr_apply

```

16.6.7 Unit tests

Test module, followed by the corresponding implementation module.

<sf_isr_ut.f90>≡
<File header>

```

module sf_isr_ut
    use unit_tests
    use sf_isr_uti

```

<Standard module head>

<SF isr: public test>

contains

<SF isr: test driver>

```

end module sf_isr_ut

```

<sf_isr_uti.f90>≡
<File header>

```

module sf_isr_uti

```

<Use kinds>

<Use strings>

```

    use io_units
    use format_defs, only: FMT_12
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use interactions, only: interaction_t
    use model_data
    use sf_aux, only: KEEP_ENERGY
    use sf_mappings
    use sf_base

```

```

    use sf_isr

```

```

    <Standard module head>

    <SF isr: test declarations>

contains

    <SF isr: tests>

end module sf_isr_util
API: driver for the unit tests below.
<SF isr: public test>≡
    public :: sf_isr_test
<SF isr: test driver>≡
    subroutine sf_isr_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF isr: execute tests>
end subroutine sf_isr_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF isr: execute tests>≡
    call test (sf_isr_1, "sf_isr_1", &
        "structure function configuration", &
        u, results)
<SF isr: test declarations>≡
    public :: sf_isr_1
<SF isr: tests>≡
    subroutine sf_isr_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t) :: pdg_in
        type(pdg_array_t), dimension(1) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        class(sf_data_t), allocatable :: data

        write (u, "(A)")  "* Test output: sf_isr_1"
        write (u, "(A)")  "* Purpose: initialize and display &
            &test structure function data"
        write (u, "(A)")

        write (u, "(A)")  "* Create empty data object"
        write (u, "(A)")

        call model%init_qed_test ()
        pdg_in = ELECTRON

        allocate (isr_data_t :: data)
        call data%write (u)
    end subroutine sf_isr_1

```

```

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

select type (data)
type is (isr_data_t)
  call data%init (model, pdg_in, 1./137._default, 10._default, &
    0.000511_default, order = 3, recoil = .false.)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_1"

end subroutine sf_isr_1

```

Structure function without mapping

Direct ISR evaluation. This is the use case for a double-beam structure function. The parameter pair is mapped in the calling program.

```

<SF isr: execute tests>+≡
  call test (sf_isr_2, "sf_isr_2", &
    "no ISR mapping", &
    u, results)

<SF isr: test declarations>+≡
  public :: sf_isr_2

<SF isr: tests>+≡
  subroutine sf_isr_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, f_isr

    write (u, "(A)")  "* Test output: sf_isr_2"

```

```

write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
pdg_in = ELECTRON
call flv%init (ELECTRON, model)

call reset_interaction_counter ()

allocate (isr_data_t :: data)
select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 500._default, &
        0.000511_default, order = 3, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.9, no ISR mapping, &
                  &collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.9_default
rb = 1 - r
write (u, "(A,9(1x," // FMT_12 // "))")  "r =", r
write (u, "(A,9(1x," // FMT_12 // "))")  "rb=", rb

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))")  "x =", x

```

```

write (u, "(A,9(1x," // FMT_12 // "))") "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Re-evaluate structure function, leading order"
write (u, "(A)")

select type (sf_int)
type is (isr_t)
    call sf_int%set_order (0)
end select
call sf_int%apply (scale = 100._default)
f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_2"

end subroutine sf_isr_2

```

Structure function with mapping

Apply the optimal ISR mapping. This is the use case for a single-beam structure function.

```
<SF isr: execute tests>+≡
    call test (sf_isr_3, "sf_isr_3", &
               "ISR mapping", &
               u, results)

<SF isr: test declarations>+≡
    public :: sf_isr_3

<SF isr: tests>+≡
    subroutine sf_isr_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f, f_isr

        write (u, "(A)")  "* Test output: sf_isr_3"
        write (u, "(A)")  "*   Purpose: initialize and fill &
                           &test structure function object"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize configuration data"
        write (u, "(A)")

        call model%init_qed_test ()
        call flv%init (ELECTRON, model)
        pdg_in = ELECTRON

        call reset_interaction_counter ()

        allocate (isr_data_t :: data)
        select type (data)
        type is (isr_data_t)
            call data%init (model, pdg_in, 1./137._default, 500._default, &
                           0.000511_default, order = 3, recoil = .false.)
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")

        call data%allocate_sf_int (sf_int)
        call sf_int%init (data)
        call sf_int%set_beam_index ([1])

        write (u, "(A)")  "* Initialize incoming momentum with E=500"
        write (u, "(A)")
```

```

E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.7, with ISR mapping, &
    &collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.7_default
rb = 1 - r
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))") "x =", x
write (u, "(A,9(1x," // FMT_12 // "))") "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")

```



```

write (u, "(A)")  "* Re-evaluate structure function, leading order"
write (u, "(A)")

select type (sf_int)
type is (isr_t)
  call sf_int%set_order (0)
end select
call sf_int%apply (scale = 100._default)
f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))")  "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))")  "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_3"

end subroutine sf_isr_3

```

Non-collinear ISR splitting

Construct and display a structure function object based on the ISR structure function. We blank out numerical fluctuations for 32bit.

```

<SF isr: execute tests>+≡
  call test (sf_isr_4, "sf_isr_4", &
    "ISR non-collinear", &
    u, results)

<SF isr: test declarations>+≡
  public :: sf_isr_4

<SF isr: tests>+≡
  subroutine sf_isr_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, f_isr
    character(len=80) :: buffer
    integer :: u_scratch, iostat

    write (u, "(A)")  "* Test output: sf_isr_4"

```

```

write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
call flv%init (ELECTRON, model)
pdg_in = ELECTRON

call reset_interaction_counter ()

write (u, "(A)")
write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

allocate (isr_data_t :: data)
select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 500._default, &
        0.000511_default, order = 3, recoil = .true.)
end select

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.25, with ISR mapping, "
write (u, "(A)")  "          non-coll., keeping energy"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%pacify_momenta (1e-10_default)

write (u, "(A,9(1x,F10.7))")  "x =", x

```

```

write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%pacify_momenta (1e-10_default)
call sf_int%apply (scale = 10._default)
u_scratch = free_unit ()
open (u_scratch, status="scratch", action = "readwrite")
call sf_int%write (u_scratch, testflag = .true.)
rewind (u_scratch)
do
  read (u_scratch, "(A)", iostat=iostat) buffer
  if (iostat /= 0) exit
  if (buffer(1:25) == " P =  0.000000E+00  9.57") then
    buffer = replace (buffer, 26, "XXXX")
  end if
  if (buffer(1:25) == " P =  0.000000E+00 -9.57") then
    buffer = replace (buffer, 26, "XXXX")
  end if
  write (u, "(A)") buffer
end do
close (u_scratch)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

```

```

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_4"

end subroutine sf_isr_4

```

Structure function pair with mapping

Apply the ISR mapping for a ISR pair. structure function.

```

<SF isr: execute tests>+≡
  call test (sf_isr_5, "sf_isr_5", &
    "ISR pair mapping", &
    u, results)

<SF isr: test declarations>+≡
  public :: sf_isr_5

<SF isr: tests>+≡
  subroutine sf_isr_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_mapping_t), allocatable :: mapping
    class(sf_int_t), dimension(:), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k
    real(default) :: E, f_map
    real(default), dimension(:), allocatable :: p, pb, r, rb, x, xb
    real(default), dimension(2) :: f, f_isr
    integer :: i

    write (u, "(A)")  "* Test output: sf_isr_5"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv%init (ELECTRON, model)
    pdg_in = ELECTRON

    call reset_interaction_counter ()

```

```

allocate (isr_data_t :: data)
select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 500._default, &
        0.000511_default, order = 3, recoil = .false.)
end select

allocate (sf_ip_mapping_t :: mapping)
select type (mapping)
type is (sf_ip_mapping_t)
    select type (data)
    type is (isr_data_t)
        call mapping%init (eps = data%get_eps ())
    end select
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

allocate (isr_t :: sf_int (2))

do i = 1, 2
    call sf_int(i)%init (data)
    call sf_int(i)%set_beam_index ([i])
end do

write (u, "(A)")  "* Initialize incoming momenta with E=500"
write (u, "(A)")
E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
k(2) = vector4_moving (E, - sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
do i = 1, 2
    call vector4_write (k(i), u)
    call sf_int(i)%seed_kinematics (k(i:i))
end do

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for p=[0.7,0.4], collinear"
write (u, "(A)")

allocate (p (2 * data%get_n_par ()))
allocate (pb(size (p)))
allocate (r (size (p)))
allocate (rb(size (p)))
allocate (x (size (p)))
allocate (xb(size (p)))

p = [0.7_default, 0.4_default]

```

```

pb= 1 - p
call mapping%compute (r, rb, f_map, p, pb)

write (u, "(A,9(1x," // FMT_12 // "))") "p =", p
write (u, "(A,9(1x," // FMT_12 // "))") "pb=", pb
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))") "fm=", f_map

do i = 1, 2
    call sf_int(i)%complete_kinematics (x(i:i), xb(i:i), f(i), r(i:i), rb(i:i), &
        map=.false.)
end do

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))") "x =", x
write (u, "(A,9(1x," // FMT_12 // "))") "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

do i = 1, 2
    call sf_int(i)%inverse_kinematics (x(i:i), xb(i:i), f(i), r(i:i), rb(i:i), &
        map=.false.)
end do
call mapping%inverse (r, rb, f_map, p, pb)

write (u, "(A,9(1x," // FMT_12 // "))") "p =", p
write (u, "(A,9(1x," // FMT_12 // "))") "pb=", pb
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))") "fm=", f_map

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"

call sf_int(1)%apply (scale = 100._default)
call sf_int(2)%apply (scale = 100._default)

write (u, "(A)")
write (u, "(A)")  "* Structure function #1"
write (u, "(A)")
call sf_int(1)%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Structure function #2"
write (u, "(A)")
call sf_int(2)%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

```

```

do i = 1, 2
    f_isr(i) = sf_int(i)%get_matrix_element (1)
end do

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", &
    product (f_isr)
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", &
    product (f_isr * f) * f_map

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

do i = 1, 2
    call sf_int(i)%final ()
end do
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_5"

end subroutine sf_isr_5

```

16.7 EPA

```
<sf_epa.f90>≡
  <File header>

  module sf_epa

    <Use kinds>
    <Use strings>
    use lorentz
    use pdg_arrays
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use polarizations
    use interactions
    use sf_aux
    use sf_base

    <Standard module head>

    <SF epa: public>

    <SF epa: parameters>

    <SF epa: types>

    interface
    <SF epa: sub interfaces>
    end interface

    contains

    <SF epa: main procedures>

  end module sf_epa

<sf_epa_sub.f90>≡
  <File header>

  submodule (sf_epa) sf_epa_s

    use io_units
    use constants, only: pi
    use format_defs, only: FMT_17, FMT_19
    use numeric_utils
    use diagnostics
    use physics_defs, only: PHOTON
    use colors

    implicit none

    contains
```


$\langle SF \text{ epa: procedures} \rangle$

end submodule sf_epa_s

16.7.1 Physics

The EPA structure function for a photon inside an (elementary) particle p with energy E , mass m and charge q_p (e.g., electron) is given by ($\bar{x} \equiv 1 - x$)

There are several variants of the EPA, which are steered by the `\$epa_mode` switch. The formula (6.17b) from the report by Budnev et al. is given by

$$f(x) = \frac{\alpha}{\pi} q_p^2 \frac{1}{x} \left[\left(\bar{x} + \frac{x^2}{2} \right) \ln \frac{Q_{\max}^2}{Q_{\min}^2} - \left(1 - \frac{x}{2} \right)^2 \ln \frac{x^2 + \frac{Q_{\max}^2}{E^2}}{\frac{Q_{\min}^2}{E^2}} - x^2 \frac{m^2}{Q_{\min}^2} \left(1 - \frac{Q_{\min}^2}{Q_{\max}^2} \right) \right]. \quad (16.39)$$

If no explicit Q bounds are provided, the kinematical bounds are

$$-Q_{\max}^2 = t_0 = -2\bar{x}(E^2 + p\bar{p}) + 2m^2 \approx -4\bar{x}E^2, \quad (16.40)$$

$$-Q_{\min}^2 = t_1 = -2\bar{x}(E^2 - p\bar{p}) + 2m^2 \approx -\frac{x^2}{\bar{x}}m^2. \quad (16.41)$$

The second and third terms in (16.39) are negative definite (and subleading). Noting that $\bar{x} + x^2/2$ is bounded between $1/2$ and 1 , we derive that $f(x)$ is always smaller than

$$\bar{f}(x) = \frac{\alpha}{\pi} q_p^2 \frac{L - 2 \ln x}{x} \quad \text{where} \quad L = \ln \frac{\min(4E_{\max}^2, Q_{\max}^2)}{\max(m^2, Q_{\min}^2)}, \quad (16.42)$$

where we allow for explicit Q bounds that narrow the kinematical range. Therefore, we generate this distribution:

$$\int_{x_0}^{x_1} dx \bar{f}(x) = C(x_0, x_1) \int_0^1 dx' \quad (16.43)$$

We set

$$\ln x = \frac{1}{2} \left\{ L - \sqrt{L^2 - 4[x' \ln x_1 (L - \ln x_1) + \bar{x}' \ln x_0 (L - \ln x_0)]} \right\} \quad (16.44)$$

such that $x(0) = x_0$ and $x(1) = x_1$ and

$$\frac{dx}{dx'} = \left(\frac{\alpha}{\pi} q_p^2 \right)^{-1} x \frac{C(x_0, x_1)}{L - 2 \ln x} \quad (16.45)$$

with

$$C(x_0, x_1) = \frac{\alpha}{\pi} q_p^2 [\ln x_1 (L - \ln x_1) - \ln x_0 (L - \ln x_0)] \quad (16.46)$$

such that (16.43) is satisfied. Finally, we have

$$\int_{x_0}^{x_1} dx f(x) = C(x_0, x_1) \int_0^1 dx' \frac{f(x(x'))}{\bar{f}(x(x'))} \quad (16.47)$$

where x' is calculated from x via (16.44).

The structure of the mapping is most obvious from:

$$x'(x) = \frac{\log x(L - \log x) - \log x_0(L - \log x_0)}{\log x_1(L - \log x_1) - \log x_0(L - \log x_0)} . \quad (16.48)$$

Taking the Eq. (6.16e) from the Budnev et al. report, and integrating it over q^2 yields the modified result

$$f(x) = \frac{\alpha}{\pi} q_p^2 \frac{1}{x} \left[\left(\bar{x} + \frac{x^2}{2} \right) \ln \frac{Q_{\max}^2}{Q_{\min}^2} - x^2 \frac{m^2}{Q_{\min}^2} \left(1 - \frac{Q_{\min}^2}{Q_{\max}^2} \right) \right]. \quad (16.49)$$

This is closer to many standard papers from LEP times, and to textbook formulae like e.g. in Peskin/Schroeder. For historical reasons, we keep Eq. (16.39) as the default in WHIZARD.

16.7.2 The EPA data block

The EPA parameters are: α , E_{\max} , m , Q_{\min} , and x_{\min} . Instead of m we can use the incoming particle PDG code as input; from this we can deduce the mass and charge.

Internally we store in addition $C_{0/1} = \frac{\alpha}{\pi} q_e^2 \ln x_{0/1}(L - \ln x_{0/1})$, the c.m. energy squared and the incoming particle mass.

$\langle SF \text{ epa: public} \rangle \equiv$

```
public :: EPA_MODE_DEFAULT
public :: EPA_MODE_BUDNEV_617
public :: EPA_MODE_BUDNEV_616E
public :: EPA_MODE_LOG_POWER
public :: EPA_MODE_LOG_SIMPLE
public :: EPA_MODE_LOG
```

$\langle SF \text{ epa: parameters} \rangle \equiv$

```
integer, parameter :: EPA_MODE_DEFAULT = 0
integer, parameter :: EPA_MODE_BUDNEV_617 = 0
integer, parameter :: EPA_MODE_BUDNEV_616E = 1
integer, parameter :: EPA_MODE_LOG_POWER = 2
integer, parameter :: EPA_MODE_LOG_SIMPLE = 3
integer, parameter :: EPA_MODE_LOG = 4
```

$\langle SF \text{ epa: public} \rangle + \equiv$

```
public :: epa_data_t
```

$\langle SF \text{ epa: types} \rangle \equiv$

```
type, extends(sf_data_t) :: epa_data_t
private
class(model_data_t), pointer :: model => null ()
type(flavor_t), dimension(:), allocatable :: flv_in
real(default) :: alpha
real(default) :: x_min
real(default) :: x_max
real(default) :: q_min
real(default) :: q_max
real(default) :: E_max
real(default) :: mass
```

```

    real(default) :: log
    real(default) :: a
    real(default) :: c0
    real(default) :: c1
    real(default) :: dc
    integer :: mode = EPA_MODE_DEFAULT
    integer :: error = NONE
    logical :: recoil = .false.
    logical :: keep_energy = .true.
contains
    <SF epa: epa_data: TBP>
end type epa_data_t

```

Error codes

```

<SF epa: parameters>+=
    integer, parameter :: NONE = 0
    integer, parameter :: ZERO_QMIN = 1
    integer, parameter :: Q_MAX_TOO_SMALL = 2
    integer, parameter :: ZERO_XMIN = 3
    integer, parameter :: MASS_MIX = 4
    integer, parameter :: NO_EPA = 5

<SF epa: epa_data: TBP>=
    procedure :: init => epa_data_init

<SF epa: sub interfaces>=
    module subroutine epa_data_init (data, model, mode, pdg_in, alpha, &
        x_min, q_min, q_max, mass, recoil, keep_energy)
        class(epa_data_t), intent(inout) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), intent(in) :: pdg_in
        integer, intent(in) :: mode
        real(default), intent(in) :: alpha, x_min, q_min, q_max
        real(default), intent(in), optional :: mass
        logical, intent(in), optional :: recoil
        logical, intent(in), optional :: keep_energy
    end subroutine epa_data_init

<SF epa: procedures>=
    module subroutine epa_data_init (data, model, mode, pdg_in, alpha, &
        x_min, q_min, q_max, mass, recoil, keep_energy)
        class(epa_data_t), intent(inout) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), intent(in) :: pdg_in
        integer, intent(in) :: mode
        real(default), intent(in) :: alpha, x_min, q_min, q_max
        real(default), intent(in), optional :: mass
        logical, intent(in), optional :: recoil
        logical, intent(in), optional :: keep_energy
        integer :: n_flv, i
        data%model => model
        data%mode = mode
        n_flv = pdg_in%get_length ()
        allocate (data%flv_in (n_flv))
        do i = 1, n_flv

```

```

        call data%flv_in(i)%init (pdg_in%get (i), model)
    end do
    data%alpha = alpha
    data%E_max = q_max / 2
    data%x_min = x_min
    data%x_max = 1
    if (vanishes (data%x_min)) then
        data%error = ZERO_XMIN; return
    end if
    data%q_min = q_min
    data%q_max = q_max
    select case (char (data%model%get_name ()))
    case ("QCD", "Test")
        data%error = NO_EPA; return
    end select
    if (present (recoil)) then
        data%recoil = recoil
    end if
    if (present (keep_energy)) then
        data%keep_energy = keep_energy
    end if
    if (present (mass)) then
        data%mass = mass
    else
        data%mass = data%flv_in(1)%get_mass ()
        if (any (data%flv_in%get_mass () /= data%mass)) then
            data%error = MASS_MIX; return
        end if
    end if
    if (max (data%mass, data%q_min) == 0) then
        data%error = ZERO_QMIN; return
    else if (max (data%mass, data%q_min) >= data%E_max) then
        data%error = Q_MAX_TOO_SMALL; return
    end if
    data%log = log ((data%q_max / max (data%mass, data%q_min)) ** 2 )
    data%a = data%alpha / pi
    data%c0 = log (data%x_min) * (data%log - log (data%x_min))
    data%c1 = log (data%x_max) * (data%log - log (data%x_max))
    data%dc = data%c1 - data%c0
end subroutine epa_data_init

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.

```

<SF epa: epa_data: TBP>+≡
    procedure :: check => epa_data_check

<SF epa: sub interfaces>+≡
    module subroutine epa_data_check (data)
        class(epa_data_t), intent(in) :: data
    end subroutine epa_data_check

<SF epa: procedures>+≡
    module subroutine epa_data_check (data)
        class(epa_data_t), intent(in) :: data
        select case (data%error)

```

```

case (NO_EPA)
  call msg_fatal ("EPA structure function not available for model " &
    // char (data%model%get_name ()) // ".")
case (ZERO_QMIN)
  call msg_fatal ("EPA: Particle mass is zero")
case (Q_MAX_TOO_SMALL)
  call msg_fatal ("EPA: Particle mass exceeds Qmax")
case (ZERO_XMIN)
  call msg_fatal ("EPA: x_min must be larger than zero")
case (MASS_MIX)
  call msg_fatal ("EPA: incoming particle masses must be uniform")
end select
end subroutine epa_data_check

```

Output

<SF epa: epa data: TBP>+≡

```
procedure :: write => epa_data_write
```

<SF epa: sub interfaces>+≡

```

module subroutine epa_data_write (data, unit, verbose)
  class(epa_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
end subroutine epa_data_write

```

<SF epa: procedures>+≡

```

module subroutine epa_data_write (data, unit, verbose)
  class(epa_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "EPA data:"
  if (allocated (data%flv_in)) then
    write (u, "(3x,A)", advance="no") " flavor = "
    do i = 1, size (data%flv_in)
      if (i > 1) write (u, "(',',1x)", advance="no")
      call data%flv_in(i)%write (u)
    end do
    write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") " alpha = ", data%alpha
    write (u, "(3x,A," // FMT_19 // ")") " x_min = ", data%x_min
    write (u, "(3x,A," // FMT_19 // ")") " x_max = ", data%x_max
    write (u, "(3x,A," // FMT_19 // ")") " q_min = ", data%q_min
    write (u, "(3x,A," // FMT_19 // ")") " q_max = ", data%q_max
    write (u, "(3x,A," // FMT_19 // ")") " E_max = ", data%e_max
    write (u, "(3x,A," // FMT_19 // ")") " mass = ", data%mass
    write (u, "(3x,A," // FMT_19 // ")") " a = ", data%a
    write (u, "(3x,A," // FMT_19 // ")") " c0 = ", data%c0
    write (u, "(3x,A," // FMT_19 // ")") " c1 = ", data%c1
    write (u, "(3x,A," // FMT_19 // ")") " log = ", data%log
    write (u, "(3x,A,L2)") " recoil = ", data%recoil
    write (u, "(3x,A,L2)") " keep en. = ", data%keep_energy
  else
    write (u, "(3x,A)") "[undefined]"
  end if
end subroutine epa_data_write

```

```

        end if
    end subroutine epa_data_write

```

The number of kinematic parameters.

```

<SF epa: epa data: TBP>+≡
    procedure :: get_n_par => epa_data_get_n_par

<SF epa: sub interfaces>+≡
    module function epa_data_get_n_par (data) result (n)
        class(epa_data_t), intent(in) :: data
        integer :: n
    end function epa_data_get_n_par

<SF epa: procedures>+≡
    module function epa_data_get_n_par (data) result (n)
        class(epa_data_t), intent(in) :: data
        integer :: n
        if (data%recoil) then
            n = 3
        else
            n = 1
        end if
    end function epa_data_get_n_par

```

Return the outgoing particles PDG codes. The outgoing particle is always the photon while the radiated particle is identical to the incoming one.

```

<SF epa: epa data: TBP>+≡
    procedure :: get_pdg_out => epa_data_get_pdg_out

<SF epa: sub interfaces>+≡
    module subroutine epa_data_get_pdg_out (data, pdg_out)
        class(epa_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine epa_data_get_pdg_out

<SF epa: procedures>+≡
    module subroutine epa_data_get_pdg_out (data, pdg_out)
        class(epa_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        pdg_out(1) = PHOTON
    end subroutine epa_data_get_pdg_out

```

Allocate the interaction record. Gfortran 7/8/9 bug, has to remain in module.

```

<SF epa: epa data: TBP>+≡
    procedure :: allocate_sf_int => epa_data_allocate_sf_int

<SF epa: main procedures>≡
    subroutine epa_data_allocate_sf_int (data, sf_int)
        class(epa_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (epa_t :: sf_int)
    end subroutine epa_data_allocate_sf_int

```

16.7.3 The EPA object

The `epa_t` data type is a $1 \rightarrow 2$ interaction. We should be able to handle several flavors in parallel, since EPA is not necessarily applied immediately after beam collision: Photons may be radiated from quarks. In that case, the partons are massless and q_{\min} applies instead, so we do not need to generate several kinematical configurations in parallel.

The squared charge values multiply the matrix elements, depending on the flavour. We scan the interaction after building it, so we have the correct assignments.

The particles are ordered as (incoming, radiated, photon), where the photon initiates the hard interaction.

We generate an unpolarized photon and transfer initial polarization to the radiated parton. Color is transferred in the same way.

```

<SF epa: types>+=
  type, extends (sf_int_t) :: epa_t
    type(epa_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: xb = 0
    real(default) :: E = 0
    real(default), dimension(:), allocatable :: charge2
  contains
    <SF epa: epa: TBP>
  end type epa_t

```

Type string: has to be here, but there is no string variable on which EPA depends. Hence, a dummy routine.

```

<SF epa: epa: TBP>=
  procedure :: type_string => epa_type_string

<SF epa: sub interfaces>+=
  module function epa_type_string (object) result (string)
    class(epa_t), intent(in) :: object
    type(string_t) :: string
  end function epa_type_string

<SF epa: procedures>+=
  module function epa_type_string (object) result (string)
    class(epa_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "EPA: equivalent photon approx."
    else
      string = "EPA: [undefined]"
    end if
  end function epa_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF epa: epa: TBP>+=
  procedure :: write => epa_write

<SF epa: sub interfaces>+=
  module subroutine epa_write (object, unit, testflag)

```

```

        class(epa_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine epa_write

<SF epa: procedures>+≡
module subroutine epa_write (object, unit, testflag)
    class(epa_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
        call object%data%write (u)
        if (object%status >= SF_DONE_KINEMATICS) then
            write (u, "(1x,A)") "SF parameters:"
            write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
            if (object%status >= SF_FAILED_EVALUATION) then
                write (u, "(3x,A," // FMT_17 // ")") "E =", object%E
            end if
        end if
        call object%base_write (u, testflag)
    else
        write (u, "(1x,A)") "EPA data: [undefined]"
    end if
end subroutine epa_write

```

Prepare the interaction object. We have to construct transition matrix elements for all flavor and helicity combinations.

```

<SF epa: epa: TBP>+≡
    procedure :: init => epa_init

<SF epa: sub interfaces>+≡
    module subroutine epa_init (sf_int, data)
        class(epa_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
    end subroutine epa_init

<SF epa: procedures>+≡
module subroutine epa_init (sf_int, data)
    class(epa_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    integer, dimension(3) :: hel_lock
    type(polarization_t), target :: pol
    type(quantum_numbers_t), dimension(1) :: qn_fc
    type(flavor_t) :: flv_photon
    type(color_t) :: col_photon
    type(quantum_numbers_t) :: qn_hel, qn_photon, qn, qn_rad
    type(polarization_iterator_t) :: it_hel
    integer :: i
    mask = quantum_numbers_mask (.false., .false., &
        mask_h = [.false., .false., .true.])
    hel_lock = [2, 1, 0]
    select type (data)

```



```

type is (epa_data_t)
  call sf_int%base_init (mask, [data%mass**2], &
    [data%mass**2], [0._default], hel_lock = hel_lock)
  sf_int%data => data
  call flv_photon%init (PHOTON, data%model)
  call col_photon%init ()
  call qn_photon%init (flv_photon, col_photon)
  do i = 1, size (data%flv_in)
    call pol%init_generic (data%flv_in(i))
    call qn_fc(1)%init ( &
      flv = data%flv_in(i), &
      col = color_from_flavor (data%flv_in(i), 1))
    call it_hel%init (pol)
    do while (it_hel%is_valid ())
      qn_hel = it_hel%get_quantum_numbers ()
      qn = qn_hel .merge. qn_fc(1)
      qn_rad = qn
      call qn_rad%tag_radiated ()
      call sf_int%add_state ([qn, qn_rad, qn_photon])
      call it_hel%advance ()
    end do
    ! call pol%final ()
  end do
  call sf_int%freeze ()
  if (data%keep_energy) then
    sf_int%on_shell_mode = KEEP_ENERGY
  else
    sf_int%on_shell_mode = KEEP_MOMENTUM
  end if
  call sf_int%set_incoming ([1])
  call sf_int%set_radiated ([2])
  call sf_int%set_outgoing ([3])
end select
end subroutine epa_init

```

Prepare the charge array. This is separate from the previous routine since the state matrix may be helicity-contracted.

<SF epa: epa: TBP>+≡

```

procedure :: setup_constants => epa_setup_constants

```

<SF epa: sub interfaces>+≡

```

module subroutine epa_setup_constants (sf_int)
  class(epa_t), intent(inout), target :: sf_int
end subroutine epa_setup_constants

```

<SF epa: procedures>+≡

```

module subroutine epa_setup_constants (sf_int)
  class(epa_t), intent(inout), target :: sf_int
  type(state_iterator_t) :: it
  type(flavor_t) :: flv
  integer :: i, n_me
  n_me = sf_int%get_n_matrix_elements ()
  allocate (sf_int%charge2 (n_me))
  call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
  do while (it%is_valid ())

```

```

        i = it%get_me_index ()
        flv = it%get_flavor (1)
        sf_int%charge2(i) = flv%get_charge () ** 2
        call it%advance ()
    end do
    sf_int%status = SF_INITIAL
end subroutine epa_setup_constants

```

16.7.4 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

The EPA structure function allows for a straightforward mapping of the unit interval. The x value is transformed, and the mapped structure function becomes unity at its upper boundary.

The structure function implementation applies the above mapping to the input (random) number `r` to generate the momentum fraction `x` and the function value `f`. For numerical stability reasons, we also output `xb`, which is $\bar{x} = 1 - x$.

<SF epa: epa: TBP>+≡

```

    procedure :: complete_kinematics => epa_complete_kinematics

```

<SF epa: sub interfaces>+≡

```

    module subroutine epa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
    end subroutine epa_complete_kinematics

```

<SF epa: procedures>+≡

```

    module subroutine epa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        real(default) :: delta, sqrt_delta, lx
        if (map) then
            associate (data => sf_int%data)
                delta = data%log ** 2 - 4 * (r(1) * data%c1 + rb(1) * data%c0)
                if (delta > 0) then
                    sqrt_delta = sqrt (delta)
                    lx = (data%log - sqrt_delta) / 2
                else
                    sf_int%status = SF_FAILED_KINEMATICS
                    f = 0
                    return
                end if
            end associate
        end if
    end subroutine epa_complete_kinematics

```

```

        x(1) = exp (lx)
        f = x(1) * data%dc / sqrt_delta
    end associate
else
    x(1) = r(1)
    if (sf_int%data%x_min < x(1) .and. x(1) < sf_int%data%x_max) then
        f = 1
    else
        sf_int%status = SF_FAILED_KINEMATICS
        f = 0
        return
    end if
end if
xb(1) = 1 - x(1)
if (size(x) == 3) then
    x(2:3) = r(2:3)
    xb(2:3) = rb(2:3)
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_DONE_KINEMATICS)
    sf_int%x = x(1)
    sf_int%xb= xb(1)
    sf_int%E = energy (sf_int%get_momentum (1))
case (SF_FAILED_KINEMATICS)
    sf_int%x = 0
    sf_int%xb= 0
    f = 0
end select
end subroutine epa_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum configuration. In the specific case of EPA, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

Note: the extraction of \bar{x} is not numerically safe, but it cannot be as long as the base `recover_x` is not.

(SF epa: epa: TBP)+≡

```

    procedure :: recover_x => sf_epa_recover_x

```

(SF epa: sub interfaces)+≡

```

    module subroutine sf_epa_recover_x (sf_int, x, xb, x_free)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_epa_recover_x

```

(SF epa: procedures)+≡

```

    module subroutine sf_epa_recover_x (sf_int, x, xb, x_free)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(inout), optional :: x_free
        call sf_int%base_recover_x (x, xb, x_free)
    end subroutine sf_epa_recover_x

```

```

    sf_int%x = x(1)
    sf_int%xb = xb(1)
end subroutine sf_epa_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF epa: epa: TBP>+≡
    procedure :: inverse_kinematics => epa_inverse_kinematics

<SF epa: sub interfaces>+≡
    module subroutine epa_inverse_kinematics &
        (sf_int, x, xb, f, r, rb, map, set_momenta)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(in) :: x
        real(default), dimension(:), intent(in) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: r
        real(default), dimension(:), intent(out) :: rb
        logical, intent(in) :: map
        logical, intent(in), optional :: set_momenta
    end subroutine epa_inverse_kinematics

<SF epa: procedures>+≡
    module subroutine epa_inverse_kinematics &
        (sf_int, x, xb, f, r, rb, map, set_momenta)
        class(epa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(in) :: x
        real(default), dimension(:), intent(in) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: r
        real(default), dimension(:), intent(out) :: rb
        logical, intent(in) :: map
        logical, intent(in), optional :: set_momenta
        real(default) :: lx, delta, sqrt_delta, c
        logical :: set_mom
        set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
        if (map) then
            associate (data => sf_int%data)
                lx = log (x(1))
                sqrt_delta = data%log - 2 * lx
                delta = sqrt_delta ** 2
                c = (data%log ** 2 - delta) / 4
                r (1) = (c - data%c0) / data%dc
                rb(1) = (data%c1 - c) / data%dc
                f = x(1) * data%dc / sqrt_delta
            end associate
        else
            r (1) = x(1)
            rb(1) = xb(1)
            if (sf_int%data%x_min < x(1) .and. x(1) < sf_int%data%x_max) then
                f = 1
            else
                f = 0
            end if
        end if
    end subroutine epa_inverse_kinematics

```

```

        end if
    end if
    if (size(r) == 3) then
        r (2:3) = x(2:3)
        rb(2:3) = xb(2:3)
    end if
    if (set_mom) then
        call sf_int%split_momentum (x, xb)
        select case (sf_int%status)
            case (SF_FAILED_KINEMATICS); f = 0
        end select
    end if
    sf_int%E = energy (sf_int%get_momentum (1))
end subroutine epa_inverse_kinematics

```

16.7.5 EPA application

For EPA, we can in principle compute kinematics and function value in a single step. In order to be able to reweight events, kinematics and structure function application are separated. This function works on a single beam, assuming that the input momentum has been set. We need three random numbers as input: one for x , and two for the polar and azimuthal angles. Alternatively, for the no-recoil case, we can skip p_T generation; in this case, we only need one.

For obtaining splitting kinematics, we rely on the assumption that all in-particles are mass-degenerate (or there is only one), so the generated x values are identical.

Fix 2020-03-10: Divide by two if there is polarization. In the polarized case, the outgoing electron/positron retains the incoming polarization. The latter is summed over when convoluting with the beam, but there are still two states with different outgoing polarization but identical structure-function value. This leads to double-counting for the overall cross section.

Fix 2022-02-18: The above fix was wrong! The structure function was divided by 4 because there are four entries in the complete electron density matrix. Now it is divided by 2 if there is more than one entry, unchanged otherwise.

```

<SF epa: epa: TBP>+=
    procedure :: apply => epa_apply

<SF epa: sub interfaces>+=
    module subroutine epa_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(epa_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
    end subroutine epa_apply

<SF epa: procedures>+=
    module subroutine epa_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(epa_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale

```

```

integer, intent(in), optional :: i_sub
real(default) :: x, xb, qminsq, qmaxsq, f, E, m2
associate (data => sf_int%data)
  x = sf_int%x
  xb = sf_int%xb
  E = sf_int%E
  m2 = data%mass ** 2
  qminsq = max (x ** 2 / xb * data%mass ** 2, data%q_min ** 2)
  select case (data%mode)
  case (0)
    qmaxsq = min (4 * xb * E ** 2, data%q_max ** 2)
    if (qminsq < qmaxsq) then
      f = data%a / x &
        * ((xb + x ** 2 / 2) * log (qmaxsq / qminsq) &
          - (1 - x / 2) ** 2 &
          * log ((x**2 + qmaxsq / E ** 2) / (x**2 + qminsq / E ** 2)) &
          - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
    else
      f = 0
    end if
  case (1)
    qmaxsq = min (4 * xb * E ** 2, data%q_max ** 2)
    if (qminsq < qmaxsq) then
      f = data%a / x &
        * ((xb + x ** 2 / 2) * log (qmaxsq / qminsq) &
          - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
    else
      f = 0
    end if
  case (2)
    qmaxsq = data%q_max ** 2
    if (data%mass ** 2 < qmaxsq) then
      f = data%a / x &
        * ((xb + x ** 2 / 2) * log (qmaxsq / m2) &
          - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
    else
      f = 0
    end if
  case (3)
    qmaxsq = data%q_max ** 2
    if (data%mass ** 2 < qmaxsq) then
      f = data%a / x &
        * ((xb + x ** 2 / 2) * log (qmaxsq / m2) &
          - x ** 2 * (1 - m2 / qmaxsq))
    else
      f = 0
    end if
  case (4)
    qmaxsq = data%q_max ** 2
    if (data%mass ** 2 < qmaxsq) then
      f = data%a / x &
        * ((xb + x ** 2 / 2) * log (qmaxsq / m2))
    else
      f = 0
    end if
  end select
end associate

```

```

        end if
    end select
    if (sf_int%get_n_matrix_elements () > 1) then
        f = f / 2
    end if
    call sf_int%set_matrix_element &
        (cmplx (f, kind=default) * sf_int%charge2)
    end associate
    sf_int%status = SF_EVALUATED
end subroutine epa_apply

```

16.7.6 Unit tests

Test module, followed by the corresponding implementation module.

<sf_epa_ut.f90>≡
<File header>

```

module sf_epa_ut
    use unit_tests
    use sf_epa_uti

```

<Standard module head>

<SF epa: public test>

contains

<SF epa: test driver>

```

end module sf_epa_ut

```

<sf_epa_uti.f90>≡
<File header>

```

module sf_epa_uti

```

<Use kinds>

```

    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_aux
    use sf_base

```

```

    use sf_epa

```

<Standard module head>

<SF epa: test declarations>

contains

<SF epa: tests>

end module sf_epa_util

API: driver for the unit tests below.

<SF epa: public test>≡

public :: sf_epa_test

<SF epa: test driver>≡

subroutine sf_epa_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SF epa: execute tests>

end subroutine sf_epa_test

Test structure function data

Construct and display a test structure function data object.

<SF epa: execute tests>≡

call test (sf_epa_1, "sf_epa_1", &
"structure function configuration", &
u, results)

<SF epa: test declarations>≡

public :: sf_epa_1

<SF epa: tests>≡

subroutine sf_epa_1 (u)

integer, intent(in) :: u

type(model_data_t), target :: model

type(pdg_array_t) :: pdg_in

type(pdg_array_t), dimension(1) :: pdg_out

integer, dimension(:), allocatable :: pdg1

class(sf_data_t), allocatable :: data

write (u, "(A)") "* Test output: sf_epa_1"

write (u, "(A)") "* Purpose: initialize and display &
 &test structure function data"

write (u, "(A)")

write (u, "(A)") "* Create empty data object"

write (u, "(A)")

call model%init_qed_test ()

pdg_in = ELECTRON

allocate (epa_data_t :: data)

call data%write (u)

write (u, "(A)")

write (u, "(A)") "* Initialize"

write (u, "(A)")

select type (data)


```

type is (epa_data_t)
  call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
    10._default, 100._default, 0.000511_default, recoil = .false.)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_1"

end subroutine sf_epa_1

```

Test and probe structure function

Construct and display a structure function object based on the EPA structure function.

```

<SF epa: execute tests>+≡
  call test (sf_epa_2, "sf_epa_2", &
    "structure function instance", &
    u, results)

<SF epa: test declarations>+≡
  public :: sf_epa_2

<SF epa: tests>+≡
  subroutine sf_epa_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_epa_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"

```

```

write (u, "(A)")

call model%init_qed_test ()
call flv%init (ELECTRON, model)
pdg_in = ELECTRON

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

```

```

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_2"

end subroutine sf_epa_2

```

Standard mapping

Construct and display a structure function object based on the EPA structure function, applying the standard single-particle mapping.

```

<SF epa: execute tests>+≡
    call test (sf_epa_3, "sf_epa_3", &
        "apply mapping", &
        u, results)

<SF epa: test declarations>+≡
    public :: sf_epa_3

<SF epa: tests>+≡
    subroutine sf_epa_3 (u)

```

```

integer, intent(in) :: u
type(model_data_t), target :: model
type(flavor_t) :: flv
type(pdg_array_t) :: pdg_in
class(sf_data_t), allocatable, target :: data
class(sf_int_t), allocatable :: sf_int
type(vector4_t) :: k
type(vector4_t), dimension(2) :: q
real(default) :: E
real(default), dimension(:), allocatable :: r, rb, x, xb
real(default) :: f

write (u, "(A)")  "* Test output: sf_epa_3"
write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
call flv%init (ELECTRON, model)
pdg_in = ELECTRON

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, with EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))

```

```

allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_3"

```

```
end subroutine sf_epa_3
```

Non-collinear case

Construct and display a structure function object based on the EPA structure function.

```
<SF epa: execute tests>+≡
  call test (sf_epa_4, "sf_epa_4", &
    "non-collinear", &
    u, results)

<SF epa: test declarations>+≡
  public :: sf_epa_4

<SF epa: tests>+≡
  subroutine sf_epa_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E, m
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_epa_4"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv%init (ELECTRON, model)
    pdg_in = ELECTRON

    call reset_interaction_counter ()

    allocate (epa_data_t :: data)
    select type (data)
    type is (epa_data_t)
      call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 5.0_default, recoil = .true.)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")
```

```

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500, me = 5 GeV"
write (u, "(A)")
E = 500
m = 5
k = vector4_moving (E, sqrt (E**2 - m**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.5/0.5/0.25, with EPA mapping, "
write (u, "(A)")  "          non-coll., keeping energy, me = 5 GeV"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%pacify_momenta (1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)

```

```

call sf_int%pacify_momenta (1e-10_default)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_4"

end subroutine sf_epa_4

```

Structure function for multiple flavors

Construct and display a structure function object based on the EPA structure function. The incoming state has multiple particles with non-uniform charge.

```

<SF epa: execute tests>+≡
  call test (sf_epa_5, "sf_epa_5", &
    "multiple flavors", &
    u, results)

<SF epa: test declarations>+≡
  public :: sf_epa_5

<SF epa: tests>+≡
  subroutine sf_epa_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_epa_5"
    write (u, "(A)")  "* Purpose: initialize and fill &

```



```

        &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_sm_test ()
call flv%init (1, model)
pdg_in = [1, 2, -1, -2]

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
    call data%check ()
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

```

```

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_5"

end subroutine sf_epa_5

```

16.8 EWA

```
<sf_ewa.f90>≡  
  <File header>  
  
  module sf_ewa  
  
    <Use kinds>  
    <Use strings>  
    use pdg_arrays  
    use model_data  
    use flavors  
    use quantum_numbers  
    use state_matrices  
    use polarizations  
    use interactions  
    use sf_aux  
    use sf_base  
  
    <Standard module head>  
  
    <SF ewa: public>  
  
    <SF ewa: parameters>  
  
    <SF ewa: types>  
  
    interface  
    <SF ewa: sub interfaces>  
    end interface  
  
    contains  
  
    <SF ewa: main procedures>  
  
  end module sf_ewa  
<sf_ewa_sub.f90>≡  
  <File header>  
  
  submodule (sf_ewa) sf_ewa_s  
  
    use io_units  
    use constants, only: pi  
    use format_defs, only: FMT_17, FMT_19  
    use numeric_utils  
    use diagnostics  
    use physics_defs, only: W_BOSON, Z_BOSON  
    use lorentz  
    use colors  
  
    implicit none  
  
    contains
```

⟨SF ewa: procedures⟩

`end submodule sf_ewa_s`

16.8.1 Physics

The EWA structure function for a Z or W inside a fermion (lepton or quark) depends on the vector-boson polarization. We distinguish transversal (\pm) and longitudinal (0) polarization.

$$F_+(x) = \frac{1}{16\pi^2} \frac{(v-a)^2 + (v+a)^2 \bar{x}^2}{x} \left[\ln \left(\frac{p_{\perp,\max}^2 + \bar{x}M^2}{\bar{x}M^2} \right) - \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \right] \quad (16.50)$$

$$F_-(x) = \frac{1}{16\pi^2} \frac{(v+a)^2 + (v-a)^2 \bar{x}^2}{x} \left[\ln \left(\frac{p_{\perp,\max}^2 + \bar{x}M^2}{\bar{x}M^2} \right) - \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \right] \quad (16.51)$$

$$F_0(x) = \frac{v^2 + a^2}{8\pi^2} \frac{2\bar{x}}{x} \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \quad (16.52)$$

where $p_{\perp,\max}$ is the cutoff in transversal momentum, M is the vector-boson mass, v and a are the vector and axial-vector couplings, and $\bar{x} \equiv 1-x$. Note that the longitudinal structure function is finite for large cutoff, while the transversal structure function is logarithmically divergent.

The maximal transverse momentum is given by the kinematical limit, it is

$$p_{\perp,\max} = \bar{x}\sqrt{s}/2. \quad (16.53)$$

The vector and axial couplings for a fermion branching into a W are

$$v_W = \frac{g}{2\sqrt{2}}, \quad a_W = \frac{g}{2\sqrt{2}}. \quad (16.54)$$

For Z emission, this is replaced by

$$v_Z = \frac{g}{2\cos\theta_w} (t_3 - 2q\sin^2\theta_w), \quad a_Z = \frac{g}{2\cos\theta_w} t_3, \quad (16.55)$$

where $t_3 = \pm\frac{1}{2}$ is the fermion isospin, and q its charge.

For an initial antifermion, the signs of the axial couplings are inverted. Note that a common sign change of v and a is irrelevant.

The EWA depends on the parameters g , $\sin^2\theta_w$, M_W , and M_Z . These can all be taken from the SM input, and the prefactors are calculated from those and the incoming particle type.

Since these structure functions have a $1/x$ singularity (which is not really relevant in practice, however, since the vector boson mass is finite), we map this singularity allowing for nontrivial x bounds:

$$x = \exp(\bar{r} \ln x_0 + r \ln x_1) \quad (16.56)$$

such that

$$\int_{x_0}^{x_1} \frac{dx}{x} = (\ln x_1 - \ln x_0) \int_0^1 dr. \quad (16.57)$$

As a user parameter, we have the cutoff $p_{\perp, \max}$. The divergence $1/x$ also requires a x_0 cutoff; and for completeness we introduce a corresponding x_1 . Physically, the minimal sensible value of x is M^2/s , although the approximation loses its value already at higher x values.

16.8.2 The EWA data block

The EWA parameters are: $p_{T, \max}$, c_V , c_A , and m . Instead of m we can use the incoming particle PDG code as input; from this we can deduce the mass and charges. In the initialization phase it is not yet determined whether a W or a Z is radiated, hence we set the vector and axial-vector couplings equal to the common prefactors $g/2 = e/2/\sin \theta_W$.

In principle, for EWA it would make sense to allow the user to also set the upper bound for x , x_{\max} , but we fix it to one here.

```

<SF ewa: public>≡
  public :: ewa_data_t

<SF ewa: types>≡
  type, extends(sf_data_t) :: ewa_data_t
    private
      class(model_data_t), pointer :: model => null ()
      type(flavor_t), dimension(:), allocatable :: flv_in
      type(flavor_t), dimension(:), allocatable :: flv_out
      real(default) :: pt_max
      real(default) :: sqrts
      real(default) :: x_min
      real(default) :: x_max
      real(default) :: mass
      real(default) :: m_out
      real(default) :: q_min
      real(default) :: cv
      real(default) :: ca
      real(default) :: costhw
      real(default) :: sinthw
      real(default) :: mW
      real(default) :: mZ
      real(default) :: coeff
      logical :: mass_set = .false.
      logical :: recoil = .false.
      logical :: keep_energy = .false.
      integer :: id = 0
      integer :: error = NONE
    contains
      <SF ewa: ewa data: TBP>
    end type ewa_data_t

```

Error codes

```

<SF ewa: parameters>≡
  integer, parameter :: NONE = 0

```

```

integer, parameter :: ZERO_QMIN = 1
integer, parameter :: Q_MAX_TOO_SMALL = 2
integer, parameter :: ZERO_XMIN = 3
integer, parameter :: MASS_MIX = 4
integer, parameter :: ZERO_SW = 5
integer, parameter :: ISOSPIN_MIX = 6
integer, parameter :: WRONG_PRT = 7
integer, parameter :: MASS_MIX_OUT = 8
integer, parameter :: NO_EWA = 9

<SF ewa: ewa data: TBP>≡
  procedure :: init => ewa_data_init

<SF ewa: sub interfaces>≡
  module subroutine ewa_data_init (data, model, pdg_in, x_min, pt_max, &
    sqrts, recoil, keep_energy, mass)
    class(ewa_data_t), intent(inout) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: x_min, pt_max, sqrts
    logical, intent(in) :: recoil, keep_energy
    real(default), intent(in), optional :: mass
  end subroutine ewa_data_init

<SF ewa: procedures>≡
  module subroutine ewa_data_init (data, model, pdg_in, x_min, pt_max, &
    sqrts, recoil, keep_energy, mass)
    class(ewa_data_t), intent(inout) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: x_min, pt_max, sqrts
    logical, intent(in) :: recoil, keep_energy
    real(default), intent(in), optional :: mass
    real(default) :: g, ee
    integer :: n_flv, i
    data%model => model
    if (.not. any (pdg_in .match. &
      [1,2,3,4,5,6,11,13,15,-1,-2,-3,-4,-5,-6,-11,-13,-15])) then
      data%error = WRONG_PRT; return
    end if
    n_flv = pdg_in%get_length ()
    allocate (data%flv_in (n_flv))
    allocate (data%flv_out(n_flv))
    do i = 1, n_flv
      call data%flv_in(i)%init (pdg_in%get (i), model)
    end do
    data%pt_max = pt_max
    data%sqrts = sqrts
    data%x_min = x_min
    data%x_max = 1
    if (vanishes (data%x_min)) then
      data%error = ZERO_XMIN; return
    end if
    select case (char (data%model%get_name ()))
    case ("QCD","QED","Test")
      data%error = NO_EWA; return

```

```

end select
ee = data%model%get_real (var_str ("ee"))
data%sinthw = data%model%get_real (var_str ("sw"))
data%costhw = data%model%get_real (var_str ("cw"))
data%mZ = data%model%get_real (var_str ("mZ"))
data%mW = data%model%get_real (var_str ("mW"))
if (data%sinthw /= 0) then
  g = ee / data%sinthw
else
  data%error = ZERO_SW; return
end if
data%cv = g / 2._default
data%ca = g / 2._default
data%coeff = 1._default / (8._default * PI**2)
data%recoil = recoil
data%keep_energy = keep_energy
if (present (mass)) then
  data%mass = mass
  data%m_out = mass
  data%mass_set = .true.
else
  data%mass = data%flv_in(1)%get_mass ()
  if (any (data%flv_in%get_mass () /= data%mass)) then
    data%error = MASS_MIX; return
  end if
end if
end subroutine ewa_data_init

```

Set the vector boson ID for distinguishing W and Z bosons.

```

<SF ewa: ewa data: TBP>+≡
  procedure :: set_id => ewa_set_id

<SF ewa: sub interfaces>+≡
  module subroutine ewa_set_id (data, id)
    class(ewa_data_t), intent(inout) :: data
    integer, intent(in) :: id
  end subroutine ewa_set_id

<SF ewa: procedures>+≡
  module subroutine ewa_set_id (data, id)
    class(ewa_data_t), intent(inout) :: data
    integer, intent(in) :: id
    integer :: i, isospin, pdg
    if (.not. allocated (data%flv_in)) &
      call msg_bug ("EWA: incoming particles not set")
    data%id = id
    select case (data%id)
    case (23)
      data%m_out = data%mass
      data%flv_out = data%flv_in
    case (24)
      do i = 1, size (data%flv_in)
        pdg = data%flv_in(i)%get_pdg ()
        isospin = data%flv_in(i)%get_isospin_type ()
        if (isospin > 0) then

```

```

        !!! up-type quark or neutrinos
        if (data%flv_in(i)%is_antiparticle ()) then
            call data%flv_out(i)%init (pdg + 1, data%model)
        else
            call data%flv_out(i)%init (pdg - 1, data%model)
        end if
    else
        !!! down-type quark or lepton
        if (data%flv_in(i)%is_antiparticle ()) then
            call data%flv_out(i)%init (pdg - 1, data%model)
        else
            call data%flv_out(i)%init (pdg + 1, data%model)
        end if
    end if
end do
if (.not. data%mass_set) then
    data%m_out = data%flv_out(1)%get_mass ()
    if (any (data%flv_out%get_mass () /= data%m_out)) then
        data%error = MASS_MIX_OUT; return
    end if
end if
end select
end subroutine ewa_set_id

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.

<SF ewa: ewa data: TBP>+≡

```

    procedure :: check => ewa_data_check

```

<SF ewa: sub interfaces>+≡

```

    module subroutine ewa_data_check (data)
        class(ewa_data_t), intent(in) :: data
    end subroutine ewa_data_check

```

<SF ewa: procedures>+≡

```

    module subroutine ewa_data_check (data)
        class(ewa_data_t), intent(in) :: data
        select case (data%error)
        case (WRONG_PRT)
            call msg_fatal ("EWA structure function only accessible for " &
                // "SM quarks and leptons.")
        case (NO_EWA)
            call msg_fatal ("EWA structure function not available for model " &
                // char (data%model%get_name ()))
        case (ZERO_SW)
            call msg_fatal ("EWA: Vanishing value of sin(theta_w)")
        case (ZERO_QMIN)
            call msg_fatal ("EWA: Particle mass is zero")
        case (Q_MAX_TOO_SMALL)
            call msg_fatal ("EWA: Particle mass exceeds Qmax")
        case (ZERO_XMIN)
            call msg_fatal ("EWA: x_min must be larger than zero")
        case (MASS_MIX)
            call msg_fatal ("EWA: incoming particle masses must be uniform")
        case (MASS_MIX_OUT)

```



```

        call msg_fatal ("EWA: outgoing particle masses must be uniform")
    case (ISOSPIN_MIX)
        call msg_fatal ("EWA: incoming particle isospins must be uniform")
    end select
end subroutine ewa_data_check

```

Output

```

<SF ewa: ewa data: TBP>+≡
    procedure :: write => ewa_data_write

<SF ewa: sub interfaces>+≡
    module subroutine ewa_data_write (data, unit, verbose)
        class(ewa_data_t), intent(in) :: data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine ewa_data_write

<SF ewa: procedures>+≡
    module subroutine ewa_data_write (data, unit, verbose)
        class(ewa_data_t), intent(in) :: data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)") "EWA data:"
        if (allocated (data%flv_in) .and. allocated (data%flv_out)) then
            write (u, "(3x,A)", advance="no") " flavor(in) = "
            do i = 1, size (data%flv_in)
                if (i > 1) write (u, "(',',1x)", advance="no")
                call data%flv_in(i)%write (u)
            end do
            write (u, *)
            write (u, "(3x,A)", advance="no") " flavor(out) = "
            do i = 1, size (data%flv_out)
                if (i > 1) write (u, "(',',1x)", advance="no")
                call data%flv_out(i)%write (u)
            end do
            write (u, *)
            write (u, "(3x,A," // FMT_19 // ")") " x_min = ", data%x_min
            write (u, "(3x,A," // FMT_19 // ")") " x_max = ", data%x_max
            write (u, "(3x,A," // FMT_19 // ")") " pt_max = ", data%pt_max
            write (u, "(3x,A," // FMT_19 // ")") " sqrts = ", data%sqrts
            write (u, "(3x,A," // FMT_19 // ")") " mass = ", data%mass
            write (u, "(3x,A," // FMT_19 // ")") " cv = ", data%cv
            write (u, "(3x,A," // FMT_19 // ")") " ca = ", data%ca
            write (u, "(3x,A," // FMT_19 // ")") " coeff = ", data%coeff
            write (u, "(3x,A," // FMT_19 // ")") " costhw = ", data%costhw
            write (u, "(3x,A," // FMT_19 // ")") " sinthw = ", data%sinthw
            write (u, "(3x,A," // FMT_19 // ")") " mZ = ", data%mZ
            write (u, "(3x,A," // FMT_19 // ")") " mW = ", data%mW
            write (u, "(3x,A,L2)") " recoil = ", data%recoil
            write (u, "(3x,A,L2)") " keep en. = ", data%keep_energy
            write (u, "(3x,A,I2)") " PDG (VB) = ", data%id
        else
            write (u, "(3x,A)") "[undefined]"
        end if
    end subroutine ewa_data_write

```

```

        end if
    end subroutine ewa_data_write

```

The number of parameters is one for collinear splitting, in case the `recoil` option is set, we take the recoil into account.

```

<SF ewa: ewa data: TBP>+≡
    procedure :: get_n_par => ewa_data_get_n_par

<SF ewa: sub interfaces>+≡
    module function ewa_data_get_n_par (data) result (n)
        class(ewa_data_t), intent(in) :: data
        integer :: n
    end function ewa_data_get_n_par

<SF ewa: procedures>+≡
    module function ewa_data_get_n_par (data) result (n)
        class(ewa_data_t), intent(in) :: data
        integer :: n
        if (data%recoil) then
            n = 3
        else
            n = 1
        end if
    end function ewa_data_get_n_par

```

Return the outgoing particles PDG codes. This depends, whether this is a charged-current or neutral-current interaction.

```

<SF ewa: ewa data: TBP>+≡
    procedure :: get_pdg_out => ewa_data_get_pdg_out

<SF ewa: sub interfaces>+≡
    module subroutine ewa_data_get_pdg_out (data, pdg_out)
        class(ewa_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine ewa_data_get_pdg_out

<SF ewa: procedures>+≡
    module subroutine ewa_data_get_pdg_out (data, pdg_out)
        class(ewa_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        integer :: i, n_flv
        if (allocated (data%flv_out)) then
            n_flv = size (data%flv_out)
        else
            n_flv = 0
        end if
        allocate (pdg1 (n_flv))
        do i = 1, n_flv
            pdg1(i) = data%flv_out(i)%get_pdg ()
        end do
        pdg_out(1) = pdg1
    end subroutine ewa_data_get_pdg_out

```

Allocate the interaction record. Due to a gfortran 7/8/9 bug, this has to remain in the main module.

```

<SF ewa: ewa data: TBP>+≡
  procedure :: allocate_sf_int => ewa_data_allocate_sf_int

<SF ewa: main procedures>≡
  subroutine ewa_data_allocate_sf_int (data, sf_int)
    class(ewa_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (ewa_t :: sf_int)
  end subroutine ewa_data_allocate_sf_int

```

16.8.3 The EWA object

The `ewa_t` data type is a $1 \rightarrow 2$ interaction. We should be able to handle several flavors in parallel, since EWA is not necessarily applied immediately after beam collision: W/Z bosons may be radiated from quarks. In that case, the partons are massless and q_{\min} applies instead, so we do not need to generate several kinematical configurations in parallel.

The particles are ordered as (incoming, radiated, W/Z), where the W/Z initiates the hard interaction.

In the case of EPA, we generated an unpolarized photon and transferred initial polarization to the radiated parton. Color is transferred in the same way. I do not know whether the same can/should be done for EWA, as the structure functions depend on the W/Z polarization. If we are having Z bosons, both up- and down-type fermions can participate. Otherwise, with a W^+ an up-type fermion is transferred to a down-type fermion, and the other way round.

```

<SF ewa: types>+≡
  type, extends (sf_int_t) :: ewa_t
    type(ewa_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: xb = 0
    integer :: n_me = 0
    real(default), dimension(:), allocatable :: cv
    real(default), dimension(:), allocatable :: ca
  contains
    <SF ewa: ewa: TBP>
  end type ewa_t

```

Type string: has to be here, but there is no string variable on which EWA depends. Hence, a dummy routine.

```

<SF ewa: ewa: TBP>≡
  procedure :: type_string => ewa_type_string

<SF ewa: sub interfaces>+≡
  module function ewa_type_string (object) result (string)
    class(ewa_t), intent(in) :: object
    type(string_t) :: string
  end function ewa_type_string

```

```

<SF ewa: procedures>+≡
module function ewa_type_string (object) result (string)
  class(ewa_t), intent(in) :: object
  type(string_t) :: string
  if (associated (object%data)) then
    string = "EWA: equivalent W/Z approx."
  else
    string = "EWA: [undefined]"
  end if
end function ewa_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF ewa: ewa: TBP>+≡
  procedure :: write => ewa_write

<SF ewa: sub interfaces>+≡
  module subroutine ewa_write (object, unit, testflag)
    class(ewa_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine ewa_write

<SF ewa: procedures>+≡
  module subroutine ewa_write (object, unit, testflag)
    class(ewa_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
        write (u, "(3x,A," // FMT_17 // ")") "xb=", object%xb
      end if
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "EWA data: [undefined]"
    end if
  end subroutine ewa_write

```

The current implementation requires uniform isospin for all incoming particles, therefore we need to probe only the first one.

```

<SF ewa: ewa: TBP>+≡
  procedure :: init => ewa_init

<SF ewa: sub interfaces>+≡
  module subroutine ewa_init (sf_int, data)
    class(ewa_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
  end subroutine ewa_init

```

(SF ewa: procedures)+≡

```

module subroutine ewa_init (sf_int, data)
  class(ewa_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  type(quantum_numbers_mask_t), dimension(3) :: mask
  integer, dimension(3) :: hel_lock
  type(polarization_t), target :: pol
  type(quantum_numbers_t), dimension(1) :: qn_fc, qn_fc_fin
  type(flavor_t) :: flv_z, flv_wp, flv_wm
  type(color_t) :: col0
  type(quantum_numbers_t) :: qn_hel, qn_z, qn_wp, qn_wm, qn, qn_rad, qn_w
  type(polarization_iterator_t) :: it_hel
  integer :: i, isospin
  select type (data)
  type is (ewa_data_t)
    mask = quantum_numbers_mask (.false., .false., &
      mask_h = [.false., .false., .true.])
    hel_lock = [2, 1, 0]
    call col0%init ()
    select case (data%id)
    case (23)
      !!! Z boson, flavor is not changing
      call sf_int%base_init (mask, [data%mass**2], [data%mass**2], &
        [data%mZ**2], hel_lock = hel_lock)
      sf_int%data => data
      call flv_z%init (Z_BOSON, data%model)
      call qn_z%init (flv_z, col0)
      do i = 1, size (data%flv_in)
        call pol%init_generic (data%flv_in(i))
        call qn_fc(1)%init ( &
          flv = data%flv_in(i), &
          col = color_from_flavor (data%flv_in(i), 1))
        call it_hel%init (pol)
        do while (it_hel%is_valid ())
          qn_hel = it_hel%get_quantum_numbers ()
          qn = qn_hel .merge. qn_fc(1)
          qn_rad = qn
          call qn_rad%tag_radiated ()
          call sf_int%add_state ([qn, qn_rad, qn_z])
          call it_hel%advance ()
        end do
        ! call pol%final ()
      end do
    case (24)
      call sf_int%base_init (mask, [data%mass**2], [data%m_out**2], &
        [data%mW**2], hel_lock = hel_lock)
      sf_int%data => data
      call flv_wp%init (W_BOSON, data%model)
      call flv_wm%init (- W_BOSON, data%model)
      call qn_wp%init (flv_wp, col0)
      call qn_wm%init (flv_wm, col0)
      do i = 1, size (data%flv_in)
        isospin = data%flv_in(i)%get_isospin_type ()
        if (isospin > 0) then

```

```

        !!! up-type quark or neutrinos
        if (data%flv_in(i)%is_antiparticle ()) then
            qn_w = qn_wm
        else
            qn_w = qn_wp
        end if
    else
        !!! down-type quark or lepton
        if (data%flv_in(i)%is_antiparticle ()) then
            qn_w = qn_wp
        else
            qn_w = qn_wm
        end if
    end if
    call pol%init_generic (data%flv_in(i))
    call qn_fc(1)%init ( &
        flv = data%flv_in(i), &
        col = color_from_flavor (data%flv_in(i), 1))
    call qn_fc_fin(1)%init ( &
        flv = data%flv_out(i), &
        col = color_from_flavor (data%flv_out(i), 1))
    call it_hel%init (pol)
    do while (it_hel%is_valid ())
        qn_hel = it_hel%get_quantum_numbers ()
        qn = qn_hel .merge. qn_fc(1)
        qn_rad = qn_hel .merge. qn_fc_fin(1)
        call qn_rad%tag_radiated ()
        call sf_int%add_state ([qn, qn_rad, qn_w])
        call it_hel%advance ()
    end do
    ! call pol%final ()
end do
case default
    call msg_fatal ("EWA initialization failed: wrong particle type.")
end select
call sf_int%freeze ()
if (data%keep_energy) then
    sf_int%on_shell_mode = KEEP_ENERGY
else
    sf_int%on_shell_mode = KEEP_MOMENTUM
end if
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
end select
end subroutine ewa_init

```

Prepare the coupling arrays. This is separate from the previous routine since the state matrix may be helicity-contracted.

```

<SF ewa: ewa: TBP>+≡
    procedure :: setup_constants => ewa_setup_constants

<SF ewa: sub interfaces>+≡
    module subroutine ewa_setup_constants (sf_int)

```

```

        class(ewa_t), intent(inout), target :: sf_int
    end subroutine ewa_setup_constants

<SF ewa: procedures>+=
module subroutine ewa_setup_constants (sf_int)
    class(ewa_t), intent(inout), target :: sf_int
    type(state_iterator_t) :: it
    type(flavor_t) :: flv
    real(default) :: q, t3
    integer :: i
    sf_int%n_me = sf_int%get_n_matrix_elements ()
    allocate (sf_int%cv (sf_int%n_me))
    allocate (sf_int%ca (sf_int%n_me))
    associate (data => sf_int%data)
        select case (data%id)
            case (23)
                call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
                do while (it%is_valid ())
                    i = it%get_me_index ()
                    flv = it%get_flavor (1)
                    q = flv%get_charge ()
                    t3 = flv%get_isospin ()
                    if (flv%is_antiparticle ()) then
                        sf_int%cv(i) = - data%cv &
                            * (t3 - 2._default * q * data%sinthw**2) / data%costhw
                        sf_int%ca(i) = data%ca * t3 / data%costhw
                    else
                        sf_int%cv(i) = data%cv &
                            * (t3 - 2._default * q * data%sinthw**2) / data%costhw
                        sf_int%ca(i) = data%ca * t3 / data%costhw
                    end if
                    call it%advance ()
                end do
            case (24)
                call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
                do while (it%is_valid ())
                    i = it%get_me_index ()
                    flv = it%get_flavor (1)
                    if (flv%is_antiparticle ()) then
                        sf_int%cv(i) = data%cv / sqrt(2._default)
                        sf_int%ca(i) = - data%ca / sqrt(2._default)
                    else
                        sf_int%cv(i) = data%cv / sqrt(2._default)
                        sf_int%ca(i) = data%ca / sqrt(2._default)
                    end if
                    call it%advance ()
                end do
            end select
        end associate
    sf_int%status = SF_INITIAL
end subroutine ewa_setup_constants

```

16.8.4 Kinematics

Set kinematics. The EWA structure function allows for a straightforward mapping of the unit interval. So, to leading order, the structure function value is unity, but the x value is transformed. Higher orders affect the function value. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, the exponential mapping for the $1/x$ singularity discussed above is applied.

```

(SF ewa: ewa: TBP)+≡
  procedure :: complete_kinematics => ewa_complete_kinematics

(SF ewa: sub interfaces)+≡
  module subroutine ewa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
  end subroutine ewa_complete_kinematics

(SF ewa: procedures)+≡
  module subroutine ewa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    real(default) :: e_1
    real(default) :: x0, x1, lx0, lx1, lx
    e_1 = energy (sf_int%get_momentum (1))
    if (sf_int%data%recoil) then
      select case (sf_int%data%id)
        case (23)
          x0 = max (sf_int%data%x_min, sf_int%data%mz / e_1)
        case (24)
          x0 = max (sf_int%data%x_min, sf_int%data%mw / e_1)
        end select
      end if
    else
      x0 = sf_int%data%x_min
    end if
    x1 = sf_int%data%x_max
    if ( x0 >= x1) then
      f = 0
      sf_int%status = SF_FAILED_KINEMATICS
      return
    end if
    if (map) then
      lx0 = log (x0)
      lx1 = log (x1)
      lx = lx1 * r(1) + lx0 * rb(1)
      x(1) = exp(lx)
    end if
  end subroutine ewa_complete_kinematics

```



```

        f = x(1) * (lx1 - lx0)
    else
        x(1) = r(1)
        if (x0 < x(1) .and. x(1) < x1) then
            f = 1
        else
            sf_int%status = SF_FAILED_KINEMATICS
            f = 0
            return
        end if
    end if
    xb(1) = 1 - x(1)
    if (size(x) == 3) then
        x(2:3) = r(2:3)
        xb(2:3) = rb(2:3)
    end if
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_DONE_KINEMATICS)
        sf_int%x = x(1)
        sf_int%xb = xb(1)
    case (SF_FAILED_KINEMATICS)
        sf_int%x = 0
        sf_int%xb = 0
        f = 0
    end select
end subroutine ewa_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum configuration. In the specific case of EWA, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

```

<SF ewa: ewa: TBP>+≡
    procedure :: recover_x => sf_ewa_recover_x

<SF ewa: sub interfaces>+≡
    module subroutine sf_ewa_recover_x (sf_int, x, xb, x_free)
        class(ewa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_ewa_recover_x

<SF ewa: procedures>+≡
    module subroutine sf_ewa_recover_x (sf_int, x, xb, x_free)
        class(ewa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(inout), optional :: x_free
        call sf_int%base_recover_x (x, xb, x_free)
        sf_int%x = x(1)
        sf_int%xb = xb(1)
    end subroutine sf_ewa_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF ewa: ewa: TBP>+≡
  procedure :: inverse_kinematics => ewa_inverse_kinematics

<SF ewa: sub interfaces>+≡
  module subroutine ewa_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine ewa_inverse_kinematics

<SF ewa: procedures>+≡
  module subroutine ewa_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default) :: x0, x1, lx0, lx1, lx, e_1
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    e_1 = energy (sf_int%get_momentum (1))
    if (sf_int%data%recoil) then
      select case (sf_int%data%id)
        case (23)
          x0 = max (sf_int%data%x_min, sf_int%data% mz / e_1)
        case (24)
          x0 = max (sf_int%data%x_min, sf_int%data% mw / e_1)
        end select
    else
      x0 = sf_int%data%x_min
    end if
    x1 = sf_int%data%x_max
    if (map) then
      lx0 = log (x0)
      lx1 = log (x1)
      lx = log (x(1))
      r(1) = (lx - lx0) / (lx1 - lx0)
      rb(1) = (lx1 - lx) / (lx1 - lx0)
      f = x(1) * (lx1 - lx0)
    else
      r (1) = x(1)
      rb(1) = 1 - x(1)
    end if
  end subroutine ewa_inverse_kinematics

```

```

        if (x0 < x(1) .and. x(1) < x1) then
            f = 1
        else
            f = 0
        end if
    end if
    if (size(r) == 3) then
        r (2:3) = x(2:3)
        rb(2:3) = xb(2:3)
    end if
    if (set_mom) then
        call sf_int%split_momentum (x, xb)
        select case (sf_int%status)
            case (SF_FAILED_KINEMATICS); f = 0
        end select
    end if
end subroutine ewa_inverse_kinematics

```

16.8.5 EWA application

For EWA, we can compute kinematics and function value in a single step. This function works on a single beam, assuming that the input momentum has been set. We need four random numbers as input: one for x , one for Q^2 , and two for the polar and azimuthal angles. Alternatively, we can skip p_T generation; in this case, we only need one.

For obtaining splitting kinematics, we rely on the assumption that all in-particles are mass-degenerate (or there is only one), so the generated x values are identical.

```

<SF ewa: ewa: TBP>+≡
    procedure :: apply => ewa_apply

<SF ewa: sub interfaces>+≡
    module subroutine ewa_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(ewa_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
    end subroutine ewa_apply

<SF ewa: procedures>+≡
    module subroutine ewa_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(ewa_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
        real(default) :: x, xb, pt2, c1, c2
        real(default) :: cv, ca
        real(default) :: f, fm, fp, fL
        integer :: i
        associate (data => sf_int%data)
            x = sf_int%x

```

```

xb = sf_int%xb
pt2 = min ((data%pt_max)**2, (xb * data%sqrts / 2)**2)
select case (data%id)
case (23)
    !!! Z boson structure function
    c1 = log (1 + pt2 / (xb * (data%mZ)**2))
    c2 = 1 / (1 + (xb * (data%mZ)**2) / pt2)
case (24)
    !!! W boson structure function
    c1 = log (1 + pt2 / (xb * (data%mW)**2))
    c2 = 1 / (1 + (xb * (data%mW)**2) / pt2)
end select
do i = 1, sf_int%n_me
    cv = sf_int%cv(i)
    ca = sf_int%ca(i)
    fm = data%coeff * &
        ((cv + ca)**2 + ((cv - ca) * xb)**2) * (c1 - c2) / (2 * x)
    fp = data%coeff * &
        ((cv - ca)**2 + ((cv + ca) * xb)**2) * (c1 - c2) / (2 * x)
    fL = data%coeff * &
        (cv**2 + ca**2) * (2 * xb / x) * c2
    f = fp + fm + fL
    if (.not. vanishes (f)) then
        fp = fp / f
        fm = fm / f
        fL = fL / f
    end if
    call sf_int%set_matrix_element (i, cmplx (f, kind=default))
end do
end associate
sf_int%status = SF_EVALUATED
end subroutine ewa_apply

```

16.8.6 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_ewa_ut.f90⟩≡
⟨File header⟩

module sf_ewa_ut
    use unit_tests
    use sf_ewa_ut

    ⟨Standard module head⟩

    ⟨SF ewa: public test⟩

contains

    ⟨SF ewa: test driver⟩

end module sf_ewa_ut

```

```

⟨sf_ewa_util.f90⟩≡
  ⟨File header⟩

  module sf_ewa_util

    ⟨Use kinds⟩
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_aux
    use sf_base

    use sf_ewa

    ⟨Standard module head⟩

    ⟨SF ewa: test declarations⟩

    contains

    ⟨SF ewa: tests⟩

  end module sf_ewa_util

```

API: driver for the unit tests below.

```

⟨SF ewa: public test⟩≡
  public :: sf_ewa_test

⟨SF ewa: test driver⟩≡
  subroutine sf_ewa_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨SF ewa: execute tests⟩
  end subroutine sf_ewa_test

```

Test structure function data

Construct and display a test structure function data object.

```

⟨SF ewa: execute tests⟩≡
  call test (sf_ewa_1, "sf_ewa_1", &
    "structure function configuration", &
    u, results)

⟨SF ewa: test declarations⟩≡
  public :: sf_ewa_1

⟨SF ewa: tests⟩≡
  subroutine sf_ewa_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1

```

```

class(sf_data_t), allocatable :: data

write (u, "(A)")  "* Test output: sf_ewa_1"
write (u, "(A)")  "* Purpose: initialize and display &
                  &test structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_sm_test ()
pdg_in = 2

allocate (ewa_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize for Z boson"
write (u, "(A)")

select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
                    500._default, 5000._default, .false., .false.)
    call data%set_id (23)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

write (u, "(A)")
write (u, "(A)")  "* Initialize for W boson"
write (u, "(A)")

deallocate (data)
allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
                    500._default, 5000._default, .false., .false.)
    call data%set_id (24)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"

```

```

call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_1"

end subroutine sf_ewa_1

```

Test and probe structure function

Construct and display a structure function object based on the EWA structure function.

```

<SF ewa: execute tests>+≡
  call test (sf_ewa_2, "sf_ewa_2", &
    "structure function instance", &
    u, results)

<SF ewa: test declarations>+≡
  public :: sf_ewa_2

<SF ewa: tests>+≡
  subroutine sf_ewa_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_ewa_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_sm_test ()
    call flv%init (2, model)
    pdg_in = 2

    call reset_interaction_counter ()

    allocate (ewa_data_t :: data)
    select type (data)

```

```

type is (ewa_data_t)
  call data%init (model, pdg_in, 0.01_default, &
    500._default, 3000._default, .false., .true.)
  call data%set_id (24)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

```



```

call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_2"

end subroutine sf_ewa_2

```

Standard mapping

Construct and display a structure function object based on the EWA structure function, applying the standard single-particle mapping.

```

<SF ewa: execute tests>+≡
    call test (sf_ewa_3, "sf_ewa_3", &
        "apply mapping", &
        u, results)

<SF ewa: test declarations>+≡
    public :: sf_ewa_3

<SF ewa: tests>+≡
    subroutine sf_ewa_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int

```

```

type(vector4_t) :: k
type(vector4_t), dimension(2) :: q
real(default) :: E
real(default), dimension(:), allocatable :: r, rb, x, xb
real(default) :: f

write (u, "(A)")  "* Test output: sf_ewa_3"
write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_sm_test ()
call flv%init (2, model)
pdg_in = 2

call reset_interaction_counter ()

allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
                    500._default, 3000._default, .false., .true.)
    call data%set_id (24)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, with EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))

```

```

allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_3"

end subroutine sf_ewa_3

```

Non-collinear case

Construct and display a structure function object based on the EPA structure function.

```
<SF ewa: execute tests>+=  
  call test (sf_ewa_4, "sf_ewa_4", &  
    "non-collinear", &  
    u, results)  
  
<SF ewa: test declarations>+=  
  public :: sf_ewa_4  
  
<SF ewa: tests>+=  
  subroutine sf_ewa_4 (u)  
    integer, intent(in) :: u  
    type(model_data_t), target :: model  
    type(flavor_t) :: flv  
    type(pdg_array_t) :: pdg_in  
    class(sf_data_t), allocatable, target :: data  
    class(sf_int_t), allocatable :: sf_int  
    type(vector4_t) :: k  
    type(vector4_t), dimension(2) :: q  
    real(default) :: E  
    real(default), dimension(:), allocatable :: r, rb, x, xb  
    real(default) :: f  
  
    write (u, "(A)")  "* Test output: sf_ewa_4"  
    write (u, "(A)")  "* Purpose: initialize and fill &  
      &test structure function object"  
    write (u, "(A)")  
  
    write (u, "(A)")  "* Initialize configuration data"  
    write (u, "(A)")  
  
    call model%init_sm_test ()  
    call flv%init (2, model)  
    pdg_in = 2  
  
    call reset_interaction_counter ()  
  
    allocate (ewa_data_t :: data)  
    select type (data)  
    type is (ewa_data_t)  
      call data%init (model, pdg_in, 0.01_default, &  
        500._default, 3000.0_default, .true., .true.)  
      call data%set_id (24)  
    end select  
  
    write (u, "(A)")  "* Initialize structure-function object"  
    write (u, "(A)")  
  
    call data%allocate_sf_int (sf_int)
```

```

call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.5/0.5/0.25, with EWA mapping, "
write (u, "(A)")  "          non-coll., keeping energy"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%pacify_momenta (1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)
call sf_int%pacify_momenta (1e-10_default)

```

```

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 1500._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_4"

end subroutine sf_ewa_4

```

Structure function for multiple flavors

Construct and display a structure function object based on the EWA structure function. The incoming state has multiple particles with non-uniform quantum numbers.

```

<SF ewa: execute tests>+≡
  call test (sf_ewa_5, "sf_ewa_5", &
    "structure function instance", &
    u, results)

<SF ewa: test declarations>+≡
  public :: sf_ewa_5

<SF ewa: tests>+≡
  subroutine sf_ewa_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_ewa_5"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"

```

```

write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_sm_test ()
call flv%init (2, model)
pdg_in = [1, 2, -1, -2]

call reset_interaction_counter ()

allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
        500._default, 3000._default, .false., .true.)
    call data%set_id (24)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb (size (r)))
allocate (x (size (r)))
allocate (xb (size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x

```

```

write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_5"

end subroutine sf_ewa_5

```


16.9 Energy-scan spectrum

This spectrum is actually a trick that allows us to plot the c.m. energy dependence of a cross section without scanning the input energy. We start with the observation that a spectrum $f(x)$, applied to one of the incoming beams only, results in a cross section

$$\sigma = \int dx f(x) \hat{\sigma}(xs). \quad (16.58)$$

We want to compute the distribution of $E = \sqrt{\hat{s}} = \sqrt{xs}$, i.e.,

$$\frac{d\sigma}{dE} = \frac{2\sqrt{x}}{\sqrt{s}} \frac{d\sigma}{dx} = \frac{2\sqrt{x}}{\sqrt{s}} f(x) \hat{\sigma}(xs), \quad (16.59)$$

so if we set

$$f(x) = \frac{\sqrt{s}}{2\sqrt{x}}, \quad (16.60)$$

we get the distribution

$$\frac{d\sigma}{dE} = \hat{\sigma}(\hat{s} = E^2). \quad (16.61)$$

We implement this as a spectrum with a single parameter x . The parameters for the individual beams are computed as $x_i = \sqrt{x}$, so they are equal and the kinematics is always symmetric.

`<sf_escan.f90>≡`
`<File header>`

`module sf_escan`

`<Use kinds>`

`<Use strings>`

`use pdg_arrays`

`use model_data`

`use flavors`

`use quantum_numbers`

`use state_matrices`

`use polarizations`

`use sf_base`

`<Standard module head>`

`<SF_escan: public>`

`<SF_escan: types>`

`interface`

`<SF_escan: sub interfaces>`

`end interface`

`contains`

`<SF_escan: main procedures>`

`end module sf_escan`

```

⟨sf_escan_sub.f90⟩≡
  ⟨File header⟩

  submodule (sf_escan) sf_escan_s

    use io_units
    use format_defs, only: FMT_12
    use numeric_utils
    use diagnostics
    use lorentz

    implicit none

  contains

  ⟨SF_escan: procedures⟩

end submodule sf_escan_s

```

16.9.1 Data type

The `norm` is unity if the total cross section should be normalized to one, and \sqrt{s} if it should be normalized to the total energy. In the latter case, the differential distribution $d\sigma/d\sqrt{\hat{s}}$ coincides with the partonic cross section $\hat{\sigma}$ as a function of $\sqrt{\hat{s}}$.

```

⟨SF_escan: public⟩≡
  public :: escan_data_t

⟨SF_escan: types⟩≡
  type, extends(sf_data_t) :: escan_data_t
    private
    type(flavor_t), dimension(:, :), allocatable :: flv_in
    integer, dimension(2) :: n_flv = 0
    real(default) :: norm = 1
  contains
  ⟨SF_escan: escan_data: TBP⟩
end type escan_data_t

⟨SF_escan: escan_data: TBP⟩≡
  procedure :: init => escan_data_init

⟨SF_escan: sub interfaces⟩≡
  module subroutine escan_data_init (data, model, pdg_in, norm)
    class(escan_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(2), intent(in) :: pdg_in
    real(default), intent(in), optional :: norm
  end subroutine escan_data_init

⟨SF_escan: procedures⟩≡
  module subroutine escan_data_init (data, model, pdg_in, norm)
    class(escan_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model

```

```

type(pdg_array_t), dimension(2), intent(in) :: pdg_in
real(default), intent(in), optional :: norm
real(default), dimension(2) :: m2
integer :: i, j
data%n_flv = pdg_in%get_length ()
allocate (data%flv_in (maxval (data%n_flv), 2))
do i = 1, 2
  do j = 1, data%n_flv(i)
    call data%flv_in(j, i)%init (pdg_in(i)%get (j), model)
  end do
end do
m2 = data%flv_in(1,:)%get_mass ()
do i = 1, 2
  if (.not. any (nearly_equal (data%flv_in(1:data%n_flv(i),i)%get_mass (), m2(i)))) then
    call msg_fatal ("Energy scan: incoming particle mass must be uniform")
  end if
end do
if (present (norm)) data%norm = norm
end subroutine escan_data_init

```

Output

```

<SF escan: escan data: TBP>+≡
  procedure :: write => escan_data_write

<SF escan: sub interfaces>+≡
  module subroutine escan_data_write (data, unit, verbose)
    class(escan_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine escan_data_write

<SF escan: procedures>+≡
  module subroutine escan_data_write (data, unit, verbose)
    class(escan_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i, j
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Energy-scan data:"
    write (u, "(3x,A)", advance="no") "prt_in = "
    do i = 1, 2
      if (i > 1) write (u, "(',',1x)", advance="no")
      do j = 1, data%n_flv(i)
        if (j > 1) write (u, "(::)", advance="no")
        write (u, "(A)", advance="no") char (data%flv_in(j,i)%get_name ())
      end do
    end do
    write (u, *)
    write (u, "(3x,A," // FMT_12 // ")") "norm  =", data%norm
  end subroutine escan_data_write

```

Kinematics is completely collinear, hence there is only one parameter for a pair spectrum.

```

<SF escan: escan data: TBP>+≡

```

```

    procedure :: get_n_par => escan_data_get_n_par
<SF escan: sub interfaces>+≡
    module function escan_data_get_n_par (data) result (n)
        class(escan_data_t), intent(in) :: data
        integer :: n
    end function escan_data_get_n_par
<SF escan: procedures>+≡
    module function escan_data_get_n_par (data) result (n)
        class(escan_data_t), intent(in) :: data
        integer :: n
        n = 1
    end function escan_data_get_n_par

```

Return the outgoing particles PDG codes. This is always the same as the incoming particle, where we use two indices for the two beams.

```

<SF escan: escan data: TBP>+≡
    procedure :: get_pdg_out => escan_data_get_pdg_out
<SF escan: sub interfaces>+≡
    module subroutine escan_data_get_pdg_out (data, pdg_out)
        class(escan_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine escan_data_get_pdg_out
<SF escan: procedures>+≡
    module subroutine escan_data_get_pdg_out (data, pdg_out)
        class(escan_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer :: i, n
        n = 2
        do i = 1, n
            pdg_out(i) = data%flv_in(1:data%n_flv(i),i)%get_pdg ()
        end do
    end subroutine escan_data_get_pdg_out

```

Allocate the interaction record. Due to a gfortran 7/8/9 this has to remain in the main module.

```

<SF escan: escan data: TBP>+≡
    procedure :: allocate_sf_int => escan_data_allocate_sf_int
<SF escan: main procedures>≡
    subroutine escan_data_allocate_sf_int (data, sf_int)
        class(escan_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (escan_t :: sf_int)
    end subroutine escan_data_allocate_sf_int

```

16.9.2 The Energy-scan object

This is a spectrum, not a radiation. We create an interaction with two incoming and two outgoing particles, flavor, color, and helicity being carried through. x

nevertheless is only one-dimensional, as we are always using only one beam parameter.

```

<SF escan: types>+≡
  type, extends (sf_int_t) :: escan_t
    type(escan_data_t), pointer :: data => null ()
  contains
    <SF escan: escan: TBP>
  end type escan_t

```

Type string: for the energy scan this is just a dummy function.

```

<SF escan: escan: TBP>≡
  procedure :: type_string => escan_type_string
<SF escan: sub interfaces>+≡
  module function escan_type_string (object) result (string)
    class(escan_t), intent(in) :: object
    type(string_t) :: string
  end function escan_type_string
<SF escan: procedures>+≡
  module function escan_type_string (object) result (string)
    class(escan_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "Escan: energy scan"
    else
      string = "Escan: [undefined]"
    end if
  end function escan_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF escan: escan: TBP>+≡
  procedure :: write => escan_write
<SF escan: sub interfaces>+≡
  module subroutine escan_write (object, unit, testflag)
    class(escan_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine escan_write
<SF escan: procedures>+≡
  module subroutine escan_write (object, unit, testflag)
    class(escan_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "Energy scan data: [undefined]"
    end if
  end subroutine escan_write

```

```

<SF escan: escan: TBP>+=
    procedure :: init => escan_init

<SF escan: sub interfaces>+=
    module subroutine escan_init (sf_int, data)
        class(escan_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
    end subroutine escan_init

<SF escan: procedures>+=
module subroutine escan_init (sf_int, data)
    class(escan_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(4) :: mask
    integer, dimension(4) :: hel_lock
    real(default), dimension(2) :: m2
    real(default), dimension(0) :: mr2
    type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
    type(polarization_t), target :: pol1, pol2
    type(polarization_iterator_t) :: it_hel1, it_hel2
    integer :: j1, j2
    select type (data)
    type is (escan_data_t)
        hel_lock = [3, 4, 1, 2]
        m2 = data%flv_in(1,:)%get_mass ()
        call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
        sf_int%data => data
        do j1 = 1, data%n_flv(1)
            call qn_fc(1)%init ( &
                flv = data%flv_in(j1,1), &
                col = color_from_flavor (data%flv_in(j1,1)))
            call qn_fc(3)%init ( &
                flv = data%flv_in(j1,1), &
                col = color_from_flavor (data%flv_in(j1,1)))
            call pol1%init_generic (data%flv_in(j1,1))
        do j2 = 1, data%n_flv(2)
            call qn_fc(2)%init ( &
                flv = data%flv_in(j2,2), &
                col = color_from_flavor (data%flv_in(j2,2)))
            call qn_fc(4)%init ( &
                flv = data%flv_in(j2,2), &
                col = color_from_flavor (data%flv_in(j2,2)))
            call pol2%init_generic (data%flv_in(j2,2))
            call it_hel1%init (pol1)
            do while (it_hel1%is_valid ())
                qn_hel(1) = it_hel1%get_quantum_numbers ()
                qn_hel(3) = it_hel1%get_quantum_numbers ()
                call it_hel2%init (pol2)
                do while (it_hel2%is_valid ())
                    qn_hel(2) = it_hel2%get_quantum_numbers ()
                    qn_hel(4) = it_hel2%get_quantum_numbers ()
                    qn = qn_hel .merge. qn_fc
                    call sf_int%add_state (qn)
                    call it_hel2%advance ()
                end do
            end do
        end do
    end select
end module

```

```

        call it_hell1%advance ()
    end do
    ! call pol2%final ()
end do
! call pol1%final ()
end do
call sf_int%set_incoming ([1,2])
call sf_int%set_outgoing ([3,4])
call sf_int%freeze ()
sf_int%status = SF_INITIAL
end select
end subroutine escan_init

```

16.9.3 Kinematics

Set kinematics. We have a single parameter, but reduce both beams. The map flag is ignored.

```

<SF escan: escan: TBP>+≡
    procedure :: complete_kinematics => escan_complete_kinematics

<SF escan: sub interfaces>+≡
    module subroutine escan_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(escan_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default) :: sqrt_x
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
    end subroutine escan_complete_kinematics

<SF escan: procedures>+≡
    module subroutine escan_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(escan_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default) :: sqrt_x
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        x = r
        xb= rb
        sqrt_x = sqrt (x(1))
        if (sqrt_x > 0) then
            f = 1 / (2 * sqrt_x)
        else
            f = 0
            sf_int%status = SF_FAILED_KINEMATICS
            return
        end if
        call sf_int%reduce_momenta ([sqrt_x, sqrt_x])
    end subroutine

```

```
end subroutine escan_complete_kinematics
```

Recover x . The base procedure should return two momentum fractions for the two beams, while we have only one parameter. This is the product of the extracted momentum fractions.

```
(SF escan: escan: TBP)+≡
  procedure :: recover_x => escan_recover_x

(SF escan: sub interfaces)+≡
  module subroutine escan_recover_x (sf_int, x, xb, x_free)
    class(escan_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
  end subroutine escan_recover_x

(SF escan: procedures)+≡
  module subroutine escan_recover_x (sf_int, x, xb, x_free)
    class(escan_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: xi, xib
    call sf_int%base_recover_x (xi, xib, x_free)
    x = product (xi)
    xb= 1 - x
  end subroutine escan_recover_x
```

Compute inverse kinematics.

```
(SF escan: escan: TBP)+≡
  procedure :: inverse_kinematics => escan_inverse_kinematics

(SF escan: sub interfaces)+≡
  module subroutine escan_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(escan_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine escan_inverse_kinematics

(SF escan: procedures)+≡
  module subroutine escan_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(escan_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
```



```

logical, intent(in), optional :: set_momenta
real(default) :: sqrt_x
logical :: set_mom

set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
sqrt_x = sqrt (x(1))
if (sqrt_x > 0) then
  f = 1 / (2 * sqrt_x)
else
  f = 0
  sf_int%status = SF_FAILED_KINEMATICS
  return
end if
r = x
rb = xb
if (set_mom) then
  call sf_int%reduce_momenta ([sqrt_x, sqrt_x])
end if
end subroutine escan_inverse_kinematics

```

16.9.4 Energy scan application

Here, we insert the predefined norm.

```

<SF escan: escan: TBP>+≡
  procedure :: apply => escan_apply

<SF escan: sub interfaces>+≡
  module subroutine escan_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(escan_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine escan_apply

<SF escan: procedures>+≡
  module subroutine escan_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(escan_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f
    associate (data => sf_int%data)
      f = data%norm
    end associate
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine escan_apply

```

16.9.5 Unit tests

Test module, followed by the corresponding implementation module.

```
<sf_escan_ut.f90>≡  
  <File header>  
  
  module sf_escan_ut  
    use unit_tests  
    use sf_escan_ut_i  
  
    <Standard module head>  
  
    <SF escan: public test>  
  
    contains  
  
    <SF escan: test driver>  
  
  end module sf_escan_ut  
  
<sf_escan_ut_i.f90>≡  
  <File header>  
  
  module sf_escan_ut_i  
  
    <Use kinds>  
    use physics_defs, only: ELECTRON  
    use lorentz  
    use pdg_arrays  
    use flavors  
    use interactions, only: reset_interaction_counter  
    use model_data  
    use sf_aux  
    use sf_base  
  
    use sf_escan  
  
    <Standard module head>  
  
    <SF escan: test declarations>  
  
    contains  
  
    <SF escan: tests>  
  
  end module sf_escan_ut_i  
API: driver for the unit tests below.  
<SF escan: public test>≡  
  public :: sf_escan_test  
<SF escan: test driver>≡  
  subroutine sf_escan_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <SF escan: execute tests>
```

```
end subroutine sf_escan_test
```

Test structure function data

Construct and display a test structure function data object.

```
<SF escan: execute tests>≡
  call test (sf_escan_1, "sf_escan_1", &
    "structure function configuration", &
    u, results)

<SF escan: test declarations>≡
  public :: sf_escan_1

<SF escan: tests>≡
  subroutine sf_escan_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t), dimension(2) :: pdg_in
    type(pdg_array_t), dimension(2) :: pdg_out
    integer, dimension(:), allocatable :: pdg1, pdg2
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_escan_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &energy-scan structure function data"
    write (u, "(A)")

    call model%init_qed_test ()
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    allocate (escan_data_t :: data)
    select type (data)
    type is (escan_data_t)
      call data%init (model, pdg_in, norm = 2._default)
    end select

    call data%write (u)

    write (u, "(A)")

    write (u, "(1x,A)") "Outgoing particle codes:"
    call data%get_pdg_out (pdg_out)
    pdg1 = pdg_out(1)
    pdg2 = pdg_out(2)
    write (u, "(2x,99(1x,I0))")  pdg1, pdg2

    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sf_escan_1"

  end subroutine sf_escan_1
```

g@

Probe the structure-function object

Active the beam event reader, generate an event.

```
<SF escan: execute tests>+≡
  call test (sf_escan_2, "sf_escan_2", &
    "generate event", &
    u, results)

<SF escan: test declarations>+≡
  public :: sf_escan_2

<SF escan: tests>+≡
  subroutine sf_escan_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: x_free, f

    write (u, "(A)")  "* Test output: sf_escan_2"
    write (u, "(A)")  "*   Purpose: initialize and display &
      &beam-events structure function data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv(1)%init (ELECTRON, model)
    call flv(2)%init (-ELECTRON, model)
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    call reset_interaction_counter ()

    allocate (escan_data_t :: data)
    select type (data)
    type is (escan_data_t)
      call data%init (model, pdg_in)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)
    call sf_int%set_beam_index ([1,2])

    write (u, "(A)")  "* Initialize incoming momentum with E=500"
    write (u, "(A)")
    E = 250
```

```

k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E,-sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set dummy parameters and generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.8
rb = 1 - r
x_free = 1

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call sf_int%recover_x (x, xb, x_free)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_escan_2"

end subroutine sf_escan_2

```

16.10 Gaussian beam spread

Instead of an analytic beam description, beam data may be provided in form of an event file. In its most simple form, the event file contains pairs of x values, relative to nominal beam energies. More advanced formats may include polarization, etc. The current implementation carries beam polarization through, if specified.

The code is very similar to the energy scan described above.

However, we must include a file-handle manager for the beam-event files. Two different processes may access a given beam-event file at the same time (i.e., serially but alternating). Accessing an open file from two different units is non-standard and not supported by all compilers. Therefore, we keep a global registry of open files, associated units, and reference counts. The `gaussian_t` objects act as proxies to this registry.

```

<sf_gaussian.f90>≡
  <File header>

  module sf_gaussian

    <Use kinds>
    <Use strings>
    use rng_base
    use pdg_arrays
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use polarizations
    use sf_base

    <Standard module head>

    <SF gaussian: public>

    <SF gaussian: types>

    interface
    <SF gaussian: sub interfaces>
    end interface

    contains

    <SF gaussian: main procedures>

  end module sf_gaussian

```

```

⟨sf_gaussian_sub.f90⟩≡
  ⟨File header⟩

  submodule (sf_gaussian) sf_gaussian_s

    use io_units
    use format_defs, only: FMT_12
    use file_registries
    use diagnostics
    use lorentz

    implicit none

  contains

  ⟨SF gaussian: procedures⟩

end submodule sf_gaussian_s

```

16.10.1 The beam-data file registry

We manage data files via the `file_registries` module. To this end, we keep the registry as a private module variable here.

```

⟨CCC SF gaussian: variables⟩≡
  type(file_registry_t), save :: beam_file_registry

```

16.10.2 Data type

We store the spread for each beam, as a relative number related to the beam energy. For the actual generation, we include an (abstract) random-number generator factory.

```

⟨SF gaussian: public⟩≡
  public :: gaussian_data_t

⟨SF gaussian: types⟩≡
  type, extends(sf_data_t) :: gaussian_data_t
    private
    type(flavor_t), dimension(2) :: flv_in
    real(default), dimension(2) :: spread
    class(rng_factory_t), allocatable :: rng_factory
  contains
    ⟨SF gaussian: gaussian data: TBP⟩
  end type gaussian_data_t

⟨SF gaussian: gaussian data: TBP⟩≡
  procedure :: init => gaussian_data_init

⟨SF gaussian: sub interfaces⟩≡
  module subroutine gaussian_data_init &
    (data, model, pdg_in, spread, rng_factory)
    class(gaussian_data_t), intent(out) :: data

```

```

        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), dimension(2), intent(in) :: pdg_in
        real(default), dimension(2), intent(in) :: spread
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
    end subroutine gaussian_data_init
<SF gaussian: procedures>≡
    module subroutine gaussian_data_init &
        (data, model, pdg_in, spread, rng_factory)
        class(gaussian_data_t), intent(out) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), dimension(2), intent(in) :: pdg_in
        real(default), dimension(2), intent(in) :: spread
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
        if (any (spread < 0)) then
            call msg_fatal ("Gaussian beam spread: must not be negative")
        end if
        call data%flv_in(1)%init (pdg_in(1)%get (1), model)
        call data%flv_in(2)%init (pdg_in(2)%get (1), model)
        data%spread = spread
        call move_alloc (from = rng_factory, to = data%rng_factory)
    end subroutine gaussian_data_init

```

Return true since this spectrum is always in generator mode.

```

<SF gaussian: gaussian data: TBP>+≡
    procedure :: is_generator => gaussian_data_is_generator
<SF gaussian: sub interfaces>+≡
    module function gaussian_data_is_generator (data) result (flag)
        class(gaussian_data_t), intent(in) :: data
        logical :: flag
    end function gaussian_data_is_generator
<SF gaussian: procedures>+≡
    module function gaussian_data_is_generator (data) result (flag)
        class(gaussian_data_t), intent(in) :: data
        logical :: flag
        flag = .true.
    end function gaussian_data_is_generator

```

The number of parameters is two. They are free parameters.

```

<SF gaussian: gaussian data: TBP>+≡
    procedure :: get_n_par => gaussian_data_get_n_par
<SF gaussian: sub interfaces>+≡
    module function gaussian_data_get_n_par (data) result (n)
        class(gaussian_data_t), intent(in) :: data
        integer :: n
    end function gaussian_data_get_n_par
<SF gaussian: procedures>+≡
    module function gaussian_data_get_n_par (data) result (n)
        class(gaussian_data_t), intent(in) :: data
        integer :: n
        n = 2
    end function gaussian_data_get_n_par

```



```

<SF gaussian: gaussian data: TBP>+≡
  procedure :: get_pdg_out => gaussian_data_get_pdg_out

<SF gaussian: sub interfaces>+≡
  module subroutine gaussian_data_get_pdg_out (data, pdg_out)
    class(gaussian_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  end subroutine gaussian_data_get_pdg_out

<SF gaussian: procedures>+≡
  module subroutine gaussian_data_get_pdg_out (data, pdg_out)
    class(gaussian_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      pdg_out(i) = data%flv_in(i)%get_pdg ()
    end do
  end subroutine gaussian_data_get_pdg_out

```

Allocate the interaction record. Due to a gfortran 7/8/9 bug has to remain in the main module.

```

<SF gaussian: gaussian data: TBP>+≡
  procedure :: allocate_sf_int => gaussian_data_allocate_sf_int

<SF gaussian: main procedures>≡
  subroutine gaussian_data_allocate_sf_int (data, sf_int)
    class(gaussian_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (gaussian_t :: sf_int)
  end subroutine gaussian_data_allocate_sf_int

```

Output

```

<SF gaussian: gaussian data: TBP>+≡
  procedure :: write => gaussian_data_write

<SF gaussian: sub interfaces>+≡
  module subroutine gaussian_data_write (data, unit, verbose)
    class(gaussian_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine gaussian_data_write

<SF gaussian: procedures>+≡
  module subroutine gaussian_data_write (data, unit, verbose)
    class(gaussian_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Gaussian beam spread data:"
    write (u, "(3x,A,A,A,A)") "prt_in = ", &
      char (data%flv_in(1)%get_name ()), &
      ", ", char (data%flv_in(2)%get_name ())
    write (u, "(3x,A,2(1x," // FMT_12 // ")") "spread =", data%spread

```

```

        call data%rng_factory%write (u)
    end subroutine gaussian_data_write

```

16.10.3 The gaussian object

Flavor and polarization carried through, no radiated particles. The generator needs a random-number generator, obviously.

```

<SF gaussian: public>+≡
    public :: gaussian_t

<SF gaussian: types>+≡
    type, extends (sf_int_t) :: gaussian_t
        type(gaussian_data_t), pointer :: data => null ()
        class(rng_t), allocatable :: rng
    contains
        <SF gaussian: gaussian: TBP>
    end type gaussian_t

```

Type string: show gaussian file.

```

<SF gaussian: gaussian: TBP>≡
    procedure :: type_string => gaussian_type_string

<SF gaussian: sub interfaces>+≡
    module function gaussian_type_string (object) result (string)
        class(gaussian_t), intent(in) :: object
        type(string_t) :: string
    end function gaussian_type_string

<SF gaussian: procedures>+≡
    module function gaussian_type_string (object) result (string)
        class(gaussian_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "Gaussian: gaussian beam-energy spread"
        else
            string = "Gaussian: [undefined]"
        end if
    end function gaussian_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: write => gaussian_write

<SF gaussian: sub interfaces>+≡
    module subroutine gaussian_write (object, unit, testflag)
        class(gaussian_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine gaussian_write

```

```

<SF gaussian: procedures>+=
module subroutine gaussian_write (object, unit, testflag)
  class(gaussian_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  if (associated (object%data)) then
    call object%data%write (u)
    call object%rng%write (u)
    call object%base_write (u, testflag)
  else
    write (u, "(1x,A)") "gaussian data: [undefined]"
  end if
end subroutine gaussian_write

<SF gaussian: gaussian: TBP>+=
procedure :: init => gaussian_init

<SF gaussian: sub interfaces>+=
module subroutine gaussian_init (sf_int, data)
  class(gaussian_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
end subroutine gaussian_init

<SF gaussian: procedures>+=
module subroutine gaussian_init (sf_int, data)
  class(gaussian_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  real(default), dimension(2) :: m2
  real(default), dimension(0) :: mr2
  type(quantum_numbers_mask_t), dimension(4) :: mask
  integer, dimension(4) :: hel_lock
  type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
  type(polarization_t), target :: pol1, pol2
  type(polarization_iterator_t) :: it_hel1, it_hel2
  integer :: i
  select type (data)
  type is (gaussian_data_t)
    m2 = data%flv_in%get_mass () ** 2
    hel_lock = [3, 4, 1, 2]
    mask = quantum_numbers_mask (.false., .false., .false.)
    call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
    sf_int%data => data
    do i = 1, 2
      call qn_fc(i)%init ( &
        flv = data%flv_in(i), &
        col = color_from_flavor (data%flv_in(i)))
      call qn_fc(i+2)%init ( &
        flv = data%flv_in(i), &
        col = color_from_flavor (data%flv_in(i)))
    end do
    call pol1%init_generic (data%flv_in(1))
    call it_hel1%init (pol1)
    do while (it_hel1%is_valid ())

```

```

        qn_hel(1) = it_hel1%get_quantum_numbers ()
        qn_hel(3) = it_hel1%get_quantum_numbers ()
        call pol2%init_generic (data%flv_in(2))
        call it_hel2%init (pol2)
        do while (it_hel2%is_valid ())
            qn_hel(2) = it_hel2%get_quantum_numbers ()
            qn_hel(4) = it_hel2%get_quantum_numbers ()
            qn = qn_hel .merge. qn_fc
            call sf_int%add_state (qn)
            call it_hel2%advance ()
        end do
        ! call pol2%final ()
        call it_hel1%advance ()
    end do
    ! call pol1%final ()
    call sf_int%freeze ()
    call sf_int%set_incoming ([1,2])
    call sf_int%set_outgoing ([3,4])
    sf_int%status = SF_INITIAL
end select
call sf_int%data%rng_factory%make (sf_int%rng)
end subroutine gaussian_init

```

This spectrum type needs a finalizer, which closes the data file.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: final => sf_gaussian_final

<SF gaussian: sub interfaces>+≡
    module subroutine sf_gaussian_final (object)
        class(gaussian_t), intent(inout) :: object
    end subroutine sf_gaussian_final

<SF gaussian: procedures>+≡
    module subroutine sf_gaussian_final (object)
        class(gaussian_t), intent(inout) :: object
        call object%interaction_t%final ()
    end subroutine sf_gaussian_final

```

16.10.4 Kinematics

Refer to the data component.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: is_generator => gaussian_is_generator

<SF gaussian: sub interfaces>+≡
    module function gaussian_is_generator (sf_int) result (flag)
        class(gaussian_t), intent(in) :: sf_int
        logical :: flag
    end function gaussian_is_generator

<SF gaussian: procedures>+≡
    module function gaussian_is_generator (sf_int) result (flag)
        class(gaussian_t), intent(in) :: sf_int
        logical :: flag

```

```

        flag = sf_int%data%is_generator ()
    end function gaussian_is_generator

```

Generate free parameters. The x value should be distributed with mean 1 and σ given by the spread. We reject negative x values. (This cut slightly biases the distribution, but for reasonable (small) spreads negative r should not occur.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: generate_free => gaussian_generate_free

<SF gaussian: sub interfaces>+≡
    module subroutine gaussian_generate_free (sf_int, r, rb, x_free)
        class(gaussian_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
    end subroutine gaussian_generate_free

<SF gaussian: procedures>+≡
    module subroutine gaussian_generate_free (sf_int, r, rb, x_free)
        class(gaussian_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        real(default), dimension(size(r)) :: z
        associate (data => sf_int%data)
            do
                call sf_int%rng%generate_gaussian (z)
                rb = z * data%spread
                r = 1 - rb
                x_free = x_free * product (r)
                if (all (r > 0)) exit
            end do
        end associate
    end subroutine gaussian_generate_free

```

Set kinematics. Trivial transfer since this is a pure generator. The map flag doesn't apply.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: complete_kinematics => gaussian_complete_kinematics

<SF gaussian: sub interfaces>+≡
    module subroutine gaussian_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(gaussian_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
    end subroutine gaussian_complete_kinematics

<SF gaussian: procedures>+≡
    module subroutine gaussian_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(gaussian_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x

```

```

real(default), dimension(:), intent(out) :: xb
real(default), intent(out) :: f
real(default), dimension(:), intent(in) :: r
real(default), dimension(:), intent(in) :: rb
logical, intent(in) :: map
if (map) then
  call msg_fatal ("gaussian: map flag not supported")
else
  x = r
  xb= rb
  f = 1
end if
call sf_int%reduce_momenta (x)
end subroutine gaussian_complete_kinematics

```

Compute inverse kinematics. Trivial in this case.

(SF gaussian: gaussian: TBP)+≡

```

procedure :: inverse_kinematics => gaussian_inverse_kinematics

```

(SF gaussian: sub interfaces)+≡

```

module subroutine gaussian_inverse_kinematics &
  (sf_int, x, xb, f, r, rb, map, set_momenta)
  class(gaussian_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: r
  real(default), dimension(:), intent(out) :: rb
  logical, intent(in) :: map
  logical, intent(in), optional :: set_momenta
end subroutine gaussian_inverse_kinematics

```

(SF gaussian: procedures)+≡

```

module subroutine gaussian_inverse_kinematics &
  (sf_int, x, xb, f, r, rb, map, set_momenta)
  class(gaussian_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: r
  real(default), dimension(:), intent(out) :: rb
  logical, intent(in) :: map
  logical, intent(in), optional :: set_momenta
  logical :: set_mom
  set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
  if (map) then
    call msg_fatal ("gaussian: map flag not supported")
  else
    r = x
    rb= xb
    f = 1
  end if
  if (set_mom) then
    call sf_int%reduce_momenta (x)
  end if

```

```
end subroutine gaussian_inverse_kinematics
```

16.10.5 gaussian application

Trivial, just set the unit weight.

```
<SF gaussian: gaussian: TBP>+≡
  procedure :: apply => gaussian_apply

<SF gaussian: sub interfaces>+≡
  module subroutine gaussian_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(gaussian_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine gaussian_apply

<SF gaussian: procedures>+≡
  module subroutine gaussian_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(gaussian_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f
    f = 1
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine gaussian_apply
```

16.10.6 Unit tests

Test module, followed by the corresponding implementation module.

```
<sf_gaussian_ut.f90>≡
  <File header>

  module sf_gaussian_ut
    use unit_tests
    use sf_gaussian_uti

  <Standard module head>

  <SF gaussian: public test>

  contains

  <SF gaussian: test driver>

  end module sf_gaussian_ut
```

```

⟨sf_gaussian_util.f90⟩≡
  ⟨File header⟩

  module sf_gaussian_util

    ⟨Use kinds⟩
    use numeric_utils, only: pacify
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use rng_base
    use sf_aux
    use sf_base

    use sf_gaussian

    use rng_base_util, only: rng_test_factory_t

  ⟨Standard module head⟩

  ⟨SF gaussian: test declarations⟩

  contains

  ⟨SF gaussian: tests⟩

  end module sf_gaussian_util
API: driver for the unit tests below.
⟨SF gaussian: public test⟩≡
  public :: sf_gaussian_test
⟨SF gaussian: test driver⟩≡
  subroutine sf_gaussian_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  ⟨SF gaussian: execute tests⟩
  end subroutine sf_gaussian_test

```

Test structure function data

Construct and display a test structure function data object.

```

⟨SF gaussian: execute tests⟩≡
  call test (sf_gaussian_1, "sf_gaussian_1", &
    "structure function configuration", &
    u, results)
⟨SF gaussian: test declarations⟩≡
  public :: sf_gaussian_1

```



```

<SF gaussian: tests>≡
subroutine sf_gaussian_1 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(pdg_array_t), dimension(2) :: pdg_in
  type(pdg_array_t), dimension(2) :: pdg_out
  integer, dimension(:), allocatable :: pdg1, pdg2
  class(sf_data_t), allocatable :: data
  class(rng_factory_t), allocatable :: rng_factory

  write (u, "(A)")  "* Test output: sf_gaussian_1"
  write (u, "(A)")  "* Purpose: initialize and display &
    &gaussian-spread structure function data"
  write (u, "(A)")

  call model%init_qed_test ()
  pdg_in(1) = ELECTRON
  pdg_in(2) = -ELECTRON

  allocate (gaussian_data_t :: data)
  allocate (rng_test_factory_t :: rng_factory)
  select type (data)
  type is (gaussian_data_t)
    call data%init (model, pdg_in, [1e-2_default, 2e-2_default], rng_factory)
  end select

  call data%write (u)

  write (u, "(A)")

  write (u, "(1x,A)") "Outgoing particle codes:"
  call data%get_pdg_out (pdg_out)
  pdg1 = pdg_out(1)
  pdg2 = pdg_out(2)
  write (u, "(2x,99(1x,I0))") pdg1, pdg2

  call model%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: sf_gaussian_1"

end subroutine sf_gaussian_1

```

Probe the structure-function object

Active the beam event reader, generate an event.

```

<SF gaussian: execute tests>+≡
  call test (sf_gaussian_2, "sf_gaussian_2", &
    "generate event", &
    u, results)

<SF gaussian: test declarations>+≡
  public :: sf_gaussian_2

```

```

<SF gaussian: tests>+=
subroutine sf_gaussian_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t), dimension(2) :: flv
  type(pdg_array_t), dimension(2) :: pdg_in
  class(sf_data_t), allocatable, target :: data
  class(rng_factory_t), allocatable :: rng_factory
  class(sf_int_t), allocatable :: sf_int
  type(vector4_t) :: k1, k2
  real(default) :: E
  real(default), dimension(:), allocatable :: r, rb, x, xb
  real(default) :: x_free, f
  integer :: i

  write (u, "(A)")  "* Test output: sf_gaussian_2"
  write (u, "(A)")  "*   Purpose: initialize and display &
    &gaussian-spread structure function data"
  write (u, "(A)")

  call model%init_qed_test ()
  call flv(1)%init (ELECTRON, model)
  call flv(2)%init (-ELECTRON, model)
  pdg_in(1) = ELECTRON
  pdg_in(2) = -ELECTRON

  call reset_interaction_counter ()

  allocate (gaussian_data_t :: data)
  allocate (rng_test_factory_t :: rng_factory)
  select type (data)
  type is (gaussian_data_t)
    call data%init (model, pdg_in, [1e-2_default, 2e-2_default], rng_factory)
  end select

  write (u, "(A)")  "* Initialize structure-function object"
  write (u, "(A)")

  call data%allocate_sf_int (sf_int)
  call sf_int%init (data)
  call sf_int%set_beam_index ([1,2])

  write (u, "(A)")  "* Initialize incoming momentum with E=500"
  write (u, "(A)")
  E = 250
  k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
  k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
  call vector4_write (k1, u)
  call vector4_write (k2, u)
  call sf_int%seed_kinematics ([k1, k2])

  write (u, "(A)")
  write (u, "(A)")  "* Set dummy parameters and generate x."
  write (u, "(A)")

```

```

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call pacify (rb, 1.e-8_default)
call pacify (xb, 1.e-8_default)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)") "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)") "* Generate more events"
write (u, "(A)")

select type (sf_int)
type is (gaussian_t)
  do i = 1, 3
    call sf_int%generate_free (r, rb, x_free)
    write (u, "(A,9(1x,F10.7))") "r =", r
  end do
end select

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_gaussian_2"

end subroutine sf_gaussian_2

```

16.11 Using beam event data

Instead of an analytic beam description, beam data may be provided in form of an event file. In its most simple form, the event file contains pairs of x values, relative to nominal beam energies. More advanced formats may include polarization, etc. The current implementation carries beam polarization through, if specified.

The code is very similar to the energy scan described above.

However, we must include a file-handle manager for the beam-event files. Two different processes may access a given beam-event file at the same time (i.e., serially but alternating). Accessing an open file from two different units is non-standard and not supported by all compilers. Therefore, we keep a global registry of open files, associated units, and reference counts. The `beam_events_t` objects act as proxies to this registry.

```
(sf_beam_events.f90)≡
  <File header>

  module sf_beam_events

    <Use kinds>
    <Use strings>
    use file_registries
    use pdg_arrays
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use polarizations
    use sf_base

    <Standard module head>

    <SF beam events: public>

    <SF beam events: types>

    <SF beam events: variables>

    interface
    <SF beam events: sub interfaces>
    end interface

    contains

    <SF beam events: main procedures>

  end module sf_beam_events

(sf_beam_events_sub.f90)≡
  <File header>

  submodule (sf_beam_events) sf_beam_events_s
```

```

    use io_units
    use diagnostics
    use lorentz

    implicit none

contains

    <SF beam events: procedures>

end submodule sf_beam_events_s

```

16.11.1 The beam-data file registry

We manage data files via the `file_registries` module. To this end, we keep the registry as a private module variable here.

This is public only for the unit tests.

```

    <SF beam events: public>≡
        public :: beam_file_registry

    <SF beam events: variables>≡
        type(file_registry_t), save :: beam_file_registry

```

16.11.2 Data type

```

    <SF beam events: public>+≡
        public :: beam_events_data_t

    <SF beam events: types>≡
        type, extends(sf_data_t) :: beam_events_data_t
        private
            type(flavor_t), dimension(2) :: flv_in
            type(string_t) :: dir
            type(string_t) :: file
            type(string_t) :: fqname
            integer :: unit = 0
            logical :: warn_eof = .true.
        contains
            <SF beam events: beam events data: TBP>
        end type beam_events_data_t

    <SF beam events: beam events data: TBP>≡
        procedure :: init => beam_events_data_init

    <SF beam events: sub interfaces>≡
        module subroutine beam_events_data_init &
            (data, model, pdg_in, dir, file, warn_eof)
            class(beam_events_data_t), intent(out) :: data
            class(model_data_t), intent(in), target :: model
            type(pdg_array_t), dimension(2), intent(in) :: pdg_in
            type(string_t), intent(in) :: dir
            type(string_t), intent(in) :: file

```

```

        logical, intent(in), optional :: warn_eof
    end subroutine beam_events_data_init

<SF beam events: procedures>≡
module subroutine beam_events_data_init &
    (data, model, pdg_in, dir, file, warn_eof)
    class(beam_events_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(2), intent(in) :: pdg_in
    type(string_t), intent(in) :: dir
    type(string_t), intent(in) :: file
    logical, intent(in), optional :: warn_eof
    if (any (pdg_in%get_length () /= 1)) then
        call msg_fatal ("Beam events: incoming beam particles must be unique")
    end if
    call data%flv_in(1)%init (pdg_in(1)%get (1), model)
    call data%flv_in(2)%init (pdg_in(2)%get (1), model)
    data%dir = dir
    data%file = file
    if (present (warn_eof)) data%warn_eof = warn_eof
end subroutine beam_events_data_init

```

Return true since this spectrum is always in generator mode.

```

<SF beam events: beam events data: TBP>+≡
    procedure :: is_generator => beam_events_data_is_generator

<SF beam events: sub interfaces>+≡
    module function beam_events_data_is_generator (data) result (flag)
        class(beam_events_data_t), intent(in) :: data
        logical :: flag
    end function beam_events_data_is_generator

<SF beam events: procedures>+≡
    module function beam_events_data_is_generator (data) result (flag)
        class(beam_events_data_t), intent(in) :: data
        logical :: flag
        flag = .true.
    end function beam_events_data_is_generator

```

The number of parameters is two. They are free parameters.

```

<SF beam events: beam events data: TBP>+≡
    procedure :: get_n_par => beam_events_data_get_n_par

<SF beam events: sub interfaces>+≡
    module function beam_events_data_get_n_par (data) result (n)
        class(beam_events_data_t), intent(in) :: data
        integer :: n
    end function beam_events_data_get_n_par

<SF beam events: procedures>+≡
    module function beam_events_data_get_n_par (data) result (n)
        class(beam_events_data_t), intent(in) :: data
        integer :: n
        n = 2
    end function beam_events_data_get_n_par

```

```

<SF beam events: beam events data: TBP>+≡
  procedure :: get_pdg_out => beam_events_data_get_pdg_out

<SF beam events: sub interfaces>+≡
  module subroutine beam_events_data_get_pdg_out (data, pdg_out)
    class(beam_events_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  end subroutine beam_events_data_get_pdg_out

<SF beam events: procedures>+≡
  module subroutine beam_events_data_get_pdg_out (data, pdg_out)
    class(beam_events_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      pdg_out(i) = data%flv_in(i)%get_pdg ()
    end do
  end subroutine beam_events_data_get_pdg_out

```

Allocate the interaction record. Due to a gfortran 7/8/9 bug has to remain in the main module.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: allocate_sf_int => beam_events_data_allocate_sf_int

<SF beam events: main procedures>≡
  subroutine beam_events_data_allocate_sf_int (data, sf_int)
    class(beam_events_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (beam_events_t :: sf_int)
  end subroutine beam_events_data_allocate_sf_int

```

Output

```

<SF beam events: beam events data: TBP>+≡
  procedure :: write => beam_events_data_write

<SF beam events: sub interfaces>+≡
  module subroutine beam_events_data_write (data, unit, verbose)
    class(beam_events_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine beam_events_data_write

<SF beam events: procedures>+≡
  module subroutine beam_events_data_write (data, unit, verbose)
    class(beam_events_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Beam-event file data:"
    write (u, "(3x,A,A,A,A)") "prt_in = ", &
      char (data%flv_in(1)%get_name ()), &
      ", ", char (data%flv_in(2)%get_name ())
    write (u, "(3x,A,A,A)") "file   = ", char (data%file), ""

```

```

write (u, "(3x,A,I0)") "unit   = ", data%unit
write (u, "(3x,A,L1)") "warn   = ", data%warn_eof
end subroutine beam_events_data_write

```

The data file needs to be opened and closed explicitly. The open/close message is communicated to the file handle registry, which does the actual work.

We determine first whether to look in the local directory or in the given system directory.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: open => beam_events_data_open
  procedure :: close => beam_events_data_close

<SF beam events: sub interfaces>+≡
  module subroutine beam_events_data_open (data)
    class(beam_events_data_t), intent(inout) :: data
  end subroutine beam_events_data_open
  module subroutine beam_events_data_close (data)
    class(beam_events_data_t), intent(inout) :: data
  end subroutine beam_events_data_close

<SF beam events: procedures>+≡
  module subroutine beam_events_data_open (data)
    class(beam_events_data_t), intent(inout) :: data
    logical :: exist
    if (data%unit == 0) then
      data%fqn = data%file
      if (data%fqn == "") &
        call msg_fatal ("Beam events: $beam_events_file is not set")
      inquire (file = char (data%fqn), exist = exist)
      if (.not. exist) then
        data%fqn = data%dir // "/" // data%file
        inquire (file = char (data%fqn), exist = exist)
        if (.not. exist) then
          data%fqn = ""
          call msg_fatal ("Beam events: file '" &
            // char (data%file) // "' not found")
          return
        end if
      end if
      call msg_message ("Beam events: reading from file '" &
        // char (data%file) // "'")
      call beam_file_registry%open (data%fqn, data%unit)
    else
      call msg_bug ("Beam events: file '" &
        // char (data%file) // "' is already open")
    end if
  end subroutine beam_events_data_open

  module subroutine beam_events_data_close (data)
    class(beam_events_data_t), intent(inout) :: data
    if (data%unit /= 0) then
      call beam_file_registry%close (data%fqn)
      call msg_message ("Beam events: closed file '" &
        // char (data%file) // "'")
    end if
  end subroutine beam_events_data_close

```



```

        data%unit = 0
    end if
end subroutine beam_events_data_close

```

Return the beam event file.

```

<SF beam events: beam events data: TBP>+≡
    procedure :: get_beam_file => beam_events_data_get_beam_file

<SF beam events: sub interfaces>+≡
    module function beam_events_data_get_beam_file (data) result (file)
        class(beam_events_data_t), intent(in) :: data
        type(string_t) :: file
    end function beam_events_data_get_beam_file

<SF beam events: procedures>+≡
    module function beam_events_data_get_beam_file (data) result (file)
        class(beam_events_data_t), intent(in) :: data
        type(string_t) :: file
        file = "Beam events: " // data%file
    end function beam_events_data_get_beam_file

```

16.11.3 The beam events object

Flavor and polarization carried through, no radiated particles.

```

<SF beam events: public>+≡
    public :: beam_events_t

<SF beam events: types>+≡
    type, extends (sf_int_t) :: beam_events_t
        type(beam_events_data_t), pointer :: data => null ()
        integer :: count = 0
    contains
        <SF beam events: beam events: TBP>
    end type beam_events_t

```

Type string: show beam events file.

```

<SF beam events: beam events: TBP>≡
    procedure :: type_string => beam_events_type_string

<SF beam events: sub interfaces>+≡
    module function beam_events_type_string (object) result (string)
        class(beam_events_t), intent(in) :: object
        type(string_t) :: string
    end function beam_events_type_string

<SF beam events: procedures>+≡
    module function beam_events_type_string (object) result (string)
        class(beam_events_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "Beam events: " // object%data%file
        else
            string = "Beam events: [undefined]"
        end if
    end function

```

```
end function beam_events_type_string
```

Output. Call the interaction routine after displaying the configuration.

```
<SF beam events: beam events: TBP>+≡
```

```
procedure :: write => beam_events_write
```

```
<SF beam events: sub interfaces>+≡
```

```
module subroutine beam_events_write (object, unit, testflag)
  class(beam_events_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
end subroutine beam_events_write
```

```
<SF beam events: procedures>+≡
```

```
module subroutine beam_events_write (object, unit, testflag)
  class(beam_events_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  if (associated (object%data)) then
    call object%data%write (u)
    call object%base_write (u, testflag)
  else
    write (u, "(1x,A)") "Beam events data: [undefined]"
  end if
end subroutine beam_events_write
```

```
<SF beam events: beam events: TBP>+≡
```

```
procedure :: init => beam_events_init
```

```
<SF beam events: sub interfaces>+≡
```

```
module subroutine beam_events_init (sf_int, data)
  class(beam_events_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
end subroutine beam_events_init
```

```
<SF beam events: procedures>+≡
```

```
module subroutine beam_events_init (sf_int, data)
  class(beam_events_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  real(default), dimension(2) :: m2
  real(default), dimension(0) :: mr2
  type(quantum_numbers_mask_t), dimension(4) :: mask
  integer, dimension(4) :: hel_lock
  type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
  type(polarization_t), target :: pol1, pol2
  type(polarization_iterator_t) :: it_hel1, it_hel2
  integer :: i
  select type (data)
  type is (beam_events_data_t)
    m2 = data%flv_in%get_mass () ** 2
    hel_lock = [3, 4, 1, 2]
    mask = quantum_numbers_mask (.false., .false., .false.)
    call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
```

```

sf_int%data => data
do i = 1, 2
  call qn_fc(i)%init ( &
    flv = data%flv_in(i), &
    col = color_from_flavor (data%flv_in(i)))
  call qn_fc(i+2)%init ( &
    flv = data%flv_in(i), &
    col = color_from_flavor (data%flv_in(i)))
end do
call pol1%init_generic (data%flv_in(1))
call it_hel1%init (pol1)
do while (it_hel1%is_valid ())
  qn_hel(1) = it_hel1%get_quantum_numbers ()
  qn_hel(3) = it_hel1%get_quantum_numbers ()
  call pol2%init_generic (data%flv_in(2))
  call it_hel2%init (pol2)
  do while (it_hel2%is_valid ())
    qn_hel(2) = it_hel2%get_quantum_numbers ()
    qn_hel(4) = it_hel2%get_quantum_numbers ()
    qn = qn_hel .merge. qn_fc
    call sf_int%add_state (qn)
    call it_hel2%advance ()
  end do
  ! call pol2%final ()
  call it_hel1%advance ()
end do
! call pol1%final ()
call sf_int%freeze ()
call sf_int%set_incoming ([1,2])
call sf_int%set_outgoing ([3,4])
call sf_int%data%open ()
sf_int%status = SF_INITIAL
end select
end subroutine beam_events_init

```

This spectrum type needs a finalizer, which closes the data file.

```

<SF beam events: beam events: TBP>+≡
  procedure :: final => sf_beam_events_final

<SF beam events: sub interfaces>+≡
  module subroutine sf_beam_events_final (object)
    class(beam_events_t), intent(inout) :: object
  end subroutine sf_beam_events_final

<SF beam events: procedures>+≡
  module subroutine sf_beam_events_final (object)
    class(beam_events_t), intent(inout) :: object
    call object%data%close ()
    call object%interaction_t%final ()
  end subroutine sf_beam_events_final

```

16.11.4 Kinematics

Refer to the data component.

```
<SF beam events: beam events: TBP>+≡
    procedure :: is_generator => beam_events_is_generator

<SF beam events: sub interfaces>+≡
    module function beam_events_is_generator (sf_int) result (flag)
        class(beam_events_t), intent(in) :: sf_int
        logical :: flag
    end function beam_events_is_generator

<SF beam events: procedures>+≡
    module function beam_events_is_generator (sf_int) result (flag)
        class(beam_events_t), intent(in) :: sf_int
        logical :: flag
        flag = sf_int%data%is_generator ()
    end function beam_events_is_generator
```

Generate free parameters. We read them from file.

```
<SF beam events: beam events: TBP>+≡
    procedure :: generate_free => beam_events_generate_free

<SF beam events: sub interfaces>+≡
    recursive module subroutine beam_events_generate_free &
        (sf_int, r, rb, x_free)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
    end subroutine beam_events_generate_free

<SF beam events: procedures>+≡
    recursive module subroutine beam_events_generate_free &
        (sf_int, r, rb, x_free)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        integer :: iostat
        associate (data => sf_int%data)
            if (data%unit /= 0) then
                read (data%unit, fmt=*, iostat=iostat) r
                if (iostat > 0) then
                    write (msg_buffer, "(A,I0,A)") &
                        "Beam events: I/O error after reading ", sf_int%count, &
                        " events"
                    call msg_fatal ()
                else if (iostat < 0) then
                    if (sf_int%count == 0) then
                        call msg_fatal ("Beam events: file is empty")
                    else if (sf_int%data%warn_eof) then
                        write (msg_buffer, "(A,I0,A)") &
                            "Beam events: End of file after reading ", sf_int%count, &
                            " events, rewinding"
                        call msg_warning ()
                    end if
                end if
                rewind (data%unit)
            end if
        end associate
    end subroutine beam_events_generate_free
```

```

        sf_int%count = 0
        call sf_int%generate_free (r, rb, x_free)
    else
        sf_int%count = sf_int%count + 1
        rb = 1 - r
        x_free = x_free * product (r)
    end if
else
    call msg_bug ("Beam events: file is not open for reading")
end if
end associate
end subroutine beam_events_generate_free

```

Set kinematics. Trivial transfer since this is a pure generator. The map flag doesn't apply.

```

<SF beam events: beam events: TBP>+≡
    procedure :: complete_kinematics => beam_events_complete_kinematics

<SF beam events: sub interfaces>+≡
    module subroutine beam_events_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
    end subroutine beam_events_complete_kinematics

<SF beam events: procedures>+≡
    module subroutine beam_events_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        if (map) then
            call msg_fatal ("Beam events: map flag not supported")
        else
            x = r
            xb = rb
            f = 1
        end if
        call sf_int%reduce_momenta (x)
    end subroutine beam_events_complete_kinematics

```

Compute inverse kinematics. Trivial in this case.

```

<SF beam events: beam events: TBP>+≡
    procedure :: inverse_kinematics => beam_events_inverse_kinematics

```

```

<SF beam events: sub interfaces>+≡
  module subroutine beam_events_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(beam_events_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine beam_events_inverse_kinematics

<SF beam events: procedures>+≡
  module subroutine beam_events_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(beam_events_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
      call msg_fatal ("Beam events: map flag not supported")
    else
      r = x
      rb= xb
      f = 1
    end if
    if (set_mom) then
      call sf_int%reduce_momenta (x)
    end if
  end subroutine beam_events_inverse_kinematics

```

16.11.5 Beam events application

Trivial, just set the unit weight.

```

<SF beam events: beam events: TBP>+≡
  procedure :: apply => beam_events_apply

<SF beam events: sub interfaces>+≡
  module subroutine beam_events_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(beam_events_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine beam_events_apply

```

```

⟨SF beam events: procedures⟩+≡
  module subroutine beam_events_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(beam_events_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f
    f = 1
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine beam_events_apply

```

16.11.6 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_beam_events_ut.f90⟩≡
  ⟨File header⟩

  module sf_beam_events_ut
    use unit_tests
    use sf_beam_events_uti

    ⟨Standard module head⟩

    ⟨SF beam events: public test⟩

    contains

    ⟨SF beam events: test driver⟩

  end module sf_beam_events_ut

⟨sf_beam_events_uti.f90⟩≡
  ⟨File header⟩

  module sf_beam_events_uti

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use numeric_utils, only: pacify
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_aux
    use sf_base

    use sf_beam_events

```

<Standard module head>

<SF beam events: test declarations>

contains

<SF beam events: tests>

end module sf_beam_events_util

API: driver for the unit tests below.

<SF beam events: public test>≡

public :: sf_beam_events_test

<SF beam events: test driver>≡

subroutine sf_beam_events_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SF beam events: execute tests>

end subroutine sf_beam_events_test

Test structure function data

Construct and display a test structure function data object.

<SF beam events: execute tests>≡

**call test (sf_beam_events_1, "sf_beam_events_1", &
"structure function configuration", &
u, results)**

<SF beam events: test declarations>≡

public :: sf_beam_events_1

<SF beam events: tests>≡

subroutine sf_beam_events_1 (u)

integer, intent(in) :: u

type(model_data_t), target :: model

type(pdg_array_t), dimension(2) :: pdg_in

type(pdg_array_t), dimension(2) :: pdg_out

integer, dimension(:), allocatable :: pdg1, pdg2

class(sf_data_t), allocatable :: data

write (u, "(A)") **"* Test output: sf_beam_events_1"**

write (u, "(A)") **"* Purpose: initialize and display &
&beam-events structure function data"**

write (u, "(A)")

call model%init_qed_test ()

pdg_in(1) = ELECTRON

pdg_in(2) = -ELECTRON

allocate (beam_events_data_t :: data)

select type (data)

type is (beam_events_data_t)

call data%init (model, pdg_in, var_str (""), var_str ("beam_events.dat"))


```

end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))") pdg1, pdg2

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_beam_events_1"

end subroutine sf_beam_events_1

```

Probe the structure-function object

Active the beam event reader, generate an event.

```

<SF beam events: execute tests>+≡
  call test (sf_beam_events_2, "sf_beam_events_2", &
    "generate event", &
    u, results)

<SF beam events: test declarations>+≡
  public :: sf_beam_events_2

<SF beam events: tests>+≡
  subroutine sf_beam_events_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: x_free, f
    integer :: i

    write (u, "(A)")  "* Test output: sf_beam_events_2"
    write (u, "(A)")  "* Purpose: initialize and display &
      &beam-events structure function data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv(1)%init (ELECTRON, model)
    call flv(2)%init (-ELECTRON, model)
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

```

```

call reset_interaction_counter ()

allocate (beam_events_data_t :: data)
select type (data)
type is (beam_events_data_t)
    call data%init (model, pdg_in, &
        var_str (""), var_str ("test_beam_events.dat"))
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set dummy parameters and generate x."
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free
select type (sf_int)
type is (beam_events_t)
    write (u, "(A,1x,I0)")  "count =", sf_int%count
end select

write (u, "(A)")
write (u, "(A)")  "* Evaluate"

```

```

write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate more events, rewind"
write (u, "(A)")

select type (sf_int)
type is (beam_events_t)
  do i = 1, 3
    call sf_int%generate_free (r, rb, x_free)
    write (u, "(A,9(1x,F10.7))") "r =", r
    write (u, "(A,1x,I0)") "count =", sf_int%count
  end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_beam_events_2"

end subroutine sf_beam_events_2

```

Check the file handle registry

Open and close some files, checking the registry contents.

```

<SF beam events: execute tests>+≡
  call test (sf_beam_events_3, "sf_beam_events_3", &
    "check registry", &
    u, results)

<SF beam events: test declarations>+≡
  public :: sf_beam_events_3

<SF beam events: tests>+≡
  subroutine sf_beam_events_3 (u)
    integer, intent(in) :: u
    integer :: u1

    write (u, "(A)")  "* Test output: sf_beam_events_2"
    write (u, "(A)")  "* Purpose: check file handle registry"
    write (u, "(A)")

    write (u, "(A)")  "* Create some empty files"
    write (u, "(A)")

    u1 = free_unit ()
    open (u1, file = "sf_beam_events_fl.tmp", action="write", status="new")

```

```

close (u1)
open (u1, file = "sf_beam_events_f2.tmp", action="write", status="new")
close (u1)
open (u1, file = "sf_beam_events_f3.tmp", action="write", status="new")
close (u1)

write (u, "(A)")  "* Empty registry"
write (u, "(A)")

call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Insert three entries"
write (u, "(A)")

call beam_file_registry%open (var_str ("sf_beam_events_f3.tmp"))
call beam_file_registry%open (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%open (var_str ("sf_beam_events_f1.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Open a second channel"
write (u, "(A)")

call beam_file_registry%open (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Close second entry twice"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%close (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Close last entry"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f3.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Close remaining entry"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f1.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

open (u1, file = "sf_beam_events_f1.tmp", action="write")
close (u1, status = "delete")

```

```
open (u1, file = "sf_beam_events_f2.tmp", action="write")
close (u1, status = "delete")
open (u1, file = "sf_beam_events_f3.tmp", action="write")
close (u1, status = "delete")

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_beam_events_3"

end subroutine sf_beam_events_3
```

16.12 Lepton collider beamstrahlung: CIRCE1

```
<sf_circe1.f90>≡
  <File header>

  module sf_circe1

    <Use kinds>
    use kinds, only: double
    <Use strings>
    use rng_base
    use pdg_arrays
    use model_data
    use flavors
    use polarizations
    use sf_mappings
    use sf_base
    use circe1, circe1_rng_t => rng_type !NODEP!

    <Standard module head>

    <SF circe1: public>

    <SF circe1: types>

    interface
    <SF circe1: sub interfaces>
    end interface

    contains

    <SF circe1: main procedures>

  end module sf_circe1

<sf_circe1_sub.f90>≡
  <File header>

  submodule (sf_circe1) sf_circe1_s

    use io_units
    use format_defs, only: FMT_17, FMT_19
    use diagnostics
    use physics_defs, only: ELECTRON, PHOTON
    use lorentz
    use colors
    use quantum_numbers
    use state_matrices

    implicit none

    contains

    <SF circe1: procedures>
```

```
end submodule sf_circe1_s
```

16.12.1 Physics

Beamstrahlung is applied before ISR. The **CIRCE1** implementation has a single structure function for both beams (which makes sense since it has to be switched on or off for both beams simultaneously). Nevertheless it is factorized:

The functional form in the **CIRCE1** parameterization is defined for electrons or photons

$$f(x) = \alpha x^\beta (1-x)^\gamma \quad (16.62)$$

for $x < 1 - \epsilon$ (resp. $x > \epsilon$ in the photon case). In the remaining interval, the standard form is zero, with a delta singularity at $x = 1$ (resp. $x = 0$). Equivalently, the delta part may be distributed uniformly among this interval. This latter form is implemented in the **kirke** version of the **CIRCE1** subroutines, and is used here.

The parameter **circe1_eps** sets the peak mapping of the **CIRCE1** structure function. Its default value is 10^{-5} . The other parameters are the parameterization version and revision number, the accelerator type, and the \sqrt{s} value used by **CIRCE1**. The chattiness can also be set.

Since the energy is distributed in a narrow region around unity (for electrons) or zero (for photons), it is advantageous to map the interval first. The mapping is controlled by the parameter **circe1_epsilon** which is taken from the **CIRCE1** internal data structure.

The \sqrt{s} value, if not explicitly set, is taken from the process data. Note that interpolating \sqrt{s} is not recommended; one should rather choose one of the distinct values known to **CIRCE1**.

16.12.2 The CIRCE1 data block

The **CIRCE1** parameters are: The incoming flavors, the flags whether the photon or the lepton is the parton in the hard interaction, the flags for the generation mode (generator/mapping/no mapping), the mapping parameter ϵ , \sqrt{s} and several steering parameters: **ver**, **rev**, **acc**, **chat**.

In generator mode, the x values are actually discarded and a random number generator is used instead.

```
<SF circe1: public>≡
  public :: circe1_data_t

<SF circe1: types>≡
  type, extends (sf_data_t) :: circe1_data_t
  private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(2) :: flv_in
    integer, dimension(2) :: pdg_in
    real(default), dimension(2) :: m_in = 0
    logical, dimension(2) :: photon = .false.
    logical :: generate = .false.
    class(rng_factory_t), allocatable :: rng_factory
    real(default) :: sqrts = 0
    real(default) :: eps = 0
```

```

integer :: ver = 0
integer :: rev = 0
character(6) :: acc = "?"
integer :: chat = 0
logical :: with_radiation = .false.
contains
  <SF circe1: circe1 data: TBP>
end type circe1_data_t

```

<SF circe1: circe1 data: TBP>≡

```

procedure :: init => circe1_data_init

```

<SF circe1: sub interfaces>≡

```

module subroutine circe1_data_init &
  (data, model, pdg_in, sqrts, eps, out_photon, &
   ver, rev, acc, chat, with_radiation)
  class(circe1_data_t), intent(out) :: data
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t), dimension(2), intent(in) :: pdg_in
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: eps
  logical, dimension(2), intent(in) :: out_photon
  character(*), intent(in) :: acc
  integer, intent(in) :: ver, rev, chat
  logical, intent(in) :: with_radiation
end subroutine circe1_data_init

```

<SF circe1: procedures>≡

```

module subroutine circe1_data_init &
  (data, model, pdg_in, sqrts, eps, out_photon, &
   ver, rev, acc, chat, with_radiation)
  class(circe1_data_t), intent(out) :: data
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t), dimension(2), intent(in) :: pdg_in
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: eps
  logical, dimension(2), intent(in) :: out_photon
  character(*), intent(in) :: acc
  integer, intent(in) :: ver, rev, chat
  logical, intent(in) :: with_radiation
  data%model => model
  if (any (pdg_in%get_length () /= 1)) then
    call msg_fatal ("CIRCE1: incoming beam particles must be unique")
  end if
  call data%flv_in(1)%init (pdg_in(1)%get (1), model)
  call data%flv_in(2)%init (pdg_in(2)%get (1), model)
  data%pdg_in = data%flv_in%get_pdg ()
  data%m_in = data%flv_in%get_mass ()
  data%sqrts = sqrts
  data%eps = eps
  data%photon = out_photon
  data%ver = ver
  data%rev = rev
  data%acc = acc
  data%chat = chat

```



```

data%with_radiation = with_radiation
call data%check ()
call circex (0.d0, 0.d0, dble (data%sqrts), &
            data%acc, data%ver, data%rev, data%chat)
end subroutine circe1_data_init

```

Activate the generator mode. We import a RNG factory into the data type, which can then spawn RNG generator objects.

```

<SF circe1: circe1 data: TBP>+=
  procedure :: set_generator_mode => circe1_data_set_generator_mode

<SF circe1: sub interfaces>+=
  module subroutine circe1_data_set_generator_mode (data, rng_factory)
    class(circe1_data_t), intent(inout) :: data
    class(rng_factory_t), intent(inout), allocatable :: rng_factory
  end subroutine circe1_data_set_generator_mode

<SF circe1: procedures>+=
  module subroutine circe1_data_set_generator_mode (data, rng_factory)
    class(circe1_data_t), intent(inout) :: data
    class(rng_factory_t), intent(inout), allocatable :: rng_factory
    data%generate = .true.
    call move_alloc (from = rng_factory, to = data%rng_factory)
  end subroutine circe1_data_set_generator_mode

```

Handle error conditions.

```

<SF circe1: circe1 data: TBP>+=
  procedure :: check => circe1_data_check

<SF circe1: sub interfaces>+=
  module subroutine circe1_data_check (data)
    class(circe1_data_t), intent(in) :: data
  end subroutine circe1_data_check

<SF circe1: procedures>+=
  module subroutine circe1_data_check (data)
    class(circe1_data_t), intent(in) :: data
    type(flavor_t) :: flv_electron, flv_photon
    call flv_electron%init (ELECTRON, data%model)
    call flv_photon%init (PHOTON, data%model)
    if (.not. flv_electron%is_defined () &
        .or. .not. flv_photon%is_defined ()) then
      call msg_fatal ("CIRCE1: model must contain photon and electron")
    end if
    if (any (abs (data%pdg_in) /= ELECTRON) &
        .or. (data%pdg_in(1) /= - data%pdg_in(2))) then
      call msg_fatal ("CIRCE1: applicable only for e+e- or e-e+ collisions")
    end if
    if (data%eps <= 0) then
      call msg_error ("CIRCE1: circe1_eps = 0: integration will &
                     &miss x=1 peak")
    end if
  end subroutine circe1_data_check

```

Output

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: write => circe1_data_write

<SF circe1: sub interfaces>+≡
  module subroutine circe1_data_write (data, unit, verbose)
    class(circe1_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine circe1_data_write

<SF circe1: procedures>+≡
  module subroutine circe1_data_write (data, unit, verbose)
    class(circe1_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    logical :: verb
    verb = .false.; if (present (verbose)) verb = verbose
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "CIRCE1 data:"
    write (u, "(3x,A,2(1x,A))") "prt_in  =", &
      char (data%flv_in(1)%get_name ()), &
      char (data%flv_in(2)%get_name ())
    write (u, "(3x,A,2(1x,L1))") "photon  =", data%photon
    write (u, "(3x,A,L1)") "generate =", data%generate
    write (u, "(3x,A,2(1x," // FMT_19 // ")") "m_in    =", data%m_in
    write (u, "(3x,A," // FMT_19 // ")") "sqrts   =", data%sqrts
    write (u, "(3x,A," // FMT_19 // ")") "eps     =", data%eps
    write (u, "(3x,A,I0)") "ver      =", data%ver
    write (u, "(3x,A,I0)") "rev      =", data%rev
    write (u, "(3x,A,A)") "acc      =", data%acc
    write (u, "(3x,A,I0)") "chat     =", data%chat
    write (u, "(3x,A,L1)") "with rad.=", data%with_radiation
    if (data%generate) then
      if (verb) then
        call data%rng_factory%write (u)
      end if
    end if
  end subroutine circe1_data_write

```

Return true if this structure function is in generator mode. In that case, all parameters are free, otherwise bound. (We do not support mixed cases.) Default is: no generator.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: is_generator => circe1_data_is_generator

<SF circe1: sub interfaces>+≡
  module function circe1_data_is_generator (data) result (flag)
    class(circe1_data_t), intent(in) :: data
    logical :: flag
  end function circe1_data_is_generator

<SF circe1: procedures>+≡
  module function circe1_data_is_generator (data) result (flag)

```

```

class(circe1_data_t), intent(in) :: data
logical :: flag
flag = data%generate
end function circe1_data_is_generator

```

The number of parameters is two, collinear splitting for the two beams.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_n_par => circe1_data_get_n_par

<SF circe1: sub interfaces>+≡
  module function circe1_data_get_n_par (data) result (n)
    class(circe1_data_t), intent(in) :: data
    integer :: n
  end function circe1_data_get_n_par

<SF circe1: procedures>+≡
  module function circe1_data_get_n_par (data) result (n)
    class(circe1_data_t), intent(in) :: data
    integer :: n
    n = 2
  end function circe1_data_get_n_par

```

Return the outgoing particles PDG codes. This is either the incoming particle (if a photon is radiated), or the photon if that is the particle of the hard interaction. The latter is determined via the photon flag. There are two entries for the two beams.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_pdg_out => circe1_data_get_pdg_out

<SF circe1: sub interfaces>+≡
  module subroutine circe1_data_get_pdg_out (data, pdg_out)
    class(circe1_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  end subroutine circe1_data_get_pdg_out

<SF circe1: procedures>+≡
  module subroutine circe1_data_get_pdg_out (data, pdg_out)
    class(circe1_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      if (data%photon(i)) then
        pdg_out(i) = PHOTON
      else
        pdg_out(i) = data%pdg_in(i)
      end if
    end do
  end subroutine circe1_data_get_pdg_out

```

This variant is not inherited, it returns integers.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_pdg_int => circe1_data_get_pdg_int

```

```

<SF circe1: sub interfaces>+≡
    module function circe1_data_get_pdg_int (data) result (pdg)
        class(circe1_data_t), intent(in) :: data
        integer, dimension(2) :: pdg
    end function circe1_data_get_pdg_int

<SF circe1: procedures>+≡
    module function circe1_data_get_pdg_int (data) result (pdg)
        class(circe1_data_t), intent(in) :: data
        integer, dimension(2) :: pdg
        integer :: i
        do i = 1, 2
            if (data%photon(i)) then
                pdg(i) = PHOTON
            else
                pdg(i) = data%pdg_in(i)
            end if
        end do
    end function circe1_data_get_pdg_int

```

Allocate the interaction record. Due to the gfortran 7/8/9 bug this has to remain in the main module.

```

<SF circe1: circe1 data: TBP>+≡
    procedure :: allocate_sf_int => circe1_data_allocate_sf_int

<SF circe1: main procedures>≡
    subroutine circe1_data_allocate_sf_int (data, sf_int)
        class(circe1_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (circe1_t :: sf_int)
    end subroutine circe1_data_allocate_sf_int

```

Return the accelerator type.

```

<SF circe1: circe1 data: TBP>+≡
    procedure :: get_beam_file => circe1_data_get_beam_file

<SF circe1: sub interfaces>+≡
    module function circe1_data_get_beam_file (data) result (file)
        class(circe1_data_t), intent(in) :: data
        type(string_t) :: file
    end function circe1_data_get_beam_file

<SF circe1: procedures>+≡
    module function circe1_data_get_beam_file (data) result (file)
        class(circe1_data_t), intent(in) :: data
        type(string_t) :: file
        file = "CIRCE1: " // data%acc
    end function circe1_data_get_beam_file

```

16.12.3 Random Number Generator for CIRCE

The CIRCE implementation now supports a generic random-number generator object that allows for a local state as a component. To support this, we must

extend the abstract type provided by CIRCE and delegate the generator call to the (also abstract) RNG used by WHIZARD.

```

<SF circe1: types>+≡
  type, extends (circe1_rng_t) :: rng_obj_t
    class(rng_t), allocatable :: rng
    contains
      procedure :: generate => rng_obj_generate
    end type rng_obj_t

<SF circe1: sub interfaces>+≡
  module subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(double), intent(out) :: u
  end subroutine rng_obj_generate

<SF circe1: procedures>+≡
  module subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(double), intent(out) :: u
    real(default) :: x
    call rng_obj%rng%generate (x)
    u = x
  end subroutine rng_obj_generate

```

16.12.4 The CIRCE1 object

This is a $2 \rightarrow 4$ interaction, where, depending on the parameters, any two of the four outgoing particles are connected to the hard interactions, the others are radiated. Knowing that all particles are colorless, we do not have to deal with color.

The flavors are sorted such that the first two particles are the incoming leptons, the next two are the radiated particles, and the last two are the partons initiating the hard interaction.

CIRCE1 does not support polarized beams explicitly. For simplicity, we nevertheless carry beam polarization through to the outgoing electrons and make the photons unpolarized.

In the case that no radiated particle is kept (which actually is the default), polarization is always transferred to the electrons, too. If there is a recoil photon in the event, the radiated particles are 3 and 4, respectively, and 5 and 6 are the outgoing ones (triggering the hard scattering process), while in the case of no radiation, the outgoing particles are 3 and 4, respectively. In the case of the electron being the radiated particle, helicity is not kept.

```

<SF circe1: public>+≡
  public :: circe1_t

<SF circe1: types>+≡
  type, extends (sf_int_t) :: circe1_t
    type(circe1_data_t), pointer :: data => null ()
    real(default), dimension(2) :: x = 0
    real(default), dimension(2) :: xb= 0
    real(default) :: f = 0

```

```

        logical, dimension(2) :: continuum = .true.
        logical, dimension(2) :: peak = .true.
        type(rng_obj_t) :: rng_obj
    contains
        <SF circe1: circe1: TBP>
    end type circe1_t

```

Type string: has to be here, but there is no string variable on which CIRCE1 depends. Hence, a dummy routine.

```

<SF circe1: circe1: TBP>≡
    procedure :: type_string => circe1_type_string

<SF circe1: sub interfaces>+≡
    module function circe1_type_string (object) result (string)
        class(circe1_t), intent(in) :: object
        type(string_t) :: string
    end function circe1_type_string

<SF circe1: procedures>+≡
    module function circe1_type_string (object) result (string)
        class(circe1_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "CIRCE1: beamstrahlung"
        else
            string = "CIRCE1: [undefined]"
        end if
    end function circe1_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF circe1: circe1: TBP>+≡
    procedure :: write => circe1_write

<SF circe1: sub interfaces>+≡
    module subroutine circe1_write (object, unit, testflag)
        class(circe1_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine circe1_write

<SF circe1: procedures>+≡
    module subroutine circe1_write (object, unit, testflag)
        class(circe1_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
            if (object%data%generate) call object%rng_obj%rng%write (u)
            if (object%status >= SF_DONE_KINEMATICS) then
                write (u, "(3x,A,2(1x," // FMT_17 // "))") "x =", object%x
                write (u, "(3x,A,2(1x," // FMT_17 // "))") "xb=", object%xb
                if (object%status >= SF_FAILED_EVALUATION) then
                    write (u, "(3x,A,1x," // FMT_17 // ")") "f =", object%f

```

```

        end if
    end if
    call object%base_write (u, testflag)
else
    write (u, "(1x,A)") "CIRCE1 data: [undefined]"
end if
end subroutine circe1_write

```

<SF circe1: circe1: TBP>+≡

```

    procedure :: init => circe1_init

```

<SF circe1: sub interfaces>+≡

```

    module subroutine circe1_init (sf_int, data)
        class(circe1_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
    end subroutine circe1_init

```

<SF circe1: procedures>+≡

```

    module subroutine circe1_init (sf_int, data)
        class(circe1_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
        logical, dimension(6) :: mask_h
        type(quantum_numbers_mask_t), dimension(6) :: mask
        integer, dimension(6) :: hel_lock
        type(polarization_t), target :: pol1, pol2
        type(quantum_numbers_t), dimension(1) :: qn_fc1, qn_fc2
        type(flavor_t) :: flv_photon
        type(color_t) :: col0
        real(default), dimension(2) :: mi2, mr2, mo2
        type(quantum_numbers_t) :: qn_hel1, qn_hel2, qn_photon, qn1, qn2
        type(quantum_numbers_t), dimension(6) :: qn
        type(polarization_iterator_t) :: it_hel1, it_hel2
        hel_lock = 0
        mask_h = .false.
        select type (data)
        type is (circe1_data_t)
            mi2 = data%m_in**2
            if (data%with_radiation) then
                if (data%photon(1)) then
                    hel_lock(1) = 3; hel_lock(3) = 1; mask_h(5) = .true.
                    mr2(1) = mi2(1)
                    mo2(1) = 0._default
                else
                    hel_lock(1) = 5; hel_lock(5) = 1; mask_h(3) = .true.
                    mr2(1) = 0._default
                    mo2(1) = mi2(1)
                end if
            if (data%photon(2)) then
                hel_lock(2) = 4; hel_lock(4) = 2; mask_h(6) = .true.
                mr2(2) = mi2(2)
                mo2(2) = 0._default
            else
                hel_lock(2) = 6; hel_lock(6) = 2; mask_h(4) = .true.
                mr2(2) = 0._default
                mo2(2) = mi2(2)
            end if
        end type
    end subroutine

```

```

end if
mask = quantum_numbers_mask (.false., .false., mask_h)
call sf_int%base_init (mask, mi2, mr2, mo2, &
    hel_lock = hel_lock)
sf_int%data => data
call flv_photon%init (PHOTON, data%model)
call col0%init ()
call qn_photon%init (flv_photon, col0)
call pol1%init_generic (data%flv_in(1))
call qn_fc1(1)%init (flv = data%flv_in(1), col = col0)
call pol2%init_generic (data%flv_in(2))
call qn_fc2(1)%init (flv = data%flv_in(2), col = col0)
call it_hel1%init (pol1)

do while (it_hel1%is_valid ())
    qn_hel1 = it_hel1%get_quantum_numbers ()
    qn1 = qn_hel1 .merge. qn_fc1(1)
    qn(1) = qn1
    if (data%photon(1)) then
        qn(3) = qn1; qn(5) = qn_photon
    else
        qn(3) = qn_photon; qn(5) = qn1
    end if
    call it_hel2%init (pol2)
    do while (it_hel2%is_valid ())
        qn_hel2 = it_hel2%get_quantum_numbers ()
        qn2 = qn_hel2 .merge. qn_fc2(1)
        qn(2) = qn2
        if (data%photon(2)) then
            qn(4) = qn2; qn(6) = qn_photon
        else
            qn(4) = qn_photon; qn(6) = qn2
        end if
        call qn(3:4)%tag_radiated ()
        call sf_int%add_state (qn)
        call it_hel2%advance ()
    end do
    call it_hel1%advance ()
end do
!
!
call pol1%final ()
call pol2%final ()
call sf_int%freeze ()
call sf_int%set_incoming ([1,2])
call sf_int%set_radiated ([3,4])
call sf_int%set_outgoing ([5,6])
else
    if (data%photon(1)) then
        mask_h(3) = .true.
        mo2(1) = 0._default
    else
        hel_lock(1) = 3; hel_lock(3) = 1
        mo2(1) = mi2(1)
    end if
    if (data%photon(2)) then

```



```

        mask_h(4) = .true.
        mo2(2) = 0._default
    else
        hel_lock(2) = 4; hel_lock(4) = 2
        mo2(2) = mi2(2)
    end if
    mask = quantum_numbers_mask (.false., .false., mask_h)
    call sf_int%base_init (mask(1:4), mi2, [real(default) :: ], mo2, &
        hel_lock = hel_lock(1:4))
    sf_int%data => data
    call flv_photon%init (PHOTON, data%model)
    call col0%init ()
    call qn_photon%init (flv_photon, col0)
    call pol1%init_generic (data%flv_in(1))
    call qn_fc1(1)%init (flv = data%flv_in(1), col = col0)
    call pol2%init_generic (data%flv_in(2))
    call qn_fc2(1)%init (flv = data%flv_in(2), col = col0)
    call it_hel1%init (pol1)

    do while (it_hel1%is_valid ())
        qn_hel1 = it_hel1%get_quantum_numbers ()
        qn1 = qn_hel1 .merge. qn_fc1(1)
        qn(1) = qn1
        if (data%photon(1)) then
            qn(3) = qn_photon
        else
            qn(3) = qn1
        end if
        call it_hel2%init (pol2)
        do while (it_hel2%is_valid ())
            qn_hel2 = it_hel2%get_quantum_numbers ()
            qn2 = qn_hel2 .merge. qn_fc2(1)
            qn(2) = qn2
            if (data%photon(2)) then
                qn(4) = qn_photon
            else
                qn(4) = qn2
            end if
            call sf_int%add_state (qn(1:4))
            call it_hel2%advance ()
        end do
        call it_hel1%advance ()
    end do
!       call pol1%final ()
!       call pol2%final ()
    call sf_int%freeze ()
    call sf_int%set_incoming ([1,2])
    call sf_int%set_outgoing ([3,4])
end if
sf_int%status = SF_INITIAL
end select
if (sf_int%data%generate) then
    call sf_int%data%rng_factory%make (sf_int%rng_obj%rng)
end if

```

```
end subroutine circe1_init
```

16.12.5 Kinematics

Refer to the data component.

```
<SF circe1: circe1: TBP>+≡
  procedure :: is_generator => circe1_is_generator

<SF circe1: sub interfaces>+≡
  module function circe1_is_generator (sf_int) result (flag)
    class(circe1_t), intent(in) :: sf_int
    logical :: flag
  end function circe1_is_generator

<SF circe1: procedures>+≡
  module function circe1_is_generator (sf_int) result (flag)
    class(circe1_t), intent(in) :: sf_int
    logical :: flag
    flag = sf_int%data%is_generator ()
  end function circe1_is_generator
```

Generate free parameters, if generator mode is on. Otherwise, the parameters will be discarded.

```
<SF circe1: circe1: TBP>+≡
  procedure :: generate_free => circe1_generate_free

<SF circe1: sub interfaces>+≡
  module subroutine circe1_generate_free (sf_int, r, rb, x_free)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free
  end subroutine circe1_generate_free

<SF circe1: procedures>+≡
  module subroutine circe1_generate_free (sf_int, r, rb, x_free)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free

    if (sf_int%data%generate) then
      call circe_generate (r, sf_int%data%get_pdg_int (), sf_int%rng_obj)
      rb = 1 - r
      x_free = x_free * product (r)
    else
      r = 0
      rb = 1
    end if
  end subroutine circe1_generate_free
```

Generator mode: depending on the particle codes, call one of the available `girce` generators. Illegal particle code combinations should have been caught during data initialization.

```
<SF circe1: procedures>+≡
```

```

subroutine circe_generate (x, pdg, rng_obj)
  real(default), dimension(2), intent(out) :: x
  integer, dimension(2), intent(in) :: pdg
  class(rng_obj_t), intent(inout) :: rng_obj
  real(double) :: xc1, xc2
  select case (abs (pdg(1)))
  case (ELECTRON)
    select case (abs (pdg(2)))
    case (ELECTRON)
      call gircee (xc1, xc2, rng_obj = rng_obj)
    case (PHOTON)
      call girceg (xc1, xc2, rng_obj = rng_obj)
    end select
  case (PHOTON)
    select case (abs (pdg(2)))
    case (ELECTRON)
      call girceg (xc2, xc1, rng_obj = rng_obj)
    case (PHOTON)
      call gircgg (xc1, xc2, rng_obj = rng_obj)
    end select
  end select
  x = [xc1, xc2]
end subroutine circe_generate

```

Set kinematics. The r values (either from integration or from the generator call above) are copied to x unchanged, and f is unity. We store the x values, so we can use them for the evaluation later.

```

<SF circe1: circe1: TBP>+≡
  procedure :: complete_kinematics => circe1_complete_kinematics

<SF circe1: sub interfaces>+≡
  module subroutine circe1_complete_kinematics &
    (sf_int, x, xb, f, r, rb, map)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
  end subroutine circe1_complete_kinematics

<SF circe1: procedures>+≡
  module subroutine circe1_complete_kinematics &
    (sf_int, x, xb, f, r, rb, map)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    x = r
    xb = rb
    sf_int%x = x

```

```

sf_int%xb= xb
f = 1
if (sf_int%data%with_radiation) then
  call sf_int%split_momenta (x, xb)
else
  call sf_int%reduce_momenta (x)
end if
select case (sf_int%status)
case (SF_FAILED_KINEMATICS); f = 0
end select
end subroutine circe1_complete_kinematics

```

Compute inverse kinematics. In generator mode, the r values are meaningless, but we copy them anyway.

```

<SF circe1: circe1: TBP>+≡
  procedure :: inverse_kinematics => circe1_inverse_kinematics
<SF circe1: sub interfaces>+≡
  module subroutine circe1_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine circe1_inverse_kinematics
<SF circe1: procedures>+≡
  module subroutine circe1_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    r = x
    rb = xb
    sf_int%x = x
    sf_int%xb= xb
    f = 1
    if (set_mom) then
      call sf_int%split_momenta (x, xb)
      select case (sf_int%status)
      case (SF_FAILED_KINEMATICS); f = 0
      end select
    end if
  end subroutine circe1_inverse_kinematics

```

16.12.6 CIRCE1 application

CIRCE is applied for the two beams at once. We can safely assume that no structure functions are applied before this, so the incoming particles are on-shell electrons/positrons.

The scale is ignored.

```
<SF circe1: circe1: TBP>+≡
  procedure :: apply => circe1_apply

<SF circe1: sub interfaces>+≡
  module subroutine circe1_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(circe1_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine circe1_apply

<SF circe1: procedures>+≡
  module subroutine circe1_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(circe1_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default), dimension(2) :: xb
    real(double), dimension(2) :: xc
    real(double), parameter :: one = 1
    associate (data => sf_int%data)
      xc = sf_int%x
      xb = sf_int%xb
      if (data%generate) then
        sf_int%f = 1
      else
        sf_int%f = 0
        if (all (sf_int%continuum)) then
          sf_int%f = circe (xc(1), xc(2), data%pdg_in(1), data%pdg_in(2))
        end if
        if (sf_int%continuum(2) .and. sf_int%peak(1)) then
          sf_int%f = sf_int%f &
            + circe (one, xc(2), data%pdg_in(1), data%pdg_in(2)) &
            * peak (xb(1), data%eps)
        end if
        if (sf_int%continuum(1) .and. sf_int%peak(2)) then
          sf_int%f = sf_int%f &
            + circe (xc(1), one, data%pdg_in(1), data%pdg_in(2)) &
            * peak (xb(2), data%eps)
        end if
        if (all (sf_int%peak)) then
          sf_int%f = sf_int%f &
            + circe (one, one, data%pdg_in(1), data%pdg_in(2)) &
            * peak (xb(1), data%eps) * peak (xb(2), data%eps)
        end if
      end associate
    end module
```

```

        end if
    end if
    end associate
    call sf_int%set_matrix_element (cmplx (sf_int%f, kind=default))
    sf_int%status = SF_EVALUATED
end subroutine circe1_apply

```

This is a smeared delta peak at zero, as an endpoint singularity. We choose an exponentially decreasing function, starting at zero, with integral (from 0 to 1) $1 - e^{-1/\epsilon}$. For small ϵ , this reduces to one.

```

⟨SF circe1: procedures⟩+=
function peak (x, eps) result (f)
    real(default), intent(in) :: x, eps
    real(default) :: f
    f = exp (-x / eps) / eps
end function peak

```

16.12.7 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_circe1_ut.f90⟩≡
    ⟨File header⟩

    module sf_circe1_ut
        use unit_tests
        use sf_circe1_utl

    ⟨Standard module head⟩

    ⟨SF circe1: public test⟩

    contains

    ⟨SF circe1: test driver⟩

    end module sf_circe1_ut

⟨sf_circe1_uti.f90⟩≡
    ⟨File header⟩

    module sf_circe1_uti

    ⟨Use kinds⟩
        use physics_defs, only: ELECTRON
        use lorentz
        use pdg_arrays
        use flavors
        use interactions, only: reset_interaction_counter
        use model_data
        use rng_base
        use sf_aux
        use sf_base

```

```

use sf_circe1

use rng_base_ut, only: rng_test_factory_t

<Standard module head>

<SF circe1: test declarations>

contains

<SF circe1: tests>

end module sf_circe1_utl
API: driver for the unit tests below.
<SF circe1: public test>≡
public :: sf_circe1_test
<SF circe1: test driver>≡
subroutine sf_circe1_test (u, results)
integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
<SF circe1: execute tests>
end subroutine sf_circe1_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF circe1: execute tests>≡
call test (sf_circe1_1, "sf_circe1_1", &
"structure function configuration", &
u, results)
<SF circe1: test declarations>≡
public :: sf_circe1_1
<SF circe1: tests>≡
subroutine sf_circe1_1 (u)
integer, intent(in) :: u
type(model_data_t), target :: model
type(pdg_array_t), dimension(2) :: pdg_in
type(pdg_array_t), dimension(2) :: pdg_out
integer, dimension(:), allocatable :: pdg1, pdg2
class(sf_data_t), allocatable :: data

write (u, "(A)")  "* Test output: sf_circe1_1"
write (u, "(A)")  "* Purpose: initialize and display &
&CIRCE structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_qed_test ()

```

```

pdg_in(1) = ELECTRON
pdg_in(2) = -ELECTRON

allocate (circe1_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

select type (data)
type is (circe1_data_t)
  call data%init (model, pdg_in, &
    sqrts = 500._default, &
    eps = 1e-6_default, &
    out_photon = [.false., .false.], &
    ver = 0, &
    rev = 0, &
    acc = "SBAND", &
    chat = 0, &
    with_radiation = .true.)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))") pdg1, pdg2

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_1"

end subroutine sf_circe1_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```

<SF circe1: execute tests>+≡
  call test (sf_circe1_2, "sf_circe1_2", &
    "structure function instance", &
    u, results)

<SF circe1: test declarations>+≡
  public :: sf_circe1_2

<SF circe1: tests>+≡

```



```

subroutine sf_circe1_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t), dimension(2) :: flv
  type(pdg_array_t), dimension(2) :: pdg_in
  class(sf_data_t), allocatable, target :: data
  class(sf_int_t), allocatable :: sf_int
  type(vector4_t) :: k1, k2
  type(vector4_t), dimension(4) :: q
  real(default) :: E
  real(default), dimension(:), allocatable :: r, rb, x, xb
  real(default) :: f

  write (u, "(A)")  "* Test output: sf_circe1_2"
  write (u, "(A)")  "* Purpose: initialize and fill &
    &circe1 structure function object"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize configuration data"
  write (u, "(A)")

  call model%init_qed_test ()
  call flv(1)%init (ELECTRON, model)
  call flv(2)%init (-ELECTRON, model)
  pdg_in(1) = ELECTRON
  pdg_in(2) = -ELECTRON

  call reset_interaction_counter ()

  allocate (circe1_data_t :: data)
  select type (data)
  type is (circe1_data_t)
    call data%init (model, pdg_in, &
      sqrts = 500._default, &
      eps = 1e-6_default, &
      out_photon = [.false., .false.], &
      ver = 0, &
      rev = 0, &
      acc = "SBAND", &
      chat = 0, &
      with_radiation = .true.)
  end select

  write (u, "(A)")  "* Initialize structure-function object"
  write (u, "(A)")

  call data%allocate_sf_int (sf_int)
  call sf_int%init (data)
  call sf_int%set_beam_index ([1,2])

  call sf_int%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize incoming momentum with E=500"

```

```

write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E,-sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.95,0.85."
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.9_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1, 2])

call sf_int%seed_kinematics ([k1, k2])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 0._default)
call sf_int%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_2"

end subroutine sf_circe1_2

```

Generator mode

Construct and evaluate a structure function object in generator mode.

```

<SF circe1: execute tests>+≡
  call test (sf_circe1_3, "sf_circe1_3", &
    "generator mode", &
    u, results)

<SF circe1: test declarations>+≡
  public :: sf_circe1_3

<SF circe1: tests>+≡
  subroutine sf_circe1_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe1_3"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe1 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv(1)%init (ELECTRON, model)
    call flv(2)%init (-ELECTRON, model)
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    call reset_interaction_counter ()

    allocate (circe1_data_t :: data)
    allocate (rng_test_factory_t :: rng_factory)

```

```

select type (data)
type is (circe1_data_t)
    call data%init (model, pdg_in, &
        sqrts = 500._default, &
        eps = 1e-6_default, &
        out_photon = [.false., .false.], &
        ver = 0, &
        rev = 0, &
        acc = "SBAND", &
        chat = 0, &
        with_radiation = .true.)
    call data%set_generator_mode (rng_factory)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe1_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

```

```

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_3"

end subroutine sf_circe1_3

```

16.13 Lepton Collider Beamstrahlung and Photon collider: CIRCE2

```
<sf_circe2.f90>≡
  <File header>

  module sf_circe2

    <Use kinds>
    <Use strings>
    use os_interface
    use rng_base
    use selectors
    use pdg_arrays
    use model_data
    use flavors
    use polarizations
    use sf_base
    use circe2, circe2_rng_t => rng_type !NODEP!

    <Standard module head>

    <SF circe2: public>

    <SF circe2: types>

    interface
    <SF circe2: sub interfaces>
    end interface

    contains

    <SF circe2: main procedures>

  end module sf_circe2

<sf_circe2_sub.f90>≡
  <File header>

  submodule (sf_circe2) sf_circe2_s

    use io_units
    use format_defs, only: FMT_19
    use numeric_utils
    use diagnostics
    use physics_defs, only: PHOTON, ELECTRON, MUON
    use lorentz
    use colors
    use helicities
    use quantum_numbers
    use state_matrices

    implicit none
```

```
contains

<SF circe2: procedures>

end submodule sf_circe2_s
```

16.13.1 Physics

CIRCE2 describes photon spectra Beamstrahlung is applied before ISR. The CIRCE2 implementation has a single structure function for both beams (which makes sense since it has to be switched on or off for both beams simultaneously).

16.13.2 The CIRCE2 data block

The CIRCE2 parameters are: file and collider specification, incoming (= outgoing) particles. The luminosity is returned by `circe2_luminosity`.

```
<SF circe2: public>≡
  public :: circe2_data_t

<SF circe2: types>≡
  type, extends (sf_data_t) :: circe2_data_t
  private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(2) :: flv_in
    integer, dimension(2) :: pdg_in
    real(default) :: sqrts = 0
    logical :: polarized = .false.
    logical :: beams_polarized = .false.
    class(rng_factory_t), allocatable :: rng_factory
    type(string_t) :: filename
    type(string_t) :: file
    type(string_t) :: design
    real(default) :: lumi = 0
    real(default), dimension(4) :: lumi_hel_frac = 0
    integer, dimension(0:4) :: h1 = [0, -1, -1, 1, 1]
    integer, dimension(0:4) :: h2 = [0, -1, 1, -1, 1]
    integer :: error = 1
  contains
    <SF circe2: circe2 data: TBP>
  end type circe2_data_t

<SF circe2: types>+≡
  type(circe2_state) :: circe2_global_state

<SF circe2: circe2 data: TBP>≡
  procedure :: init => circe2_data_init

<SF circe2: sub interfaces>≡
  module subroutine circe2_data_init (data, os_data, model, pdg_in, &
    sqrts, polarized, beam_pol, file, design)
    class(circe2_data_t), intent(out) :: data
    type(os_data_t), intent(in) :: os_data
```

```

        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), dimension(2), intent(in) :: pdg_in
        real(default), intent(in) :: sqrts
        logical, intent(in) :: polarized, beam_pol
        type(string_t), intent(in) :: file, design
    end subroutine circe2_data_init
<SF circe2: procedures>≡
    module subroutine circe2_data_init (data, os_data, model, pdg_in, &
        sqrts, polarized, beam_pol, file, design)
        class(circe2_data_t), intent(out) :: data
        type(os_data_t), intent(in) :: os_data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), dimension(2), intent(in) :: pdg_in
        real(default), intent(in) :: sqrts
        logical, intent(in) :: polarized, beam_pol
        type(string_t), intent(in) :: file, design
        integer :: h
        data%model => model
        if (any (pdg_in%get_length () /= 1)) then
            call msg_fatal ("CIRCE2: incoming beam particles must be unique")
        end if
        call data%flv_in(1)%init (pdg_in(1)%get (1), model)
        call data%flv_in(2)%init (pdg_in(2)%get (1), model)
        data%pdg_in = data%flv_in%get_pdg ()
        data%sqrts = sqrts
        data%polarized = polarized
        data%beams_polarized = beam_pol
        data%filename = file
        data%design = design
        call data%check_file (os_data)
        call circe2_load (circe2_global_state, trim (char(data%file)), &
            trim (char(data%design)), data%sqrts, data%error)
        call data%check ()
        data%lumi = circe2_luminosity (circe2_global_state, data%pdg_in, [0, 0])
        if (vanishes (data%lumi)) then
            call msg_fatal ("CIRCE2: luminosity vanishes for specified beams.")
        end if
        if (data%polarized) then
            do h = 1, 4
                data%lumi_hel_frac(h) = &
                    circe2_luminosity (circe2_global_state, data%pdg_in, &
                        [data%h1(h), data%h2(h)]) &
                    / data%lumi
            end do
        end if
    end subroutine circe2_data_init

```

Activate the generator mode. We import a RNG factory into the data type, which can then spawn RNG generator objects.

```

<SF circe2: circe2 data: TBP>+≡
    procedure :: set_generator_mode => circe2_data_set_generator_mode
<SF circe2: sub interfaces>+≡
    module subroutine circe2_data_set_generator_mode (data, rng_factory)

```



```

        class(circe2_data_t), intent(inout) :: data
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
    end subroutine circe2_data_set_generator_mode

<SF circe2: procedures>+≡
    module subroutine circe2_data_set_generator_mode (data, rng_factory)
        class(circe2_data_t), intent(inout) :: data
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
        call move_alloc (from = rng_factory, to = data%rng_factory)
    end subroutine circe2_data_set_generator_mode

```

Check whether the requested data file is in the system directory or in the current directory.

```

<SF circe2: circe2 data: TBP>+≡
    procedure :: check_file => circe2_check_file

<SF circe2: sub interfaces>+≡
    module subroutine circe2_check_file (data, os_data)
        class(circe2_data_t), intent(inout) :: data
        type(os_data_t), intent(in) :: os_data
    end subroutine circe2_check_file

<SF circe2: procedures>+≡
    module subroutine circe2_check_file (data, os_data)
        class(circe2_data_t), intent(inout) :: data
        type(os_data_t), intent(in) :: os_data
        logical :: exist
        type(string_t) :: file
        file = data%filename
        if (file == "") &
            call msg_fatal ("CIRCE2: $circe2_file is not set")
        inquire (file = char (file), exist = exist)
        if (exist) then
            data%file = file
        else
            file = os_data%whizard_circe2path // "/" // data%filename
            inquire (file = char (file), exist = exist)
            if (exist) then
                data%file = file
            else
                call msg_fatal ("CIRCE2: data file '" // char (data%filename) &
                    // "' not found")
            end if
        end if
    end subroutine circe2_check_file

```

Handle error conditions.

```

<SF circe2: circe2 data: TBP>+≡
    procedure :: check => circe2_data_check

<SF circe2: sub interfaces>+≡
    module subroutine circe2_data_check (data)
        class(circe2_data_t), intent(in) :: data
    end subroutine circe2_data_check

```

```

<SF circe2: procedures>+≡
module subroutine circe2_data_check (data)
  class(circe2_data_t), intent(in) :: data
  type(flavor_t) :: flv_photon, flv_electron, flv_muon
  call flv_photon%init (PHOTON, data%model)
  if (.not. flv_photon%is_defined ()) then
    call msg_fatal ("CIRCE2: model must contain photon")
  end if
  if (any (abs (data%pdg_in) /= PHOTON .and. abs (data%pdg_in) /= &
    ELECTRON .and. abs (data%pdg_in) /= MUON)) then
    call msg_fatal ("CIRCE2: applicable only for e+e-, mu+mu- or " // &
      "photon collisions")
  end if
  if (any (abs (data%pdg_in) == ELECTRON)) then
    call flv_electron%init (ELECTRON, data%model)
    if (.not. flv_electron%is_defined ()) then
      call msg_fatal ("CIRCE2: model must contain electron")
    end if
  end if
  if (any (abs (data%pdg_in) == MUON)) then
    call flv_muon%init (MUON, data%model)
    if (.not. flv_muon%is_defined ()) then
      call msg_fatal ("CIRCE2: model must contain muon")
    end if
  end if
  select case (data%error)
  case (-1)
    call msg_fatal ("CIRCE2: data file not found.")
  case (-2)
    call msg_fatal ("CIRCE2: beam setup does not match data file.")
  case (-3)
    call msg_fatal ("CIRCE2: invalid format of data file.")
  case (-4)
    call msg_fatal ("CIRCE2: data file too large.")
  end select
end subroutine circe2_data_check

```

Output

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: write => circe2_data_write

<SF circe2: sub interfaces>+≡
  module subroutine circe2_data_write (data, unit, verbose)
    class(circe2_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine circe2_data_write

<SF circe2: procedures>+≡
module subroutine circe2_data_write (data, unit, verbose)
  class(circe2_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: u, h
  logical :: verb

```

```

verb = .false.; if (present (verbose)) verb = verbose
u = given_output_unit (unit)
write (u, "(1x,A)") "CIRCE2 data:"
write (u, "(3x,A,A)")      "file   = ", char(data%filename)
write (u, "(3x,A,A)")      "design  = ", char(data%design)
write (u, "(3x,A," // FMT_19 // ")") "sqrts = ", data%sqrts
write (u, "(3x,A,A,A,A)")    "prt_in = ", &
    char (data%flv_in(1)%get_name ()), &
    ", ", char (data%flv_in(2)%get_name ())
write (u, "(3x,A,L1)")      "polarized = ", data%polarized
write (u, "(3x,A,L1)")      "beams pol. = ", data%beams_polarized
write (u, "(3x,A," // FMT_19 // ")") "luminosity = ", data%lumi
if (data%polarized) then
    do h = 1, 4
        write (u, "(6x,'(,I2,1x,I2,')',1x,'=',1x)", advance="no") &
            data%h1(h), data%h2(h)
        write (u, "(6x," // FMT_19 // ")") data%lumi_hel_frac(h)
    end do
end if
if (verb) then
    call data%rng_factory%write (u)
end if
end subroutine circe2_data_write

```

This is always in generator mode.

```

<SF circe2: circe2 data: TBP>+≡
    procedure :: is_generator => circe2_data_is_generator

<SF circe2: sub interfaces>+≡
    module function circe2_data_is_generator (data) result (flag)
        class(circe2_data_t), intent(in) :: data
        logical :: flag
    end function circe2_data_is_generator

<SF circe2: procedures>+≡
    module function circe2_data_is_generator (data) result (flag)
        class(circe2_data_t), intent(in) :: data
        logical :: flag
        flag = .true.
    end function circe2_data_is_generator

```

The number of parameters is two, collinear splitting for the two beams.

```

<SF circe2: circe2 data: TBP>+≡
    procedure :: get_n_par => circe2_data_get_n_par

<SF circe2: sub interfaces>+≡
    module function circe2_data_get_n_par (data) result (n)
        class(circe2_data_t), intent(in) :: data
        integer :: n
    end function circe2_data_get_n_par

<SF circe2: procedures>+≡
    module function circe2_data_get_n_par (data) result (n)
        class(circe2_data_t), intent(in) :: data
        integer :: n
    end function circe2_data_get_n_par

```

```

      n = 2
    end function circe2_data_get_n_par

```

Return the outgoing particles PDG codes. They are equal to the incoming ones.

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: get_pdg_out => circe2_data_get_pdg_out

<SF circe2: sub interfaces>+≡
  module subroutine circe2_data_get_pdg_out (data, pdg_out)
    class(circe2_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  end subroutine circe2_data_get_pdg_out

<SF circe2: procedures>+≡
  module subroutine circe2_data_get_pdg_out (data, pdg_out)
    class(circe2_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      pdg_out(i) = data%pdg_in(i)
    end do
  end subroutine circe2_data_get_pdg_out

```

Allocate the interaction record. Due to gfortran 7/8/9 bug has to remain in the main module.

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: allocate_sf_int => circe2_data_allocate_sf_int

<SF circe2: main procedures>≡
  subroutine circe2_data_allocate_sf_int (data, sf_int)
    class(circe2_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (circe2_t :: sf_int)
  end subroutine circe2_data_allocate_sf_int

```

Return the beam file.

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: get_beam_file => circe2_data_get_beam_file

<SF circe2: sub interfaces>+≡
  module function circe2_data_get_beam_file (data) result (file)
    class(circe2_data_t), intent(in) :: data
    type(string_t) :: file
  end function circe2_data_get_beam_file

<SF circe2: procedures>+≡
  module function circe2_data_get_beam_file (data) result (file)
    class(circe2_data_t), intent(in) :: data
    type(string_t) :: file
    file = "CIRCE2: " // data%filename
  end function circe2_data_get_beam_file

```

16.13.3 Random Number Generator for CIRCE

The CIRCE implementation now supports a generic random-number generator object that allows for a local state as a component. To support this, we must extend the abstract type provided by CIRCE and delegate the generator call to the (also abstract) RNG used by WHIZARD.

```
<SF circe2: types>+≡
  type, extends (circe2_rng_t) :: rng_obj_t
    class(rng_t), allocatable :: rng
  contains
    procedure :: generate => rng_obj_generate
  end type rng_obj_t

<SF circe2: sub interfaces>+≡
  module subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(default), intent(out) :: u
  end subroutine rng_obj_generate

<SF circe2: procedures>+≡
  module subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(default), intent(out) :: u
    real(default) :: x
    call rng_obj%rng%generate (x)
    u = x
  end subroutine rng_obj_generate
```

16.13.4 The CIRCE2 object

For CIRCE2 spectra it does not make sense to describe the state matrix as a radiation interaction, even if photons originate from laser backscattering. Instead, it is a $2 \rightarrow 2$ interaction where the incoming particles are identical to the outgoing ones.

The current implementation of CIRCE2 does support polarization and classical correlations, but no entanglement, so the density matrix of the outgoing particles is diagonal. The incoming particles are unpolarized (user-defined polarization for beams is meaningless, since polarization is described by the data file). The outgoing particles are polarized or polarization-averaged, depending on user request.

When assigning matrix elements, we scan the previously initialized state matrix. For each entry, we extract helicity and call the structure function. In the unpolarized case, the helicity is undefined and replaced by value zero. In the polarized case, there are four entries. If the generator is used, only one entry is nonzero in each call. Which one, is determined by comparing with a previously (randomly, distributed by relative luminosity) selected pair of helicities.

```
<SF circe2: public>+≡
  public :: circe2_t
```

```

<SF circe2: types>+≡
  type, extends (sf_int_t) :: circe2_t
    type(circe2_data_t), pointer :: data => null ()
    type(rng_obj_t) :: rng_obj
    type(selector_t) :: selector
    integer :: h_sel = 0
  contains
    <SF circe2: circe2: TBP>
  end type circe2_t

```

Type string: show file and design of CIRCE2 structure function.

```

<SF circe2: circe2: TBP>≡
  procedure :: type_string => circe2_type_string

<SF circe2: sub interfaces>+≡
  module function circe2_type_string (object) result (string)
    class(circe2_t), intent(in) :: object
    type(string_t) :: string
  end function circe2_type_string

<SF circe2: procedures>+≡
  module function circe2_type_string (object) result (string)
    class(circe2_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "CIRCE2: " // object%data%design
    else
      string = "CIRCE2: [undefined]"
    end if
  end function circe2_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF circe2: circe2: TBP>+≡
  procedure :: write => circe2_write

<SF circe2: sub interfaces>+≡
  module subroutine circe2_write (object, unit, testflag)
    class(circe2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine circe2_write

<SF circe2: procedures>+≡
  module subroutine circe2_write (object, unit, testflag)
    class(circe2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "CIRCE2 data: [undefined]"
    end if
  end subroutine circe2_write

```

```

end subroutine circe2_write

<SF circe2: circe2: TBP>+≡
  procedure :: init => circe2_init

<SF circe2: sub interfaces>+≡
  module subroutine circe2_init (sf_int, data)
    class(circe2_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
  end subroutine circe2_init

<SF circe2: procedures>+≡
  module subroutine circe2_init (sf_int, data)
    class(circe2_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    logical, dimension(4) :: mask_h
    real(default), dimension(2) :: m2_array
    real(default), dimension(0) :: null_array
    type(quantum_numbers_mask_t), dimension(4) :: mask
    type(quantum_numbers_t), dimension(4) :: qn
    type(helicity_t) :: hel
    type(color_t) :: col0
    integer :: h
    select type (data)
    type is (circe2_data_t)
      if (data%polarized .and. data%beams_polarized) then
        call msg_fatal ("CIRCE2: Beam polarization can't be set &
          &for polarized data file")
      else if (data%beams_polarized) then
        call msg_warning ("CIRCE2: User-defined beam polarization set &
          &for unpolarized CIRCE2 data file")
      end if
      mask_h(1:2) = .not. data%beams_polarized
      mask_h(3:4) = .not. (data%polarized .or. data%beams_polarized)
      mask = quantum_numbers_mask (.false., .false., mask_h)
      m2_array(:) = (data%flv_in(:)%get_mass ())**2
      call sf_int%base_init (mask, m2_array, null_array, m2_array)
      sf_int%data => data
      if (data%polarized) then
        if (vanishes (sum (data%lumi_hel_frac)) .or. &
          any (data%lumi_hel_frac < 0)) then
          call msg_fatal ("CIRCE2: Helicity-dependent lumi " &
            // "fractions all vanish or", &
            [var_str ("are negative: Please inspect the " &
              // "CIRCE2 file or "), &
              var_str ("switch off the polarized" // &
                " option for CIRCE2.")])
        else
          call sf_int%selector%init (data%lumi_hel_frac)
        end if
      end if
      call col0%init ()
      if (data%beams_polarized) then
        do h = 1, 4
          call hel%init (data%h1(h))
        end do
      end if
    end type
  end module

```

```

        call qn(1)%init &
            (flv = data%flv_in(1), col = col0, hel = hel)
        call qn(3)%init &
            (flv = data%flv_in(1), col = col0, hel = hel)
        call hel%init (data%h2(h))
        call qn(2)%init &
            (flv = data%flv_in(2), col = col0, hel = hel)
        call qn(4)%init &
            (flv = data%flv_in(2), col = col0, hel = hel)
        call sf_int%add_state (qn)
    end do
else if (data%polarized) then
    call qn(1)%init (flv = data%flv_in(1), col = col0)
    call qn(2)%init (flv = data%flv_in(2), col = col0)
    do h = 1, 4
        call hel%init (data%h1(h))
        call qn(3)%init &
            (flv = data%flv_in(1), col = col0, hel = hel)
        call hel%init (data%h2(h))
        call qn(4)%init &
            (flv = data%flv_in(2), col = col0, hel = hel)
        call sf_int%add_state (qn)
    end do
else
    call qn(1)%init (flv = data%flv_in(1), col = col0)
    call qn(2)%init (flv = data%flv_in(2), col = col0)
    call qn(3)%init (flv = data%flv_in(1), col = col0)
    call qn(4)%init (flv = data%flv_in(2), col = col0)
    call sf_int%add_state (qn)
end if
call sf_int%freeze ()
call sf_int%set_incoming ([1,2])
call sf_int%set_outgoing ([3,4])
call sf_int%data%rng_factory%make (sf_int%rng_obj%rng)
sf_int%status = SF_INITIAL
end select
end subroutine circe2_init

```

16.13.5 Kinematics

Refer to the data component.

```

<SF circe2: circe2: TBP>+≡
    procedure :: is_generator => circe2_is_generator

<SF circe2: sub interfaces>+≡
    module function circe2_is_generator (sf_int) result (flag)
        class(circe2_t), intent(in) :: sf_int
        logical :: flag
    end function circe2_is_generator

<SF circe2: procedures>+≡
    module function circe2_is_generator (sf_int) result (flag)
        class(circe2_t), intent(in) :: sf_int

```



```

logical :: flag
flag = sf_int%data%is_generator ()
end function circe2_is_generator

```

Generate free parameters. We first select a helicity, which we have to store, then generate x values for that helicity.

```

<SF circe2: circe2: TBP>+≡
  procedure :: generate_free => circe2_generate_whizard_free

<SF circe2: sub interfaces>+≡
  module subroutine circe2_generate_whizard_free (sf_int, r, rb, x_free)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free
  end subroutine circe2_generate_whizard_free

<SF circe2: procedures>+≡
  module subroutine circe2_generate_whizard_free (sf_int, r, rb, x_free)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free
    integer :: h_sel
    if (sf_int%data%polarized) then
      call sf_int%selector%generate (sf_int%rng_obj%rng, h_sel)
    else
      h_sel = 0
    end if
    sf_int%h_sel = h_sel
    call circe2_generate_whizard (r, sf_int%data%pdg_in, &
      [sf_int%data%h1(h_sel), sf_int%data%h2(h_sel)], &
      sf_int%rng_obj)
    rb = 1 - r
    x_free = x_free * product (r)
  end subroutine circe2_generate_whizard_free

```

Generator mode: call the CIRCE2 generator for the given particles and helicities. (For unpolarized generation, helicities are zero.)

```

<SF circe2: sub interfaces>+≡
  module subroutine circe2_generate_whizard (x, pdg, hel, rng_obj)
    real(default), dimension(2), intent(out) :: x
    integer, dimension(2), intent(in) :: pdg
    integer, dimension(2), intent(in) :: hel
    class(rng_obj_t), intent(inout) :: rng_obj
  end subroutine circe2_generate_whizard

<SF circe2: procedures>+≡
  module subroutine circe2_generate_whizard (x, pdg, hel, rng_obj)
    real(default), dimension(2), intent(out) :: x
    integer, dimension(2), intent(in) :: pdg
    integer, dimension(2), intent(in) :: hel
    class(rng_obj_t), intent(inout) :: rng_obj
    call circe2_generate (circe2_global_state, rng_obj, x, pdg, hel)
  end subroutine circe2_generate_whizard

```

Set kinematics. Trivial here.

```

<SF circe2: circe2: TBP>+≡
  procedure :: complete_kinematics => circe2_complete_kinematics

<SF circe2: sub interfaces>+≡
  module subroutine circe2_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
  end subroutine circe2_complete_kinematics

<SF circe2: procedures>+≡
  module subroutine circe2_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    if (map) then
      call msg_fatal ("CIRCE2: map flag not supported")
    else
      x = r
      xb= rb
      f = 1
    end if
    call sf_int%reduce_momenta (x)
  end subroutine circe2_complete_kinematics

```

Compute inverse kinematics.

```

<SF circe2: circe2: TBP>+≡
  procedure :: inverse_kinematics => circe2_inverse_kinematics

<SF circe2: sub interfaces>+≡
  module subroutine circe2_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine circe2_inverse_kinematics

<SF circe2: procedures>+≡
  module subroutine circe2_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(circe2_t), intent(inout) :: sf_int

```

```

real(default), dimension(:), intent(in) :: x
real(default), dimension(:), intent(in) :: xb
real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: r
real(default), dimension(:), intent(out) :: rb
logical, intent(in) :: map
logical, intent(in), optional :: set_momenta
logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
if (map) then
    call msg_fatal ("CIRCE2: map flag not supported")
else
    r = x
    rb= xb
    f = 1
end if
if (set_mom) then
    call sf_int%reduce_momenta (x)
end if
end subroutine circe2_inverse_kinematics

```

16.13.6 CIRCE2 application

This function works on both beams. In polarized mode, we set only the selected helicity. In unpolarized mode, the interaction has only one entry, and the factor is unity.

```

<SF circe2: circe2: TBP>+≡
    procedure :: apply => circe2_apply

<SF circe2: sub interfaces>+≡
    module subroutine circe2_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(circe2_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
    end subroutine circe2_apply

<SF circe2: procedures>+≡
    module subroutine circe2_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(circe2_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
        complex(default) :: f
        associate (data => sf_int%data)
            f = 1
            if (data%beams_polarized) then
                call sf_int%set_matrix_element (f)
            else if (data%polarized) then
                call sf_int%set_matrix_element (sf_int%h_sel, f)
            else

```

```

        call sf_int%set_matrix_element (1, f)
    end if
end associate
sf_int%status = SF_EVALUATED
end subroutine circe2_apply

```

16.13.7 Unit tests

Test module, followed by the corresponding implementation module.

<sf_circe2_ut.f90>≡

<File header>

```

module sf_circe2_ut
  use unit_tests
  use sf_circe2_ut

```

<Standard module head>

<SF circe2: public test>

contains

<SF circe2: test driver>

```

end module sf_circe2_ut

```

<sf_circe2_ut.f90>≡

<File header>

```

module sf_circe2_ut

```

<Use kinds>

<Use strings>

```

  use os_interface
  use physics_defs, only: PHOTON
  use lorentz
  use pdg_arrays
  use flavors
  use interactions, only: reset_interaction_counter
  use model_data
  use rng_base
  use sf_aux
  use sf_base

  use sf_circe2

```

```

  use rng_base_ut, only: rng_test_factory_t

```

<Standard module head>

<SF circe2: test declarations>

contains

<SF circe2: tests>

end module sf_circe2_util

API: driver for the unit tests below.

<SF circe2: public test>≡

public :: sf_circe2_test

<SF circe2: test driver>≡

subroutine sf_circe2_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SF circe2: execute tests>

end subroutine sf_circe2_test

Test structure function data

Construct and display a test structure function data object.

<SF circe2: execute tests>≡

call test (sf_circe2_1, "sf_circe2_1", &
"structure function configuration", &
u, results)

<SF circe2: test declarations>≡

public :: sf_circe2_1

<SF circe2: tests>≡

subroutine sf_circe2_1 (u)

integer, intent(in) :: u

type(os_data_t) :: os_data

type(model_data_t), target :: model

type(pdg_array_t), dimension(2) :: pdg_in

type(pdg_array_t), dimension(2) :: pdg_out

integer, dimension(:), allocatable :: pdg1, pdg2

class(sf_data_t), allocatable :: data

class(rng_factory_t), allocatable :: rng_factory

write (u, "(A)") "*" Test output: sf_circe2_1

write (u, "(A)") "*" Purpose: initialize and display &
&CIRCE structure function data"

write (u, "(A)")

write (u, "(A)") "*" Create empty data object"

write (u, "(A)")

call os_data%init ()

call model%init_qed_test ()

pdg_in(1) = PHOTON

pdg_in(2) = PHOTON

allocate (circe2_data_t :: data)

allocate (rng_test_factory_t :: rng_factory)

write (u, "(A)")

```

write (u, "(A)")  "* Initialize (unpolarized)"
write (u, "(A)")

select type (data)
type is (circe2_data_t)
  call data%init (os_data, model, pdg_in, &
    sqrts = 500._default, &
    polarized = .false., &
    beam_pol = .false., &
    file = var_str ("teslagg_500_polavg.circe"), &
    design = var_str ("TESLA/GG"))
  call data%set_generator_mode (rng_factory)
end select

call data%write (u, verbose = .true.)

write (u, "(A)")

write (u, "(1x,A)")  "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))")  pdg1, pdg2

write (u, "(A)")
write (u, "(A)")  "* Initialize (polarized)"
write (u, "(A)")

allocate (rng_test_factory_t :: rng_factory)

select type (data)
type is (circe2_data_t)
  call data%init (os_data, model, pdg_in, &
    sqrts = 500._default, &
    polarized = .true., &
    beam_pol = .false., &
    file = var_str ("teslagg_500.circe"), &
    design = var_str ("TESLA/GG"))
  call data%set_generator_mode (rng_factory)
end select

call data%write (u, verbose = .true.)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_1"

end subroutine sf_circe2_1

```

Generator mode, unpolarized

Construct and evaluate a structure function object in generator mode.

```

<SF circe2: execute tests>+≡
  call test (sf_circe2_2, "sf_circe2_2", &
    "generator, unpolarized", &
    u, results)

<SF circe2: test declarations>+≡
  public :: sf_circe2_2

<SF circe2: tests>+≡
  subroutine sf_circe2_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe2_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe2 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call os_data%init ()
    call model%init_qed_test ()
    call flv(1)%init (PHOTON, model)
    call flv(2)%init (PHOTON, model)
    pdg_in(1) = PHOTON
    pdg_in(2) = PHOTON

    call reset_interaction_counter ()

    allocate (circe2_data_t :: data)
    allocate (rng_test_factory_t :: rng_factory)
    select type (data)
    type is (circe2_data_t)
      call data%init (os_data, model, pdg_in, &
        sqrts = 500._default, &
        polarized = .false., &
        beam_pol = .false., &
        file = var_str ("teslagg_500_polavg.circe"), &
        design = var_str ("TESLA/GG"))
      call data%set_generator_mode (rng_factory)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

```

```

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe2_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_2"

```



```
end subroutine sf_circe2_2
```

Generator mode, polarized

Construct and evaluate a structure function object in generator mode.

```
<SF circe2: execute tests>+≡
  call test (sf_circe2_3, "sf_circe2_3", &
    "generator, polarized", &
    u, results)

<SF circe2: test declarations>+≡
  public :: sf_circe2_3

<SF circe2: tests>+≡
  subroutine sf_circe2_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe2_3"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe2 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call os_data%init ()
    call model%init_qed_test ()
    call flv(1)%init (PHOTON, model)
    call flv(2)%init (PHOTON, model)
    pdg_in(1) = PHOTON
    pdg_in(2) = PHOTON

    call reset_interaction_counter ()

    allocate (circe2_data_t :: data)
    allocate (rng_test_factory_t :: rng_factory)
    select type (data)
    type is (circe2_data_t)
      call data%init (os_data, model, pdg_in, &
        sqrts = 500._default, &
        polarized = .true., &
        beam_pol = .false., &
        file = var_str ("teslagg_500.circe"), &
```

```

        design = var_str ("TESLA/GG"))
    call data%set_generator_mode (rng_factory)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe2_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```
call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_3"

end subroutine sf_circe2_3
```

16.14 HOPPET interface

Interface to the HOPPET wrapper necessary to perform the LO vs. NLO matching of processes containing an initial b quark.

```
<hoppet_interface.f90>≡  
  <File header>  
  
  module hoppet_interface  
    use lhpdf !NODEP!  
  
    <Standard module head>  
  
    public :: hoppet_init, hoppet_eval  
  
  contains  
  
    subroutine hoppet_init (pdf_builtin, pdf, pdf_id)  
      logical, intent(in) :: pdf_builtin  
      type(lhpdf_pdf_t), intent(inout), optional :: pdf  
      integer, intent(in), optional :: pdf_id  
      external InitForWhizard  
      call InitForWhizard (pdf_builtin, pdf, pdf_id)  
    end subroutine hoppet_init  
  
    subroutine hoppet_eval (x, q, f)  
      double precision, intent(in) :: x, q  
      double precision, intent(out) :: f(-6:6)  
      external EvalForWhizard  
      call EvalForWhizard (x, q, f)  
    end subroutine hoppet_eval  
  
  end module hoppet_interface
```

16.15 Builtin PDF sets

For convenience in order not to depend on the external package LHAPDF, we ship some PDFs with WHIZARD.

16.15.1 The module

```
<sf_pdf_builtin.f90>≡
  <File header>

  module sf_pdf_builtin

    <Use kinds>
    use kinds, only: double
    <Use strings>
    use sm_qcd
    use pdg_arrays
    use model_data
    use flavors
    use polarizations
    use sf_base

    <Standard module head>

    <SF pdf builtin: public>

    <SF pdf builtin: types>

    interface
    <SF pdf builtin: sub interfaces>
    end interface

    contains

    <SF pdf builtin: main procedures>

  end module sf_pdf_builtin

<sf_pdf_builtin_sub.f90>≡
  <File header>

  submodule (sf_pdf_builtin) sf_pdf_builtin_s

    use io_units
    use format_defs, only: FMT_17
    use diagnostics
    use os_interface
    use physics_defs, only: PROTON, PHOTON, GLUON
    use physics_defs, only: HADRON_REMNANT_SINGLET
    use physics_defs, only: HADRON_REMNANT_TRIPLET
    use physics_defs, only: HADRON_REMNANT_OCTET
    use lorentz
    use colors
    use quantum_numbers
```

```

    use state_matrices
    use pdf_builtin !NODEP!
    use hoppet_interface

    implicit none

    <SF pdf builtin: parameters>

    contains

    <SF pdf builtin: procedures>

    end submodule sf_pdf_builtin_s

```

16.15.2 Codes for default PDF sets

```

<SF pdf builtin: parameters>≡
    character(*), parameter :: PDF_BUILTIN_DEFAULT_PROTON = "CTEQ6L"
    ! character(*), parameter :: PDF_BUILTIN_DEFAULT_PION   = "NONE"
    ! character(*), parameter :: PDF_BUILTIN_DEFAULT_PHOTON = "MRST2004QEDp"

```

16.15.3 The PDF builtin data block

The data block holds the incoming flavor (which has to be proton, pion, or photon), the corresponding pointer to the global access data (1, 2, or 3), the flag `invert` which is set for an antiproton, the bounds as returned by LHAPDF for the specified set, and a mask that determines which partons will be actually in use.

```

<SF pdf builtin: public>≡
    public :: pdf_builtin_data_t

<SF pdf builtin: types>≡
    type, extends (sf_data_t) :: pdf_builtin_data_t
    private
    integer :: id = -1
    type (string_t) :: name
    class(model_data_t), pointer :: model => null ()
    type(flavor_t) :: flv_in
    logical :: invert
    logical :: has_photon
    logical :: photon
    logical, dimension(-6:6) :: mask
    logical :: mask_photon
    logical :: hoppet_b_matching = .false.
    contains
    <SF pdf builtin: pdf builtin data: TBP>
    end type pdf_builtin_data_t

```

Generate PDF data and initialize the requested set. Pion and photon PDFs are disabled at the moment until we ship appropriate structure functions. needed.

```

<SF pdf builtin: pdf builtin data: TBP>≡
    procedure :: init => pdf_builtin_data_init

```

<SF pdf builtin: sub interfaces>≡

```

module subroutine pdf_builtin_data_init (data, &
    model, pdg_in, name, path, hoppet_b_matching)
    class(pdf_builtin_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: path
    logical, intent(in), optional :: hoppet_b_matching
end subroutine pdf_builtin_data_init

```

<SF pdf builtin: procedures>≡

```

module subroutine pdf_builtin_data_init (data, &
    model, pdg_in, name, path, hoppet_b_matching)
    class(pdf_builtin_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: path
    logical, intent(in), optional :: hoppet_b_matching
    data%model => model
    if (pdg_in%get_length () /= 1) &
        call msg_fatal ("PDF: incoming particle must be unique")
    call data%flv_in%init (pdg_in%get (1), model)
    data%mask = .true.
    data%mask_photon = .true.
    select case (pdg_in%get (1))
    case (PROTON)
        data%name = var_str (PDF_BUILTIN_DEFAULT_PROTON)
        data%invert = .false.
        data%photon = .false.
    case (-PROTON)
        data%name = var_str (PDF_BUILTIN_DEFAULT_PROTON)
        data%invert = .true.
        data%photon = .false.
        ! case (PIPLUS)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PION)
        !     data%invert = .false.
        !     data%photon = .false.
        ! case (-PIPLUS)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PION)
        !     data%invert = .true.
        !     data%photon = .false.
        ! case (PHOTON)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PHOTON)
        !     data%invert = .false.
        !     data%photon = .true.
    case default
        call msg_fatal ("PDF: " &
            // "incoming particle must either proton or antiproton.")
        return
    end select
    data%name = name
    data%id = pdf_get_id (data%name)
    if (data%id < 0) call msg_fatal ("unknown PDF set " // char (data%name))

```

```

data%has_photon = pdf_provides_photon (data%id)
if (present (hoppet_b_matching)) data%hoppet_b_matching = hoppet_b_matching
call pdf_init (data%id, path)
if (data%hoppet_b_matching) call hoppet_init (.true., pdf_id = data%id)
end subroutine pdf_builtin_data_init

```

Enable/disable partons explicitly. If a mask entry is true, applying the PDF will generate the corresponding flavor on output.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
  procedure :: set_mask => pdf_builtin_data_set_mask

<SF pdf builtin: sub interfaces>+≡
  module subroutine pdf_builtin_data_set_mask (data, mask)
    class(pdf_builtin_data_t), intent(inout) :: data
    logical, dimension(-6:6), intent(in) :: mask
  end subroutine pdf_builtin_data_set_mask

<SF pdf builtin: procedures>+≡
  module subroutine pdf_builtin_data_set_mask (data, mask)
    class(pdf_builtin_data_t), intent(inout) :: data
    logical, dimension(-6:6), intent(in) :: mask
    data%mask = mask
  end subroutine pdf_builtin_data_set_mask

```

Output.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
  procedure :: write => pdf_builtin_data_write

<SF pdf builtin: sub interfaces>+≡
  module subroutine pdf_builtin_data_write (data, unit, verbose)
    class(pdf_builtin_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine pdf_builtin_data_write

<SF pdf builtin: procedures>+≡
  module subroutine pdf_builtin_data_write (data, unit, verbose)
    class(pdf_builtin_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "PDF builtin data:"
    if (data%id < 0) then
      write (u, "(3x,A)") "[undefined]"
      return
    end if
    write (u, "(3x,A)", advance="no") "flavor      = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A,A)") "name          = ", char (data%name)
    write (u, "(3x,A,L1)") "invert       = ", data%invert
    write (u, "(3x,A,L1)") "has photon   = ", data%has_photon
    write (u, "(3x,A,6(1x,L1),1x,A,1x,L1,1x,A,6(1x,L1))") &
      "mask      = ", &
      data%mask(-6:-1), " * ", data%mask(0), " * ", data%mask(1:6)
  end subroutine pdf_builtin_data_write

```



```

        write (u, "(3x,A,L1)") "photon mask = ", data%mask_photon
        write (u, "(3x,A,L1)") "hoppet_b = ", data%hoppet_b_matching
    end subroutine pdf_builtin_data_write

```

The number of parameters is one. We do not generate transverse momentum.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
    procedure :: get_n_par => pdf_builtin_data_get_n_par

<SF pdf builtin: sub interfaces>+≡
    module function pdf_builtin_data_get_n_par (data) result (n)
        class(pdf_builtin_data_t), intent(in) :: data
        integer :: n
    end function pdf_builtin_data_get_n_par

<SF pdf builtin: procedures>+≡
    module function pdf_builtin_data_get_n_par (data) result (n)
        class(pdf_builtin_data_t), intent(in) :: data
        integer :: n
        n = 1
    end function pdf_builtin_data_get_n_par

```

Return the outgoing particle PDG codes. This is based on the mask.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
    procedure :: get_pdg_out => pdf_builtin_data_get_pdg_out

<SF pdf builtin: sub interfaces>+≡
    module subroutine pdf_builtin_data_get_pdg_out (data, pdg_out)
        class(pdf_builtin_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine pdf_builtin_data_get_pdg_out

<SF pdf builtin: procedures>+≡
    module subroutine pdf_builtin_data_get_pdg_out (data, pdg_out)
        class(pdf_builtin_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        integer :: n, np, i
        n = count (data%mask)
        np = 0; if (data%has_photon .and. data%mask_photon) np = 1
        allocate (pdg1 (n + np))
        pdg1(1:n) = pack ([i, i = -6, 6], data%mask)
        if (np == 1) pdg1(n+np) = PHOTON
        pdg_out(1) = pdg1
    end subroutine pdf_builtin_data_get_pdg_out

```

Allocate the interaction record. Due to gfortran 7/8/9 bug this has to remain in the main module.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
    procedure :: allocate_sf_int => pdf_builtin_data_allocate_sf_int

<SF pdf builtin: main procedures>≡
    subroutine pdf_builtin_data_allocate_sf_int (data, sf_int)
        class(pdf_builtin_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (pdf_builtin_t :: sf_int)
    end subroutine pdf_builtin_data_allocate_sf_int

```

```
end subroutine pdf_builtin_data_allocate_sf_int
```

Return the numerical PDF set index.

```
<SF pdf builtin: pdf builtin data: TBP>+≡
  procedure :: get_pdf_set => pdf_builtin_data_get_pdf_set

<SF pdf builtin: sub interfaces>+≡
  elemental module function pdf_builtin_data_get_pdf_set &
    (data) result (pdf_set)
    class(pdf_builtin_data_t), intent(in) :: data
    integer :: pdf_set
  end function pdf_builtin_data_get_pdf_set

<SF pdf builtin: procedures>+≡
  elemental module function pdf_builtin_data_get_pdf_set &
    (data) result (pdf_set)
    class(pdf_builtin_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = data%id
  end function pdf_builtin_data_get_pdf_set
```

16.15.4 The PDF object

The PDF $1 \rightarrow 2$ interaction which describes the splitting of an (anti)proton into a parton and a beam remnant. We stay in the strict forward-splitting limit, but allow some invariant mass for the beam remnant such that the outgoing parton is exactly massless. For a real event, we would replace this by a parton cascade, where the outgoing partons have virtuality as dictated by parton-shower kinematics, and transverse momentum is generated.

The PDF application is a $1 \rightarrow 2$ splitting process, where the particles are ordered as (hadron, remnant, parton).

Polarization is ignored completely. The beam particle is colorless, while partons and beam remnant carry color. The remnant gets a special flavor code.

```
<SF pdf builtin: public>+≡
  public :: pdf_builtin_t

<SF pdf builtin: types>+≡
  type, extends (sf_int_t) :: pdf_builtin_t
    type(pdf_builtin_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: q = 0
  contains
    <SF pdf builtin: pdf builtin: TBP>
  end type pdf_builtin_t
```

Type string: display the chosen PDF set.

```
<SF pdf builtin: pdf builtin: TBP>≡
  procedure :: type_string => pdf_builtin_type_string
```

```

<SF pdf builtin: sub interfaces>+≡
    module function pdf_builtin_type_string (object) result (string)
        class(pdf_builtin_t), intent(in) :: object
        type(string_t) :: string
    end function pdf_builtin_type_string

<SF pdf builtin: procedures>+≡
    module function pdf_builtin_type_string (object) result (string)
        class(pdf_builtin_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "PDF builtin: " // object%data%name
        else
            string = "PDF builtin: [undefined]"
        end if
    end function pdf_builtin_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF pdf builtin: pdf builtin: TBP>+≡
    procedure :: write => pdf_builtin_write

<SF pdf builtin: sub interfaces>+≡
    module subroutine pdf_builtin_write (object, unit, testflag)
        class(pdf_builtin_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine pdf_builtin_write

<SF pdf builtin: procedures>+≡
    module subroutine pdf_builtin_write (object, unit, testflag)
        class(pdf_builtin_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
            if (object%status >= SF_DONE_KINEMATICS) then
                write (u, "(1x,A)") "SF parameters:"
                write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
                if (object%status >= SF_FAILED_EVALUATION) then
                    write (u, "(3x,A," // FMT_17 // ")") "Q =", object%q
                end if
            end if
        end if
        call object%base_write (u, testflag)
    else
        write (u, "(1x,A)") "PDF builtin data: [undefined]"
    end if
end subroutine pdf_builtin_write

```

Initialize. We know that `data` will be of concrete type `sf_test_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

<SF pdf builtin: pdf builtin: TBP>+≡
  procedure :: init => pdf_builtin_init

<SF pdf builtin: sub interfaces>+≡
  module subroutine pdf_builtin_init (sf_int, data)
    class(pdf_builtin_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
  end subroutine pdf_builtin_init

<SF pdf builtin: procedures>+≡
  module subroutine pdf_builtin_init (sf_int, data)
    class(pdf_builtin_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    type(flavor_t) :: flv, flv_remnant
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(3) :: qn
    integer :: i
    select type (data)
    type is (pdf_builtin_data_t)
      mask = quantum_numbers_mask (.false., .false., .true.)
      call col0%init ()
      call sf_int%base_init (mask, [0._default], [0._default], [0._default])
      sf_int%data => data
      do i = -6, 6
        if (data%mask(i)) then
          call qn(1)%init (data%flv_in, col = col0)
          if (i == 0) then
            call flv%init (GLUON, data%model)
            call flv_remnant%init (HADRON_REMNANT_OCTET, data%model)
          else
            call flv%init (i, data%model)
            call flv_remnant%init &
              (sign (HADRON_REMNANT_TRIPLET, -i), data%model)
          end if
          call qn(2)%init ( &
            flv = flv_remnant, col = color_from_flavor (flv_remnant, 1))
          call qn(2)%tag_radiated ()
          call qn(3)%init ( &
            flv = flv, col = color_from_flavor (flv, 1, reverse=.true.))
          call sf_int%add_state (qn)
        end if
      end do
    type is (pdf_builtin_data_t_photon)
      if (data%has_photon .and. data%mask_photon) then
        call flv%init (PHOTON, data%model)
        call flv_remnant%init (HADRON_REMNANT_SINGLET, data%model)
        call qn(2)%init (flv = flv_remnant, &
          col = color_from_flavor (flv_remnant, 1))
        call qn(2)%tag_radiated ()
        call qn(3)%init (flv = flv, &
          col = color_from_flavor (flv, 1, reverse = .true.))
        call sf_int%add_state (qn)
      end if
    end select
  end subroutine pdf_builtin_init

```

```

        call sf_int%freeze ()
        call sf_int%set_incoming ([1])
        call sf_int%set_radiated ([2])
        call sf_int%set_outgoing ([3])
        sf_int%status = SF_INITIAL
    end select
end subroutine pdf_builtin_init

```

16.15.5 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
    procedure :: complete_kinematics => pdf_builtin_complete_kinematics

⟨SF pdf builtin: sub interfaces⟩+≡
    module subroutine pdf_builtin_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(pdf_builtin_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
    end subroutine pdf_builtin_complete_kinematics

⟨SF pdf builtin: procedures⟩+≡
    module subroutine pdf_builtin_complete_kinematics &
        (sf_int, x, xb, f, r, rb, map)
        class(pdf_builtin_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        if (map) then
            call msg_fatal ("PDF builtin: map flag not supported")
        else
            x(1) = r(1)
            xb(1) = rb(1)
            f = 1
        end if
        call sf_int%split_momentum (x, xb)
        select case (sf_int%status)
        case (SF_DONE_KINEMATICS)
            sf_int%x = x(1)
        case (SF_FAILED_KINEMATICS)
            sf_int%x = 0
            f = 0
        end select
    end subroutine pdf_builtin_complete_kinematics

```

```

end select
end subroutine pdf_builtin_complete_kinematics

```

Overriding the default method: we compute the x value from the momentum configuration. In this specific case, we also set the internally stored x value, so it can be used in the following routine.

```

<SF pdf_builtin: pdf_builtin: TBP>+≡
  procedure :: recover_x => pdf_builtin_recover_x

<SF pdf_builtin: sub interfaces>+≡
  module subroutine pdf_builtin_recover_x (sf_int, x, xb, x_free)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
  end subroutine pdf_builtin_recover_x

<SF pdf_builtin: procedures>+≡
  module subroutine pdf_builtin_recover_x (sf_int, x, xb, x_free)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
  end subroutine pdf_builtin_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF pdf_builtin: pdf_builtin: TBP>+≡
  procedure :: inverse_kinematics => pdf_builtin_inverse_kinematics

<SF pdf_builtin: sub interfaces>+≡
  module subroutine pdf_builtin_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
  end subroutine pdf_builtin_inverse_kinematics

<SF pdf_builtin: procedures>+≡
  module subroutine pdf_builtin_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb

```

```

logical, intent(in) :: map
logical, intent(in), optional :: set_momenta
logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
if (map) then
  call msg_fatal ("PDF builtin: map flag not supported")
else
  r(1) = x(1)
  rb(1)= xb(1)
  f = 1
end if
if (set_mom) then
  call sf_int%split_momentum (x, xb)
  select case (sf_int%status)
  case (SF_FAILED_KINEMATICS); f = 0
  end select
end if
end subroutine pdf_builtin_inverse_kinematics

```

16.15.6 Structure function

Once the scale is also known, we can actually call the PDF and set the values. Contrary to LHAPDF, the wrapper already takes care of adjusting to the x and Q bounds. Account for the Jacobian.

The parameter `negative_sf` is necessary to determine if we allow for negative PDF values. The class `rescale` gives rescaling prescription for NLO convolution of the structure function in combination with `i_sub`.

```

<SF pdf builtin: pdf builtin: TBP>+≡
  procedure :: apply => pdf_builtin_apply

<SF pdf builtin: sub interfaces>+≡
  module subroutine pdf_builtin_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine pdf_builtin_apply

<SF pdf builtin: procedures>+≡
  module subroutine pdf_builtin_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default), dimension(-6:6) :: ff
    real(double), dimension(-6:6) :: ff_dbl
    real(default) :: x, fph
    real(double) :: xx, qq
    complex(default), dimension(:), allocatable :: fc

```

```

integer :: i, j_sub, i_sub_opt
logical :: negative_sf_opt
i_sub_opt = 0; if (present (i_sub)) i_sub_opt = i_sub
negative_sf_opt = .false.; if (present(negative_sf)) negative_sf_opt = negative_sf
associate (data => sf_int%data)
  sf_int%q = scale
  x = sf_int%x
  if (present (rescale)) call rescale%apply (x)
  if (debug2_active (D_BEAMS)) then
    call msg_debug2 (D_BEAMS, "pdf_builtin_apply")
    call msg_debug2 (D_BEAMS, "rescale: ", present(rescale))
    call msg_debug2 (D_BEAMS, "i_sub: ", i_sub_opt)
    call msg_debug2 (D_BEAMS, "x: ", x)
  end if
  xx = x
  qq = scale
  if (data%invert) then
    if (data%has_photon) then
      call pdf_evolve (data%id, x, scale, ff(6:-6:-1), fph)
    else
      if (data%hoppet_b_matching) then
        call hoppet_eval (xx, qq, ff_dbl(6:-6:-1))
        ff = ff_dbl
      else
        call pdf_evolve (data%id, x, scale, ff(6:-6:-1))
      end if
    end if
  else
    if (data%has_photon) then
      call pdf_evolve (data%id, x, scale, ff, fph)
    else
      if (data%hoppet_b_matching) then
        call hoppet_eval (xx, qq, ff_dbl)
        ff = ff_dbl
      else
        call pdf_evolve (data%id, x, scale, ff)
      end if
    end if
  end if
  if (data%has_photon) then
    allocate (fc (count ([data%mask, data%mask_photon])))
    if (negative_sf_opt) then
      fc = pack ([ff, fph], [data%mask, data%mask_photon])
    else
      fc = max( pack ([ff, fph], [data%mask, data%mask_photon]), 0._default)
    end if
  else
    allocate (fc (count (data%mask)))
    if (negative_sf_opt) then
      fc = pack (ff, data%mask)
    else
      fc = max( pack (ff, data%mask), 0._default)
    end if
  end if
end if

```



```

end associate
if (debug_active (D_BEAMS)) print *, 'Set pdfs: ', real (fc)
call sf_int%set_matrix_element (fc, [(i_sub_opt * size(fc) + i, i = 1, size(fc))])
sf_int%status = SF_EVALUATED
end subroutine pdf_builtin_apply

```

16.15.7 Strong Coupling

Since the PDF codes provide a function for computing the running α_s value, we make this available as an implementation of the abstract `alpha_qcd_t` type, which is used for matrix element evaluation.

```

<SF pdf builtin: public>+≡
    public :: alpha_qcd_pdf_builtin_t
<SF pdf builtin: types>+≡
    type, extends (alpha_qcd_t) :: alpha_qcd_pdf_builtin_t
        type(string_t) :: pdfset_name
        integer :: pdfset_id = -1
    contains
        <SF pdf builtin: alpha qcd: TBP>
    end type alpha_qcd_pdf_builtin_t

```

Output.

```

<SF pdf builtin: alpha qcd: TBP>≡
    procedure :: write => alpha_qcd_pdf_builtin_write
<SF pdf builtin: sub interfaces>+≡
    module subroutine alpha_qcd_pdf_builtin_write (object, unit)
        class(alpha_qcd_pdf_builtin_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine alpha_qcd_pdf_builtin_write
<SF pdf builtin: procedures>+≡
    module subroutine alpha_qcd_pdf_builtin_write (object, unit)
        class(alpha_qcd_pdf_builtin_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A)") "QCD parameters (pdf_builtin):"
        write (u, "(5x,A,A)") "PDF set = ", char (object%pdfset_name)
        write (u, "(5x,A,I0)") "PDF ID = ", object%pdfset_id
    end subroutine alpha_qcd_pdf_builtin_write

```

Calculation: the numeric ID selects the correct PDF set, which must be properly initialized.

```

<SF pdf builtin: alpha qcd: TBP>+≡
    procedure :: get => alpha_qcd_pdf_builtin_get
<SF pdf builtin: sub interfaces>+≡
    module function alpha_qcd_pdf_builtin_get (alpha_qcd, scale) result (alpha)
        class(alpha_qcd_pdf_builtin_t), intent(in) :: alpha_qcd
        real(default), intent(in) :: scale
        real(default) :: alpha
    end function alpha_qcd_pdf_builtin_get

```

```

<SF pdf builtin: procedures>+≡
  module function alpha_qcd_pdf_builtin_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_pdf_builtin_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = pdf_alphas (alpha_qcd%pdfset_id, scale)
  end function alpha_qcd_pdf_builtin_get

```

Initialization. We need to access the global initialization status.

```

<SF pdf builtin: alpha qcd: TBP>+≡
  procedure :: init => alpha_qcd_pdf_builtin_init

<SF pdf builtin: sub interfaces>+≡
  module subroutine alpha_qcd_pdf_builtin_init (alpha_qcd, name, path)
    class(alpha_qcd_pdf_builtin_t), intent(out) :: alpha_qcd
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: path
  end subroutine alpha_qcd_pdf_builtin_init

<SF pdf builtin: procedures>+≡
  module subroutine alpha_qcd_pdf_builtin_init (alpha_qcd, name, path)
    class(alpha_qcd_pdf_builtin_t), intent(out) :: alpha_qcd
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: path
    alpha_qcd%pdfset_name = name
    alpha_qcd%pdfset_id = pdf_get_id (name)
    if (alpha_qcd%pdfset_id < 0) &
      call msg_fatal ("QCD parameter initialization: PDF set " &
        // char (name) // " is unknown")
    call pdf_init (alpha_qcd%pdfset_id, path)
  end subroutine alpha_qcd_pdf_builtin_init

```

16.15.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_pdf_builtin_ut.f90>≡
  <File header>

  module sf_pdf_builtin_ut
    use unit_tests
    use sf_pdf_builtin_uti

    <Standard module head>

    <SF pdf builtin: public test>

    contains

    <SF pdf builtin: test driver>

  end module sf_pdf_builtin_ut

```

```

<sf_pdf_builtin_uti.f90>≡
  <File header>

  module sf_pdf_builtin_uti

    <Use kinds>
    <Use strings>
    use os_interface
    use physics_defs, only: PROTON
    use sm_qcd
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_base

    use sf_pdf_builtin

    <Standard module head>

    <SF pdf builtin: test declarations>

    contains

    <SF pdf builtin: tests>

  end module sf_pdf_builtin_uti
API: driver for the unit tests below.
<SF pdf builtin: public test>≡
  public :: sf_pdf_builtin_test
<SF pdf builtin: test driver>≡
  subroutine sf_pdf_builtin_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SF pdf builtin: execute tests>
  end subroutine sf_pdf_builtin_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF pdf builtin: execute tests>≡
  call test (sf_pdf_builtin_1, "sf_pdf_builtin_1", &
    "structure function configuration", &
    u, results)
<SF pdf builtin: test declarations>≡
  public :: sf_pdf_builtin_1
<SF pdf builtin: tests>≡
  subroutine sf_pdf_builtin_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data

```

```

type(model_data_t), target :: model
type(pdg_array_t) :: pdg_in
type(pdg_array_t), dimension(1) :: pdg_out
integer, dimension(:), allocatable :: pdg1
class(sf_data_t), allocatable :: data
type(string_t) :: name

write (u, "(A)")  "* Test output: sf_pdf_builtin_1"
write (u, "(A)")  "* Purpose: initialize and display &
                  &test structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call os_data%init ()

call model%init_sm_test ()
pdg_in = PROTON

allocate (pdf_builtin_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

name = "CTEQ6L"

select type (data)
type is (pdf_builtin_data_t)
    call data%init (model, pdg_in, name, &
                  os_data%pdf_builtin_datapath)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_pdf_builtin_1"

end subroutine sf_pdf_builtin_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```
<SF pdf builtin: execute tests>+≡
    call test (sf_pdf_builtin_2, "sf_pdf_builtin_2", &
               "structure function instance", &
               u, results)

<SF pdf builtin: test declarations>+≡
    public :: sf_pdf_builtin_2

<SF pdf builtin: tests>+≡
    subroutine sf_pdf_builtin_2 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(string_t) :: name
        type(vector4_t) :: k
        type(vector4_t), dimension(2) :: q
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f

        write (u, "(A)")  "* Test output: sf_pdf_builtin_2"
        write (u, "(A)")  "* Purpose: initialize and fill &
                           &test structure function object"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize configuration data"
        write (u, "(A)")

        call os_data%init ()
        call model%init_sm_test ()
        call flv%init (PROTON, model)
        pdg_in = PROTON

        call reset_interaction_counter ()

        name = "CTEQ6L"

        allocate (pdf_builtin_data_t :: data)
        select type (data)
        type is (pdf_builtin_data_t)
            call data%init (model, pdg_in, name, &
                           os_data%pdf_builtin_datapath)
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")
```

```

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100 GeV"

```

```

write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_pdf_builtin_2"

end subroutine sf_pdf_builtin_2

```

Strong Coupling

Test α_s as an implementation of the `alpha_qcd_t` abstract type.

```

<SF pdf builtin: execute tests>+≡
  call test (sf_pdf_builtin_3, "sf_pdf_builtin_3", &
    "running alpha_s", &
    u, results)

<SF pdf builtin: test declarations>+≡
  public :: sf_pdf_builtin_3

<SF pdf builtin: tests>+≡
  subroutine sf_pdf_builtin_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(qcd_t) :: qcd
    type(string_t) :: name

    write (u, "(A)")  "* Test output: sf_pdf_builtin_3"
    write (u, "(A)")  "* Purpose: initialize and evaluate alpha_s"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call os_data%init ()

    name = "CTEQ6L"

    write (u, "(A)")  "* Initialize qcd object"
    write (u, "(A)")

    allocate (alpha_qcd_pdf_builtin_t :: qcd%alpha)
    select type (alpha => qcd%alpha)
    type is (alpha_qcd_pdf_builtin_t)
      call alpha%init (name, os_data%pdf_builtin_datapath)

```

```

end select
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100"
write (u, "(A)")

write (u, "(1x,A,F8.5)")  "alpha = ", qcd%alpha%get (100._default)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_pdf_builtin_3"

end subroutine sf_pdf_builtin_3

```


16.16 LHAPDF

Parton distribution functions (PDFs) are available via an interface to the LHAPDF standard library.

16.16.1 The module

```
<sf_lhapdf.f90>≡  
<File header>  
  
module sf_lhapdf  
  
  <Use kinds>  
  <Use strings>  
    use sm_qcd  
    use pdg_arrays  
    use model_data  
    use flavors  
    use polarizations  
    use sf_base  
    use lhapdf !NODEP!  
  
  <Standard module head>  
  
  <SF lhapdf: public>  
  
  <SF lhapdf: types>  
  
  <SF lhapdf: variables>  
  
  <SF lhapdf: interfaces>  
  
    interface  
  <SF lhapdf: sub interfaces>  
    end interface  
  
contains  
  
  <SF lhapdf: main procedures>  
  
end module sf_lhapdf  
  
<sf_lhapdf_sub.f90>≡  
<File header>  
  
submodule (sf_lhapdf) sf_lhapdf_s  
  
  use format_defs, only: FMT_17, FMT_19  
  use io_units  
  use system_dependencies, only: LHAPDF_PDFSETS_PATH  
  use system_dependencies, only: LHAPDF5_AVAILABLE  
  use system_dependencies, only: LHAPDF6_AVAILABLE  
  use diagnostics  
  use physics_defs, only: PROTON, PHOTON, PIPLUS, GLUON
```

```

use physics_defs, only: HADRON_REMNANT_SINGLET
use physics_defs, only: HADRON_REMNANT_TRIPLET
use physics_defs, only: HADRON_REMNANT_OCTET
use lorentz
use colors
use quantum_numbers
use state_matrices
use hoppet_interface

implicit none

<SF lhpdf: parameters>

contains

<SF lhpdf: procedures>

end submodule sf_lhpdf_s

```

16.16.2 Codes for default PDF sets

The default PDF for protons set is chosen to be CTEQ6ll (LO fit with LO α_s).

```

<SF lhpdf: parameters>≡
character(*), parameter :: LHAPDF5_DEFAULT_PROTON = "cteq6ll.LHpdf"
character(*), parameter :: LHAPDF5_DEFAULT_PION   = "ABFKWPI.LHgrid"
character(*), parameter :: LHAPDF5_DEFAULT_PHOTON = "GSG960.LHgrid"
character(*), parameter :: LHAPDF6_DEFAULT_PROTON = "CT10"

```

16.16.3 LHAPDF library interface

Here we specify explicit interfaces for all LHAPDF routines that we use below.

```

<SF lhpdf: interfaces>≡
interface
  subroutine InitPDFsetM (set, file)
    integer, intent(in) :: set
    character(*), intent(in) :: file
  end subroutine InitPDFsetM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine InitPDFM (set, mem)
    integer, intent(in) :: set, mem
  end subroutine InitPDFM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine numberPDFM (set, n_members)
    integer, intent(in) :: set
    integer, intent(out) :: n_members
  end subroutine numberPDFM
end interface

```

```

        end subroutine numberPDFM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine evolvePDFM (set, x, q, ff)
            integer, intent(in) :: set
            double precision, intent(in) :: x, q
            double precision, dimension(-6:6), intent(out) :: ff
        end subroutine evolvePDFM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine evolvePDFphotonM (set, x, q, ff, fphot)
            integer, intent(in) :: set
            double precision, intent(in) :: x, q
            double precision, dimension(-6:6), intent(out) :: ff
            double precision, intent(out) :: fphot
        end subroutine evolvePDFphotonM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine evolvePDFpM (set, x, q, s, scheme, ff)
            integer, intent(in) :: set
            double precision, intent(in) :: x, q, s
            integer, intent(in) :: scheme
            double precision, dimension(-6:6), intent(out) :: ff
        end subroutine evolvePDFpM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine GetXminM (set, mem, xmin)
            integer, intent(in) :: set, mem
            double precision, intent(out) :: xmin
        end subroutine GetXminM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine GetXmaxM (set, mem, xmax)
            integer, intent(in) :: set, mem
            double precision, intent(out) :: xmax
        end subroutine GetXmaxM
    end interface

    <SF lhpdf: interfaces>+≡
    interface
        subroutine GetQ2minM (set, mem, q2min)
            integer, intent(in) :: set, mem

```

```

        double precision, intent(out) :: q2min
    end subroutine GetQ2minM
end interface

<SF lhpdf: interfaces>+=
interface
    subroutine GetQ2maxM (set, mem, q2max)
        integer, intent(in) :: set, mem
        double precision, intent(out) :: q2max
    end subroutine GetQ2maxM
end interface

<SF lhpdf: interfaces>+=
interface
    function has_photon () result(flag)
        logical :: flag
    end function has_photon
end interface

```

16.16.4 The LHAPDF status

This type holds the initialization status of the LHAPDF system. Entry 1 is for proton PDFs, entry 2 for pion PDFs, entry 3 for photon PDFs.

Since it is connected to the external LHAPDF library, this is a truly global object. We implement it as a private module variable. To access it from elsewhere, the caller has to create and initialize an object of type `lhpdf_status_t`, which acts as a proxy.

```

<SF lhpdf: types>=
type :: lhpdf_global_status_t
    private
    logical, dimension(3) :: initialized = .false.
end type lhpdf_global_status_t

<SF lhpdf: variables>=
type(lhpdf_global_status_t), save :: lhpdf_global_status

<SF lhpdf: procedures>=
function lhpdf_global_status_is_initialized (set) result (flag)
    logical :: flag
    integer, intent(in), optional :: set
    if (present (set)) then
        select case (set)
            case (1:3);    flag = lhpdf_global_status%initialized(set)
            case default;  flag = .false.
        end select
    else
        flag = any (lhpdf_global_status%initialized)
    end if
end function lhpdf_global_status_is_initialized

```

```

<SF lhpdf: procedures>+≡
  subroutine lhpdf_global_status_set_initialized (set)
    integer, intent(in) :: set
    lhpdf_global_status%initialized(set) = .true.
  end subroutine lhpdf_global_status_set_initialized

```

This is the only public procedure, it tells the system to forget about previous initialization, allowing for changing the chosen PDF set. Note that such a feature works only if the global program flow is serial, so no two distinct sets are accessed simultaneously. But this applies to LHAPDF anyway.

```

<SF lhpdf: public>≡
  public :: lhpdf_global_reset

<SF lhpdf: sub interfaces>≡
  module subroutine lhpdf_global_reset ()
    end subroutine lhpdf_global_reset

<SF lhpdf: procedures>+≡
  module subroutine lhpdf_global_reset ()
    lhpdf_global_status%initialized = .false.
  end subroutine lhpdf_global_reset

```

16.16.5 LHAPDF initialization

Before using LHAPDF, we have to initialize it with a particular data set and member. This applies not just if we use structure functions, but also if we just use an α_s formula. The integer `set` should be 1 for proton, 2 for pion, and 3 for photon, but this is just convention.

It appears as if LHAPDF does not allow for multiple data sets being used concurrently (?), so multi-threaded usage with different sets (e.g., a scan) is excluded. The current setup with a global flag that indicates initialization is fine as long as Whizard itself is run in serial mode at the Sindarin level. If we introduce multithreading in any form from Sindarin, we have to rethink the implementation of the LHAPDF interface. (The same considerations apply to builtin PDFs.)

If the particular set has already been initialized, do nothing. This implies that whenever we want to change the setup for a particular set, we have to reset the LHAPDF status. `lhpdf_initialize` has an obvious name clash with `lhpdf_init`, the reason it works for `pdf_builtin` is that there things are outsourced to a separate module (inc. `lhpdf_status` etc.).

```

<SF lhpdf: public>+≡
  public :: lhpdf_initialize

<SF lhpdf: sub interfaces>+≡
  module subroutine lhpdf_initialize &
    (set, prefix, file, member, pdf, b_match)
    integer, intent(in) :: set
    type(string_t), intent(inout) :: prefix
    type(string_t), intent(inout) :: file
    type(lhpdf_pdf_t), intent(inout), optional :: pdf
    integer, intent(inout) :: member
    logical, intent(in), optional :: b_match
  end subroutine lhpdf_initialize

```

```

end subroutine lhpdf_initialize

<SF lhpdf: procedures>+=
module subroutine lhpdf_initialize &
  (set, prefix, file, member, pdf, b_match)
  integer, intent(in) :: set
  type(string_t), intent(inout) :: prefix
  type(string_t), intent(inout) :: file
  type(lhpdf_pdf_t), intent(inout), optional :: pdf
  integer, intent(inout) :: member
  logical, intent(in), optional :: b_match
  if (prefix == "") prefix = LHAPDF_PDFSETS_PATH
  if (LHAPDF5_AVAILABLE) then
    if (lhpdf_global_status_is_initialized (set)) return
    if (file == "") then
      select case (set)
        case (1); file = LHAPDF5_DEFAULT_PROTON
        case (2); file = LHAPDF5_DEFAULT_PION
        case (3); file = LHAPDF5_DEFAULT_PHOTON
      end select
    end if
    if (data_file_exists (prefix // "/" // file)) then
      call InitPDFsetM (set, char (prefix // "/" // file))
    else
      call msg_fatal ("LHAPDF: Data file '" &
        // char (file) // "' not found in '" // char (prefix) // "'.")
      return
    end if
    if (.not. dataset_member_exists (set, member)) then
      call msg_error (" LHAPDF: Chosen member does not exist for set '" &
        // char (file) // "', using default.")
      member = 0
    end if
    call InitPDFM (set, member)
  else if (LHAPDF6_AVAILABLE) then
    ! TODO: (bcn 2015-07-07) we should have a closer look why this global
    !               check must not be executed
    !   if (lhpdf_global_status_is_initialized (set) .and. &
    !       pdf%is_associated ()) return
    if (file == "") then
      select case (set)
        case (1); file = LHAPDF6_DEFAULT_PROTON
        case (2);
          call msg_fatal ("LHAPDF6: no pion PDFs supported")
        case (3);
          call msg_fatal ("LHAPDF6: no photon PDFs supported")
      end select
    end if
    if (data_file_exists (prefix // "/" // file // "/" // file // ".info")) then
      call pdf%init (char (file), member)
    else
      call msg_fatal ("LHAPDF: Data file '" &
        // char (file) // "' not found in '" // char (prefix) // "'.")
      return
    end if
  end if
end if

```

```

end if
if (present (b_match)) then
  if (b_match) then
    if (LHAPDF5_AVAILABLE) then
      call hoppet_init (.false.)
    else if (LHAPDF6_AVAILABLE) then
      call hoppet_init (.false., pdf)
    end if
  end if
end if
call lhpdf_global_status_set_initialized (set)
contains
function data_file_exists (fq_name) result (exist)
  type(string_t), intent(in) :: fq_name
  logical :: exist
  inquire (file = char(fq_name), exist = exist)
end function data_file_exists
function dataset_member_exists (set, member) result (exist)
  integer, intent(in) :: set, member
  logical :: exist
  integer :: n_members
  call numberPDFM (set, n_members)
  exist = member >= 0 .and. member <= n_members
end function dataset_member_exists
end subroutine lhpdf_initialize

```

16.16.6 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

```

<SF lhpdf: lhpdf: TBP>≡
  procedure :: complete_kinematics => lhpdf_complete_kinematics

<SF lhpdf: sub interfaces>+≡
  module subroutine lhpdf_complete_kinematics &
    (sf_int, x, xb, f, r, rb, map)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
  end subroutine lhpdf_complete_kinematics

<SF lhpdf: procedures>+≡
  module subroutine lhpdf_complete_kinematics &
    (sf_int, x, xb, f, r, rb, map)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb

```

```

real(default), intent(out) :: f
real(default), dimension(:), intent(in) :: r
real(default), dimension(:), intent(in) :: rb
logical, intent(in) :: map
if (map) then
  call msg_fatal ("LHAPDF: map flag not supported")
else
  x(1) = r(1)
  xb(1)= rb(1)
  f = 1
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_DONE_KINEMATICS)
  sf_int%x = x(1)
case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  f = 0
end select
end subroutine lhapdf_complete_kinematics

```

Overriding the default method: we compute the x value from the momentum configuration. In this specific case, we also set the internally stored x value, so it can be used in the following routine.

```

<SF lhapdf: lhapdf: TBP>+≡
  procedure :: recover_x => lhapdf_recover_x

<SF lhapdf: sub interfaces>+≡
  module subroutine lhapdf_recover_x (sf_int, x, xb, x_free)
    class(lhapdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
  end subroutine lhapdf_recover_x

<SF lhapdf: procedures>+≡
  module subroutine lhapdf_recover_x (sf_int, x, xb, x_free)
    class(lhapdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
  end subroutine lhapdf_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF lhapdf: lhapdf: TBP>+≡
  procedure :: inverse_kinematics => lhapdf_inverse_kinematics

<SF lhapdf: sub interfaces>+≡
  module subroutine lhapdf_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)

```



```

        class(lhapdf_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(in) :: x
        real(default), dimension(:), intent(in) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: r
        real(default), dimension(:), intent(out) :: rb
        logical, intent(in) :: map
        logical, intent(in), optional :: set_momenta
    end subroutine lhpdf_inverse_kinematics

<SF lhpdf: procedures>+≡
module subroutine lhpdf_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(lhapdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
        call msg_fatal ("LHAPDF: map flag not supported")
    else
        r(1) = x(1)
        rb(1) = xb(1)
        f = 1
    end if
    if (set_mom) then
        call sf_int%split_momentum (x, xb)
        select case (sf_int%status)
            case (SF_FAILED_KINEMATICS); f = 0
        end select
    end if
end subroutine lhpdf_inverse_kinematics

```

16.16.7 The LHAPDF data block

The data block holds the incoming flavor (which has to be proton, pion, or photon), the corresponding pointer to the global access data (1, 2, or 3), the flag `invert` which is set for an antiproton, the bounds as returned by LHAPDF for the specified set, and a mask that determines which partons will be actually in use.

```

<SF lhpdf: public>+≡
    public :: lhpdf_data_t

<SF lhpdf: types>+≡
    type, extends (sf_data_t) :: lhpdf_data_t
    private
    type(string_t) :: prefix
    type(string_t) :: file

```

```

type(lhapdf_pdf_t) :: pdf
integer :: member = 0
class(model_data_t), pointer :: model => null ()
type(flavor_t) :: flv_in
integer :: set = 0
logical :: invert = .false.
logical :: photon = .false.
logical :: has_photon = .false.
integer :: photon_scheme = 0
real(default) :: xmin = 0, xmax = 0
real(default) :: qmin = 0, qmax = 0
logical, dimension(-6:6) :: mask = .true.
logical :: mask_photon = .true.
logical :: hoppet_b_matching = .false.
contains
  <SF lhpdf: lhpdf data: TBP>
end type lhpdf_data_t

```

Generate PDF data. This is provided as a function, but it has the side-effect of initializing the requested PDF set. A finalizer is not needed.

The library uses double precision, so since the default precision may be extended or quadruple, we use auxiliary variables for type casting.

```

<SF lhpdf: lhpdf data: TBP>≡
  procedure :: init => lhpdf_data_init

<SF lhpdf: sub interfaces>+≡
  module subroutine lhpdf_data_init &
    (data, model, pdg_in, prefix, file, member, photon_scheme, &
     hoppet_b_matching)
    class(lhapdf_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    type(string_t), intent(in), optional :: prefix, file
    integer, intent(in), optional :: member
    integer, intent(in), optional :: photon_scheme
    logical, intent(in), optional :: hoppet_b_matching
  end subroutine lhpdf_data_init

<SF lhpdf: procedures>+≡
  module subroutine lhpdf_data_init &
    (data, model, pdg_in, prefix, file, member, photon_scheme, &
     hoppet_b_matching)
    class(lhapdf_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    type(string_t), intent(in), optional :: prefix, file
    integer, intent(in), optional :: member
    integer, intent(in), optional :: photon_scheme
    logical, intent(in), optional :: hoppet_b_matching
    double precision :: xmin, xmax, q2min, q2max
    external :: InitPDFsetM, InitPDFM, numberPDFM
    external :: GetXminM, GetXmaxM, GetQ2minM, GetQ2maxM
    if (.not. LHAPDF5_AVAILABLE .and. .not. LHAPDF6_AVAILABLE) then
      call msg_fatal ("LHAPDF requested but library is not linked")
    end if
  end subroutine lhpdf_data_init

```

```

        return
    end if
    data%model => model
    if (pdg_in%get_length () /= 1) &
        call msg_fatal ("PDF: incoming particle must be unique")
    call data%flv_in%init (pdg_in%get (1), model)
    select case (pdg_in%get (1))
    case (PROTON)
        data%set = 1
    case (-PROTON)
        data%set = 1
        data%invert = .true.
    case (PIPLUS)
        data%set = 2
    case (-PIPLUS)
        data%set = 2
        data%invert = .true.
    case (PHOTON)
        data%set = 3
        data%photon = .true.
        if (present (photon_scheme)) data%photon_scheme = photon_scheme
    case default
        call msg_fatal (" LHAPDF: " &
            // "incoming particle must be (anti)proton, pion, or photon.")
        return
    end select
    if (present (prefix)) then
        data%prefix = prefix
    else
        data%prefix = ""
    end if
    if (present (file)) then
        data%file = file
    else
        data%file = ""
    end if
    if (present (hoppet_b_matching)) data%hoppet_b_matching = hoppet_b_matching
    if (LHAPDF5_AVAILABLE) then
        call lhpdf_initialize (data%set, &
            data%prefix, data%file, data%member, &
            b_match = data%hoppet_b_matching)
        call GetXminM (data%set, data%member, xmin)
        call GetXmaxM (data%set, data%member, xmax)
        call GetQ2minM (data%set, data%member, q2min)
        call GetQ2maxM (data%set, data%member, q2max)
        data%xmin = xmin
        data%xmax = xmax
        data%qmin = sqrt (q2min)
        data%qmax = sqrt (q2max)
        data%has_photon = has_photon ()
    else if (LHAPDF6_AVAILABLE) then
        call lhpdf_initialize (data%set, &
            data%prefix, data%file, data%member, &
            data%pdf, data%hoppet_b_matching)
    end if
end

```

```

        data%xmin = data%pdf%getxmin ()
        data%xmax = data%pdf%getxmax ()
        data%qmin = sqrt(data%pdf%getq2min ())
        data%qmax = sqrt(data%pdf%getq2max ())
        data%has_photon = data%pdf%has_photon ()
    end if
end subroutine lhpdf_data_init

```

Enable/disable partons explicitly. If a mask entry is true, applying the PDF will generate the corresponding flavor on output.

```

<LHAPDF: lhpdf data: TBP>≡
    procedure :: set_mask => lhpdf_data_set_mask

<LHAPDF: procedures>≡
    subroutine lhpdf_data_set_mask (data, mask)
        class(lhpdf_data_t), intent(inout) :: data
        logical, dimension(-6:6), intent(in) :: mask
        data%mask = mask
    end subroutine lhpdf_data_set_mask

```

Return the public part of the data set.

```

<LHAPDF: public>≡
    public :: lhpdf_data_get_public_info

<LHAPDF: procedures>+≡
    subroutine lhpdf_data_get_public_info &
        (data, lhpdf_dir, lhpdf_file, lhpdf_member)
        type(lhpdf_data_t), intent(in) :: data
        type(string_t), intent(out) :: lhpdf_dir, lhpdf_file
        integer, intent(out) :: lhpdf_member
        lhpdf_dir = data%prefix
        lhpdf_file = data%file
        lhpdf_member = data%member
    end subroutine lhpdf_data_get_public_info

```

Return the number of the member of the data set.

```

<LHAPDF: public>+≡
    public :: lhpdf_data_get_set

<LHAPDF: procedures>+≡
    function lhpdf_data_get_set(data) result(set)
        type(lhpdf_data_t), intent(in) :: data
        integer :: set
        set = data%set
    end function lhpdf_data_get_set

```

Output

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: write => lhpdf_data_write

```

```

<SF lhpdf: sub interfaces>+≡
  module subroutine lhpdf_data_write (data, unit, verbose)
    class(lhpdf_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine lhpdf_data_write

<SF lhpdf: procedures>+≡
  module subroutine lhpdf_data_write (data, unit, verbose)
    class(lhpdf_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    logical :: verb
    integer :: u
    if (present (verbose)) then
      verb = verbose
    else
      verb = .false.
    end if
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "LHAPDF data:"
    if (data%set /= 0) then
      write (u, "(3x,A)", advance="no") "flavor      = "
      call data%flv_in%write (u); write (u, *)
      if (verb) then
        write (u, "(3x,A,A)")      " prefix      = ", char (data%prefix)
      else
        write (u, "(3x,A,A)")      " prefix      = ", &
          " <empty (non-verbose version)>"
      end if
      write (u, "(3x,A,A)")      " file          = ", char (data%file)
      write (u, "(3x,A,I3)")      " member       = ", data%member
      write (u, "(3x,A," // FMT_19 // ")") " x(min)       = ", data%xmin
      write (u, "(3x,A," // FMT_19 // ")") " x(max)       = ", data%xmax
      write (u, "(3x,A," // FMT_19 // ")") " Q(min)       = ", data%qmin
      write (u, "(3x,A," // FMT_19 // ")") " Q(max)       = ", data%qmax
      write (u, "(3x,A,L1)")      " invert       = ", data%invert
      if (data%photon) write (u, "(3x,A,I3)") &
        " IP2 (scheme) = ", data%photon_scheme
      write (u, "(3x,A,6(1x,L1),1x,A,1x,L1,1x,A,6(1x,L1))") &
        " mask          = ", &
        data%mask(-6:-1), " ", data%mask(0), " ", data%mask(1:6)
      write (u, "(3x,A,L1)")      " photon mask = ", data%mask_photon
      if (data%set == 1) write (u, "(3x,A,L1)") &
        " hoppet_b     = ", data%hoppet_b_matching
    else
      write (u, "(3x,A)") "[undefined]"
    end if
  end subroutine lhpdf_data_write

```

The number of parameters is one. We do not generate transverse momentum.

```

<SF lhpdf: lhpdf data: TBP>+≡
  procedure :: get_n_par => lhpdf_data_get_n_par

<SF lhpdf: sub interfaces>+≡
  module function lhpdf_data_get_n_par (data) result (n)

```

```

        class(lhapdf_data_t), intent(in) :: data
        integer :: n
    end function lhpdf_data_get_n_par
<SF lhpdf: procedures>+≡
module function lhpdf_data_get_n_par (data) result (n)
    class(lhapdf_data_t), intent(in) :: data
    integer :: n
    n = 1
end function lhpdf_data_get_n_par

```

Return the outgoing particle PDG codes. This is based on the mask.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: get_pdg_out => lhpdf_data_get_pdg_out
<SF lhpdf: sub interfaces>+≡
    module subroutine lhpdf_data_get_pdg_out (data, pdg_out)
        class(lhapdf_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine lhpdf_data_get_pdg_out
<SF lhpdf: procedures>+≡
    module subroutine lhpdf_data_get_pdg_out (data, pdg_out)
        class(lhapdf_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        integer :: n, np, i
        n = count (data%mask)
        np = 0; if (data%has_photon .and. data%mask_photon) np = 1
        allocate (pdg1 (n + np))
        pdg1(1:n) = pack ([i, i = -6, 6], data%mask)
        if (np == 1) pdg1(n+np) = PHOTON
        pdg_out(1) = pdg1
    end subroutine lhpdf_data_get_pdg_out

```

Allocate the interaction record. Due to a gfortran 7/8/9 bug this has to remain in the main module.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: allocate_sf_int => lhpdf_data_allocate_sf_int
<SF lhpdf: main procedures>≡
    subroutine lhpdf_data_allocate_sf_int (data, sf_int)
        class(lhapdf_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (lhpdf_t :: sf_int)
    end subroutine lhpdf_data_allocate_sf_int

```

Return the numerical PDF set index.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: get_pdf_set => lhpdf_data_get_pdf_set
<SF lhpdf: sub interfaces>+≡
    elemental module function lhpdf_data_get_pdf_set (data) result (pdf_set)
        class(lhapdf_data_t), intent(in) :: data
        integer :: pdf_set
    end function lhpdf_data_get_pdf_set

```

```

<SF lhpdf: procedures>+≡
  elemental module function lhpdf_data_get_pdf_set (data) result (pdf_set)
    class(lhpdf_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = data%set
  end function lhpdf_data_get_pdf_set

```

16.16.8 The LHAPDF object

The `lhpdf_t` data type is a $1 \rightarrow 2$ interaction which describes the splitting of an (anti)proton into a parton and a beam remnant. We stay in the strict forward-splitting limit, but allow some invariant mass for the beam remnant such that the outgoing parton is exactly massless. For a real event, we would replace this by a parton cascade, where the outgoing partons have virtuality as dictated by parton-shower kinematics, and transverse momentum is generated.

This is the LHAPDF object which holds input data together with the interaction. We also store the x momentum fraction and the scale, since kinematics and function value are requested at different times.

The PDF application is a $1 \rightarrow 2$ splitting process, where the particles are ordered as (hadron, remnant, parton).

Polarization is ignored completely. The beam particle is colorless, while partons and beam remnant carry color. The remnant gets a special flavor code.

```

<SF lhpdf: public>+≡
  public :: lhpdf_t

<SF lhpdf: types>+≡
  type, extends (sf_int_t) :: lhpdf_t
    type(lhpdf_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: q = 0
    real(default) :: s = 0
  contains
    <SF lhpdf: lhpdf: TBP>
  end type lhpdf_t

```

Type string: display the chosen PDF set.

```

<SF lhpdf: lhpdf: TBP>+≡
  procedure :: type_string => lhpdf_type_string

<SF lhpdf: sub interfaces>+≡
  module function lhpdf_type_string (object) result (string)
    class(lhpdf_t), intent(in) :: object
    type(string_t) :: string
  end function lhpdf_type_string

<SF lhpdf: procedures>+≡
  module function lhpdf_type_string (object) result (string)
    class(lhpdf_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "LHAPDF: " // object%data%file
    else

```

```

        string = "LHAPDF: [undefined]"
    end if
end function lhpdf_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF lhpdf: lhpdf: TBP>+≡
    procedure :: write => lhpdf_write

<SF lhpdf: sub interfaces>+≡
    module subroutine lhpdf_write (object, unit, testflag)
        class(lhpdf_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine lhpdf_write

<SF lhpdf: procedures>+≡
    module subroutine lhpdf_write (object, unit, testflag)
        class(lhpdf_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
            if (object%status >= SF_DONE_KINEMATICS) then
                write (u, "(1x,A)") "SF parameters:"
                write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
                if (object%status >= SF_FAILED_EVALUATION) then
                    write (u, "(3x,A," // FMT_17 // ")") "Q =", object%q
                end if
            end if
        end if
        call object%base_write (u, testflag)
    else
        write (u, "(1x,A)") "LHAPDF data: [undefined]"
    end if
end subroutine lhpdf_write

```

Initialize. We know that `data` will be of concrete type `sf_lhpdf_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

```

<SF lhpdf: lhpdf: TBP>+≡
    procedure :: init => lhpdf_init

<SF lhpdf: sub interfaces>+≡
    module subroutine lhpdf_init (sf_int, data)
        class(lhpdf_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
    end subroutine lhpdf_init

<SF lhpdf: procedures>+≡
    module subroutine lhpdf_init (sf_int, data)
        class(lhpdf_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
        type(quantum_numbers_mask_t), dimension(3) :: mask

```



```

type(flavor_t) :: flv, flv_remnant
type(color_t) :: col0
type(quantum_numbers_t), dimension(3) :: qn
integer :: i
select type (data)
type is (lhpdf_data_t)
  mask = quantum_numbers_mask (.false., .false., .true.)
  call col0%init ()
  call sf_int%base_init (mask, [0._default], [0._default], [0._default])
  sf_int%data => data
  do i = -6, 6
    if (data%mask(i)) then
      call qn(1)%init (data%flv_in, col = col0)
      if (i == 0) then
        call flv%init (GLUON, data%model)
        call flv_remnant%init (HADRON_REMNANT_OCTET, data%model)
      else
        call flv%init (i, data%model)
        call flv_remnant%init &
          (sign (HADRON_REMNANT_TRIPLET, -i), data%model)
      end if
      call qn(2)%init ( &
        flv = flv_remnant, col = color_from_flavor (flv_remnant, 1))
      call qn(2)%tag_radiated ()
      call qn(3)%init ( &
        flv = flv, col = color_from_flavor (flv, 1, reverse=.true.))
      call sf_int%add_state (qn)
    end if
  end do
  if (data%has_photon .and. data%mask_photon) then
    call flv%init (PHOTON, data%model)
    call flv_remnant%init (HADRON_REMNANT_SINGLET, data%model)
    call qn(2)%init (flv = flv_remnant, &
      col = color_from_flavor (flv_remnant, 1))
    call qn(2)%tag_radiated ()
    call qn(3)%init (flv = flv, &
      col = color_from_flavor (flv, 1, reverse=.true.))
    call sf_int%add_state (qn)
  end if
  call sf_int%freeze ()
  call sf_int%set_incoming ([1])
  call sf_int%set_radiated ([2])
  call sf_int%set_outgoing ([3])
  sf_int%status = SF_INITIAL
end select
end subroutine lhpdf_init

```

16.16.9 Structure function

We have to cast the LHAPDF arguments to/from double precision (possibly from/to extended/quadruple precision), if necessary. Some structure functions can yield negative results (sea quarks close to $x = 1$). In an NLO computation,

this is perfectly fine and we keep negative values. Unlike total cross sections, PDFs do not have to be positive definite. For LO however, negative PDFs would cause negative event weights so we set these values to zero instead.

```

<SF lhpdf: lhpdf: TBP>+≡
  procedure :: apply => lhpdf_apply

<SF lhpdf: sub interfaces>+≡
  module subroutine lhpdf_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
  end subroutine lhpdf_apply

<SF lhpdf: procedures>+≡
  module subroutine lhpdf_apply &
    (sf_int, scale, negative_sf, rescale, i_sub)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: x, s
    double precision :: xx, qq, ss
    double precision, dimension(-6:6) :: ff
    double precision :: fphot
    complex(default), dimension(:), allocatable :: fc
    integer :: i, i_sub_opt, j_sub
    logical :: negative_sf_opt
    external :: evolvePDFM, evolvePDFpM
    i_sub_opt = 0; if (present(i_sub)) i_sub_opt = i_sub
    negative_sf_opt = .false.; if (present(negative_sf)) negative_sf_opt = negative_sf
    associate (data => sf_int%data)
      sf_int%q = scale
      x = sf_int%x
      if (present(rescale)) call rescale%apply(x)
      s = sf_int%s
      xx = x
      if (debug2_active(D_BEAMS)) then
        call msg_debug2(D_BEAMS, "lhpdf_apply")
        call msg_debug2(D_BEAMS, "rescale: ", present(rescale))
        call msg_debug2(D_BEAMS, "i_sub: ", i_sub_opt)
        call msg_debug2(D_BEAMS, "x: ", x)
      end if
      qq = min(data%qmax, scale)
      qq = max(data%qmin, qq)
      if (.not. data%photon) then
        if (data%invert) then
          if (data%has_photon) then
            if (LHAPDF5_AVAILABLE) then
              call evolvePDFphotonM &
                (data%set, xx, qq, ff(6:-6:-1), fphot)
            else if (LHAPDF6_AVAILABLE) then

```

```

        call data%pdf%evolve_pdfphotonm &
            (xx, qq, ff(6:-6:-1), fphot)
    end if
else
    if (data%hoppet_b_matching) then
        call hoppet_eval (xx, qq, ff(6:-6:-1))
    else
        if (LHAPDF5_AVAILABLE) then
            call evolvePDFM (data%set, xx, qq, ff(6:-6:-1))
        else if (LHAPDF6_AVAILABLE) then
            call data%pdf%evolve_pdfm (xx, qq, ff(6:-6:-1))
        end if
    end if
end if
else
    if (data%has_photon) then
        if (LHAPDF5_AVAILABLE) then
            call evolvePDFphotonM (data%set, xx, qq, ff, fphot)
        else if (LHAPDF6_AVAILABLE) then
            call data%pdf%evolve_pdfphotonm (xx, qq, ff, fphot)
        end if
    else
        if (data%hoppet_b_matching) then
            call hoppet_eval (xx, qq, ff)
        else
            if (LHAPDF5_AVAILABLE) then
                call evolvePDFM (data%set, xx, qq, ff)
            else if (LHAPDF6_AVAILABLE) then
                call data%pdf%evolve_pdfm (xx, qq, ff)
            end if
        end if
    end if
end if
else
    ss = s
    if (LHAPDF5_AVAILABLE) then
        call evolvePDFpM (data%set, xx, qq, &
            ss, data%photon_scheme, ff)
    else if (LHAPDF6_AVAILABLE) then
        call data%pdf%evolve_pdfpm (xx, qq, ss, &
            data%photon_scheme, ff)
    end if
end if
if (data%has_photon) then
    allocate (fc (count ([data%mask, data%mask_photon])))
    if (negative_sf_opt) then
        fc = pack ([ff, fphot] / x, [data%mask, data%mask_photon])
    else
        fc = max( pack ([ff, fphot] / x, [data%mask, data%mask_photon]), 0._default)
    end if
end if
else
    allocate (fc (count (data%mask)))
    if (negative_sf_opt) then
        fc = pack (ff / x, data%mask)
    end if
end if

```

```

        else
            fc = max( pack (ff / x, data%mask), 0._default)
        end if
    end if
end associate
if (debug_active (D_BEAMS)) print *, 'Set pdfs: ', real (fc)
call sf_int%set_matrix_element (fc, [(i_sub_opt * size(fc) + i, i = 1, size(fc))])
sf_int%status = SF_EVALUATED
end subroutine lhpdf_apply

```

16.16.10 Strong Coupling

Since the PDF codes provide a function for computing the running α_s value, we make this available as an implementation of the abstract `alpha_qcd_t` type, which is used for matrix element evaluation.

```

<SF lhpdf: public>+≡
    public :: alpha_qcd_lhpdf_t

<SF lhpdf: types>+≡
    type, extends (alpha_qcd_t) :: alpha_qcd_lhpdf_t
        type(string_t) :: pdfset_dir
        type(string_t) :: pdfset_file
        integer :: pdfset_member = -1
        type(lhpdf_pdf_t) :: pdf
    contains
        <SF lhpdf: alpha qcd: TBP>
    end type alpha_qcd_lhpdf_t

```

Output. As in earlier versions we leave the LHAPDF path out.

```

<SF lhpdf: alpha qcd: TBP>≡
    procedure :: write => alpha_qcd_lhpdf_write

<SF lhpdf: sub interfaces>+≡
    module subroutine alpha_qcd_lhpdf_write (object, unit)
        class(alpha_qcd_lhpdf_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine alpha_qcd_lhpdf_write

<SF lhpdf: procedures>+≡
    module subroutine alpha_qcd_lhpdf_write (object, unit)
        class(alpha_qcd_lhpdf_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A)") "QCD parameters (lhpdf):"
        write (u, "(5x,A,A)") "PDF set      = ", char (object%pdfset_file)
        write (u, "(5x,A,I0)") "PDF member = ", object%pdfset_member
    end subroutine alpha_qcd_lhpdf_write

```

Calculation: the numeric member ID selects the correct PDF set, which must be properly initialized.

```

<SF lhpdf: interfaces>+≡

```

```

interface
  double precision function alphasPDF (Q)
    double precision, intent(in) :: Q
  end function alphasPDF
end interface

<SF lhpdf: alpha qcd: TBP>+≡
  procedure :: get => alpha_qcd_lhapdf_get

<SF lhpdf: sub interfaces>+≡
  module function alpha_qcd_lhapdf_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
  end function alpha_qcd_lhapdf_get

<SF lhpdf: procedures>+≡
  module function alpha_qcd_lhapdf_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    if (LHAPDF5_AVAILABLE) then
      alpha = alphasPDF (dble (scale))
    else if (LHAPDF6_AVAILABLE) then
      alpha = alpha_qcd%pdf%alphas_pdf (dble (scale))
    end if
  end function alpha_qcd_lhapdf_get

```

Initialization. We need to access the (quasi-global) initialization status.

```

<SF lhpdf: alpha qcd: TBP>+≡
  procedure :: init => alpha_qcd_lhapdf_init

<SF lhpdf: sub interfaces>+≡
  module subroutine alpha_qcd_lhapdf_init (alpha_qcd, file, member, path)
    class(alpha_qcd_lhapdf_t), intent(out) :: alpha_qcd
    type(string_t), intent(inout) :: file
    integer, intent(inout) :: member
    type(string_t), intent(inout) :: path
  end subroutine alpha_qcd_lhapdf_init

<SF lhpdf: procedures>+≡
  module subroutine alpha_qcd_lhapdf_init (alpha_qcd, file, member, path)
    class(alpha_qcd_lhapdf_t), intent(out) :: alpha_qcd
    type(string_t), intent(inout) :: file
    integer, intent(inout) :: member
    type(string_t), intent(inout) :: path
    alpha_qcd%pdfset_file = file
    alpha_qcd%pdfset_member = member
    if (alpha_qcd%pdfset_member < 0) &
      call msg_fatal ("QCD parameter initialization: PDF set " &
        // char (file) // " is unknown")
    if (LHAPDF5_AVAILABLE) then
      call lhpdf_initialize (1, path, file, member)
    else if (LHAPDF6_AVAILABLE) then
      call lhpdf_initialize &

```

```

        (1, path, file, member, alpha_qcd%pdf)
    end if
end subroutine alpha_qcd_lhapdf_init

```

Retrieves the quark masses from the PDF.

```

⟨SF lhpdf: alpha qcd: TBP⟩+≡
    procedure :: get_qmass => alpha_qcd_lhapdf_get_qmass

⟨SF lhpdf: sub interfaces⟩+≡
    module function alpha_qcd_lhapdf_get_qmass (alpha_qcd, i_q) result (mq)
        real(default) :: mq
        class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
        integer, intent(in) :: i_q
    end function alpha_qcd_lhapdf_get_qmass

⟨SF lhpdf: procedures⟩+≡
    module function alpha_qcd_lhapdf_get_qmass (alpha_qcd, i_q) result (mq)
        real(default) :: mq
        class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
        integer, intent(in) :: i_q
        mq = alpha_qcd%pdf%get_qmass (i_q)
    end function alpha_qcd_lhapdf_get_qmass

```

Retrieves the order from the PDF.

```

⟨SF lhpdf: alpha qcd: TBP⟩+≡
    procedure :: get_order => alpha_qcd_lhapdf_get_order

⟨SF lhpdf: sub interfaces⟩+≡
    module function alpha_qcd_lhapdf_get_order (alpha_qcd) result (order)
        integer :: order
        class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
    end function alpha_qcd_lhapdf_get_order

⟨SF lhpdf: procedures⟩+≡
    module function alpha_qcd_lhapdf_get_order (alpha_qcd) result (order)
        integer :: order
        class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
        order = alpha_qcd%pdf%get_order ()
    end function alpha_qcd_lhapdf_get_order

```

16.16.11 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_lhapdf_ut.f90⟩≡
    ⟨File header⟩

    module sf_lhapdf_ut
        use unit_tests
        use system_dependencies, only: LHAPDF5_AVAILABLE
        use system_dependencies, only: LHAPDF6_AVAILABLE
        use sf_lhapdf_uti

    ⟨Standard module head⟩

```

```

    <SF lhpdf: public test>

contains

    <SF lhpdf: test driver>

end module sf_lhapdf_ut
<sf_lhapdf_uti.f90>≡
    <File header>

module sf_lhapdf_uti

    <Use kinds>
    <Use strings>
    use system_dependencies, only: LHAPDF5_AVAILABLE
    use system_dependencies, only: LHAPDF6_AVAILABLE
    use os_interface
    use physics_defs, only: PROTON
    use sm_qcd
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_base

    use sf_lhapdf

    <Standard module head>

    <SF lhpdf: test declarations>

contains

    <SF lhpdf: tests>

end module sf_lhapdf_uti
API: driver for the unit tests below.
<SF lhpdf: public test>≡
    public :: sf_lhapdf_test
<SF lhpdf: test driver>≡
    subroutine sf_lhapdf_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF lhpdf: execute tests>
    end subroutine sf_lhapdf_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF lhpdf: execute tests>≡
  if (LHAPDF5_AVAILABLE) then
    call test (sf_lhapdf_1, "sf_lhapdf5_1", &
      "structure function configuration", &
      u, results)
  else if (LHAPDF6_AVAILABLE) then
    call test (sf_lhapdf_1, "sf_lhapdf6_1", &
      "structure function configuration", &
      u, results)
  end if

<SF lhpdf: test declarations>≡
  public :: sf_lhapdf_1

<SF lhpdf: tests>≡
  subroutine sf_lhapdf_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_lhapdf_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test structure function data"
    write (u, "(A)")

    write (u, "(A)")  "* Create empty data object"
    write (u, "(A)")

    call model%init_sm_test ()
    pdg_in = PROTON

    allocate (lhpdf_data_t :: data)
    call data%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize"
    write (u, "(A)")

    select type (data)
    type is (lhpdf_data_t)
      call data%init (model, pdg_in)
    end select

    call data%write (u)

    write (u, "(A)")

    write (u, "(1x,A)")  "Outgoing particle codes:"
    call data%get_pdg_out (pdg_out)
    pdg1 = pdg_out(1)
    write (u, "(2x,99(1x,I0))")  pdg1

```



```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_lhapdf_1"

end subroutine sf_lhapdf_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```

<SF lhpdf: execute tests>+≡
  if (LHAPDF5_AVAILABLE) then
    call test (sf_lhapdf_2, "sf_lhapdf5_2", &
      "structure function instance", &
      u, results)
  else if (LHAPDF6_AVAILABLE) then
    call test (sf_lhapdf_2, "sf_lhapdf6_2", &
      "structure function instance", &
      u, results)
  end if

<SF lhpdf: test declarations>+≡
  public :: sf_lhapdf_2

<SF lhpdf: tests>+≡
  subroutine sf_lhapdf_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_lhapdf_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_sm_test ()
    call flv%init (PROTON, model)
    pdg_in = PROTON
    call lhpdf_global_reset ()

    call reset_interaction_counter ()

```

```

allocate (lhpdf_data_t :: data)
select type (data)
type is (lhpdf_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

```

```

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100 GeV"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 100._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_lhapdf_2"

end subroutine sf_lhapdf_2

```

Strong Coupling

Test α_s as an implementation of the `alpha_qcd_t` abstract type.

```

<SF lhpdf: execute tests>+≡
  if (LHAPDF5_AVAILABLE) then
    call test (sf_lhapdf_3, "sf_lhapdf5_3", &
      "running alpha_s", &
      u, results)
  else if (LHAPDF6_AVAILABLE) then
    call test (sf_lhapdf_3, "sf_lhapdf6_3", &
      "running alpha_s", &
      u, results)
  end if

<SF lhpdf: test declarations>+≡
  public :: sf_lhapdf_3

<SF lhpdf: tests>+≡
  subroutine sf_lhapdf_3 (u)
    integer, intent(in) :: u
    type(qcd_t) :: qcd
    type(string_t) :: name, path
    integer :: member

    write (u, "(A)")  "* Test output: sf_lhapdf_3"
    write (u, "(A)")  "* Purpose: initialize and evaluate alpha_s"

```

```

write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call lhpdf_global_reset ()

if (LHAPDF5_AVAILABLE) then
  name = "cteq6ll.LHpdf"
  member = 1
  path = ""
else if (LHAPDF6_AVAILABLE) then
  name = "CT10"
  member = 1
  path = ""
end if

write (u, "(A)")  "* Initialize qcd object"
write (u, "(A)")

allocate (alpha_qcd_lhpdf_t :: qcd%alpha)
select type (alpha => qcd%alpha)
type is (alpha_qcd_lhpdf_t)
  call alpha%init (name, member, path)
end select
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100"
write (u, "(A)")

write (u, "(1x,A,F8.5)")  "alpha = ", qcd%alpha%get (100._default)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_lhpdf_3"

end subroutine sf_lhpdf_3

```

16.17 Easy PDF Access

For the shower, subtraction and matching, it is very useful to have direct access to $f(x, Q)$ independently of the used library.

$\langle \text{pdf.f90} \rangle \equiv$
 $\langle \text{File header} \rangle$

module pdf

$\langle \text{Use kinds with double} \rangle$

```

        use beam_structures
        use lhpdf !NODEP!
        use pdf_builtin !NODEP!

        <Standard module head>

        <PDF: public>

        <PDF: parameters>

        <PDF: types>

        interface
        <PDF: sub interfaces>
        end interface

    end module pdf

    <pdf_sub.f90>≡
    <File header>

    submodule (pdf) pdf_s

        use io_units
        use system_dependencies, only: LHAPDF5_AVAILABLE, LHAPDF6_AVAILABLE
        use diagnostics

        implicit none

    contains

    <PDF: procedures>

    end submodule pdf_s

```

We support the following implementations:

```

    <PDF: parameters>≡
        integer, parameter, public :: STRF_NONE = 0
        integer, parameter, public :: STRF_LHAPDF6 = 1
        integer, parameter, public :: STRF_LHAPDF5 = 2
        integer, parameter, public :: STRF_PDF_BUILTIN = 3

```

A container to bundle all necessary PDF data. Could be moved to a more central location.

```

    <PDF: public>≡
        public :: pdf_data_t

    <PDF: types>≡
        type :: pdf_data_t
            type(lhpdf_pdf_t) :: pdf
            real(default) :: xmin, xmax, qmin, qmax
            integer :: type = STRF_NONE
            integer :: set = 0
        contains

```

```

    <PDF: pdf data: TBP>
    end type pdf_data_t

    <PDF: pdf data: TBP>≡
    procedure :: init => pdf_data_init

    <PDF: sub interfaces>≡
    module subroutine pdf_data_init (pdf_data, pdf_data_in)
        class(pdf_data_t), intent(out) :: pdf_data
        type(pdf_data_t), target, intent(in) :: pdf_data_in
    end subroutine pdf_data_init

    <PDF: procedures>≡
    module subroutine pdf_data_init (pdf_data, pdf_data_in)
        class(pdf_data_t), intent(out) :: pdf_data
        type(pdf_data_t), target, intent(in) :: pdf_data_in
        pdf_data%xmin = pdf_data_in%xmin
        pdf_data%xmax = pdf_data_in%xmax
        pdf_data%qmin = pdf_data_in%qmin
        pdf_data%qmax = pdf_data_in%qmax
        pdf_data%set = pdf_data_in%set
        pdf_data%type = pdf_data_in%type
        if (pdf_data%type == STRF_LHAPDF6) then
            if (pdf_data_in%pdf%is_associated ()) then
                call lhapdf_copy_pointer (pdf_data_in%pdf, pdf_data%pdf)
            else
                call msg_bug ('pdf_data_init: pdf_data%pdf was not associated!')
            end if
        end if
    end subroutine pdf_data_init

    <PDF: pdf data: TBP>+≡
    procedure :: write => pdf_data_write

    <PDF: sub interfaces>+≡
    module subroutine pdf_data_write (pdf_data, unit)
        class(pdf_data_t), intent(in) :: pdf_data
        integer, intent(in), optional :: unit
    end subroutine pdf_data_write

    <PDF: procedures>+≡
    module subroutine pdf_data_write (pdf_data, unit)
        class(pdf_data_t), intent(in) :: pdf_data
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(3x,A,I0)") "PDF set = ", pdf_data%set
        write (u, "(3x,A,I0)") "PDF type = ", pdf_data%type
    end subroutine pdf_data_write

    <PDF: pdf data: TBP>+≡
    procedure :: setup => pdf_data_setup

```

```

(PDF: sub interfaces)+≡
module subroutine pdf_data_setup &
    (pdf_data, caller, beam_structure, lhpdf_member, set)
    class(pdf_data_t), intent(inout) :: pdf_data
    character(len=*), intent(in) :: caller
    type(beam_structure_t), intent(in) :: beam_structure
    integer, intent(in) :: lhpdf_member, set
end subroutine pdf_data_setup

(PDF: procedures)+≡
module subroutine pdf_data_setup &
    (pdf_data, caller, beam_structure, lhpdf_member, set)
    class(pdf_data_t), intent(inout) :: pdf_data
    character(len=*), intent(in) :: caller
    type(beam_structure_t), intent(in) :: beam_structure
    integer, intent(in) :: lhpdf_member, set
    real(default) :: xmin, xmax, q2min, q2max
    pdf_data%set = set
    if (beam_structure%contains ("lhpdf")) then
        if (LHAPDF6_AVAILABLE) then
            pdf_data%type = STRF_LHAPDF6
        else if (LHAPDF5_AVAILABLE) then
            pdf_data%type = STRF_LHAPDF5
        end if
        write (msg_buffer, "(A,I0)") caller &
            // ": interfacing LHAPDF set #", pdf_data%set
        call msg_message ()
    else if (beam_structure%contains ("pdf_builtin")) then
        pdf_data%type = STRF_PDF_BUILTIN
        write (msg_buffer, "(A,I0)") caller &
            // ": interfacing PDF builtin set #", pdf_data%set
        call msg_message ()
    end if
    select case (pdf_data%type)
    case (STRF_LHAPDF6)
        pdf_data%xmin = pdf_data%pdf%getxmin ()
        pdf_data%xmax = pdf_data%pdf%getxmax ()
        pdf_data%qmin = sqrt(pdf_data%pdf%getq2min ())
        pdf_data%qmax = sqrt(pdf_data%pdf%getq2max ())
    case (STRF_LHAPDF5)
        call GetXminM (1, lhpdf_member, xmin)
        call GetXmaxM (1, lhpdf_member, xmax)
        call GetQ2minM (1, lhpdf_member, q2min)
        call GetQ2maxM (1, lhpdf_member, q2max)
        pdf_data%xmin = xmin
        pdf_data%xmax = xmax
        pdf_data%qmin = sqrt(q2min)
        pdf_data%qmax = sqrt(q2max)
    end select
end subroutine pdf_data_setup

```

This could be overloaded with a version that only asks for a specific flavor as it is supported by LHAPDF6.

```

(PDF: pdf data: TBP)+≡

```

```

    procedure :: evolve => pdf_data_evolve
  <PDF: sub interfaces>+≡
    module subroutine pdf_data_evolve (pdf_data, x, q_in, f)
      class(pdf_data_t), intent(inout) :: pdf_data
      real(double), intent(in) :: x, q_in
      real(double), dimension(-6:6), intent(out) :: f
    end subroutine pdf_data_evolve
  <PDF: procedures>+≡
    module subroutine pdf_data_evolve (pdf_data, x, q_in, f)
      class(pdf_data_t), intent(inout) :: pdf_data
      real(double), intent(in) :: x, q_in
      real(double), dimension(-6:6), intent(out) :: f
      real(double) :: q
      select case (pdf_data%type)
      case (STRF_PDF_BUILTIN)
        call pdf_evolve_LHAPDF (pdf_data%set, x, q_in, f)
      case (STRF_LHAPDF6)
        q = min (pdf_data%qmax, q_in)
        q = max (pdf_data%qmin, q)
        call pdf_data%pdf%evolve_pdfm (x, q, f)
      case (STRF_LHAPDF5)
        q = min (pdf_data%qmax, q_in)
        q = max (pdf_data%qmin, q)
        call evolvePDFM (pdf_data%set, x, q, f)
      case default
        call msg_fatal ("PDF function: unknown PDF method.")
      end select
    end subroutine pdf_data_evolve

```

16.18 Dispatch

```

  <dispatch_beams.f90>≡
  <File header>

  module dispatch_beams

    <Use kinds>
    <Use strings>
    use constants, only: PI, one
    use numeric_utils, only: vanishes
    use diagnostics
    use os_interface, only: os_data_t
    use variables, only: var_list_t
    use rng_base, only: rng_factory_t
    use pdg_arrays
    use model_data, only: model_data_t
    use flavors, only: flavor_t
    use physics_defs, only: PHOTON
    use physics_defs, only: MZ_REF, ME_REF, ALPHA_QCD_MZ_REF, ALPHA_QED_ME_REF
    use sm_qcd, only: qcd_t, alpha_qcd_fixed_t, alpha_qcd_from_scale_t
    use sm_qcd, only: alpha_qcd_from_lambda_t
    use sm_qed, only: qed_t, alpha_qed_fixed_t, alpha_qed_from_scale_t

```



```

    use beam_structures
    use dispatch_rng, only: dispatch_rng_factory
    use dispatch_rng, only: update_rng_seed_in_var_list
    use sf_base
    use sf_mappings
    use sf_isr
    use sf_epa
    use sf_ewa
    use sf_escan
    use sf_gaussian
    use sf_beam_events
    use sf_circe1
    use sf_circe2
    use sf_pdf_builtin
    use sf_lhapdf

    <Standard module head>

    <Dispatch beams: public>

    <Dispatch beams: types>

    <Dispatch beams: variables>

    interface
    <Dispatch beams: sub interfaces>
    end interface

contains

    <Dispatch beams: main procedures>

end module dispatch_beams
<dispatch_beams_sub.f90>≡
    <File header>

    submodule (dispatch_beams) dispatch_beams_s

        implicit none

contains

    <Dispatch beams: procedures>

end submodule dispatch_beams_s

```

This data type is a container for transferring structure-function specific data from the `dispatch_sf_data` to the `dispatch_sf_channels` subroutine.

```

    <Dispatch beams: public>≡
        public :: sf_prop_t
    <Dispatch beams: types>≡
        type :: sf_prop_t
            real(default), dimension(2) :: isr_eps = 1

```

```
end type sf_prop_t
```

Allocate a structure-function configuration object according to the `sf_method` string.

The `sf_prop` object can be used to transfer structure-function specific data up and to the `dispatch_sf_channels` subroutine below, so they can be used for particular mappings.

The `var_list_global` object is used for the RNG generator seed. It is `intent(inout)` because the RNG generator seed may change during initialization.

The `pdg_in` array is the array of incoming flavors, corresponding to the upstream structure function or the beam array. This will be checked for the structure function in question and replaced by the outgoing flavors. The `pdg_prc` array is the array of incoming flavors (beam index, component index) for the hard process. Due to a bug in gfortran 7/8/9 this has to remain in the main module.

(Dispatch beams: public)+≡

```
public :: dispatch_sf_data
```

(Dispatch beams: main procedures)≡

```
subroutine dispatch_sf_data (data, sf_method, i_beam, sf_prop, &
    var_list, var_list_global, model, &
    os_data, sqrts, pdg_in, pdg_prc, polarized)
    class(sf_data_t), allocatable, intent(inout) :: data
    type(string_t), intent(in) :: sf_method
    integer, dimension(:), intent(in) :: i_beam
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_in
    type(pdg_array_t), dimension(:, :), intent(in) :: pdg_prc
    type(sf_prop_t), intent(inout) :: sf_prop
    type(var_list_t), intent(in) :: var_list
    type(var_list_t), intent(inout) :: var_list_global
    integer :: next_rng_seed
    class(model_data_t), target, intent(in) :: model
    type(os_data_t), intent(in) :: os_data
    real(default), intent(in) :: sqrts
    logical, intent(in) :: polarized
    type(pdg_array_t), dimension(:), allocatable :: pdg_out
    real(default) :: isr_alpha, isr_q_max, isr_mass
    integer :: isr_order
    logical :: isr_recoil, isr_keep_energy
    real(default) :: epa_alpha, epa_x_min, epa_q_min, epa_q_max, epa_mass
    logical :: epa_recoil, epa_keep_energy
    integer :: epa_int_mode
    type(string_t) :: epa_mode
    real(default) :: ewa_x_min, ewa_pt_max, ewa_mass
    logical :: ewa_recoil, ewa_keep_energy
    type(pdg_array_t), dimension(:), allocatable :: pdg_prc1
    integer :: ewa_id
    type(string_t) :: pdf_name
    type(string_t) :: lhpdf_dir, lhpdf_file
    type(string_t), dimension(13) :: lhpdf_photon_sets
    integer :: lhpdf_member, lhpdf_photon_scheme
    logical :: hoppet_b_matching
    class(rng_factory_t), allocatable :: rng_factory
```

```

logical :: circe1_photon1, circe1_photon2, circe1_generate, &
    circe1_with_radiation
real(default) :: circe1_sqrts, circe1_eps
integer :: circe1_version, circe1_chattiness, &
    circe1_revision
character(6) :: circe1_accelerator
logical :: circe2_polarized
type(string_t) :: circe2_design, circe2_file
real(default), dimension(2) :: gaussian_spread
logical :: beam_events_warn_eof
type(string_t) :: beam_events_dir, beam_events_file
logical :: escan_normalize
integer :: i
lhpdf_photon_sets = [var_str ("DOG0.LHgrid"), var_str ("DOG1.LHgrid"), &
    var_str ("DGG.LHgrid"), var_str ("LACG.LHgrid"), &
    var_str ("GSG0.LHgrid"), var_str ("GSG1.LHgrid"), &
    var_str ("GSG960.LHgrid"), var_str ("GSG961.LHgrid"), &
    var_str ("GRVG0.LHgrid"), var_str ("GRVG1.LHgrid"), &
    var_str ("ACFGPG.LHgrid"), var_str ("WHITG.LHgrid"), &
    var_str ("SASG.LHgrid")]
select case (char (sf_method))
case ("pdf_builtin")
    allocate (pdf_builtin_data_t :: data)
    select type (data)
    type is (pdf_builtin_data_t)
        pdf_name = &
            var_list%get_sval (var_str ("pdf_builtin_set"))
        hoppet_b_matching = &
            var_list%get_lval (var_str ("hoppet_b_matching"))
        call data%init ( &
            model, pdg_in(i_beam(1)), &
            name = pdf_name, &
            path = os_data%pdf_builtin_datapath, &
            hoppet_b_matching = hoppet_b_matching)
    end select
case ("pdf_builtin_photon")
    call msg_fatal ("Currently, there are no photon PDFs built into WHIZARD,", &
        [var_str ("for the photon content inside a proton or neutron use"), &
        var_str ("the 'lhpdf_photon' structure function.")])
case ("lhpdf")
    allocate (lhpdf_data_t :: data)
    if (pdg_in(i_beam(1))%get (1) == PHOTON) then
        call msg_fatal ("The 'lhpdf' structure is intended only for protons and", &
            [var_str ("pions, please use 'lhpdf_photon' for photon beams.")])
    end if
    lhpdf_dir = &
        var_list%get_sval (var_str ("lhpdf_dir"))
    lhpdf_file = &
        var_list%get_sval (var_str ("lhpdf_file"))
    lhpdf_member = &
        var_list%get_ival (var_str ("lhpdf_member"))
    lhpdf_photon_scheme = &
        var_list%get_ival (var_str ("lhpdf_photon_scheme"))
    hoppet_b_matching = &

```

```

        var_list%get_lval (var_str ("?hoppet_b_matching"))
select type (data)
type is (lhpdf_data_t)
    call data%init &
        (model, pdg_in(i_beam(1)), &
        lhpdf_dir, lhpdf_file, lhpdf_member, &
        lhpdf_photon_scheme, hoppet_b_matching)
end select
case ("lhpdf_photon")
    allocate (lhpdf_data_t :: data)
    if (pdg_in(i_beam(1))%get_length () /= 1 .or. &
        pdg_in(i_beam(1))%get (1) /= PHOTON) then
        call msg_fatal ("The 'lhpdf_photon' structure function is exclusively for", &
            [var_str ("photon PDFs, i.e. for photons as beam particles")])
    end if
    lhpdf_dir = &
        var_list%get_sval (var_str ("$lhpdf_dir"))
    lhpdf_file = &
        var_list%get_sval (var_str ("$lhpdf_photon_file"))
    lhpdf_member = &
        var_list%get_ival (var_str ("lhpdf_member"))
    lhpdf_photon_scheme = &
        var_list%get_ival (var_str ("lhpdf_photon_scheme"))
    if (.not. any (lhpdf_photon_sets == lhpdf_file)) then
        call msg_fatal ("This PDF set is not supported or not " // &
            "intended for photon beams.")
    end if
    select type (data)
    type is (lhpdf_data_t)
        call data%init &
            (model, pdg_in(i_beam(1)), &
            lhpdf_dir, lhpdf_file, lhpdf_member, &
            lhpdf_photon_scheme)
    end select
case ("isr")
    allocate (isr_data_t :: data)
    isr_alpha = &
        var_list%get_rval (var_str ("isr_alpha"))
    if (vanishes (isr_alpha)) then
        isr_alpha = (var_list%get_rval (var_str ("ee"))) &
            ** 2 / (4 * PI)
    end if
    isr_q_max = &
        var_list%get_rval (var_str ("isr_q_max"))
    if (vanishes (isr_q_max)) then
        isr_q_max = sqrts
    end if
    isr_mass = var_list%get_rval (var_str ("isr_mass"))
    isr_order = var_list%get_ival (var_str ("isr_order"))
    isr_recoil = var_list%get_lval (var_str ("?isr_recoil"))
    isr_keep_energy = var_list%get_lval (var_str ("?isr_keep_energy"))
    select type (data)
    type is (isr_data_t)
        call data%init &

```

```

        (model, pdg_in (i_beam(1)), isr_alpha, isr_q_max, &
        isr_mass, isr_order, recoil = isr_recoil, keep_energy = &
        isr_keep_energy)
    call data%check ()
    sf_prop%isr_eps(i_beam(1)) = data%get_eps ()
end select
case ("epa")
    allocate (epa_data_t :: data)
    epa_mode = var_list%get_sval (var_str ("epa_mode"))
    epa_int_mode = 0
    epa_alpha = var_list%get_rval (var_str ("epa_alpha"))
    if (vanishes (epa_alpha)) then
        epa_alpha = (var_list%get_rval (var_str ("ee"))) &
            ** 2 / (4 * PI)
    end if
    epa_x_min = var_list%get_rval (var_str ("epa_x_min"))
    epa_q_min = var_list%get_rval (var_str ("epa_q_min"))
    epa_q_max = var_list%get_rval (var_str ("epa_q_max"))
    if (vanishes (epa_q_max)) then
        epa_q_max = sqrts
    end if
    select case (char (epa_mode))
    case ("default", "Budnev_617")
        epa_int_mode = 0
    case ("Budnev_616e")
        epa_int_mode = 1
    case ("log_power")
        epa_int_mode = 2
        epa_q_max = sqrts
    case ("log_simple")
        epa_int_mode = 3
        epa_q_max = sqrts
    case ("log")
        epa_int_mode = 4
        epa_q_max = sqrts
    case default
        call msg_fatal ("EPA: unsupported EPA mode; please choose " // &
            "'default', 'Budnev_616', 'Budnev_616e', 'log_power', " // &
            "'log_simple', or 'log'")
    end select
    epa_mass = var_list%get_rval (var_str ("epa_mass"))
    epa_recoil = var_list%get_lval (var_str ("?epa_recoil"))
    epa_keep_energy = var_list%get_lval (var_str ("?epa_keep_energy"))
    select type (data)
    type is (epa_data_t)
        call data%init &
            (model, epa_int_mode, pdg_in (i_beam(1)), epa_alpha, &
            epa_x_min, epa_q_min, epa_q_max, epa_mass, &
            recoil = epa_recoil, keep_energy = epa_keep_energy)
        call data%check ()
    end select
case ("ewa")
    allocate (ewa_data_t :: data)
    allocate (pdg_prc1 (size (pdg_prc, 2)))

```

```

pdg_prc1 = pdg_prc(i_beam(1),:)
if (any (pdg_prc1%get_length () /= 1) &
    .or. any (pdg_prc1 /= pdg_prc1(1))) then
    call msg_fatal &
        ("EWA: process incoming particle (W/Z) must be unique")
end if
ewa_id = abs (pdg_prc1(1)%get (1))
ewa_x_min = var_list%get_rval (var_str ("ewa_x_min"))
ewa_pt_max = var_list%get_rval (var_str ("ewa_pt_max"))
if (vanishes (ewa_pt_max)) then
    ewa_pt_max = sqrts
end if
ewa_mass = var_list%get_rval (var_str ("ewa_mass"))
ewa_recoil = var_list%get_lval (&
    var_str ("?ewa_recoil"))
ewa_keep_energy = var_list%get_lval (&
    var_str ("?ewa_keep_energy"))
select type (data)
type is (ewa_data_t)
    call data%init &
        (model, pdg_in (i_beam(1)), ewa_x_min, &
        ewa_pt_max, sqrts, ewa_recoil, &
        ewa_keep_energy, ewa_mass)
    call data%set_id (ewa_id)
    call data%check ()
end select
case ("circe1")
    allocate (circe1_data_t :: data)
    select type (data)
    type is (circe1_data_t)
        circe1_photon1 = &
            var_list%get_lval (var_str ("?circe1_photon1"))
        circe1_photon2 = &
            var_list%get_lval (var_str ("?circe1_photon2"))
        circe1_sqrts = &
            var_list%get_rval (var_str ("circe1_sqrts"))
        circe1_eps = &
            var_list%get_rval (var_str ("circe1_eps"))
        if (circe1_sqrts <= 0) circe1_sqrts = sqrts
        circe1_generate = &
            var_list%get_lval (var_str ("?circe1_generate"))
        circe1_version = &
            var_list%get_ival (var_str ("circe1_ver"))
        circe1_revision = &
            var_list%get_ival (var_str ("circe1_rev"))
        circe1_accelerator = &
            char (var_list%get_sval (var_str ("$circe1_acc")))
        circe1_chattiness = &
            var_list%get_ival (var_str ("circe1_chat"))
        circe1_with_radiation = &
            var_list%get_lval (var_str ("?circe1_with_radiation"))
        call data%init (model, pdg_in, circe1_sqrts, circe1_eps, &
            [circe1_photon1, circe1_photon2], &
            circe1_version, circe1_revision, circe1_accelerator, &

```

```

        circe1_chattiness, circe1_with_radiation)
    if (circe1_generate) then
        call msg_message ("CIRCE1: activating generator mode")
        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%set_generator_mode (rng_factory)
    end if
end select
case ("circe2")
    allocate (circe2_data_t :: data)
    select type (data)
    type is (circe2_data_t)
        circe2_polarized = &
            var_list%get_lval (var_str ("?circe2_polarized"))
        circe2_file = &
            var_list%get_sval (var_str ("$circe2_file"))
        circe2_design = &
            var_list%get_sval (var_str ("$circe2_design"))
        call data%init (os_data, model, pdg_in, sqrts, &
            circe2_polarized, polarized, circe2_file, circe2_design)
        call msg_message ("CIRCE2: activating generator mode")
        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%set_generator_mode (rng_factory)
    end select
case ("gaussian")
    allocate (gaussian_data_t :: data)
    select type (data)
    type is (gaussian_data_t)
        gaussian_spread = &
            [var_list%get_rval (var_str ("gaussian_spread1")), &
            var_list%get_rval (var_str ("gaussian_spread2"))]
        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%init (model, pdg_in, gaussian_spread, rng_factory)
    end select
case ("beam_events")
    allocate (beam_events_data_t :: data)
    select type (data)
    type is (beam_events_data_t)
        beam_events_dir = os_data%whizard_beamsimpath
        beam_events_file = var_list%get_sval (&
            var_str ("$beam_events_file"))
        beam_events_warn_eof = var_list%get_lval (&
            var_str ("?beam_events_warn_eof"))
        call data%init (model, pdg_in, &
            beam_events_dir, beam_events_file, beam_events_warn_eof)
    end select
case ("energy_scan")
    escan_normalize = &
        var_list%get_lval (var_str ("?energy_scan_normalize"))

```

```

allocate (escan_data_t :: data)
select type (data)
type is (escan_data_t)
  if (escan_normalize) then
    call data%init (model, pdg_in)
  else
    call data%init (model, pdg_in, sqrts)
  end if
end select
case default
  if (associated (dispatch_sf_data_extra)) then
    call dispatch_sf_data_extra (data, sf_method, i_beam, &
      sf_prop, var_list, var_list_global, model, os_data, sqrts, pdg_in, &
      pdg_prc, polarized)
  end if
  if (.not. allocated (data)) then
    call msg_fatal ("Structure function '" &
      // char (sf_method) // "' not implemented")
  end if
end select
if (allocated (data)) then
  allocate (pdg_out (size (pdg_prc, 1)))
  call data%get_pdg_out (pdg_out)
  do i = 1, size (i_beam)
    pdg_in(i_beam(i)) = pdg_out(i)
  end do
end if
end subroutine dispatch_sf_data

```

This is a hook that allows us to inject further handlers for structure-function objects, in particular a test structure function.

```

<Dispatch beams: public>+≡
  public :: dispatch_sf_data_extra

<Dispatch beams: variables>≡
  procedure (dispatch_sf_data), pointer :: &
    dispatch_sf_data_extra => null ()

```

This is an auxiliary procedure, used by the beam-structure expansion: tell for a given structure function name, whether it corresponds to a pair spectrum ($n = 2$), a single-particle structure function ($n = 1$), or nothing ($n = 0$). Though **energy_scan** can in principle also be a pair spectrum, it always has only one parameter.

```

<Dispatch beams: public>+≡
  public :: strfun_mode

<Dispatch beams: sub interfaces>≡
  module function strfun_mode (name) result (n)
    type(string_t), intent(in) :: name
    integer :: n
  end function strfun_mode

<Dispatch beams: procedures>≡
  module function strfun_mode (name) result (n)
    type(string_t), intent(in) :: name

```



```

integer :: n
select case (char (name))
case ("none")
  n = 0
case ("sf_test_0", "sf_test_1")
  n = 1
case ("pdf_builtin", "pdf_builtin_photon", &
      "lhpdf", "lhpdf_photon")
  n = 1
case ("isr", "epa", "ewa")
  n = 1
case ("circe1", "circe2")
  n = 2
case ("gaussian")
  n = 2
case ("beam_events")
  n = 2
case ("energy_scan")
  n = 2
case default
  n = -1
  call msg_bug ("Structure function '" // char (name) &
               // "' not supported yet")
end select
end function strfun_mode

```

Dispatch a whole structure-function chain, given beam data and beam structure data.

This could be done generically, but we should look at the specific combination of structure functions in order to select appropriate mappings.

The `beam_structure` argument gets copied because we want to expand it to canonical form (one valid structure-function entry per record) before proceeding further.

The `pdg_prc` argument is the array of incoming flavors. The first index is the beam index, the second one the process component index. Each element is itself a PDG array, nontrivial if there is a flavor sum for the incoming state of this component.

The dispatcher is divided in two parts. The first part configures the structure function data themselves. After this, we can configure the phase space for the elementary process.

<Dispatch beams: public>+≡

```
public :: dispatch_sf_config
```

<Dispatch beams: sub interfaces>+≡

```

module subroutine dispatch_sf_config (sf_config, sf_prop, beam_structure, &
  var_list, var_list_global, model, os_data, sqrts, pdg_prc)
  type(sf_config_t), dimension(:), allocatable, intent(out) :: sf_config
  type(sf_prop_t), intent(out) :: sf_prop
  type(beam_structure_t), intent(inout) :: beam_structure
  type(var_list_t), intent(in) :: var_list
  type(var_list_t), intent(inout) :: var_list_global
  class(model_data_t), target, intent(in) :: model
  type(os_data_t), intent(in) :: os_data

```

```

    real(default), intent(in) :: sqrts
    class(sf_data_t), allocatable :: sf_data
    type(beam_structure_t) :: beam_structure_tmp
    type(pdg_array_t), dimension(:,:), intent(in) :: pdg_prc
    type(string_t), dimension(:), allocatable :: prt_in
    type(pdg_array_t), dimension(:), allocatable :: pdg_in
end subroutine dispatch_sf_config

<Dispatch beams: procedures>+≡
module subroutine dispatch_sf_config (sf_config, sf_prop, beam_structure, &
    var_list, var_list_global, model, os_data, sqrts, pdg_prc)
    type(sf_config_t), dimension(:), allocatable, intent(out) :: sf_config
    type(sf_prop_t), intent(out) :: sf_prop
    type(beam_structure_t), intent(inout) :: beam_structure
    type(var_list_t), intent(in) :: var_list
    type(var_list_t), intent(inout) :: var_list_global
    class(model_data_t), target, intent(in) :: model
    type(os_data_t), intent(in) :: os_data
    real(default), intent(in) :: sqrts
    class(sf_data_t), allocatable :: sf_data
    type(beam_structure_t) :: beam_structure_tmp
    type(pdg_array_t), dimension(:,:), intent(in) :: pdg_prc
    type(string_t), dimension(:), allocatable :: prt_in
    type(pdg_array_t), dimension(:), allocatable :: pdg_in
    type(flavor_t) :: flv_in
    integer :: n_beam, n_record, i
    beam_structure_tmp = beam_structure
    call beam_structure_tmp%expand (strfun_mode)
    n_record = beam_structure_tmp%get_n_record ()
    allocate (sf_config (n_record))
    n_beam = beam_structure_tmp%get_n_beam ()
    if (n_beam > 0) then
        allocate (prt_in (n_beam), pdg_in (n_beam))
        prt_in = beam_structure_tmp%get_prt ()
        do i = 1, n_beam
            call flv_in%init (prt_in(i), model)
            pdg_in(i) = flv_in%get_pdg ()
        end do
    else
        n_beam = size (pdg_prc, 1)
        allocate (pdg_in (n_beam))
        pdg_in = pdg_prc(:,1)
    end if
    do i = 1, n_record
        call dispatch_sf_data (sf_data, &
            beam_structure_tmp%get_name (i), &
            beam_structure_tmp%get_i_entry (i), &
            sf_prop, var_list, var_list_global, model, os_data, sqrts, &
            pdg_in, pdg_prc, &
            beam_structure_tmp%polarized ())
        call sf_config(i)%init (beam_structure_tmp%get_i_entry (i), sf_data)
        deallocate (sf_data)
    end do
end subroutine dispatch_sf_config

```

16.18.1 QCD and QED coupling

Allocate the `alpha` (running coupling) component of the `qcd` block with a concrete implementation, depending on the variable settings in the `global` record.

If a fixed α_s is requested, we do not allocate the `qcd%alpha` object. In this case, the matrix element code will just take the model parameter as-is, which implies fixed α_s . If the object is allocated, the α_s value is computed and updated for each matrix-element call.

Also fetch the `alphas_nf` variable from the list and store it in the QCD record. This is not used in the α_s calculation, but the QCD record thus becomes a messenger for this user parameter. Gfortran 7/8/9 bug: has to be part of main module.

```

(Dispatch beams: public)+≡
    public :: dispatch_qcd

(Dispatch beams: main procedures)+≡
    subroutine dispatch_qcd (qcd, var_list, os_data)
        type(qcd_t), intent(inout) :: qcd
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        logical :: fixed, from_mz, from_pdf_builtin, from_lhapdf, from_lambda_qcd
        real(default) :: mz, alpha_val, lambda
        integer :: nf, order, lhpdf_member
        type(string_t) :: pdfset, lhpdf_dir, lhpdf_file
        call unpack_variables ()
        if (allocated (qcd%alpha)) deallocate (qcd%alpha)
        if (from_lhapdf .and. from_pdf_builtin) then
            call msg_fatal (" Mixing alphas evolution", &
                [var_str (" from LHAPDF and builtin PDF is not permitted")])
        end if
        select case (count ([from_mz, from_pdf_builtin, from_lhapdf, from_lambda_qcd]))
        case (0)
            if (fixed) then
                allocate (alpha_qcd_fixed_t :: qcd%alpha)
            else
                call msg_fatal ("QCD alpha: no calculation mode set")
            end if
        case (2:)
            call msg_fatal ("QCD alpha: calculation mode is ambiguous")
        case (1)
            if (fixed) then
                call msg_fatal ("QCD alpha: use '?alphas_is_fixed = false' for " // &
                    "running alphas")
            else if (from_mz) then
                allocate (alpha_qcd_from_scale_t :: qcd%alpha)
            else if (from_pdf_builtin) then
                allocate (alpha_qcd_pdf_builtin_t :: qcd%alpha)
            else if (from_lhapdf) then
                allocate (alpha_qcd_lhapdf_t :: qcd%alpha)
            else if (from_lambda_qcd) then
                allocate (alpha_qcd_from_lambda_t :: qcd%alpha)
            end if
            call msg_message ("QCD alpha: using a running strong coupling")
        end select
    end subroutine

```

```

    call init_alpha ()
    qcd%n_f = var_list%get_ival (var_str ("alphas_nf"))
contains
  (Dispatch qcd: dispatch qcd: procedures)
end subroutine dispatch_qcd

```

```

(Dispatch qcd: dispatch qcd: procedures)≡
subroutine unpack_variables ()
  fixed = var_list%get_lval (var_str ("?alphas_is_fixed"))
  from_mz = var_list%get_lval (var_str ("?alphas_from_mz"))
  from_pdf_builtin = &
    var_list%get_lval (var_str ("?alphas_from_pdf_builtin"))
  from_lhapdf = &
    var_list%get_lval (var_str ("?alphas_from_lhapdf"))
  from_lambda_qcd = &
    var_list%get_lval (var_str ("?alphas_from_lambda_qcd"))
  pdfset = var_list%get_sval (var_str ("pdf_builtin_set"))
  lambda = var_list%get_rval (var_str ("lambda_qcd"))
  nf = var_list%get_ival (var_str ("alphas_nf"))
  order = var_list%get_ival (var_str ("alphas_order"))
  lhpdf_dir = var_list%get_sval (var_str ("lhpdf_dir"))
  lhpdf_file = var_list%get_sval (var_str ("lhpdf_file"))
  lhpdf_member = var_list%get_ival (var_str ("lhpdf_member"))
  if (var_list%contains (var_str ("mZ"))) then
    mz = var_list%get_rval (var_str ("mZ"))
  else
    mz = MZ_REF
  end if
  if (var_list%contains (var_str ("alphas"))) then
    alpha_val = var_list%get_rval (var_str ("alphas"))
  else
    alpha_val = ALPHA_QCD_MZ_REF
  end if
end subroutine unpack_variables

```

```

(Dispatch qcd: dispatch qcd: procedures)+≡
subroutine init_alpha ()
  select type (alpha => qcd%alpha)
  type is (alpha_qcd_fixed_t)
    alpha%val = alpha_val
  type is (alpha_qcd_from_scale_t)
    alpha%mu_ref = mz
    alpha%ref = alpha_val
    alpha%order = order
    alpha%nf = nf
  type is (alpha_qcd_from_lambda_t)
    alpha%lambda = lambda
    alpha%order = order
    alpha%nf = nf
  type is (alpha_qcd_pdf_builtin_t)
    call alpha%init (pdfset, &
      os_data%pdf_builtin_datapath)
  type is (alpha_qcd_lhapdf_t)

```

```

        call alpha%init (lhpdf_file, lhpdf_member, lhpdf_dir)
    end select
end subroutine init_alpha

```

Same for QED. Gfortran 7/8/9: has to be part of main module.

```

<Dispatch beams: public>+=
    public :: dispatch_qed

<Dispatch beams: main procedures>+=
    subroutine dispatch_qed (qed, var_list)
        type(qed_t), intent(inout) :: qed
        type(var_list_t), intent(in) :: var_list
        logical :: fixed, from_me, analytic
        real(default) :: me, alpha_val
        integer :: nf, nlep, order
        call unpack_variables ()
        if (allocated (qed%alpha)) deallocate (qed%alpha)
        select case (count ([from_me]))
        case (0)
            if (fixed) then
                allocate (alpha_qed_fixed_t :: qed%alpha)
            else
                call msg_fatal ("QED alpha: no calculation mode set")
            end if
        case (2:)
            call msg_fatal ("QED alpha: calculation mode is ambiguous")
        case (1)
            if (fixed) then
                call msg_fatal ("QED alpha: use '?alphas_is_fixed = false' for " // &
                    "running alpha")
            else if (from_me) then
                allocate (alpha_qed_from_scale_t :: qed%alpha)
            end if
            call msg_message ("QED alpha: using a running electromagnetic coupling")
        end select
        call init_alpha ()
        if (var_list%get_ival (var_str ("alpha_nf")) == -1) then
            qed%n_f = var_list%get_ival (var_str ("alphas_nf"))
        else
            qed%n_f = var_list%get_ival (var_str ("alpha_nf"))
        end if
        qed%n_lep = var_list%get_ival (var_str ("alpha_nlep"))
    contains
    <Dispatch qed: dispatch qed: procedures>
    end subroutine dispatch_qed

```

```

<Dispatch qed: dispatch qed: procedures>=
    subroutine unpack_variables ()
        fixed = var_list%get_lval (var_str ("?alpha_is_fixed"))
        from_me = var_list%get_lval (var_str ("?alpha_from_me"))
        if (var_list%get_ival (var_str ("alpha_nf")) == -1) then
            nf = var_list%get_ival (var_str ("alphas_nf"))
        else

```

```

        nf = var_list%get_ival (var_str ("alpha_nf"))
    end if
    analytic = var_list%get_lval (var_str ("?alpha_evolve_analytic"))
    nlep = var_list%get_ival (var_str ("alpha_nlep"))
    order = var_list%get_ival (var_str ("alpha_order"))
    if (var_list%contains (var_str ("me"))) then
        me = var_list%get_rval (var_str ("me"))
    else
        me = ME_REF
    end if
    if (var_list%contains (var_str ("alpha_em_i"))) then
        alpha_val = one / var_list%get_rval (var_str ("alpha_em_i"))
    else
        alpha_val = ALPHA_QED_ME_REF
    end if
end subroutine unpack_variables

```

<Dispatch qed: dispatch qed: procedures>+≡

```

subroutine init_alpha ()
    select type (alpha => qed%alpha)
    type is (alpha_qed_fixed_t)
        alpha%val = alpha_val
    type is (alpha_qed_from_scale_t)
        alpha%mu_ref = me
        alpha%ref = alpha_val
        alpha%order = order
        alpha%nf = nf
        alpha%nlep = nlep
        alpha%analytic = analytic
    end select
end subroutine init_alpha

```

Chapter 17

Interface for Matrix Element Objects

These modules manage internal and, in particular, external matrix-element code.

prc_core We define the abstract `prc_core_t` type which handles all specific features of kinematics matrix-element evaluation that depend on a particular class of processes. This abstract type supplements the `prc_core_def_t` type and related types in another module. Together, they provide a complete set of matrix-element handlers that are implemented in the concrete types below.

These are the implementations:

prc_template_me Implements matrix-element code without actual content (trivial value), but full-fledged interface. This can be used for injecting user-defined matrix-element code.

prc_omega Matrix elements calculated by O'MEGA are the default for WHIZARD. Here, we provide all necessary support.

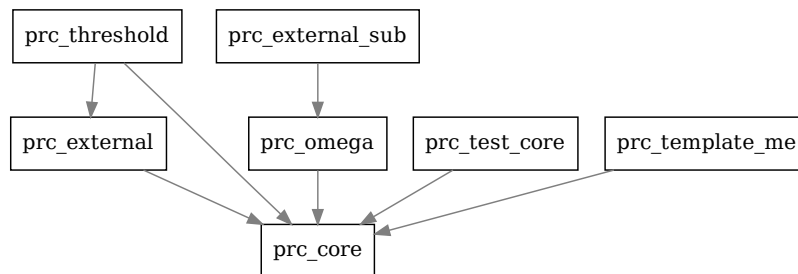


Figure 17.1: Module dependencies in `src/me_methods`.

prc_external Matrix elements provided or using external (not O’MEGA) code or libraries. This is an abstract type, with concrete extensions below:

prc_external_test Concrete implementation of the external-code type, actually using some pre-defined test matrix elements.

prc_gosam Interface for matrix elements computed using GoSam.

prc_openloops Interface for matrix elements computed using OpenLoops.

prc_recola Interface for matrix elements computed using Recola.

prc_threshold Interface for matrix elements for the top-pair threshold, that use external libraries.

17.1 Abstract process core

In this module we provide abstract data types for process classes. Each process class represents a set of processes which are handled by a common “method”, e.g., by the O’MEGA matrix-element generator. The process class is also able to select a particular implementation for the phase-space and integration modules.

For a complete implementation of a process class, we have to provide extensions of the following abstract types:

prc_core_def_t process and matrix-element configuration

prc_writer_t (optional) writing external matrix-element code

prc_driver_t accessing the matrix element (internal or external)

prc_core_t evaluating kinematics and matrix element. The process core also selects phase-space and integrator implementations as appropriate for the process class and configuration.

In the actual process-handling data structures, each process component contains an instance of such a process class as its core. This allows us to keep the **processes** module below, which supervises matrix-element evaluation, integration, and event generation, free of any reference to concrete implementations (for the process class, phase space, and integrator).

There are no unit tests, these are deferred to the **processes** module.

```
(prc_core.f90)≡
  <File header>
  module prc_core

    <Use kinds>
    <Use strings>
    use io_units
    use diagnostics
    use os_interface, only: os_data_t
    use lorentz
    use interactions
    use variables, only: var_list_t
    use model_data, only: model_data_t
```



```

    use process_constants
    use prc_core_def
    use process_libraries
    use sf_base

    <Standard module head>

    <Prc core: public>

    <Prc core: types>

    <Prc core: interfaces>

    interface
    <Prc core: sub interfaces>
    end interface

    end module prc_core
    <prc_core_sub.f90>≡
    <File header>

    submodule (prc_core) prc_core_s

        implicit none

    contains

    <Prc core: procedures>

    end submodule prc_core_s

```

17.1.1 The process core

The process core is of abstract data type. Different types of matrix elements will be represented by different implementations.

```

    <Prc core: public>≡
    public :: prc_core_t

    <Prc core: types>≡
    type, abstract :: prc_core_t
    class(prc_core_def_t), pointer :: def => null ()
    logical :: data_known = .false.
    type(process_constants_t) :: data
    class(prc_core_driver_t), allocatable :: driver
    logical :: use_color_factors = .false.
    integer :: nc = 3
    contains
    <Prc core: process core: TBP>
    end type prc_core_t

```

In any case there must be an output routine.

```

    <Prc core: process core: TBP>≡

```

```

        procedure(prc_core_write), deferred :: write
    <Prc core: interfaces>≡
    abstract interface
        subroutine prc_core_write (object, unit)
            import
            class(prc_core_t), intent(in) :: object
            integer, intent(in), optional :: unit
        end subroutine prc_core_write
    end interface

```

Just type the name of the actual core method.

```

    <Prc core: process core: TBP>+≡
        procedure(prc_core_write_name), deferred :: write_name
    <Prc core: interfaces>+≡
    abstract interface
        subroutine prc_core_write_name (object, unit)
            import
            class(prc_core_t), intent(in) :: object
            integer, intent(in), optional :: unit
        end subroutine prc_core_write_name
    end interface

```

For initialization, we assign a pointer to the process entry in the relevant library. This allows us to access all process functions via the implementation of `prc_core_t`.

We declare the object as `intent(inout)`, since just after allocation it may be useful to store some extra data in the object, which we can then use in the actual initialization. This applies to extensions of `prc_core` which override the `init` method.

```

    <Prc core: process core: TBP>+≡
        procedure :: init => prc_core_init
        procedure :: base_init => prc_core_init
    <Prc core: sub interfaces>≡
        module subroutine prc_core_init (object, def, lib, id, i_component)
            class(prc_core_t), intent(inout) :: object
            class(prc_core_def_t), intent(in), target :: def
            type(process_library_t), intent(in), target :: lib
            type(string_t), intent(in) :: id
            integer, intent(in) :: i_component
        end subroutine prc_core_init
    <Prc core: procedures>≡
        module subroutine prc_core_init (object, def, lib, id, i_component)
            class(prc_core_t), intent(inout) :: object
            class(prc_core_def_t), intent(in), target :: def
            type(process_library_t), intent(in), target :: lib
            type(string_t), intent(in) :: id
            integer, intent(in) :: i_component
            object%def => def
            call lib%connect_process (id, i_component, object%data, object%driver)
            object%data_known = .true.

```

```
end subroutine prc_core_init
```

Return true if the matrix element generation was successful. This can be tested by looking at the number of generated flavor states, which should be nonzero.

```
<Prc core: process core: TBP>+≡
  procedure :: has_matrix_element => prc_core_has_matrix_element

<Prc core: sub interfaces>+≡
  module function prc_core_has_matrix_element (object) result (flag)
    class(prc_core_t), intent(in) :: object
    logical :: flag
  end function prc_core_has_matrix_element

<Prc core: procedures>+≡
  module function prc_core_has_matrix_element (object) result (flag)
    class(prc_core_t), intent(in) :: object
    logical :: flag
    flag = object%data%n_flv /= 0
  end function prc_core_has_matrix_element
```

Return true if this process-core type needs extra code that has to be compiled and/or linked, beyond the default O'MEGA framework. This depends only on the concrete type, and the default is no.

```
<Prc core: process core: TBP>+≡
  procedure, nopass :: needs_external_code => prc_core_needs_external_code

<Prc core: sub interfaces>+≡
  module function prc_core_needs_external_code () result (flag)
    logical :: flag
  end function prc_core_needs_external_code

<Prc core: procedures>+≡
  module function prc_core_needs_external_code () result (flag)
    logical :: flag
    flag = .false.
  end function prc_core_needs_external_code
```

The corresponding procedure to create and load extra libraries. The base procedure must not be called but has to be overridden, if extra code is required.

```
<Prc core: process core: TBP>+≡
  procedure :: prepare_external_code => &
    prc_core_prepare_external_code

<Prc core: sub interfaces>+≡
  module subroutine prc_core_prepare_external_code &
    (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
    class(prc_core_t), intent(inout) :: core
    integer, intent(in), dimension(:,:), allocatable :: flv_states
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: i_core
    logical, intent(in) :: is_nlo
  end subroutine prc_core_prepare_external_code
```

```

<Prc core: procedures>+≡
  module subroutine prc_core_prepare_external_code &
    (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
    class(prc_core_t), intent(inout) :: core
    integer, intent(in), dimension(:,:), allocatable :: flv_states
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: i_core
    logical, intent(in) :: is_nlo
    call core%write ()
    call msg_bug ("prc_core_prepare_external_code called &
      &but not overridden")
  end subroutine prc_core_prepare_external_code

```

Return true if this process-core type uses the BLHA interface. This depends only on the concrete type, and the default is no.

```

<Prc core: process core: TBP>+≡
  procedure, nopass :: uses_blha => prc_core_uses_blha

```

```

<Prc core: sub interfaces>+≡
  module function prc_core_uses_blha () result (flag)
    logical :: flag
  end function prc_core_uses_blha

```

```

<Prc core: procedures>+≡
  module function prc_core_uses_blha () result (flag)
    logical :: flag
    flag = .false.
  end function prc_core_uses_blha

```

Tell whether a particular combination of flavor/helicity/color state is allowed for the matrix element.

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_is_allowed), deferred :: is_allowed

```

```

<Prc core: interfaces>+≡
  abstract interface
    function prc_core_is_allowed (object, i_term, f, h, c) result (flag)
      import
      class(prc_core_t), intent(in) :: object
      integer, intent(in) :: i_term, f, h, c
      logical :: flag
    end function prc_core_is_allowed
  end interface

```

Set the constant process data for a specific term. By default, these are the constants stored inside the object, ignoring the term index. Type extensions may override this and provide term-specific data.

```

<Prc core: process core: TBP>+≡
  procedure :: get_constants => prc_core_get_constants

```

```

<Prc core: sub interfaces>+≡
  module subroutine prc_core_get_constants (object, data, i_term)
    class(prc_core_t), intent(in) :: object
    type(process_constants_t), intent(out) :: data
    integer, intent(in) :: i_term
  end subroutine prc_core_get_constants

```

```

<Prc core: procedures>+≡
  module subroutine prc_core_get_constants (object, data, i_term)
    class(prc_core_t), intent(in) :: object
    type(process_constants_t), intent(out) :: data
    integer, intent(in) :: i_term
    data = object%data
  end subroutine prc_core_get_constants

```

The strong coupling is not among the process constants. The default implementation is to return a negative number, which indicates that α_s is not available. This may be overridden by an implementation that provides an (event-specific) value. The value can be stored in the process-specific workspace.

```

<Prc core: process core: TBP>+≡
  procedure :: get_alpha_s => prc_core_get_alpha_s

<Prc core: sub interfaces>+≡
  module function prc_core_get_alpha_s (object, core_state) result (alpha_qcd)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
  end function prc_core_get_alpha_s

<Prc core: procedures>+≡
  module function prc_core_get_alpha_s (object, core_state) result (alpha_qcd)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
    alpha_qcd = -1
  end function prc_core_get_alpha_s

```

We follow the same strategy for the electromagnetic coupling α_{em} .

```

<Prc core: process core: TBP>+≡
  procedure :: get_alpha_qed => prc_core_get_alpha_qed

<Prc core: sub interfaces>+≡
  module function prc_core_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qed
  end function prc_core_get_alpha_qed

<Prc core: procedures>+≡
  module function prc_core_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qed

```

```

        alpha_qed = -1
    end function prc_core_get_alpha_qed

```

Setup an index mapping for flavor structures and helicities that give the same matrix element. The index mapping is according to the order of flavor structures known to the `prc_core` class. This procedure here acts as a fallback in case there is no overridden procedure in the `prc_core` extension.

```

<Prc core: process core: TBP>+≡
    procedure :: set_equivalent_flv_hel_indices => &
        prc_core_set_equivalent_flv_hel_indices

<Prc core: sub interfaces>+≡
    module subroutine prc_core_set_equivalent_flv_hel_indices (object)
        class(prc_core_t), intent(inout) :: object
    end subroutine prc_core_set_equivalent_flv_hel_indices

<Prc core: procedures>+≡
    module subroutine prc_core_set_equivalent_flv_hel_indices (object)
        class(prc_core_t), intent(inout) :: object
        integer :: i, n_flv, n_hel
        n_flv = object%data%n_flv
        n_hel = object%data%n_hel
        if (.not. allocated (object%data%eqv_flv_index)) &
            allocate (object%data%eqv_flv_index(n_flv))
        if (.not. allocated (object%data%eqv_hel_index)) &
            allocate (object%data%eqv_hel_index(n_hel))
        if (size (object%data%eqv_flv_index) /= n_flv) &
            call msg_bug ("BLHA Core: Size mismatch between eqv_flv_index and number of flavors.")
        if (size (object%data%eqv_hel_index) /= n_hel) &
            call msg_bug ("BLHA Core: Size mismatch between eqv_hel_index and number of helicities.")
        object%data%eqv_flv_index = [(i, i = 1, n_flv)]
        object%data%eqv_hel_index = [(i, i = 1, n_hel)]
    end subroutine prc_core_set_equivalent_flv_hel_indices

```

Get the index mappings for flavor and helicity mappings set up in `prc_core_get_equivalent_flv_index` or any overriding variation.

```

<Prc core: process core: TBP>+≡
    procedure :: get_equivalent_flv_index => prc_core_get_equivalent_flv_index
    procedure :: get_equivalent_hel_index => prc_core_get_equivalent_hel_index

<Prc core: sub interfaces>+≡
    module function prc_core_get_equivalent_flv_index &
        (object) result (eqv_flv_index)
        class(prc_core_t), intent(in) :: object
        integer, dimension(:), allocatable :: eqv_flv_index
    end function prc_core_get_equivalent_flv_index
    module function prc_core_get_equivalent_hel_index &
        (object) result (eqv_hel_index)
        class(prc_core_t), intent(in) :: object
        integer, dimension(:), allocatable :: eqv_hel_index
    end function prc_core_get_equivalent_hel_index

<Prc core: procedures>+≡
    module function prc_core_get_equivalent_flv_index &
        (object) result (eqv_flv_index)

```

```

class(prc_core_t), intent(in) :: object
integer, dimension(:), allocatable :: eqv_flv_index
eqv_flv_index = object%data%eqv_flv_index
end function prc_core_get_equivalent_flv_index

module function prc_core_get_equivalent_hel_index &
  (object) result (eqv_hel_index)
class(prc_core_t), intent(in) :: object
integer, dimension(:), allocatable :: eqv_hel_index
eqv_hel_index = object%data%eqv_hel_index
end function prc_core_get_equivalent_hel_index

```

Allocate the workspace associated to a process component. The default is that there is no workspace, so we do nothing. A type extension may override this and allocate a workspace object of appropriate type, which can be used in further calculations.

In any case, the `intent(out)` attribute deletes any previously allocated workspace.

```

<Prc core: process core: TBP>+≡
  procedure :: allocate_workspace => prc_core_ignore_workspace

<Prc core: sub interfaces>+≡
  module subroutine prc_core_ignore_workspace (object, core_state)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_ignore_workspace

<Prc core: procedures>+≡
  module subroutine prc_core_ignore_workspace (object, core_state)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_ignore_workspace

```

Compute the momenta in the hard interaction, taking the seed kinematics as input. The `i_term` index tells us which term we want to compute. (The standard method is to just transfer the momenta to the hard interaction.)

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_hard_kinematics), deferred :: &
    compute_hard_kinematics

<Prc core: interfaces>+≡
  abstract interface
    subroutine prc_core_compute_hard_kinematics &
      (object, p_seed, i_term, int_hard, core_state)
      import
      class(prc_core_t), intent(in) :: object
      type(vector4_t), dimension(:), intent(in) :: p_seed
      integer, intent(in) :: i_term
      type(interaction_t), intent(inout) :: int_hard
      class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_core_compute_hard_kinematics
  end interface

```

Compute the momenta in the effective interaction, taking the hard kinematics as input. (This is called only if parton recombination is to be applied for the process variant.)

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_eff_kinematics), deferred :: &
    compute_eff_kinematics

<Prc core: interfaces>+≡
  abstract interface
    subroutine prc_core_compute_eff_kinematics &
      (object, i_term, int_hard, int_eff, core_state)
    import
    class(prc_core_t), intent(in) :: object
    integer, intent(in) :: i_term
    type(interaction_t), intent(in) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_compute_eff_kinematics
end interface

```

The process core must implement this function. Here, *j* is the index of the particular term we want to compute. The amplitude may depend on the factorization and renormalization scales.

The `core_state` (workspace) argument may be used if it is provided by the caller. Otherwise, the routine should compute the result directly.

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_amplitude), deferred :: compute_amplitude

<Prc core: interfaces>+≡
  abstract interface
    function prc_core_compute_amplitude &
      (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
       core_state) result (amp)
    import
    complex(default) :: amp
    class(prc_core_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: &
      core_state
  end function prc_core_compute_amplitude
end interface

```

17.1.2 Storage for intermediate results

The abstract `prc_core_state_t` type allows process cores to set up temporary workspace. The object is an extra argument for each of the individual calculations between kinematics setup and matrix-element evaluation.

```

<Prc core: public>+≡

```



```

    public :: prc_core_state_t
<Prc core: types>+≡
    type, abstract :: prc_core_state_t
    contains
        procedure(workspace_write), deferred :: write
        procedure(workspace_reset_new_kinematics), deferred :: reset_new_kinematics
    end type prc_core_state_t

```

For debugging, we should at least have an output routine.

```

<Prc core: interfaces>+≡
    abstract interface
        subroutine workspace_write (object, unit)
            import
            class(prc_core_state_t), intent(in) :: object
            integer, intent(in), optional :: unit
        end subroutine workspace_write
    end interface

```

This is used during the NLO calculation, see there for more information.

```

<Prc core: interfaces>+≡
    abstract interface
        subroutine workspace_reset_new_kinematics (object)
            import
            class(prc_core_state_t), intent(inout) :: object
        end subroutine workspace_reset_new_kinematics
    end interface

```

17.1.3 Helicity selection data

This is intended for use with O'MEGA, but may also be made available to other process methods. We set thresholds for counting the times a specific helicity amplitude is zero. When the threshold is reached, we skip this amplitude in subsequent calls.

For initializing the helicity counters, we need an object that holds the two parameters, the threshold (large real number) and the cutoff (integer).

A helicity value suppressed by more than `threshold` (a value which multiplies `epsilon`, to be compared with the average of the current amplitude, default is 10^{10}) is treated as zero. A matrix element is assumed to be zero and not called again if it has been zero `cutoff` times.

```

<Prc core: public>+≡
    public :: helicity_selection_t
<Prc core: types>+≡
    type :: helicity_selection_t
        logical :: active = .false.
        real(default) :: threshold = 0
        integer :: cutoff = 0
    contains
        <Prc core: helicity selection: TBP>
    end type helicity_selection_t

```

Output. If the selection is inactive, print nothing.

```

<Prc core: helicity selection: TBP>≡
  procedure :: write => helicity_selection_write

<Prc core: sub interfaces>+≡
  module subroutine helicity_selection_write (object, unit)
    class(helicity_selection_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine helicity_selection_write

<Prc core: procedures>+≡
  module subroutine helicity_selection_write (object, unit)
    class(helicity_selection_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (object%active) then
      write (u, "(3x,A)") "Helicity selection data:"
      write (u, "(5x,A,ES17.10)") &
        "threshold =", object%threshold
      write (u, "(5x,A,I0)") &
        "cutoff    = ", object%cutoff
    end if
  end subroutine helicity_selection_write

```

17.2 Test process type

For the following tests, we define a simple implementation of the abstract `prc_core_t`, designed such as to complement the `prc_test_t` process definition type.

Note that it is not given that the actual process is defined as `prc_test_t` type. We enforce this by calling `prc_test_create_library`. The driver component in the process core will then become of type `prc_test_t`.

```

<prc_test_core.f90>≡
  <File header>

  module prc_test_core

    <Use kinds>
    use lorentz
    use interactions
    use prc_test
    use prc_core

    <Standard module head>

    <Prc test core: public>

    <Prc test core: types>

    interface
    <Prc test core: sub interfaces>

```

```

        end interface

    end module prc_test_core

    <prc_test_core_sub.f90>≡
    <File header>

    submodule (prc_test_core) prc_test_core_s

        use io_units

        implicit none

    contains

    <Prc test core: procedures>

    end submodule prc_test_core_s

    <Prc test core: public>≡
    public :: test_t

    <Prc test core: types>≡
    type, extends (prc_core_t) :: test_t
    contains
    <Prc test core: test type: TBP>
    end type test_t

    <Prc test core: test type: TBP>≡
    procedure :: write => test_write

    <Prc test core: sub interfaces>≡
    module subroutine test_write (object, unit)
        class(test_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine test_write

    <Prc test core: procedures>≡
    module subroutine test_write (object, unit)
        class(test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A)") "test type implementing prc_test"
    end subroutine test_write

    <Prc test core: test type: TBP>+≡
    procedure :: write_name => test_write_name

    <Prc test core: sub interfaces>+≡
    module subroutine test_write_name (object, unit)
        class(test_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine test_write_name

```

```

<Prc test core: procedures>+≡
  module subroutine test_write_name (object, unit)
    class(test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(1x,A)") "Core: prc_test"
  end subroutine test_write_name

```

This process type always needs a MC parameter set and a single term. This only state is always allowed.

```

<Prc test core: test type: TBP>+≡
  procedure :: needs_mcset => test_needs_mcset
  procedure :: get_n_terms => test_get_n_terms
  procedure :: is_allowed => test_is_allowed

```

```

<Prc test core: sub interfaces>+≡
  module function test_needs_mcset (object) result (flag)
    class(test_t), intent(in) :: object
    logical :: flag
  end function test_needs_mcset
  module function test_get_n_terms (object) result (n)
    class(test_t), intent(in) :: object
    integer :: n
  end function test_get_n_terms
  module function test_is_allowed (object, i_term, f, h, c) result (flag)
    class(test_t), intent(in) :: object
    integer, intent(in) :: i_term, f, h, c
    logical :: flag
  end function test_is_allowed

```

```

<Prc test core: procedures>+≡
  module function test_needs_mcset (object) result (flag)
    class(test_t), intent(in) :: object
    logical :: flag
    flag = .true.
  end function test_needs_mcset

  module function test_get_n_terms (object) result (n)
    class(test_t), intent(in) :: object
    integer :: n
    n = 1
  end function test_get_n_terms

  module function test_is_allowed (object, i_term, f, h, c) result (flag)
    class(test_t), intent(in) :: object
    integer, intent(in) :: i_term, f, h, c
    logical :: flag
    flag = .true.
  end function test_is_allowed

```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

```

<Prc test core: test type: TBP>+≡

```

```

    procedure :: compute_hard_kinematics => test_compute_hard_kinematics
  <Prc test core: sub interfaces>+≡
    module subroutine test_compute_hard_kinematics &
      (object, p_seed, i_term, int_hard, core_state)
      class(test_t), intent(in) :: object
      type(vector4_t), dimension(:), intent(in) :: p_seed
      integer, intent(in) :: i_term
      type(interaction_t), intent(inout) :: int_hard
      class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine test_compute_hard_kinematics
  <Prc test core: procedures>+≡
    module subroutine test_compute_hard_kinematics &
      (object, p_seed, i_term, int_hard, core_state)
      class(test_t), intent(in) :: object
      type(vector4_t), dimension(:), intent(in) :: p_seed
      integer, intent(in) :: i_term
      type(interaction_t), intent(inout) :: int_hard
      class(prc_core_state_t), intent(inout), allocatable :: core_state
      call int_hard%set_momenta (p_seed)
    end subroutine test_compute_hard_kinematics

```

This procedure is not called for `test_t`, just a placeholder.

```

  <Prc test core: test type: TBP>+≡
    procedure :: compute_eff_kinematics => test_compute_eff_kinematics
  <Prc test core: sub interfaces>+≡
    module subroutine test_compute_eff_kinematics &
      (object, i_term, int_hard, int_eff, core_state)
      class(test_t), intent(in) :: object
      integer, intent(in) :: i_term
      type(interaction_t), intent(in) :: int_hard
      type(interaction_t), intent(inout) :: int_eff
      class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine test_compute_eff_kinematics
  <Prc test core: procedures>+≡
    module subroutine test_compute_eff_kinematics &
      (object, i_term, int_hard, int_eff, core_state)
      class(test_t), intent(in) :: object
      integer, intent(in) :: i_term
      type(interaction_t), intent(in) :: int_hard
      type(interaction_t), intent(inout) :: int_eff
      class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine test_compute_eff_kinematics

```

Transfer the incoming momenta of `p_seed` directly to the effective interaction, and vice versa for the outgoing momenta.

`int_hard` is left untouched since `int_eff` is an alias (via pointer) to it.

```

  <Prc test core: test type: TBP>+≡
    procedure :: recover_kinematics => test_recover_kinematics

```

```

<Prc test core: sub interfaces>+≡
  module subroutine test_recover_kinematics &
    (object, p_seed, int_hard, int_eff, core_state)
    class(test_t), intent(in) :: object
    type(vector4_t), dimension(:), intent(inout) :: p_seed
    type(interaction_t), intent(inout) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine test_recover_kinematics

```

```

<Prc test core: procedures>+≡
  module subroutine test_recover_kinematics &
    (object, p_seed, int_hard, int_eff, core_state)
    class(test_t), intent(in) :: object
    type(vector4_t), dimension(:), intent(inout) :: p_seed
    type(interaction_t), intent(inout) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    integer :: n_in
    n_in = int_eff%get_n_in ()
    call int_eff%set_momenta (p_seed(1:n_in), outgoing = .false.)
    p_seed(n_in+1:) = int_eff%get_momenta (outgoing = .true.)
  end subroutine test_recover_kinematics

```

Compute the amplitude. The driver ignores all quantum numbers and, in fact, returns a constant. Nevertheless, we properly transfer the momentum vectors.

```

<Prc test core: test type: TBP>+≡
  procedure :: compute_amplitude => test_compute_amplitude

<Prc test core: sub interfaces>+≡
  module function test_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
     core_state) result (amp)
    class(test_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: &
      core_state
    complex(default) :: amp
  end function test_compute_amplitude

<Prc test core: procedures>+≡
  module function test_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
     core_state) result (amp)
    class(test_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state

```

```

complex(default) :: amp
real(default), dimension(:,:), allocatable :: parray
integer :: i, n_tot
select type (driver => object%driver)
type is (prc_test_t)
  if (driver%scattering) then
    n_tot = 4
  else
    n_tot = 3
  end if
  allocate (parray (0:3,n_tot))
  forall (i = 1:n_tot) parray(:,i) = vector4_get_components (p(i))
  amp = driver%get_amplitude (parray)
end select
end function test_compute_amplitude

```

17.3 Template matrix elements

Here, we provide template matrix elements that are in structure very similar to O'MEGA matrix elements, but do not need its infrastructure. Per default, the matrix elements are flat, i.e. they have the constant value one. Analogous to the O'MEGA implementation, this section implements the interface to the templates (via the makefile) and the driver.

```

(prc_template_me.f90)≡
  <File header>

  module prc_template_me

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use os_interface
    use lorentz
    use interactions
    use model_data

    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def
    use process_libraries
    use prc_core

    <Standard module head>

    <Template matrix elements: public>

    <Template matrix elements: types>

    <Template matrix elements: interfaces>

```

```

    interface
    <Template matrix elements: sub interfaces>
    end interface

contains

    <Template matrix elements: main procedures>

end module prc_template_me
<prc_template_me_sub.f90>≡
<File header>

submodule (prc_template_me) prc_template_me_s

    use io_units
    use system_defs, only: TAB
    use diagnostics
    use flavors

    implicit none

contains

    <Template matrix elements: procedures>

end submodule prc_template_me_s

```

17.3.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```

<Template matrix elements: public>≡
    public :: template_me_def_t

<Template matrix elements: types>≡
    type, extends (prc_core_def_t) :: template_me_def_t
    contains
    <Template matrix elements: template ME def: TBP>
    end type template_me_def_t

<Template matrix elements: template ME def: TBP>≡
    procedure, nopass :: type_string => template_me_def_type_string

<Template matrix elements: sub interfaces>≡
    module function template_me_def_type_string () result (string)
        type(string_t) :: string
    end function template_me_def_type_string

<Template matrix elements: procedures>≡
    module function template_me_def_type_string () result (string)
        type(string_t) :: string
        string = "template"
    end function

```



```
end function template_me_def_type_string
```

Initialization: allocate the writer for the template matrix element. Also set any data for this process that the writer needs. Gfortran 7/8/9 bug, has to remain in the main module.

```
<Template matrix elements: template ME def: TBP>+≡
  procedure :: init => template_me_def_init
```

```
<Template matrix elements: main procedures>≡
  subroutine template_me_def_init &
    (object, model, prt_in, prt_out, unity)
    class(template_me_def_t), intent(out) :: object
    class(model_data_t), intent(in), target :: model
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in) :: unity
    allocate (template_me_writer_t :: object%writer)
    select type (writer => object%writer)
    type is (template_me_writer_t)
      call writer%init (model, prt_in, prt_out, unity)
    end select
  end subroutine template_me_def_init
```

Write/read process- and method-specific data.

```
<Template matrix elements: template ME def: TBP>+≡
  procedure :: write => template_me_def_write
```

```
<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_def_write (object, unit)
    class(template_me_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine template_me_def_write
```

```
<Template matrix elements: procedures>+≡
  module subroutine template_me_def_write (object, unit)
    class(template_me_def_t), intent(in) :: object
    integer, intent(in) :: unit
    select type (writer => object%writer)
    type is (template_me_writer_t)
      call writer%write (unit)
    end select
  end subroutine template_me_def_write
```

```
<Template matrix elements: template ME def: TBP>+≡
  procedure :: read => template_me_def_read
```

```
<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_def_read (object, unit)
    class(template_me_def_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine template_me_def_read
```

```

<Template matrix elements: procedures>+≡
  module subroutine template_me_def_read (object, unit)
    class(template_me_def_t), intent(out) :: object
    integer, intent(in) :: unit
    call msg_bug &
      ("WHIZARD template process definition: input not supported (yet)")
  end subroutine template_me_def_read

```

Allocate the driver for template matrix elements. Gfortran 7/8/9 bug, has to remain in the main module.

```

<Template matrix elements: template ME def: TBP>+≡
  procedure :: allocate_driver => template_me_def_allocate_driver

<Template matrix elements: main procedures>+≡
  subroutine template_me_def_allocate_driver (object, driver, basename)
    class(template_me_def_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (template_me_driver_t :: driver)
  end subroutine template_me_def_allocate_driver

```

We need code:

```

<Template matrix elements: template ME def: TBP>+≡
  procedure, nopass :: needs_code => template_me_def_needs_code

<Template matrix elements: sub interfaces>+≡
  module function template_me_def_needs_code () result (flag)
    logical :: flag
  end function template_me_def_needs_code

<Template matrix elements: procedures>+≡
  module function template_me_def_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function template_me_def_needs_code

```

These are the features that a template matrix element provides.

```

<Template matrix elements: template ME def: TBP>+≡
  procedure, nopass :: get_features => template_me_def_get_features

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
  end subroutine template_me_def_get_features

<Template matrix elements: procedures>+≡
  module subroutine template_me_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (5))
    features = [ &
      var_str ("init"), &
      var_str ("update_alpha_s"), &
      var_str ("is_allowed"), &
      var_str ("new_event"), &
      var_str ("get_amplitude")]
  end subroutine template_me_def_get_features

```

```
end subroutine template_me_def_get_features
```

The interface of the specific features.

<Template matrix elements: interfaces>≡

```
abstract interface
  subroutine init_t (par, scheme) bind(C)
  import
    real(c_default_float), dimension(*), intent(in) :: par
    integer(c_int), intent(in) :: scheme
  end subroutine init_t
end interface

abstract interface
  subroutine update_alpha_s_t (alpha_s) bind(C)
  import
    real(c_default_float), intent(in) :: alpha_s
  end subroutine update_alpha_s_t
end interface

abstract interface
  subroutine is_allowed_t (flv, hel, col, flag) bind(C)
  import
    integer(c_int), intent(in) :: flv, hel, col
    logical(c_bool), intent(out) :: flag
  end subroutine is_allowed_t
end interface

abstract interface
  subroutine new_event_t (p) bind(C)
  import
    real(c_default_float), dimension(0:3,*), intent(in) :: p
  end subroutine new_event_t
end interface

abstract interface
  subroutine get_amplitude_t (flv, hel, col, amp) bind(C)
  import
    integer(c_int), intent(in) :: flv, hel, col
    complex(c_default_complex), intent(out):: amp
  end subroutine get_amplitude_t
end interface
```

Connect the template matrix element features with the process driver.

<Template matrix elements: template ME def: TBP>+≡

```
procedure :: connect => template_me_def_connect
```

<Template matrix elements: sub interfaces>+≡

```
module subroutine template_me_def_connect (def, lib_driver, i, proc_driver)
  class(template_me_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
end subroutine template_me_def_connect
```

```

<Template matrix elements: procedures>+≡
module subroutine template_me_def_connect (def, lib_driver, i, proc_driver)
  class(template_me_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
  integer(c_int) :: pid, fid
  type(c_funptr) :: fptr
  select type (proc_driver)
  type is (template_me_driver_t)
    pid = i
    fid = 1
    call lib_driver%get_fptr (pid, fid, fptr)
    call c_f_procpointer (fptr, proc_driver%init)
    fid = 2
    call lib_driver%get_fptr (pid, fid, fptr)
    call c_f_procpointer (fptr, proc_driver%update_alpha_s)
    fid = 3
    call lib_driver%get_fptr (pid, fid, fptr)
    call c_f_procpointer (fptr, proc_driver%is_allowed)
    fid = 4
    call lib_driver%get_fptr (pid, fid, fptr)
    call c_f_procpointer (fptr, proc_driver%new_event)
    fid = 5
    call lib_driver%get_fptr (pid, fid, fptr)
    call c_f_procpointer (fptr, proc_driver%get_amplitude)
  end select
end subroutine template_me_def_connect

```

17.3.2 The Template Matrix element writer

Unlike O'MEGA, the template matrix element is directly written by the main WHIZARD program, so there will be no entry in the makefile for calling an external program. The template matrix element writer is responsible for writing interfaces and wrappers.

```

<Template matrix elements: types>+≡
type, extends (prc_writer_f_module_t) :: template_me_writer_t
  class(model_data_t), pointer :: model => null ()
  type(string_t) :: model_name
  logical :: unity
  type(string_t), dimension(:), allocatable :: prt_in
  type(string_t), dimension(:), allocatable :: prt_out
  integer :: n_in
  integer :: n_out
  integer :: n_tot
contains
  <Template matrix elements: template ME writer: TBP>
end type template_me_writer_t

```

The reported type is the same as for the `template_me_def_t` type.

```

<Template matrix elements: template ME writer: TBP>≡
procedure, nopass :: type_name => template_me_writer_type_name

```

```

<Template matrix elements: sub interfaces>+≡
  module function template_me_writer_type_name () result (string)
    type(string_t) :: string
  end function template_me_writer_type_name

<Template matrix elements: procedures>+≡
  module function template_me_writer_type_name () result (string)
    type(string_t) :: string
    string = "template"
  end function template_me_writer_type_name

```

Taking into account the prefix for template ME module names.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure, nopass :: get_module_name => template_me_writer_get_module_name

<Template matrix elements: sub interfaces>+≡
  module function template_me_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
  end function template_me_writer_get_module_name

<Template matrix elements: procedures>+≡
  module function template_me_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = "tpr_" // id
  end function template_me_writer_get_module_name

```

Output. This is called by `template_me_def_write`.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure :: write => template_me_writer_write

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_writer_write (object, unit)
    class(template_me_writer_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine template_me_writer_write

<Template matrix elements: procedures>+≡
  module subroutine template_me_writer_write (object, unit)
    class(template_me_writer_t), intent(in) :: object
    integer, intent(in) :: unit
    integer :: i, j
    write (unit, "(5x,A,I0)") "# incoming part. = ", object%n_in
    write (unit, "(7x,A)", advance="no") &
      "    Initial state: "
    do i = 1, object%n_in - 1
      write (unit, "(1x,A)", advance="no") char (object%prt_in(i))
    end do
    write (unit, "(1x,A)") char (object%prt_in(object%n_in))
    write (unit, "(5x,A,I0)") "# outgoing part. = ", object%n_out
    write (unit, "(7x,A)", advance="no") &
      "    Final state:  "
    do j = 1, object%n_out - 1
      write (unit, "(1x,A)", advance="no") char (object%prt_out(j))
    end do
  end subroutine template_me_writer_write

```

```

end do
write (unit, "(1x,A)") char (object%prt_out(object%n_out))
write (unit, "(5x,A,I0)") "# part. (total) = ", object%n_tot
end subroutine template_me_writer_write

```

Initialize with process data.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure :: init => template_me_writer_init

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_writer_init (writer, model, &
    prt_in, prt_out, unity)
    class(template_me_writer_t), intent(out) :: writer
    class(model_data_t), intent(in), target :: model
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in) :: unity
  end subroutine template_me_writer_init

<Template matrix elements: procedures>+≡
  module subroutine template_me_writer_init (writer, model, &
    prt_in, prt_out, unity)
    class(template_me_writer_t), intent(out) :: writer
    class(model_data_t), intent(in), target :: model
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in) :: unity
    writer%model => model
    writer%model_name = model%get_name ()
    writer%n_in = size (prt_in)
    writer%n_out = size (prt_out)
    writer%n_tot = size (prt_in) + size (prt_out)
    allocate (writer%prt_in (size (prt_in)), source = prt_in)
    allocate (writer%prt_out (size (prt_out)), source = prt_out)
    writer%unity = unity
  end subroutine template_me_writer_init

```

The makefile is the driver file for the test matrix elements.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure :: write_makefile_code => template_me_write_makefile_code

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)
    class(template_me_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
  end subroutine template_me_write_makefile_code

<Template matrix elements: procedures>+≡
  module subroutine template_me_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)

```

```

class(template_me_writer_t), intent(in) :: writer
integer, intent(in) :: unit
type(string_t), intent(in) :: id
type(os_data_t), intent(in) :: os_data
logical, intent(in) :: verbose
logical, intent(in), optional :: testflag
write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
write (unit, "(5A)") "clean-", char (id), ":"
if (verbose) then
    write (unit, "(5A)") TAB, "rm -f tpr-", char (id), ".mod"
    write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
else
    write (unit, "(5A)") TAB // '@echo " RM ', &
        trim (char (id)), '.mod"'
    write (unit, "(5A)") TAB, "@rm -f tpr-", char (id), ".mod"
    write (unit, "(5A)") TAB // '@echo " RM ', &
        trim (char (id)), '.lo"'
    write (unit, "(5A)") TAB, "@rm -f ", char (id), ".lo"
end if
write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
write (unit, "(5A)") "CLEAN_OBJECTS += tpr-", char (id), ".mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " FC " $@"
end if
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
end subroutine template_me_write_makefile_code

```

The source is written by this routine.

```

<Template matrix elements: template ME writer: TBP>+≡
    procedure :: write_source_code => template_me_write_source_code

<Template matrix elements: sub interfaces>+≡
    module subroutine template_me_write_source_code (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine template_me_write_source_code

<Template matrix elements: procedures>+≡
    module subroutine template_me_write_source_code (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        integer, dimension(writer%n_in) :: prt_in, mult_in, col_in
        type(flavor_t), dimension(1:writer%n_in) :: flv_in
        integer, dimension(writer%n_out) :: prt_out, mult_out
        integer, dimension(writer%n_tot) :: prt, mult
        integer, dimension(:,:), allocatable :: sxxx
        integer :: dummy, status
        type(flavor_t), dimension(1:writer%n_out) :: flv_out
        type(string_t) :: proc_str, comment_str, col_str
        integer :: u, i, j
        integer :: hel, hel_in, hel_out, fac, factor, col_fac
        type(string_t) :: filename

```

```

comment_str = ""
do i = 1, writer%n_in
    comment_str = comment_str // writer%prt_in(i) // " "
end do
do j = 1, writer%n_out
    comment_str = comment_str // writer%prt_out(j) // " "
end do
do i = 1, writer%n_in
    prt_in(i) = writer%model%get_pdg (writer%prt_in(i))
    call flv_in(i)%init (prt_in(i), writer%model)
    mult_in(i) = flv_in(i)%get_multiplicity ()
    col_in(i) = abs (flv_in(i)%get_color_type ())
    mult(i) = mult_in(i)
end do
do j = 1, writer%n_out
    prt_out(j) = writer%model%get_pdg (writer%prt_out(j))
    call flv_out(j)%init (prt_out(j), writer%model)
    mult_out(j) = flv_out(j)%get_multiplicity ()
    mult(writer%n_in + j) = mult_out(j)
end do
prt(1:writer%n_in) = prt_in(1:writer%n_in)
prt(writer%n_in+1:writer%n_tot) = prt_out(1:writer%n_out)
proc_str = converter (prt)
hel_in = product (mult_in)
hel_out = product (mult_out)
col_fac = product (col_in)
hel = hel_in * hel_out
fac = hel
dummy = 1
factor = 1
if (writer%n_out >= 3) then
    do i = 3, writer%n_out
        factor = factor * (i - 2) * (i - 1)
    end do
end if
factor = factor * col_fac
allocate (sxxx(1:hel,1:writer%n_tot))
call create_spin_table (dummy,hel,fac,mult,sxxx)
call msg_message ("Writing test matrix element for process '" &
    // char (id) // "'")
filename = id // ".f90"
u = free_unit ()
open (unit=u, file=char(filename), action="write")
write (u, "(A)") "! File generated automatically by WHIZARD"
write (u, "(A)") "! "
write (u, "(A)") "! Note that irres. of what you demanded WHIZARD"
write (u, "(A)") "! treats this as colorless process "
write (u, "(A)") "! "
write (u, "(A)") "module tpr_" // char(id)
write (u, "(A)") " "
write (u, "(A)") " use kinds"
write (u, "(A)") " use omega_color, OCF => omega_color_factor"
write (u, "(A)") " "
write (u, "(A)") " implicit none"

```



```

write (u, "(A)") " private"
write (u, "(A)") "
write (u, "(A)") " public :: md5sum"
write (u, "(A)") " public :: number_particles_in, number_particles_out"
write (u, "(A)") " public :: number_spin_states, spin_states"
write (u, "(A)") " public :: number_flavor_states, flavor_states"
write (u, "(A)") " public :: number_color_flows, color_flows"
write (u, "(A)") " public :: number_color_indices, number_color_factors, &"
write (u, "(A)") " color_factors, color_sum, openmp_supported"
write (u, "(A)") " public :: init, final, update_alpha_s"
write (u, "(A)") "
write (u, "(A)") " public :: new_event, is_allowed, get_amplitude"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
write (u, "(A)") " & conv = 0.38937966e12_default"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
write (u, "(A)") " & pi = 3.1415926535897932384626433832795028841972_default"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
if (writer%unity) then
    write (u, "(A)") " & const = 1"
else
    write (u, "(A,1x,I0,A)") " & const = (16 * pi / conv) * " &
    // "(16 * pi**2)**(", writer%n_out, "-2) "
end if
write (u, "(A)") "
write (u, "(A,1x,I0)") " integer, parameter, private :: n_prt = ", &
    writer%n_tot
write (u, "(A,1x,I0)") " integer, parameter, private :: n_in = ", &
    writer%n_in
write (u, "(A,1x,I0)") " integer, parameter, private :: n_out = ", &
    writer%n_out
write (u, "(A)") " integer, parameter, private :: n_cflow = 1"
write (u, "(A)") " integer, parameter, private :: n_cindex = 2"
write (u, "(A)") " !!! We ignore tensor products and take only one flavor state."
write (u, "(A)") " integer, parameter, private :: n_flg = 1"
write (u, "(A,1x,I0)") " integer, parameter, private :: n_hel = ", hel
write (u, "(A)") "
write (u, "(A)") " logical, parameter, private :: T = .true."
write (u, "(A)") " logical, parameter, private :: F = .false."
write (u, "(A)") "
do i = 1, hel
    write (u, "(A)") " integer, dimension(n_prt), parameter, private :: &"
    write (u, "(A)") " " // s_conv(i) // " = [ " // &
    char(converter(sxxx(i,1:writer%n_tot))) // " ]"
end do
write (u, "(A)") " integer, dimension(n_prt,n_hel), parameter, private :: table_spin_states =
write (u, "(A)") " reshape ( [ & "
do i = 1, hel-1
    write (u, "(A)") " " // s_conv(i) // ", & "
end do
write (u, "(A)") " " // s_conv(hel) // " & "
write (u, "(A)") " ], [ n_prt, n_hel ] )"

```

```

write (u, "(A)") "
write (u, "(A)") " integer, dimension(n_prt), parameter, private :: &"
write (u, "(A)") " f0001 = [ " // char(proc_str) // " ] ! " // char(comment_str)
write (u, "(A)") " integer, dimension(n_prt,n_flv), parameter, private :: table_flavor_states
write (u, "(A)") " reshape ( [ f0001 ], [ n_prt, n_flv ] )"
write (u, "(A)") "
write (u, "(A)") " integer, dimension(n_cindex, n_prt), parameter, private :: &"
!!! This produces non-matching color flows, better keep it completely colorless
! write (u, "(A)") " c0001 = reshape ( [ " // char (dummy_colorizer (flv_in)) // &
! " " // &
select case (writer%n_in)
case (1)
col_str = "0,0,"
case (2)
col_str = "0,0,0,0,"
end select
write (u, "(A)") " c0001 = reshape ( [ " // char (col_str) // &
(repeat ("0,0, ", writer%n_out-1)) // "0,0 ], " // " [ n_cindex, n_prt ] )"
write (u, "(A)") " integer, dimension(n_cindex, n_prt, n_cflow), parameter, private :: &"
write (u, "(A)") " table_color_flows = reshape ( [ c0001 ], [ n_cindex, n_prt, n_cflow ] )"
write (u, "(A)") "
write (u, "(A)") " logical, dimension(n_prt), parameter, private :: & "
write (u, "(A)") " g0001 = [ " // (repeat ("F, ", writer%n_tot-1)) // "F ] "
write (u, "(A)") " logical, dimension(n_prt, n_cflow), parameter, private " &
// ":: table_ghost_flags = &"
write (u, "(A)") " reshape ( [ g0001 ], [ n_prt, n_cflow ] )"
write (u, "(A)") "
write (u, "(A)") " integer, parameter, private :: n_cfactors = 1"
write (u, "(A)") " type(OCF), dimension(n_cfactors), parameter, private :: &"
write (u, "(A)") " table_color_factors = [ OCF(1,1,+1._default) ]"
write (u, "(A)") "
write (u, "(A)") " logical, dimension(n_flv), parameter, private :: a0001 = [ T ]"
write (u, "(A)") " logical, dimension(n_flv, n_cflow), parameter, private :: &"
write (u, "(A)") " flv_col_is_allowed = reshape ( [ a0001 ], [ n_flv, n_cflow ] )"
write (u, "(A)") "
write (u, "(A)") " complex(default), dimension (n_flv, n_hel, n_cflow), private, save :: amp"
write (u, "(A)") "
write (u, "(A)") " logical, dimension(n_hel), private, save :: hel_is_allowed = T"
write (u, "(A)") "
write (u, "(A)") "contains"
write (u, "(A)") "
write (u, "(A)") " pure function md5sum ()"
write (u, "(A)") " character(len=32) :: md5sum"
write (u, "(A)") " ! DON'T EVEN THINK of modifying the following line!"
write (u, "(A)") " md5sum = "" // writer%md5sum // ""
write (u, "(A)") " end function md5sum"
write (u, "(A)") "
write (u, "(A)") " subroutine init (par, scheme)"
write (u, "(A)") " real(default), dimension(*), intent(in) :: par"
write (u, "(A)") " integer, intent(in) :: scheme"
write (u, "(A)") " end subroutine init"
write (u, "(A)") "
write (u, "(A)") " subroutine final ()"
write (u, "(A)") " end subroutine final"

```

```

write (u, "(A)") "
write (u, "(A)") " subroutine update_alpha_s (alpha_s)"
write (u, "(A)") "   real(default), intent(in) :: alpha_s"
write (u, "(A)") " end subroutine update_alpha_s"
write (u, "(A)") "
write (u, "(A)") " pure function number_particles_in () result (n)"
write (u, "(A)") "   integer :: n"
write (u, "(A)") "   n = n_in"
write (u, "(A)") " end function number_particles_in"
write (u, "(A)") "
write (u, "(A)") " pure function number_particles_out () result (n)"
write (u, "(A)") "   integer :: n"
write (u, "(A)") "   n = n_out"
write (u, "(A)") " end function number_particles_out"
write (u, "(A)") "
write (u, "(A)") " pure function number_spin_states () result (n)"
write (u, "(A)") "   integer :: n"
write (u, "(A)") "   n = size (table_spin_states, dim=2)"
write (u, "(A)") " end function number_spin_states"
write (u, "(A)") "
write (u, "(A)") " pure subroutine spin_states (a)"
write (u, "(A)") "   integer, dimension(:,,:), intent(out) :: a"
write (u, "(A)") "   a = table_spin_states"
write (u, "(A)") " end subroutine spin_states"
write (u, "(A)") "
write (u, "(A)") " pure function number_flavor_states () result (n)"
write (u, "(A)") "   integer :: n"
write (u, "(A)") "   n = 1"
write (u, "(A)") " end function number_flavor_states"
write (u, "(A)") "
write (u, "(A)") " pure subroutine flavor_states (a)"
write (u, "(A)") "   integer, dimension(:,,:), intent(out) :: a"
write (u, "(A)") "   a = table_flavor_states"
write (u, "(A)") " end subroutine flavor_states"
write (u, "(A)") "
write (u, "(A)") " pure function number_color_indices () result (n)"
write (u, "(A)") "   integer :: n"
write (u, "(A)") "   n = size(table_color_flows, dim=1)"
write (u, "(A)") " end function number_color_indices"
write (u, "(A)") "
write (u, "(A)") " pure subroutine color_factors (cf)"
write (u, "(A)") "   type(OCF), dimension(:,), intent(out) :: cf"
write (u, "(A)") "   cf = table_color_factors"
write (u, "(A)") " end subroutine color_factors"
write (u, "(A)") "
!pure unless OpenMP
!write (u, "(A)") " pure function color_sum (flv, hel) result (amp2)"
write (u, "(A)") " function color_sum (flv, hel) result (amp2)"
write (u, "(A)") "   integer, intent(in) :: flv, hel"
write (u, "(A)") "   real(kind=default) :: amp2"
write (u, "(A)") "   amp2 = real (omega_color_sum (flv, hel, amp, table_color_factors))"
write (u, "(A)") " end function color_sum"
write (u, "(A)") "
write (u, "(A)") " pure function number_color_flows () result (n)"

```

```

write (u, "(A)") "      integer :: n"
write (u, "(A)") "      n = size (table_color_flows, dim=3)"
write (u, "(A)") " end function number_color_flows"
write (u, "(A)") " "
write (u, "(A)") " pure subroutine color_flows (a, g)"
write (u, "(A)") "      integer, dimension(:, :, :), intent(out) :: a"
write (u, "(A)") "      logical, dimension(:, :), intent(out) :: g"
write (u, "(A)") "      a = table_color_flows"
write (u, "(A)") "      g = table_ghost_flags"
write (u, "(A)") " end subroutine color_flows"
write (u, "(A)") " "
write (u, "(A)") " pure function number_color_factors () result (n)"
write (u, "(A)") "      integer :: n"
write (u, "(A)") "      n = size (table_color_factors)"
write (u, "(A)") " end function number_color_factors"
write (u, "(A)") " "
write (u, "(A)") " pure function openmp_supported () result (status)"
write (u, "(A)") "      logical :: status"
write (u, "(A)") "      status = .false."
write (u, "(A)") " end function openmp_supported"
write (u, "(A)") " "
write (u, "(A)") " subroutine new_event (p)"
write (u, "(A)") "      real(default), dimension(0:3,*), intent(in) :: p"
write (u, "(A)") "      call calculate_amplitudes (amp, p)"
write (u, "(A)") " end subroutine new_event"
write (u, "(A)") " "
write (u, "(A)") " pure function is_allowed (flv, hel, col) result (yorn)"
write (u, "(A)") "      logical :: yorn"
write (u, "(A)") "      integer, intent(in) :: flv, hel, col"
write (u, "(A)") "      yorn = hel_is_allowed(hel) .and. flv_col_is_allowed(flv,col)"
write (u, "(A)") " end function is_allowed"
write (u, "(A)") " "
write (u, "(A)") " pure function get_amplitude (flv, hel, col) result (amp_result)"
write (u, "(A)") "      complex(default) :: amp_result"
write (u, "(A)") "      integer, intent(in) :: flv, hel, col"
write (u, "(A)") "      amp_result = amp (flv, hel, col)"
write (u, "(A)") " end function get_amplitude"
write (u, "(A)") " "
write (u, "(A)") " pure subroutine calculate_amplitudes (amp, k)"
write (u, "(A)") "      complex(default), dimension(:, :, :), intent(out) :: amp"
write (u, "(A)") "      real(default), dimension(0:3,*), intent(in) :: k"
write (u, "(A)") "      real(default) :: fac"
write (u, "(A)") "      integer :: i"
write (u, "(A)") "      ! We give all helicities the same weight!"
if (writer%unity) then
    write (u, "(A,1x,I0,1x,A)") "      fac = ", col_fac
    write (u, "(A)") "      amp = const * sqrt(fac)"
else
    write (u, "(A,1x,I0,1x,A)") "      fac = ", factor
    write (u, "(A)") "      amp = sqrt((2 * (k(0,1)*k(0,2) &
    write (u, "(A,1x,I0,A)") "      - dot_product (k(1:,1), k(1:,2)))) ** (3-", &
    writer%n_out, ")) * sqrt(const * fac)"
end if
write (u, "(A,1x,I0,A)") "      amp = amp / sqrt(", hel_out, "._default)"

```

```

write (u, "(A)") " end subroutine calculate_amplitudes"
write (u, "(A)") "
write (u, "(A)") "end module tpr_" // char(id)
close (u, iostat=status)
deallocate (sxxx)
contains
function s_conv (num) result (chrt)
  integer, intent(in) :: num
  character(len=10) :: chrt
  write (chrt, "(I10)") num
  chrt = trim(adjustl(chrt))
  if (num < 10) then
    chrt = "s000" // chrt
  else if (num < 100) then
    chrt = "s00" // chrt
  else if (num < 1000) then
    chrt = "s0" // chrt
  else
    chrt = "s" // chrt
  end if
end function s_conv
function converter (flv) result (str)
  integer, dimension(:), intent(in) :: flv
  type(string_t) :: str
  character(len=150), dimension(size(flv)) :: chrt
  integer :: i
  str = ""
  do i = 1, size(flv) - 1
    write (chrt(i), "(I10)") flv(i)
    str = str // var_str(trim(adjustl(chrt(i)))) // ", "
  end do
  write (chrt(size(flv)), "(I10)") flv(size(flv))
  str = str // trim(adjustl(chrt(size(flv))))
end function converter
integer function sj (j,m)
  integer, intent(in) :: j, m
  if (((j == 1) .and. (m == 1)) .or. &
      ((j == 2) .and. (m == 2)) .or. &
      ((j == 3) .and. (m == 3)) .or. &
      ((j == 4) .and. (m == 3)) .or. &
      ((j == 5) .and. (m == 4))) then
    sj = 1
  else if (((j == 2) .and. (m == 1)) .or. &
      ((j == 3) .and. (m == 1)) .or. &
      ((j == 4) .and. (m == 2)) .or. &
      ((j == 5) .and. (m == 2))) then
    sj = -1
  else if (((j == 3) .and. (m == 2)) .or. &
      ((j == 5) .and. (m == 3))) then
    sj = 0
  else if (((j == 4) .and. (m == 1)) .or. &
      ((j == 5) .and. (m == 1))) then
    sj = -2
  else if (((j == 4) .and. (m == 4)) .or. &

```

```

        ((j == 5) .and. (m == 5))) then
            sj = 2
        else
            call msg_fatal ("template_me_write_source_code: Wrong spin type")
        end if
    end function sj
recursive subroutine create_spin_table (index, nhel, fac, mult, inta)
    integer, intent(inout) :: index, fac
    integer, intent(in) :: nhel
    integer, dimension(:), intent(in) :: mult
    integer, dimension(nhel,size(mult)), intent(out) :: inta
    integer :: j
    if (index > size(mult)) return
    fac = fac / mult(index)
    do j = 1, nhel
        inta(j,index) = sj (mult(index),mod(((j-1)/fac),mult(index))+1)
    end do
    index = index + 1
    call create_spin_table (index, nhel, fac, mult, inta)
end subroutine create_spin_table
function dummy_colorizer (flv) result (str)
    type(flavor_t), dimension(:), intent(in) :: flv
    type(string_t) :: str
    integer :: i, k
    str = ""
    k = 0
    do i = 1, size(flz)
        k = k + 1
        select case (flv(i)%get_color_type ())
        case (1,-1)
            str = str // "0,0, "
        case (3)
            str = str // int2string(k) // ",0, "
        case (-3)
            str = str // "0," // int2string(-k) // ", "
        case (8)
            str = str // int2string(k) // "," // int2string(-k-1) // ", "
            k = k + 1
        case default
            call msg_error ("Color type not supported.")
        end select
    end do
    str = adjustl(trim(str))
end function dummy_colorizer
end subroutine template_me_write_source_code

```

Nothing to be done here.

<Template matrix elements: template ME writer: TBP>+≡

```

    procedure :: before_compile => template_me_before_compile
    procedure :: after_compile => template_me_after_compile

```

<Template matrix elements: sub interfaces>+≡

```

    module subroutine template_me_before_compile (writer, id)
        class(template_me_writer_t), intent(in) :: writer

```

```

        type(string_t), intent(in) :: id
    end subroutine template_me_before_compile
    module subroutine template_me_after_compile (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine template_me_after_compile
<Template matrix elements: procedures>+≡
    module subroutine template_me_before_compile (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine template_me_before_compile

    module subroutine template_me_after_compile (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine template_me_after_compile

Return the name of a procedure that implements a given feature, as it is provided by the template matrix-element code. Template ME names are chosen completely in analogy to the O'MEGA matrix element conventions.
<Template matrix elements: template ME writer: TBP>+≡
    procedure, nopass :: get_procname => template_me_writer_get_procname
<Template matrix elements: sub interfaces>+≡
    module function template_me_writer_get_procname (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
    end function template_me_writer_get_procname
<Template matrix elements: procedures>+≡
    module function template_me_writer_get_procname (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
        select case (char (feature))
        case ("n_in");   name = "number_particles_in"
        case ("n_out");  name = "number_particles_out"
        case ("n_flv");  name = "number_flavor_states"
        case ("n_hel");  name = "number_spin_states"
        case ("n_col");  name = "number_color_flows"
        case ("n_cin");  name = "number_color_indices"
        case ("n_cf");   name = "number_color_factors"
        case ("flv_state"); name = "flavor_states"
        case ("hel_state"); name = "spin_states"
        case ("col_state"); name = "color_flows"
        case default
            name = feature
        end select
    end function template_me_writer_get_procname

```

The interfaces for the template-specific features.

```

<Template matrix elements: template ME writer: TBP>+≡
    procedure :: write_interface => template_me_write_interface

```

<Template matrix elements: sub interfaces>+≡

```

module subroutine template_me_write_interface (writer, unit, id, feature)
  class(template_me_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(string_t), intent(in) :: feature
end subroutine template_me_write_interface

```

<Template matrix elements: procedures>+≡

```

module subroutine template_me_write_interface (writer, unit, id, feature)
  class(template_me_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(string_t), intent(in) :: feature
  type(string_t) :: name
  name = writer%get_c_procname (id, feature)
  write (unit, "(2x,9A)") "interface"
  select case (char (feature))
  case ("init")
    write (unit, "(5x,9A)") "subroutine ", char (name), &
      " (par, scheme) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
      &intent(in) :: par"
    write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
  case ("update_alpha_s")
    write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
  case ("is_allowed")
    write (unit, "(5x,9A)") "subroutine ", char (name), " &
      &(flv, hel, col, flag) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
  case ("new_event")
    write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &
      &intent(in) :: p"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
  case ("get_amplitude")
    write (unit, "(5x,9A)") "subroutine ", char (name), " &
      &(flv, hel, col, amp) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
      &:: amp"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
  end select
  write (unit, "(2x,9A)") "end interface"
end subroutine template_me_write_interface

```


The wrappers have to take into account conversion between C and Fortran data types.

NOTE: The case `c_default_float` \neq `default` is not yet covered.

<Template matrix elements: template ME writer: TBP>+≡

```
procedure :: write_wrapper => template_me_write_wrapper
```

<Template matrix elements: sub interfaces>+≡

```
module subroutine template_me_write_wrapper (writer, unit, id, feature)
  class(template_me_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
end subroutine template_me_write_wrapper
```

<Template matrix elements: procedures>+≡

```
module subroutine template_me_write_wrapper (writer, unit, id, feature)
  class(template_me_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  type(string_t) :: name
  name = writer%get_c_procname (id, feature)
  write (unit, *)
  select case (char (feature))
  case ("init")
    write (unit, "(9A)") "subroutine ", char (name), &
      " (par, scheme) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use tpr_", char (id)
    write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
      &intent(in) :: par"
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
    if (c_default_float == default .and. c_int == kind(1)) then
      write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
  case ("update_alpha_s")
    write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use tpr_", char (id)
    if (c_default_float == default) then
      write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
        &:: alpha_s"
      write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
  case ("is_allowed")
    write (unit, "(9A)") "subroutine ", char (name), &
      " (flv, hel, col, flag) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use tpr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
```

```

write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
write (unit, "(2x,9A)") "flag = ", char (feature), &
    " (int (flv), int (hel), int (col))"
write (unit, "(9A)") "end subroutine ", char (name)
case ("new_event")
write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
if (c_default_float == default) then
    write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
        &intent(in) :: p"
    write (unit, "(2x,9A)") "call ", char (feature), " (p)"
end if
write (unit, "(9A)") "end subroutine ", char (name)
case ("get_amplitude")
write (unit, "(9A)") "subroutine ", char (name), &
    " (flv, hel, col, amp) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
    &:: amp"
write (unit, "(2x,9A)") "amp = ", char (feature), &
    " (int (flv), int (hel), int (col))"
write (unit, "(9A)") "end subroutine ", char (name)
end select
end subroutine template_me_write_wrapper

```

17.3.3 Driver

```

<Template matrix elements: public>+≡
public :: template_me_driver_t

<Template matrix elements: types>+≡
type, extends (prc_core_driver_t) :: template_me_driver_t
    procedure(init_t), nopass, pointer :: &
        init => null ()
    procedure(update_alpha_s_t), nopass, pointer :: &
        update_alpha_s => null ()
    procedure(is_allowed_t), nopass, pointer :: &
        is_allowed => null ()
    procedure(new_event_t), nopass, pointer :: &
        new_event => null ()
    procedure(get_amplitude_t), nopass, pointer :: &
        get_amplitude => null ()
contains
    <Template matrix elements: template ME driver: TBP>
end type template_me_driver_t

```

The reported type is the same as for the `template_me_def_t` type.

<Template matrix elements: template ME driver: TBP>≡

```

    procedure, nopass :: type_name => template_me_driver_type_name
<Template matrix elements: sub interfaces>+≡
    module function template_me_driver_type_name () result (string)
        type(string_t) :: string
    end function template_me_driver_type_name
<Template matrix elements: procedures>+≡
    module function template_me_driver_type_name () result (string)
        type(string_t) :: string
        string = "template"
    end function template_me_driver_type_name

```

17.3.4 High-level process definition

This procedure wraps the details filling a process-component definition entry as appropriate for an template matrix element. Gfortran 7/8/9 bug, remains in main module.

```

<Template matrix elements: public>+≡
    public :: template_me_make_process_component
<Template matrix elements: main procedures>+≡
    subroutine template_me_make_process_component (entry, component_index, &
        model, model_name, prt_in, prt_out, unity)
        class(process_def_entry_t), intent(inout) :: entry
        integer, intent(in) :: component_index
        type(string_t), intent(in) :: model_name
        class(model_data_t), intent(in), target :: model
        type(string_t), dimension(:), intent(in) :: prt_in
        type(string_t), dimension(:), intent(in) :: prt_out
        logical, intent(in) :: unity
        class(prc_core_def_t), allocatable :: def
        allocate (template_me_def_t :: def)
        select type (def)
        type is (template_me_def_t)
            call def%init (model, prt_in, prt_out, unity)
        end select
        call entry%import_component (component_index, &
            n_out = size (prt_out), &
            prt_in = new_prt_spec (prt_in), &
            prt_out = new_prt_spec (prt_out), &
            method = var_str ("template"), &
            variant = def)
    end subroutine template_me_make_process_component

```

17.3.5 The prc_template_me_t wrapper

This is an instance of the generic prc_core_t object. It contains a pointer to the process definition (template_me_def_t), a data component (process_constants_t), and the matrix-element driver (template_me_driver_t).

```

<Template matrix elements: public>+≡
    public :: prc_template_me_t

```

```

<Template matrix elements: types>+≡
  type, extends (prc_core_t) :: prc_template_me_t
    real(default), dimension(:), allocatable :: par
    integer :: scheme = 0
  contains
    <Template matrix elements: prc template ME: TBP>
  end type prc_template_me_t

```

The workspace associated to a `prc_template_me_t` object contains a single flag. The flag is used to suppress re-evaluating the matrix element for each quantum-number combination, after the first amplitude belonging to a given kinematics has been computed.

We can also store the value of a running coupling once it has been calculated for an event. The default value is negative, which indicates an undefined value in this context.

```

<Template matrix elements: types>+≡
  type, extends (prc_core_state_t) :: template_me_state_t
    logical :: new_kinematics = .true.
    real(default) :: alpha_qcd = -1
    real(default) :: alpha_qed = -1
  contains
    procedure :: write => template_me_state_write
    procedure :: reset_new_kinematics => template_me_state_reset_new_kinematics
  end type template_me_state_t

```

```

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_state_write (object, unit)
    class(template_me_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine template_me_state_write

```

```

<Template matrix elements: procedures>+≡
  module subroutine template_me_state_write (object, unit)
    class(template_me_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,L1)") "Template ME state: new kinematics = ", &
      object%new_kinematics
  end subroutine template_me_state_write

```

```

<Template matrix elements: sub interfaces>+≡
  module subroutine template_me_state_reset_new_kinematics (object)
    class(template_me_state_t), intent(inout) :: object
  end subroutine template_me_state_reset_new_kinematics

```

```

<Template matrix elements: procedures>+≡
  module subroutine template_me_state_reset_new_kinematics (object)
    class(template_me_state_t), intent(inout) :: object
  end subroutine template_me_state_reset_new_kinematics

```

Allocate the workspace with the above specific type. Gfortran 7/8/9 bug, has to remain in the main module.

```

<Template matrix elements: prc template ME: TBP>≡
    procedure :: allocate_workspace => prc_template_me_allocate_workspace

<Template matrix elements: main procedures>+≡
    subroutine prc_template_me_allocate_workspace (object, core_state)
        class(prc_template_me_t), intent(in) :: object
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        allocate (template_me_state_t :: core_state)
    end subroutine prc_template_me_allocate_workspace

```

The following procedures are inherited from the base type as deferred, thus must be implemented. The corresponding unit tests are skipped here; the procedures are tested when called from the `processes` module.

Output: print just the ID of the associated matrix element. Then display any stored parameters.

```

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: write => prc_template_me_write

<Template matrix elements: sub interfaces>+≡
    module subroutine prc_template_me_write (object, unit)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_template_me_write

<Template matrix elements: procedures>+≡
    module subroutine prc_template_me_write (object, unit)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(3x,A)", advance="no") "Template process core:"
        if (object%data_known) then
            write (u, "(1x,A)") char (object%data%id)
        else
            write (u, "(1x,A)") "[undefined]"
        end if
        if (allocated (object%par)) then
            write (u, "(3x,A)") "Parameter array:"
            do i = 1, size (object%par)
                write (u, "(5x,I0,1x,ES17.10)") i, object%par(i)
            end do
        end if
    end subroutine prc_template_me_write

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: write_name => prc_template_me_write_name

<Template matrix elements: sub interfaces>+≡
    module subroutine prc_template_me_write_name (object, unit)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_template_me_write_name

```

```

<Template matrix elements: procedures>+≡
module subroutine prc_template_me_write_name (object, unit)
  class(prc_template_me_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u,"(1x,A)") "Core: template"
end subroutine prc_template_me_write_name

```

Temporarily store the parameter array inside the `prc_template_me` object, so we can use it later during the actual initialization.

```

<Template matrix elements: prc template ME: TBP>+≡
  procedure :: set_parameters => prc_template_me_set_parameters

<Template matrix elements: sub interfaces>+≡
  module subroutine prc_template_me_set_parameters (prc_template_me, model)
    class(prc_template_me_t), intent(inout) :: prc_template_me
    class(model_data_t), intent(in), target, optional :: model
  end subroutine prc_template_me_set_parameters

<Template matrix elements: procedures>+≡
module subroutine prc_template_me_set_parameters (prc_template_me, model)
  class(prc_template_me_t), intent(inout) :: prc_template_me
  class(model_data_t), intent(in), target, optional :: model
  if (present (model)) then
    if (.not. allocated (prc_template_me%par)) &
      allocate (prc_template_me%par (model%get_n_real ()))
    call model%real_parameters_to_array (prc_template_me%par)
    prc_template_me%scheme = model%get_scheme_num ()
  end if
end subroutine prc_template_me_set_parameters

```

To fully initialize the process core, we perform base initialization, then initialize the external matrix element code.

This procedure overrides the `init` method of the base type, which we nevertheless can access via its binding `base_init`. When done, we have an allocated driver. The driver will call the `init` procedure for the external matrix element, and thus transfer the parameter set to where it finally belongs.

```

<Template matrix elements: prc template ME: TBP>+≡
  procedure :: init => prc_template_me_init

<Template matrix elements: sub interfaces>+≡
  module subroutine prc_template_me_init (object, def, lib, id, i_component)
    class(prc_template_me_t), intent(inout) :: object
    class(prc_core_def_t), intent(in), target :: def
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: id
    integer, intent(in) :: i_component
  end subroutine prc_template_me_init

<Template matrix elements: procedures>+≡
  module subroutine prc_template_me_init (object, def, lib, id, i_component)
    class(prc_template_me_t), intent(inout) :: object
    class(prc_core_def_t), intent(in), target :: def

```

```

type(process_library_t), intent(in), target :: lib
type(string_t), intent(in) :: id
integer, intent(in) :: i_component
call object%base_init (def, lib, id, i_component)
call object%activate_parameters ()
end subroutine prc_template_me_init

```

Activate the stored parameters by transferring them to the external matrix element.

```

<Template matrix elements: prc template ME: TBP>+≡
  procedure :: activate_parameters => prc_template_me_activate_parameters

<Template matrix elements: sub interfaces>+≡
  module subroutine prc_template_me_activate_parameters (object)
    class (prc_template_me_t), intent(inout) :: object
  end subroutine prc_template_me_activate_parameters

<Template matrix elements: procedures>+≡
  module subroutine prc_template_me_activate_parameters (object)
    class (prc_template_me_t), intent(inout) :: object
    if (allocated (object%driver)) then
      if (allocated (object%par)) then
        select type (driver => object%driver)
          type is (template_me_driver_t)
            if (associated (driver%init)) then
              call driver%init (object%par, object%scheme)
            end if
          end select
        else
          call msg_bug ("prc_template_me_activate: parameter set is not allocated")
        end if
      else
        call msg_bug ("prc_template_me_activate: driver is not allocated")
      end if
    end subroutine prc_template_me_activate_parameters

```

Tell whether a particular combination of flavor, helicity, color is allowed. Here we have to consult the matrix-element driver.

```

<Template matrix elements: prc template ME: TBP>+≡
  procedure :: is_allowed => prc_template_me_is_allowed

<Template matrix elements: sub interfaces>+≡
  module function prc_template_me_is_allowed &
    (object, i_term, f, h, c) result (flag)
    class(prc_template_me_t), intent(in) :: object
    integer, intent(in) :: i_term, f, h, c
    logical :: flag
  end function prc_template_me_is_allowed

<Template matrix elements: procedures>+≡
  module function prc_template_me_is_allowed &
    (object, i_term, f, h, c) result (flag)
    class(prc_template_me_t), intent(in) :: object
    integer, intent(in) :: i_term, f, h, c
    logical :: flag

```

```

logical(c_bool) :: cflag
select type (driver => object%driver)
type is (template_me_driver_t)
    call driver%is_allowed (f, h, c, cflag)
    flag = cflag
end select
end function prc_template_me_is_allowed

```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

```

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: compute_hard_kinematics => &
        prc_template_me_compute_hard_kinematics

<Template matrix elements: sub interfaces>+≡
    module subroutine prc_template_me_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(prc_template_me_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_template_me_compute_hard_kinematics

<Template matrix elements: procedures>+≡
    module subroutine prc_template_me_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(prc_template_me_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        call int_hard%set_momenta (p_seed)
    end subroutine prc_template_me_compute_hard_kinematics

```

This procedure is not called for `prc_template_me_t`, just a placeholder.

```

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: compute_eff_kinematics => &
        prc_template_me_compute_eff_kinematics

<Template matrix elements: sub interfaces>+≡
    module subroutine prc_template_me_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in) :: i_term
        type(interaction_t), intent(in) :: int_hard
        type(interaction_t), intent(inout) :: int_eff
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_template_me_compute_eff_kinematics

<Template matrix elements: procedures>+≡
    module subroutine prc_template_me_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in) :: i_term

```



```

type(interaction_t), intent(in) :: int_hard
type(interaction_t), intent(inout) :: int_eff
class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine prc_template_me_compute_eff_kinematics

```

Compute the amplitude. For the tree-level process, we can ignore the scale settings. The term index j is also irrelevant.

We first call `new_event` for the given momenta (which we must unpack), then retrieve the amplitude value for the given quantum numbers.

If the `core_state` status flag is present, we can make sure that we call `new_event` only once for a given kinematics. After the first call, we unset the `new_kinematics` flag.

```

<Template matrix elements: prc template ME: TBP>+≡
  procedure :: compute_amplitude => prc_template_me_compute_amplitude

<Template matrix elements: sub interfaces>+≡
  module function prc_template_me_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
     core_state) result (amp)
    class(prc_template_me_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: &
      core_state
    complex(default) :: amp
  end function prc_template_me_compute_amplitude

<Template matrix elements: procedures>+≡
  module function prc_template_me_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
     core_state) result (amp)
    class(prc_template_me_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    complex(default) :: amp
    integer :: n_tot, i
    real(c_default_float), dimension(:,:), allocatable :: parray
    complex(c_default_complex) :: camp
    logical :: new_event
    select type (driver => object%driver)
    type is (template_me_driver_t)
      new_event = .true.
      if (present (core_state)) then
        if (allocated (core_state)) then
          select type (core_state)
          type is (template_me_state_t)
            new_event = core_state%new_kinematics

```

```

        core_state%new_kinematics = .false.
    end select
end if
end if
if (new_event) then
    n_tot = object%data%n_in + object%data%n_out
    allocate (parray (0:3, n_tot))
    forall (i = 1:n_tot) parray(:,i) = vector4_get_components (p(i))
    call driver%new_event (parray)
end if
if (object%is_allowed (1, f, h, c)) then
    call driver%get_amplitude &
        (int (f, c_int), int (h, c_int), int (c, c_int), camp)
    amp = camp
else
    amp = 0
end if
end select
end function prc_template_me_compute_amplitude

```

We do not overwrite the `prc_core_t` routine for α_s .

17.3.6 Unit Test

Test module, followed by the corresponding implementation module.

`<prc_template_me_ut.f90>`≡
<File header>

```

module prc_template_me_ut
    use unit_tests
    use prc_template_me_util

```

<Standard module head>

<Template matrix elements: public test>

contains

<Template matrix elements: test driver>

```

end module prc_template_me_ut

```

`<prc_template_me_util.f90>`≡
<File header>

```

module prc_template_me_util

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
<Use strings>
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use model_data

```

```

    use prc_core_def
    use process_constants
    use process_libraries
    use model_testbed, only: prepare_model, cleanup_model

    use prc_template_me

    <Standard module head>

    <Template matrix elements: test declarations>

contains

    <Template matrix elements: tests>

end module prc_template_me_util
API: driver for the unit tests below.
<Template matrix elements: public test>≡
    public :: prc_template_me_test
<Template matrix elements: test driver>≡
    subroutine prc_template_me_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Template matrix elements: execute tests>
end subroutine prc_template_me_test

```

Generate, compile and load a simple process matrix element

The process is $e^+e^- \rightarrow \mu^+\mu^-$ for vanishing masses and $e = 0.3$. We initialize the process, build the library, and compute a particular matrix element for momenta of unit energy and right-angle scattering. The matrix element, as it happens, is equal to e^2 . (Note that are no conversion factors applied, so this result is exact.)

For GNU make, makeflags is set to -j1. This eliminates a potential clash with a -j<n> flag if this test is called from a parallel make.

```

<Template matrix elements: execute tests>≡
    call test (prc_template_me_1, "prc_template_me_1", &
        "build and load simple template process", &
        u, results)

<Template matrix elements: test declarations>≡
    public :: prc_template_me_1

<Template matrix elements: tests>≡
    subroutine prc_template_me_1 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        class(model_data_t), pointer :: model
        type(string_t) :: model_name

```

```

type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(process_constants_t) :: data
class(prc_core_driver_t), allocatable :: driver
integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(4) :: par
real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i

write (u, "(A)")  "* Test output: prc_template_me_1"
write (u, "(A)")  "*   Purpose: create a template matrix element,"
write (u, "(A)")  "*               normalized to give unit integral,"
write (u, "(A)")  "*               build a library, link, load, and &
               &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("template_me1"))
call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

allocate (template_me_def_t :: def)
select type (def)
type is (template_me_def_t)
    call def%init (model, prt_in, prt_out, unity = .false.)
end select
allocate (entry)
call entry%init (var_str ("template_me1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

```

```

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active           = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes         = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of template_me1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("template_me1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID      = ", char (data%id)
write (u, "(1x,A,A)")  "model name        = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum           = '", data%md5sum, "'"
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
do i = 2, 16
    write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set parameters for template_me1_a and initialize:"
write (u, "(A)")

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]

```

```

write (u, "(2x,A,F6.4)") "ee = ", par(1)
write (u, "(2x,A,F6.4)") "me = ", par(2)
write (u, "(2x,A,F6.4)") "mmu = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

select type (driver)
type is (template_me_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()
call cleanup_model (model)
deallocate (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_template_me_1"

end subroutine prc_template_me_1

<Template matrix elements: execute tests>+≡
call test (prc_template_me_2, "prc_template_me_2", &
    "build and load simple template_unity process", &
    u, results)

<Template matrix elements: test declarations>+≡
public :: prc_template_me_2

<Template matrix elements: tests>+≡
subroutine prc_template_me_2 (u)

```

```

integer, intent(in) :: u
type(process_library_t) :: lib
class(prc_core_def_t), allocatable :: def
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
class(model_data_t), pointer :: model
type(string_t) :: model_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(process_constants_t) :: data
class(prc_core_driver_t), allocatable :: driver
integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(4) :: par
real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i

write (u, "(A)")  "* Test output: prc_template_me_1"
write (u, "(A)")  "*   Purpose: create a template matrix element,"
write (u, "(A)")  "*               being identical to unity,"
write (u, "(A)")  "*               build a library, link, load, and &
               &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("template_me2"))
call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

allocate (template_me_def_t :: def)
select type (def)
type is (template_me_def_t)
   call def%init (model, prt_in, prt_out, unity = .true.)
end select
allocate (entry)
call entry%init (var_str ("template_me2_a"), model_name = model_name, &
   n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
   prt_in = new_prt_spec (prt_in), &
   prt_out = new_prt_spec (prt_out), &
   method = var_str ("template_unity"), &
   variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"

```

```

write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active                = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes              = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of template_me2_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("template_me2_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID      = ", char (data%id)
write (u, "(1x,A,A)")  "model name        = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum          = '", data%md5sum, "'"
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
do i = 2, 16
    write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors

```



```

write (u, "(1x,A,10(1x,I0))") "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set parameters for template_me2_a and initialize:"
write (u, "(A)")

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]
write (u, "(2x,A,F6.4)") "ee  = ", par(1)
write (u, "(2x,A,F6.4)") "me  = ", par(2)
write (u, "(2x,A,F6.4)") "mmu  = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

select type (driver)
type is (template_me_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()
call cleanup_model (model)
deallocate (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_template_me_2"

end subroutine prc_template_me_2

```

17.4 O’MEGA Interface

The standard method for process computation with WHIZARD is the O’MEGA matrix element generator.

This section implements the interface to the code generator (via the makefile) and the driver for the features provided by the O’MEGA matrix element.

There are actually two different methods steered by this interface, the traditional one which delivers compiled Fortran code, while the O’MEGA virtual machine (OVM) produces bytecode with look-up tables.

```
<prc_omega.f90>≡
  <File header>

  module prc_omega

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use constants, only: one
    use os_interface
    use diagnostics
    use lorentz
    use sm_qcd
    use sm_qed
    use interactions
    use model_data

    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def
    use process_libraries
    use prc_core

    <Standard module head>

    <Omega interface: public>

    <Omega interface: types>

    <Omega interface: interfaces>

    interface
    <Omega interface: sub interfaces>
    end interface

    contains

    <Omega interface: main procedures>

  end module prc_omega

<prc_omega_sub.f90>≡
  <File header>
```

```

submodule (prc_omega) prc_omega_s

  use io_units
  use system_defs, only: TAB

  implicit none

contains

  <Omega interface: procedures>

end submodule prc_omega_s

```

17.4.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```

<Omega interface: public>≡
  public :: omega_def_t

<Omega interface: types>≡
  type, extends (prc_core_def_t) :: omega_def_t
    logical :: ufo = .false.
    logical :: ovm = .false.
  contains
    <Omega interface: omega def: TBP>
  end type omega_def_t

<Omega interface: omega def: TBP>≡
  procedure, nopass :: type_string => omega_def_type_string

<Omega interface: sub interfaces>≡
  module function omega_def_type_string () result (string)
    type(string_t) :: string
  end function omega_def_type_string

<Omega interface: procedures>≡
  module function omega_def_type_string () result (string)
    type(string_t) :: string
    string = "omega"
  end function omega_def_type_string

```

Initialization: allocate the writer for the O'MEGA matrix element. The writer type depends on the settings of the `ufo` and `ovm` flags. Also set any data for this process that the writer needs. Gfortran 7/8/9 bug, has to remain in the main module.

```

<Omega interface: omega def: TBP>+≡
  procedure :: init => omega_def_init

```

```

<Omega interface: main procedures>≡
  subroutine omega_def_init (object, &
    model_name, prt_in, prt_out, &
    ovm, ufo, ufo_path, &
    restrictions, cms_scheme, &
    openmp_support, report_progress, write_phs_output, extra_options, diags, diags_color)
  class(omega_def_t), intent(out) :: object
  type(string_t), intent(in) :: model_name
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  logical, intent(in) :: ovm
  logical, intent(in) :: ufo
  type(string_t), intent(in), optional :: ufo_path
  type(string_t), intent(in), optional :: restrictions
  logical, intent(in), optional :: cms_scheme
  logical, intent(in), optional :: openmp_support
  logical, intent(in), optional :: report_progress
  logical, intent(in), optional :: write_phs_output
  type(string_t), intent(in), optional :: extra_options
  logical, intent(in), optional :: diags, diags_color
  object%ufo = ufo
  object%ovm = ovm
  if (object%ufo) then
    if (object%ovm) then
      call msg_fatal ("Omega process: OVM method does not support UFO model")
    else
      allocate (omega_ufo_writer_t :: object%writer)
    end if
  else
    if (object%ovm) then
      allocate (omega_ovm_writer_t :: object%writer)
    else
      allocate (omega_omega_writer_t :: object%writer)
    end if
  end if
  select type (writer => object%writer)
  class is (omega_writer_t)
    call writer%init (model_name, prt_in, prt_out, &
      ufo_path, restrictions, cms_scheme, &
      openmp_support, report_progress, write_phs_output, extra_options, diags, diags_color)
  end select
end subroutine omega_def_init

```

Write/read process- and method-specific data.

```

<Omega interface: omega def: TBP>+≡
  procedure :: write => omega_def_write

<Omega interface: sub interfaces>+≡
  module subroutine omega_def_write (object, unit)
    class(omega_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine omega_def_write

<Omega interface: procedures>+≡
  module subroutine omega_def_write (object, unit)

```

```

class(omega_def_t), intent(in) :: object
integer, intent(in) :: unit
select type (writer => object%writer)
class is (omega_writer_t)
    call writer%write (unit)
end select
end subroutine omega_def_write

```

```

<Omega interface: omega def: TBP>+≡
    procedure :: read => omega_def_read

```

```

<Omega interface: sub interfaces>+≡
    module subroutine omega_def_read (object, unit)
        class(omega_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine omega_def_read

```

```

<Omega interface: procedures>+≡
    module subroutine omega_def_read (object, unit)
        class(omega_def_t), intent(out) :: object
        integer, intent(in) :: unit
        call msg_bug ("O'Mega process definition: input not supported yet")
    end subroutine omega_def_read

```

Allocate the driver for O'MEGAmatrix elements. Gfortran 7/8/9 bug, has to remain in the main module.

```

<Omega interface: omega def: TBP>+≡
    procedure :: allocate_driver => omega_def_allocate_driver

<Omega interface: main procedures>+≡
    subroutine omega_def_allocate_driver (object, driver, basename)
        class(omega_def_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        allocate (omega_driver_t :: driver)
    end subroutine omega_def_allocate_driver

```

We need code:

```

<Omega interface: omega def: TBP>+≡
    procedure, nopass :: needs_code => omega_def_needs_code

<Omega interface: sub interfaces>+≡
    module function omega_def_needs_code () result (flag)
        logical :: flag
    end function omega_def_needs_code

<Omega interface: procedures>+≡
    module function omega_def_needs_code () result (flag)
        logical :: flag
        flag = .true.
    end function omega_def_needs_code

```

These are the features that an O'MEGA matrix element provides.

```

<Omega interface: omega def: TBP>+≡
    procedure, nopass :: get_features => omega_def_get_features

```

```

<Omega interface: sub interfaces>+≡
  module subroutine omega_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
  end subroutine omega_def_get_features

<Omega interface: procedures>+≡
  module subroutine omega_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (6))
    features = [ &
      var_str ("init"), &
      var_str ("update_alpha_s"), &
      var_str ("reset_helicity_selection"), &
      var_str ("is_allowed"), &
      var_str ("new_event"), &
      var_str ("get_amplitude")]
  end subroutine omega_def_get_features

```

The interface of the specific features.

```

<Omega interface: interfaces>≡
  abstract interface
    subroutine init_t (par, scheme) bind(C)
    import
    real(c_default_float), dimension(*), intent(in) :: par
    integer(c_int), intent(in) :: scheme
  end subroutine init_t
end interface

  abstract interface
    subroutine update_alpha_s_t (alpha_s) bind(C)
    import
    real(c_default_float), intent(in) :: alpha_s
  end subroutine update_alpha_s_t
end interface

  abstract interface
    subroutine reset_helicity_selection_t (threshold, cutoff) bind(C)
    import
    real(c_default_float), intent(in) :: threshold
    integer(c_int), intent(in) :: cutoff
  end subroutine reset_helicity_selection_t
end interface

  abstract interface
    subroutine is_allowed_t (flv, hel, col, flag) bind(C)
    import
    integer(c_int), intent(in) :: flv, hel, col
    logical(c_bool), intent(out) :: flag
  end subroutine is_allowed_t
end interface

  abstract interface
    subroutine new_event_t (p) bind(C)
    import

```

```

        real(c_default_float), dimension(0:3,*), intent(in) :: p
    end subroutine new_event_t
end interface

abstract interface
    subroutine get_amplitude_t (flv, hel, col, amp) bind(C)
        import
        integer(c_int), intent(in) :: flv, hel, col
        complex(c_default_complex), intent(out):: amp
    end subroutine get_amplitude_t
end interface

```

Connect the O'MEGA features with the process driver.

(Omega interface: omega def: TBP)+≡

```

procedure :: connect => omega_def_connect

```

(Omega interface: sub interfaces)+≡

```

module subroutine omega_def_connect (def, lib_driver, i, proc_driver)
    class(omega_def_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
end subroutine omega_def_connect

```

(Omega interface: procedures)+≡

```

module subroutine omega_def_connect (def, lib_driver, i, proc_driver)
    class(omega_def_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
    integer(c_int) :: pid, fid
    type(c_funptr) :: fptr
    select type (proc_driver)
    type is (omega_driver_t)
        pid = i
        fid = 1
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%init)
        fid = 2
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%update_alpha_s)
        fid = 3
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%reset_helicity_selection)
        fid = 4
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%is_allowed)
        fid = 5
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%new_event)
        fid = 6
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%get_amplitude)
    end select
end subroutine omega_def_connect

```

17.4.2 The O'MEGA writer

The O'MEGA writer is responsible for inserting the appropriate lines in the make-file that call O'MEGA, and for writing interfaces and wrappers.

```
<Omega interface: types>+≡
  type, extends (prc_writer_f_module_t), abstract :: omega_writer_t
    type(string_t) :: model_name
    type(string_t) :: process_mode
    type(string_t) :: process_string
    type(string_t) :: restrictions
    logical :: openmp_support = .false.
    logical :: report_progress = .false.
    logical :: diags = .false.
    logical :: diags_color = .false.
    logical :: complex_mass_scheme = .false.
    logical :: write_phs_output = .false.
    type(string_t) :: extra_options
  contains
    <Omega interface: omega writer: TBP>
  end type omega_writer_t
```

```
<Omega interface: types>+≡
  type, extends (omega_writer_t) :: omega_omega_writer_t
  contains
    <Omega interface: omega omega writer: TBP>
  end type omega_omega_writer_t
```

```
<Omega interface: types>+≡
  type, extends (omega_omega_writer_t) :: omega_ufo_writer_t
    type(string_t) :: ufo_path
  contains
    <Omega interface: omega ufo writer: TBP>
  end type omega_ufo_writer_t
```

```
<Omega interface: types>+≡
  type, extends (omega_writer_t) :: omega_ovm_writer_t
  contains
    <Omega interface: omega ovm writer: TBP>
  end type omega_ovm_writer_t
```

```
<Omega interface: omega omega writer: TBP>≡
  procedure, nopass :: type_name => omega_omega_writer_type_name
```

```
<Omega interface: sub interfaces>+≡
  module function omega_omega_writer_type_name () result (string)
    type(string_t) :: string
  end function omega_omega_writer_type_name
```



```

<Omega interface: procedures>+≡
  module function omega_omega_writer_type_name () result (string)
    type(string_t) :: string
    string = "omega"
  end function omega_omega_writer_type_name

```

```

<Omega interface: omega ufo writer: TBP>≡
  procedure, nopass :: type_name => omega_ufo_writer_type_name

```

```

<Omega interface: sub interfaces>+≡
  module function omega_ufo_writer_type_name () result (string)
    type(string_t) :: string
  end function omega_ufo_writer_type_name

```

```

<Omega interface: procedures>+≡
  module function omega_ufo_writer_type_name () result (string)
    type(string_t) :: string
    string = "omega/UFO"
  end function omega_ufo_writer_type_name

```

```

<Omega interface: omega ovm writer: TBP>≡
  procedure, nopass :: type_name => omega_ovm_writer_type_name

```

```

<Omega interface: sub interfaces>+≡
  module function omega_ovm_writer_type_name () result (string)
    type(string_t) :: string
  end function omega_ovm_writer_type_name

```

```

<Omega interface: procedures>+≡
  module function omega_ovm_writer_type_name () result (string)
    type(string_t) :: string
    string = "ovm"
  end function omega_ovm_writer_type_name

```

Taking into account the prefix for O'MEGA module names.

```

<Omega interface: omega writer: TBP>≡
  procedure, nopass :: get_module_name => omega_writer_get_module_name

```

```

<Omega interface: sub interfaces>+≡
  module function omega_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
  end function omega_writer_get_module_name

```

```

<Omega interface: procedures>+≡
  module function omega_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = "opr_" // id
  end function omega_writer_get_module_name

```

Output. This is called by omega_def_write.

```

<Omega interface: omega writer: TBP>+≡
  procedure :: write => omega_writer_write

```

<Omega interface: sub interfaces>+≡

```
module subroutine omega_writer_write (object, unit)
  class(omega_writer_t), intent(in) :: object
  integer, intent(in) :: unit
end subroutine omega_writer_write
```

<Omega interface: procedures>+≡

```
module subroutine omega_writer_write (object, unit)
  class(omega_writer_t), intent(in) :: object
  integer, intent(in) :: unit
  write (unit, "(5x,A,A)") "Model name      = ", &
    ' ' // char (object%model_name) // ' '
  write (unit, "(5x,A,A)") "Mode string    = ", &
    ' ' // char (object%process_mode) // ' '
  write (unit, "(5x,A,A)") "Process string = ", &
    ' ' // char (object%process_string) // ' '
  write (unit, "(5x,A,A)") "Restrictions   = ", &
    ' ' // char (object%restrictions) // ' '
  write (unit, "(5x,A,L1)") "OpenMP support = ", object%openmp_support
  write (unit, "(5x,A,L1)") "Report progress = ", object%report_progress
  ! write (unit, "(5x,A,L1)") "Write phs output = ", object%write_phs_output
  write (unit, "(5x,A,A)") "Extra options  = ", &
    ' ' // char (object%extra_options) // ' '
  write (unit, "(5x,A,L1)") "Write diagrams  = ", object%diags
  write (unit, "(5x,A,L1)") "Write color diag. = ", object%diags_color
  write (unit, "(5x,A,L1)") "Complex Mass S.  = ", &
    object%complex_mass_scheme
end subroutine omega_writer_write
```

Initialize with process data.

<Omega interface: omega writer: TBP>+≡

```
procedure :: init => omega_writer_init
```

<Omega interface: sub interfaces>+≡

```
module subroutine omega_writer_init (writer, model_name, prt_in, prt_out, &
  ufo_path, restrictions, cms_scheme, openmp_support, &
  report_progress, write_phs_output, extra_options, diags, diags_color)
  class(omega_writer_t), intent(out) :: writer
  type(string_t), intent(in) :: model_name
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  type(string_t), intent(in), optional :: ufo_path
  type(string_t), intent(in), optional :: restrictions
  logical, intent(in), optional :: cms_scheme
  logical, intent(in), optional :: openmp_support
  logical, intent(in), optional :: report_progress
  logical, intent(in), optional :: write_phs_output
  type(string_t), intent(in), optional :: extra_options
  logical, intent(in), optional :: diags, diags_color
end subroutine omega_writer_init
```

<Omega interface: procedures>+≡

```
module subroutine omega_writer_init (writer, model_name, prt_in, prt_out, &
  ufo_path, restrictions, cms_scheme, openmp_support, &
  report_progress, write_phs_output, extra_options, diags, diags_color)
```

```

class(omega_writer_t), intent(out) :: writer
type(string_t), intent(in) :: model_name
type(string_t), dimension(:), intent(in) :: prt_in
type(string_t), dimension(:), intent(in) :: prt_out
type(string_t), intent(in), optional :: ufo_path
type(string_t), intent(in), optional :: restrictions
logical, intent(in), optional :: cms_scheme
logical, intent(in), optional :: openmp_support
logical, intent(in), optional :: report_progress
logical, intent(in), optional :: write_phs_output
type(string_t), intent(in), optional :: extra_options
logical, intent(in), optional :: diags, diags_color
integer :: i
writer%model_name = model_name
select type (writer)
type is (omega_ufo_writer_t)
    if (present (ufo_path)) then
        writer%ufo_path = ufo_path
    else
        call msg_fatal ("O'Mega: UFO model option is selected, but UFO model path is unset")
    end if
end select
if (present (restrictions)) then
    writer%restrictions = restrictions
else
    writer%restrictions = ""
end if
if (present (cms_scheme)) writer%complex_mass_scheme = cms_scheme
if (present (openmp_support)) writer%openmp_support = openmp_support
if (present (report_progress)) writer%report_progress = report_progress
if (present (write_phs_output)) writer%write_phs_output = write_phs_output
if (present (extra_options)) then
    writer%extra_options = " " // extra_options
else
    writer%extra_options = ""
end if
if (present (diags)) writer%diags = diags
if (present (diags_color)) writer%diags_color = diags_color
select case (size (prt_in))
case (1); writer%process_mode = " -decay"
case (2); writer%process_mode = " -scatter"
end select
associate (s => writer%process_string)
    s = " '"
    do i = 1, size (prt_in)
        if (i > 1) s = s // " "
        s = s // prt_in(i)
    end do
    s = s // " ->"
    do i = 1, size (prt_out)
        s = s // " " // prt_out(i)
    end do
    s = s // "'"
end associate

```

```
end subroutine omega_writer_init
```

The makefile implements the actual O'MEGA call. For old L^AT_EX distributions, we filter out the hyperref options for O'MEGA diagrams, at least in the testsuite.

```
<Omega interface: omega writer: TBP>+=
  procedure :: write_makefile_code => omega_write_makefile_code

<Omega interface: sub interfaces>+=
  module subroutine omega_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)
    class(omega_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
  end subroutine omega_write_makefile_code

<Omega interface: procedures>+=
  module subroutine omega_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)
    class(omega_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    type(string_t) :: omega_binary, omega_path
    type(string_t) :: restrictions_string
    type(string_t) :: openmp_string
    type(string_t) :: kmatrix_string
    type(string_t) :: progress_string
    type(string_t) :: diagrams_string
    type(string_t) :: cms_string
    type(string_t) :: write_phs_output_string
    type(string_t) :: parameter_module
    logical :: escape_hyperref
    escape_hyperref = .false.
    if (present (testflag)) escape_hyperref = testflag
    select type (writer)
    type is (omega_omega_writer_t)
      omega_binary = "omega_" // writer%model_name // ".opt"
    type is (omega_ufo_writer_t)
      omega_binary = "omega_UFO.opt"
    type is (omega_ovm_writer_t)
      select case (char (writer%model_name))
      case ("SM", "SM_CKM", "SM_Higgs", "THDM", "THDM_CKM", &
        "HSExt", "QED", "QCD", "Zprime")
      case default
        call msg_fatal ("The model " // char (writer%model_name) &
          // " is not available for the O'Mega VM.")
      end select
      omega_binary = "omega_" // writer%model_name // "_VM.opt"
    end select
    omega_path = os_data%whizard_omega_binpath // "/" // omega_binary
```

```

if (.not. verbose) omega_path = "@" // omega_path
if (writer%restrictions /= "") then
    restrictions_string = " -cascade '" // writer%restrictions // "'"
else
    restrictions_string = ""
end if
if (writer%openmp_support) then
    openmp_string = " -target:openmp"
else
    openmp_string = ""
end if
if (writer%report_progress) then
    progress_string = " -fusion:progress"
else
    progress_string = ""
end if
if (writer%diags) then
    if (writer%diags_color) then
        diagrams_string = " -diagrams:C " // char(id) // &
            "_diags -diagrams_LaTeX"
    else
        diagrams_string = " -diagrams " // char(id) // &
            "_diags -diagrams_LaTeX"
    end if
else
    if (writer%diags_color) then
        diagrams_string = " -diagrams:c " // char(id) // &
            "_diags -diagrams_LaTeX"
    else
        diagrams_string = ""
    end if
end if
if (writer%complex_mass_scheme) then
    cms_string = " -model:cms_width"
else
    cms_string = ""
end if
if (writer%write_phs_output) then
    write_phs_output_string = " -phase_space " // char (id) // ".fds"
else
    write_phs_output_string = ""
endif
select case (char (writer%model_name))
case ("SM_rx", "SSC", "NoH_rx", "AltH")
    kmatrix_string = " -target:kmatrix_2_write"
case ("SSC_2", "SSC_AltT", "SM_ul")
    kmatrix_string = " -target:kmatrix_write"
case default
    kmatrix_string = ""
end select
write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
select type (writer)
type is (omega_ovm_writer_t)
    write (unit, "(5A)") "SOURCES += ", char (id), ".hbc"

```

```

end select
if (writer%diags .or. writer%diags_color) then
  write (unit, "(5A)") "TEX_SOURCES += ", char (id), "_diags.tex"
  if (os_data%event_analysis_pdf) then
    write (unit, "(5A)") "TEX_OBJECTS += ", char (id), "_diags.pdf"
  else
    write (unit, "(5A)") "TEX_OBJECTS += ", char (id), "_diags.ps"
  end if
end if
write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
select type (writer)
type is (omega_omega_writer_t)
  write (unit, "(5A)") char (id), ".f90:"
  if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " OMEGA      ', trim (char (id)), '.f90"'
  end if
  write (unit, "(99A)") TAB, char (omega_path), &
    " -o ", char (id), ".f90", &
    " -target:whizard", &
    " -target:parameter_module parameters_", char (writer%model_name), &
    " -target:module opr_", char (id), &
    " -target:md5sum '", writer%md5sum, "'", &
    char (cms_string), &
    char (openmp_string), &
    char (progress_string), &
    char (kmatrix_string), &
    char (writer%process_mode), char (writer%process_string), &
    char (restrictions_string), char (diagrams_string), &
    char (writer%extra_options), char (write_phs_output_string)
type is (omega_ufo_writer_t)
  parameter_module = char (id) // "_par_" // replace (char (writer%model_name), &
    "-", "_", every=.true.)
  write (unit, "(5A)") char (id), ".f90: ", char (parameter_module), ".lo"
  if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " OMEGA[UFO]', trim (char (id)), '.f90"'
  end if
  write (unit, "(99A)") TAB, char (omega_path), &
    " -o ", char (id), ".f90", &
    " -model:UFO_dir ", &
    char (writer%ufo_path), "/", char (writer%model_name), &
    " -model:exec", &
    " -target:whizard", &
    " -target:parameter_module ", char (parameter_module), &
    " -target:module opr_", char (id), &
    " -target:md5sum '", writer%md5sum, "'", &
    char (cms_string), &
    char (openmp_string), &
    char (progress_string), &
    char (kmatrix_string), &
    char (writer%process_mode), char (writer%process_string), &
    char (restrictions_string), char (diagrams_string), &
    char (writer%extra_options), char (write_phs_output_string)
  write (unit, "(5A)") "SOURCES += ", char (parameter_module), ".f90"
  write (unit, "(5A)") "OBJECTS += ", char (parameter_module), ".lo"

```

```

write (unit, "(5A)") char (parameter_module), ".f90:"
write (unit, "(99A)") TAB, char (omega_path), &
    " -model:UFO_dir ", &
    char (writer%ufo_path), "/", char (writer%model_name), &
    " -model:exec", &
    " -target:parameter_module ", char (parameter_module), &
    " -params", &
    " -o $"
write (unit, "(5A)") char (parameter_module), ".lo: ", char (parameter_module), ".f90"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " FC " $@'
end if
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $"
type is (omega_ovm_writer_t)
write (unit, "(5A)") char (id), ".hbc:"
write (unit, "(99A)") TAB, char (omega_path), &
    " -o ", char (id), ".hbc", &
    char (progress_string), &
    char (cms_string), &
    char (writer%process_mode), char (writer%process_string), &
    char (restrictions_string), char (diagrams_string), &
    char (writer%extra_options), char (write_phs_output_string)
write (unit, "(5A)") char (id), ".f90:"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " OVM ', trim (char (id)), '.f90"'
end if
write (unit, "(99A)") TAB, char (omega_path), &
    " -o ", char (id), ".f90 -params", &
    " -target:whizard ", &
    " -target:bytecode_file ", char (id), ".hbc", &
    " -target:wrapper_module opr_", char (id), &
    " -target:parameter_module_external parameters-", &
    char (writer%model_name), &
    " -target:md5sum '", writer%md5sum, "'", &
    char (openmp_string)
end select
if (writer%diags .or. writer%diags_color) &
    write (unit, "(5A)") char (id), "_diags.tex: ", char (id), ".f90"
write (unit, "(5A)") "clean-", char (id), ":"
if (verbose) then
    write (unit, "(5A)") TAB, "rm -f ", char (id), ".f90"
    write (unit, "(5A)") TAB, "rm -f opr_", char (id), ".mod"
    write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
else
    write (unit, "(5A)") TAB // '@echo " RM ', &
        trim (char (id)), '.f90,.mod,.lo"'
    write (unit, "(5A)") TAB, "@rm -f ", char (id), ".f90"
    write (unit, "(5A)") TAB, "@rm -f opr_", char (id), ".mod"
    write (unit, "(5A)") TAB, "@rm -f ", char (id), ".lo"
end if
write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
select type (writer)
type is (omega_ufo_writer_t)
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (writer%model_name), ".mdl"

```

```

        write (unit, "(5A)") "CLEAN_SOURCES += ", char (parameter_module), ".f90"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (parameter_module), ".mod"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (parameter_module), ".lo"
type is (omega_ovm_writer_t)
        write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".hbc"
end select
if (writer%diags .or. writer%diags_color) then
        write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), "_diags.tex"
end if
write (unit, "(5A)") "CLEAN_OBJECTS += opr_", char (id), ".mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
if (writer%diags .or. writer%diags_color) then
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.aux"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.log"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.dvi"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.toc"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.out"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9][0-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9][0-9][0-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9][0-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9][0-9][0-9]"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.mp"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.log"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.dvi"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.ps"
        if (os_data%event_analysis_pdf) &
                write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.pdf"
end if
write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
if (writer%diags .or. writer%diags_color) then
        if (os_data%event_analysis_ps) then
                if (os_data%event_analysis_pdf) then
                        write (unit, "(5A)") char (id), "_diags.pdf: ", char (id), "_diags.tex"
                else
                        write (unit, "(5A)") char (id), "_diags.ps: ", char (id), "_diags.tex"
                end if
        end if
        if (escape_hyperref) then
                if (verbose) then
                        write (unit, "(5A)") TAB, "-cat ", char (id), "_diags.tex | \"
                else
                        write (unit, "(5A)") TAB // '@echo " HYPERREF ', &
                                trim(char (id)) // '_diags.tex"'
                        write (unit, "(5A)") TAB, "@cat ", char (id), "_diags.tex | \"
                end if
        end if
        write (unit, "(5A)") TAB, " sed -e" // &
                "'s/\\usepackage\\[colorlinks\\]{hyperref}\\./%\\usepackage" // &
                "\\[colorlinks\\]{hyperref}/' > \"
        write (unit, "(5A)") TAB, " ", char (id), "_diags.tex.tmp"
        if (verbose) then
                write (unit, "(5A)") TAB, "mv -f ", char (id), "_diags.tex.tmp \"
        else

```



```

        write (unit, "(5A)") TAB, "@mv -f ", char (id), "_diags.tex.tmp \"
    end if
    write (unit, "(5A)") TAB, "    ", char (id), "_diags.tex"
end if
if (verbose) then
    write (unit, "(5A)") TAB, "-TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
        char (id) // "_diags.tex"
    write (unit, "(5A)") TAB, "MPINPUTS=$(MP_FLAGS) $(MPOST) " // &
        char (id) // "_diags-fmf.mp"
    write (unit, "(5A)") TAB, "TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
        char (id) // "_diags.tex"
    write (unit, "(5A)") TAB, "$ (DVIPS) -o " // char (id) // "_diags.ps " // &
        char (id) // "_diags.dvi"
else
    write (unit, "(5A)") TAB // '@echo " LATEX      ', &
        trim(char (id)) // '_diags.tex"'
    write (unit, "(5A)") TAB, "@TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
        char (id) // "_diags.tex > /dev/null"
    write (unit, "(5A)") TAB // '@echo " METAPOST  ', &
        trim(char (id)) // '_diags-fmf.mp"'
    write (unit, "(5A)") TAB, "@MPINPUTS=$(MP_FLAGS) $(MPOST) " // &
        char (id) // "_diags-fmf.mp > /dev/null"
    write (unit, "(5A)") TAB // '@echo " LATEX      ', &
        trim(char (id)) // '_diags.tex"'
    write (unit, "(5A)") TAB, "@TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
        char (id) // "_diags.tex > /dev/null"
    write (unit, "(5A)") TAB // '@echo " DVIPS      ', &
        trim(char (id)) // '_diags.dvi"'
    write (unit, "(5A)") TAB, "@$(DVIPS) -q -o " // char (id) &
        // "_diags.ps " // char (id) // "_diags.dvi"
end if
if (os_data%event_analysis_pdf) then
    if (verbose) then
        write (unit, "(5A)") TAB, "$ (PS2PDF) " // char (id) // "_diags.ps"
    else
        write (unit, "(5A)") TAB // '@echo " PS2PDF      ', &
            trim(char (id)) // '_diags.ps"'
        write (unit, "(5A)") TAB, "@$(PS2PDF) " // char (id) // "_diags.ps"
    end if
end if
end if
end if
end subroutine omega_write_makefile_code

```

The source is written by the makefile, so nothing to do here.

```

<Omega interface: omega writer: TBP>+≡
    procedure :: write_source_code => omega_write_source_code

<Omega interface: sub interfaces>+≡
    module subroutine omega_write_source_code (writer, id)
        class(omega_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine omega_write_source_code

<Omega interface: procedures>+≡

```

```

module subroutine omega_write_source_code (writer, id)
  class(omega_writer_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine omega_write_source_code

```

Nothing to be done here.

```

<Omega interface: omega writer: TBP>+≡
  procedure :: before_compile => omega_before_compile
  procedure :: after_compile => omega_after_compile

<Omega interface: sub interfaces>+≡
  module subroutine omega_before_compile (writer, id)
    class(omega_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine omega_before_compile
  module subroutine omega_after_compile (writer, id)
    class(omega_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine omega_after_compile

<Omega interface: procedures>+≡
  module subroutine omega_before_compile (writer, id)
    class(omega_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine omega_before_compile

  module subroutine omega_after_compile (writer, id)
    class(omega_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine omega_after_compile

```

Return the name of a procedure that implements a given feature, as it is provided by the external matrix-element code. O'MEGA names some procedures differently, therefore we translate here and override the binding of the base type.

```

<Omega interface: omega writer: TBP>+≡
  procedure, nopass :: get_procname => omega_writer_get_procname

<Omega interface: sub interfaces>+≡
  module function omega_writer_get_procname (feature) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: feature
  end function omega_writer_get_procname

<Omega interface: procedures>+≡
  module function omega_writer_get_procname (feature) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: feature
    select case (char (feature))
    case ("n_in");   name = "number_particles_in"
    case ("n_out");  name = "number_particles_out"
    case ("n_flv");  name = "number_flavor_states"
    case ("n_hel");  name = "number_spin_states"
    case ("n_col");  name = "number_color_flows"
    case ("n_cin");  name = "number_color_indices"
    case ("n_cf");   name = "number_color_factors"

```

```

case ("flv_state"); name = "flavor_states"
case ("hel_state"); name = "spin_states"
case ("col_state"); name = "color_flows"
case default
    name = feature
end select
end function omega_writer_get_procname

```

The interfaces for the O'MEGA-specific features.

```

⟨Omega interface: omega writer: TBP⟩+≡
    procedure :: write_interface => omega_write_interface

⟨Omega interface: sub interfaces⟩+≡
    module subroutine omega_write_interface (writer, unit, id, feature)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(string_t), intent(in) :: feature
    end subroutine omega_write_interface

⟨Omega interface: procedures⟩+≡
    module subroutine omega_write_interface (writer, unit, id, feature)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(string_t), intent(in) :: feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, "(2x,9A)") "interface"
        select case (char (feature))
        case ("init")
            write (unit, "(5x,9A)") "subroutine ", char (name), &
                " (par, scheme) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
                &intent(in) :: par"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("update_alpha_s")
            write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("reset_helicity_selection")
            write (unit, "(5x,9A)") "subroutine ", char (name), " &
                &(threshold, cutoff) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: threshold"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: cutoff"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("is_allowed")
            write (unit, "(5x,9A)") "subroutine ", char (name), " &
                &(flv, hel, col, flag) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"

```

```

        write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("new_event")
        write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &
            &intent(in) :: p"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("get_amplitude")
        write (unit, "(5x,9A)") "subroutine ", char (name), " &
            &(flv, hel, col, amp) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
        write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
            &:: amp"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    end select
    write (unit, "(2x,9A)") "end interface"
end subroutine omega_write_interface

```

The wrappers have to take into account conversion between C and Fortran data types.

NOTE: The case `c_default_float` \neq default is not yet covered.

<Omega interface: omega writer: TBP>+≡

```

    procedure :: write_wrapper => omega_write_wrapper

```

<Omega interface: sub interfaces>+≡

```

    module subroutine omega_write_wrapper (writer, unit, id, feature)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
    end subroutine omega_write_wrapper

```

<Omega interface: procedures>+≡

```

    module subroutine omega_write_wrapper (writer, unit, id, feature)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, *)
        select case (char (feature))
        case ("init")
            write (unit, "(9A)") "subroutine ", char (name), &
                " (par, scheme) bind(C)"
            write (unit, "(2x,9A)") "use iso_c_binding"
            write (unit, "(2x,9A)") "use kinds"
            write (unit, "(2x,9A)") "use opr_", char (id)
            write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
                &intent(in) :: par"
            write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
            if (c_default_float == default .and. c_int == kind(1)) then
                write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
            end if

```

```

        write (unit, "(9A)") "end subroutine ", char (name)
case ("update_alpha_s")
    write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
            &:: alpha_s"
        write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("reset_helicity_selection")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (threshold, cutoff) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
            &:: threshold"
        write (unit, "(2x,9A)") "integer(c_int), intent(in) :: cutoff"
        write (unit, "(2x,9A)") "call ", char (feature), &
            " (threshold, int (cutoff))"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("is_allowed")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, flag) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
    write (unit, "(2x,9A)") "flag = ", char (feature), &
        " (int (flv), int (hel), int (col))"
    write (unit, "(9A)") "end subroutine ", char (name)
case ("new_event")
    write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
            &intent(in) :: p"
        write (unit, "(2x,9A)") "call ", char (feature), " (p)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("get_amplitude")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, amp) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)

```

```

        write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
        write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
            &:: amp"
        write (unit, "(2x,9A)") "amp = ", char (feature), &
            " (int (flv), int (hel), int (col))"
        write (unit, "(9A)") "end subroutine ", char (name)
    end select
end subroutine omega_write_wrapper

```

17.4.3 Driver

```

<Omega interface: public>+≡
    public :: omega_driver_t

<Omega interface: types>+≡
    type, extends (prc_core_driver_t) :: omega_driver_t
        procedure(init_t), nopass, pointer :: &
            init => null ()
        procedure(update_alpha_s_t), nopass, pointer :: &
            update_alpha_s => null ()
        procedure(reset_helicity_selection_t), nopass, pointer :: &
            reset_helicity_selection => null ()
        procedure(is_allowed_t), nopass, pointer :: &
            is_allowed => null ()
        procedure(new_event_t), nopass, pointer :: &
            new_event => null ()
        procedure(get_amplitude_t), nopass, pointer :: &
            get_amplitude => null ()
    contains
        <Omega interface: omega driver: TBP>
    end type omega_driver_t

```

The reported type is the same as for the `omega_def_t` type.

```

<Omega interface: omega driver: TBP>≡
    procedure, nopass :: type_name => omega_driver_type_name

<Omega interface: sub interfaces>+≡
    module function omega_driver_type_name () result (string)
        type(string_t) :: string
    end function omega_driver_type_name

<Omega interface: procedures>+≡
    module function omega_driver_type_name () result (string)
        type(string_t) :: string
        string = "omega"
    end function omega_driver_type_name

```

17.4.4 High-level process definition

This procedure wraps the details filling a process-component definition entry as appropriate for an O'MEGA matrix element. Gfortran 7/8/9 bug, has to remain

in the main module.

```

<Omega interface: public>+≡
    public :: omega_make_process_component

<Omega interface: main procedures>+≡
    subroutine omega_make_process_component (entry, component_index, &
        model_name, prt_in, prt_out, &
        ufo, ufo_path, restrictions, cms_scheme, &
        openmp_support, report_progress, write_omega_output, extra_options, diags, diags_color)
    class(process_def_entry_t), intent(inout) :: entry
    integer, intent(in) :: component_index
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    type(string_t), intent(in), optional :: restrictions
    logical, intent(in), optional :: cms_scheme
    logical, intent(in), optional :: openmp_support
    logical, intent(in), optional :: report_progress
    logical, intent(in), optional :: write_omega_output
    type(string_t), intent(in), optional :: extra_options
    logical, intent(in), optional :: diags, diags_color
    logical :: ufo_model
    class(prc_core_def_t), allocatable :: def
    ufo_model = .false.; if (present (ufo)) ufo_model = ufo
    allocate (omega_def_t :: def)
    select type (def)
    class is (omega_def_t)
        call def%init (model_name, prt_in, prt_out, &
            .false., ufo_model, ufo_path, &
            restrictions, cms_scheme, &
            openmp_support, report_progress, write_omega_output, extra_options, diags, diags_color)
    end select
    call entry%import_component (component_index, &
        n_out = size (prt_out), &
        prt_in = new_prt_spec (prt_in), &
        prt_out = new_prt_spec (prt_out), &
        method = var_str ("omega"), &
        variant = def)
    end subroutine omega_make_process_component

```

17.4.5 The prc_omega_t wrapper

This is an instance of the generic prc_core_t object. It contains a pointer to the process definition (omega_def_t), a data component (process_constants_t), and the matrix-element driver (omega_driver_t).

```

<Omega interface: public>+≡
    public :: prc_omega_t

<Omega interface: types>+≡
    type, extends (prc_core_t) :: prc_omega_t
        real(default), dimension(:), allocatable :: par

```

```

integer :: scheme = 0
type(helicity_selection_t) :: helicity_selection
type(qcd_t) :: qcd
type(qed_t) :: qed
contains
  <Omega interface: prc omega: TBP>
end type prc_omega_t

```

The workspace associated to a `prc_omega_t` object contains a single flag. The flag is used to suppress re-evaluating the matrix element for each quantum-number combination, after the first amplitude belonging to a given kinematics has been computed.

We can also store the value of a running coupling once it has been calculated for an event. The default value is negative, which indicates an undefined value in this context.

```

<Omega interface: public>+≡
  public :: omega_state_t

<Omega interface: types>+≡
  type, extends (prc_core_state_t) :: omega_state_t
    logical :: new_kinematics = .true.
    real(default) :: alpha_qcd = -1
    real(default) :: alpha_qed = -1
  contains
    <Omega interface: omega state: TBP>
  end type omega_state_t

<Omega interface: omega state: TBP>≡
  procedure :: write => omega_state_write

<Omega interface: sub interfaces>+≡
  module subroutine omega_state_write (object, unit)
    class(omega_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine omega_state_write

<Omega interface: procedures>+≡
  module subroutine omega_state_write (object, unit)
    class(omega_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,L1)") "0'Mega state: new kinematics = ", &
      object%new_kinematics
  end subroutine omega_state_write

<Omega interface: omega state: TBP>+≡
  procedure :: reset_new_kinematics => omega_state_reset_new_kinematics

<Omega interface: sub interfaces>+≡
  module subroutine omega_state_reset_new_kinematics (object)
    class(omega_state_t), intent(inout) :: object
  end subroutine omega_state_reset_new_kinematics

```



```

<Omega interface: procedures>+≡
  module subroutine omega_state_reset_new_kinematics (object)
    class(omega_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine omega_state_reset_new_kinematics

```

Allocate the workspace with the above specific type. Gfortran 7/8/9 bug, has to remain in main module.

```

<Omega interface: prc omega: TBP>≡
  procedure :: allocate_workspace => prc_omega_allocate_workspace

<Omega interface: main procedures>+≡
  subroutine prc_omega_allocate_workspace (object, core_state)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (omega_state_t :: core_state)
  end subroutine prc_omega_allocate_workspace

```

The following procedures are inherited from the base type as deferred, thus must be implemented. The corresponding unit tests are skipped here; the procedures are tested when called from the `processes` module.

Output: print just the ID of the associated matrix element. Then display any stored parameters and the helicity selection data. (The latter are printed only if active.)

```

<Omega interface: prc omega: TBP>+≡
  procedure :: write => prc_omega_write

<Omega interface: sub interfaces>+≡
  module subroutine prc_omega_write (object, unit)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine prc_omega_write

<Omega interface: procedures>+≡
  module subroutine prc_omega_write (object, unit)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(3x,A)", advance="no") "0'Mega process core:"
    if (object%data_known) then
      write (u, "(1x,A)") char (object%data%id)
    else
      write (u, "(1x,A)") "[undefined]"
    end if
    if (allocated (object%par)) then
      write (u, "(3x,A)") "Parameter array:"
      do i = 1, size (object%par)
        write (u, "(5x,I0,1x,ES17.10)") i, object%par(i)
      end do
    end if
    call object%helicity_selection%write (u)
    call object%qcd%write (u)
    call object%qed%write (u)
  end subroutine prc_omega_write

```

```
end subroutine prc_omega_write
```

<Omega interface: prc omega: TBP>+≡

```
procedure :: write_name => prc_omega_write_name
```

<Omega interface: sub interfaces>+≡

```
module subroutine prc_omega_write_name (object, unit)
  class(prc_omega_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine prc_omega_write_name
```

<Omega interface: procedures>+≡

```
module subroutine prc_omega_write_name (object, unit)
  class(prc_omega_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u,"(1x,A)") "Core: 0'Mega"
end subroutine prc_omega_write_name
```

Temporarily store the parameter array inside the `prc_omega` object, so we can use it later during the actual initialization. Also store threshold and cutoff for helicity selection. Gfortran 7/8/9 bug, has to remain in the main module.

<Omega interface: prc omega: TBP>+≡

```
procedure :: set_parameters => prc_omega_set_parameters
```

<Omega interface: main procedures>+≡

```
subroutine prc_omega_set_parameters (prc_omega, model, &
  helicity_selection, qcd, use_color_factors)
  class(prc_omega_t), intent(inout) :: prc_omega
  class(model_data_t), intent(in), target, optional :: model
  type(helicity_selection_t), intent(in), optional :: helicity_selection
  type(qcd_t), intent(in), optional :: qcd
  type(qed_t) :: qed
  logical, intent(in), optional :: use_color_factors
  if (present (model)) then
    if (.not. allocated (prc_omega%par)) &
      allocate (prc_omega%par (model%get_n_real ()))
    call model%real_parameters_to_array (prc_omega%par)
    prc_omega%scheme = model%get_scheme_num ()
    if (associated (model%get_par_data_ptr (var_str ('alpha_em_i')))) then
      allocate (alpha_qed_fixed_t :: qed%alpha)
      select type (alpha => qed%alpha)
      type is (alpha_qed_fixed_t)
        alpha%val = one / model%get_real (var_str ('alpha_em_i'))
      end select
    end if
    prc_omega%qed = qed
  end if
  if (present (helicity_selection)) then
    prc_omega%helicity_selection = helicity_selection
  end if
  if (present (qcd)) then
    prc_omega%qcd = qcd
```

```

end if
if (present (use_color_factors)) then
    prc_omega%use_color_factors = use_color_factors
end if
end subroutine prc_omega_set_parameters

```

To fully initialize the process core, we perform base initialization, then initialize the external matrix element code.

This procedure overrides the `init` method of the base type, which we nevertheless can access via its binding `base_init`. When done, we have an allocated driver. The driver will call the `init` procedure for the external matrix element, and thus transfer the parameter set to where it finally belongs.

If requested, we initialize the helicity selection counter.

```

<Omega interface: prc omega: TBP>+≡
    procedure :: init => prc_omega_init

<Omega interface: sub interfaces>+≡
    module subroutine prc_omega_init (object, def, lib, id, i_component)
        class(prc_omega_t), intent(inout) :: object
        class(prc_core_def_t), intent(in), target :: def
        type(process_library_t), intent(in), target :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
    end subroutine prc_omega_init

<Omega interface: procedures>+≡
    module subroutine prc_omega_init (object, def, lib, id, i_component)
        class(prc_omega_t), intent(inout) :: object
        class(prc_core_def_t), intent(in), target :: def
        type(process_library_t), intent(in), target :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        call object%base_init (def, lib, id, i_component)
        call object%activate_parameters ()
    end subroutine prc_omega_init

```

Activate the stored parameters by transferring them to the external matrix element. Also reset the helicity selection, if requested.

```

<Omega interface: prc omega: TBP>+≡
    procedure :: activate_parameters => prc_omega_activate_parameters

<Omega interface: sub interfaces>+≡
    module subroutine prc_omega_activate_parameters (object)
        class (prc_omega_t), intent(inout) :: object
    end subroutine prc_omega_activate_parameters

<Omega interface: procedures>+≡
    module subroutine prc_omega_activate_parameters (object)
        class (prc_omega_t), intent(inout) :: object
        if (allocated (object%driver)) then
            if (allocated (object%par)) then
                select type (driver => object%driver)
                type is (omega_driver_t)
                    if (associated (driver%init)) then

```

```

        call driver%init (object%par, object%scheme)
    end if
end select
else
    call msg_bug ("prc_omega_activate: parameter set is not allocated")
end if
call object%reset_helicity_selection ()
else
    call msg_bug ("prc_omega_activate: driver is not allocated")
end if
end subroutine prc_omega_activate_parameters

```

Tell whether a particular combination of flavor, helicity, color is allowed. Here we have to consult the matrix-element driver.

```

<Omega interface: prc_omega: TBP>+≡
    procedure :: is_allowed => prc_omega_is_allowed

<Omega interface: sub interfaces>+≡
    module function prc_omega_is_allowed (object, i_term, f, h, c) result (flag)
        class(prc_omega_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
    end function prc_omega_is_allowed

<Omega interface: procedures>+≡
    module function prc_omega_is_allowed (object, i_term, f, h, c) result (flag)
        class(prc_omega_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
        logical(c_bool) :: cflag
        select type (driver => object%driver)
        type is (omega_driver_t)
            call driver%is_allowed (f, h, c, cflag)
            flag = cflag
        end select
    end function prc_omega_is_allowed

```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

We don't reset the `new_kinematics` flag here. This has to be done explicitly by the caller (`reset_new_kinematics`) when a new kinematics configuration is to be considered.

```

<Omega interface: prc_omega: TBP>+≡
    procedure :: compute_hard_kinematics => prc_omega_compute_hard_kinematics

<Omega interface: sub interfaces>+≡
    module subroutine prc_omega_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(prc_omega_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_omega_compute_hard_kinematics

```

```

<Omega interface: procedures>+=
module subroutine prc_omega_compute_hard_kinematics &
  (object, p_seed, i_term, int_hard, core_state)
  class(prc_omega_t), intent(in) :: object
  type(vector4_t), dimension(:), intent(in) :: p_seed
  integer, intent(in) :: i_term
  type(interaction_t), intent(inout) :: int_hard
  class(prc_core_state_t), intent(inout), allocatable :: core_state
  call int_hard%set_momenta (p_seed)
end subroutine prc_omega_compute_hard_kinematics

```

This procedure is not called for `prc_omega_t`, just a placeholder.

```

<Omega interface: prc omega: TBP>+=
procedure :: compute_eff_kinematics => prc_omega_compute_eff_kinematics

```

```

<Omega interface: sub interfaces>+=
module subroutine prc_omega_compute_eff_kinematics &
  (object, i_term, int_hard, int_eff, core_state)
  class(prc_omega_t), intent(in) :: object
  integer, intent(in) :: i_term
  type(interaction_t), intent(in) :: int_hard
  type(interaction_t), intent(inout) :: int_eff
  class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine prc_omega_compute_eff_kinematics

```

```

<Omega interface: procedures>+=
module subroutine prc_omega_compute_eff_kinematics &
  (object, i_term, int_hard, int_eff, core_state)
  class(prc_omega_t), intent(in) :: object
  integer, intent(in) :: i_term
  type(interaction_t), intent(in) :: int_hard
  type(interaction_t), intent(inout) :: int_eff
  class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine prc_omega_compute_eff_kinematics

```

Reset the helicity selection counters and start counting zero helicities. We assume that the `helicity_selection` object is allocated. Otherwise, reset and switch off helicity counting.

In the test routine, the driver is allocated but the driver methods are not. Therefore, guard against a disassociated method.

```

<Omega interface: prc omega: TBP>+=
procedure :: reset_helicity_selection => prc_omega_reset_helicity_selection

```

```

<Omega interface: sub interfaces>+=
module subroutine prc_omega_reset_helicity_selection (object)
  class(prc_omega_t), intent(inout) :: object
end subroutine prc_omega_reset_helicity_selection

```

```

<Omega interface: procedures>+=
module subroutine prc_omega_reset_helicity_selection (object)
  class(prc_omega_t), intent(inout) :: object
  select type (driver => object%driver)
  type is (omega_driver_t)
    if (associated (driver%reset_helicity_selection)) then
      if (object%helicity_selection%active) then

```

```

        call driver%reset_helicity_selection &
            (real (object%helicity_selection%threshold, &
                c_default_float), &
            int (object%helicity_selection%cutoff, c_int))
    else
        call driver%reset_helicity_selection &
            (0._c_default_float, 0_c_int)
    end if
end if
end select
end subroutine prc_omega_reset_helicity_selection

```

Compute the amplitude. For the tree-level process, we can ignore the scale settings. The term index j is also irrelevant.

We first call `new_event` for the given momenta (which we must unpack), then retrieve the amplitude value for the given quantum numbers.

If the `core_state` status flag is present, we can make sure that we call `new_event` only once for a given kinematics. After the first call, we unset the `new_kinematics` flag.

The core objects computes the appropriate α_s value via the `qcd` subobject, taking into account the provided `ren_scale` value. However, if the extra parameter `alpha_qcd_forced` is allocated, it overrides this setting.

The `is_allowed` query is not redundant, since the status may change during the run if helicities are switched off.

(Omega interface: prc omega: TBP)+≡

```

procedure :: compute_amplitude => prc_omega_compute_amplitude

```

(Omega interface: sub interfaces)+≡

```

module function prc_omega_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: &
        core_state
    complex(default):: amp
end function prc_omega_compute_amplitude

```

(Omega interface: procedures)+≡

```

module function prc_omega_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    real(default) :: alpha_qcd

```

```

complex(default) :: amp
integer :: n_tot, i
real(c_default_float), dimension(:,,:), allocatable :: parray
complex(c_default_complex) :: camp
logical :: new_event
select type (driver => object%driver)
type is (omega_driver_t)
    new_event = .true.
    if (present (core_state)) then
        if (allocated (core_state)) then
            select type (core_state)
            type is (omega_state_t)
                new_event = core_state%new_kinematics
                core_state%new_kinematics = .false.
            end select
        end if
    end if
    if (new_event) then
        if (allocated (object%qcd%alpha)) then
            if (allocated (alpha_qcd_forced)) then
                alpha_qcd = alpha_qcd_forced
            else
                alpha_qcd = object%qcd%alpha%get (ren_scale)
            end if
            call driver%update_alpha_s (alpha_qcd)
            if (present (core_state)) then
                if (allocated (core_state)) then
                    select type (core_state)
                    type is (omega_state_t)
                        core_state%alpha_qcd = alpha_qcd
                    end select
                end if
            end if
        end if
        n_tot = object%data%get_n_tot ()
        allocate (parray (0:3, n_tot))
        do i = 1, n_tot
            parray(:,i) = vector4_get_components (p(i))
        end do
        call driver%new_event (parray)
    end if
    if (object%is_allowed (1, f, h, c)) then
        call driver%get_amplitude &
            (int (f, c_int), int (h, c_int), int (c, c_int), camp)
        amp = camp
    else
        amp = 0
    end if
end select
end function prc_omega_compute_amplitude

```

After the amplitude has been computed, we may read off the current value of α_s . This works only if α_s varies, and if the workspace `core_state` is present

which stores this value.

```

<Omega interface: prc omega: TBP>+=
  procedure :: get_alpha_s => prc_omega_get_alpha_s

<Omega interface: sub interfaces>+=
  module function prc_omega_get_alpha_s &
    (object, core_state) result (alpha_qcd)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
  end function prc_omega_get_alpha_s

<Omega interface: procedures>+=
  module function prc_omega_get_alpha_s &
    (object, core_state) result (alpha_qcd)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
    alpha_qcd = -1
    if (allocated (object%qcd%alpha) .and. allocated (core_state)) then
      select type (core_state)
        type is (omega_state_t)
          alpha_qcd = core_state%alpha_qcd
        end select
      end if
    end function prc_omega_get_alpha_s

```

After the amplitude has been computed, we may read off the current value of α . This works only if α varies, and if the workspace `core_state` is present which stores this value.

```

<Omega interface: prc omega: TBP>+=
  procedure :: get_alpha_qed => prc_omega_get_alpha_qed

<Omega interface: sub interfaces>+=
  module function prc_omega_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qed
  end function prc_omega_get_alpha_qed

<Omega interface: procedures>+=
  module function prc_omega_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qed
    alpha_qed = -1
    if (allocated (object%qed%alpha) .and. allocated (core_state)) then
      select type (core_state)
        type is (omega_state_t)
          alpha_qed = core_state%alpha_qed
        end select
      end if
    end function prc_omega_get_alpha_qed

```


17.4.6 Unit Test

Test module, followed by the corresponding implementation module. There is a separate test for testing O'MEGA diagram generation as this depends on a working analysis setup.

```
<prc_omega_ut.f90>≡  
  <File header>  
  
  module prc_omega_ut  
    use unit_tests  
    use prc_omega_ut  
  
    <Standard module head>  
  
    <Omega interface: public test>  
  
    contains  
  
    <Omega interface: test driver>  
  
  end module prc_omega_ut  
<prc_omega_util.f90>≡  
  <File header>  
  
  module prc_omega_util  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    use kinds  
    <Use strings>  
    use io_units  
    use file_utils, only: delete_file  
    use os_interface  
    use sm_qcd  
    use lorentz  
    use model_data  
    use var_base  
    use particle_specifiers, only: new_prt_spec  
    use prc_core_def  
    use process_constants  
    use process_libraries  
    use prc_core  
    use model_testbed, only: prepare_model, cleanup_model  
  
    use prc_omega  
  
    <Standard module head>  
  
    <Omega interface: test declarations>  
  
    contains  
  
    <Omega interface: tests>
```

```

end module prc_omega_utili
API: driver for the unit tests below.
<Omega interface: public test>≡
    public :: prc_omega_test
<Omega interface: test driver>≡
    subroutine prc_omega_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Omega interface: execute tests>
end subroutine prc_omega_test

<Omega interface: public test>+≡
    public :: prc_omega_diags_test
<Omega interface: test driver>+≡
    subroutine prc_omega_diags_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Omega interface: execute diags tests>
end subroutine prc_omega_diags_test

```

Generate, compile and load a simple process matrix element

The process is $e^+e^- \rightarrow \mu^+\mu^-$ for vanishing masses and $e = 0.3$. We initialize the process, build the library, and compute a particular matrix element for momenta of unit energy and right-angle scattering. The matrix element, as it happens, is equal to e^2 . (Note that are no conversion factors applied, so this result is exact.)

For GNU make, makeflags is set to -j1. This eliminates a potential clash with a -j<n> flag if this test is called from a parallel make.

```

<Omega interface: execute tests>≡
    call test (prc_omega_1, "prc_omega_1", &
        "build and load simple OMega process", &
        u, results)

<Omega interface: test declarations>≡
    public :: prc_omega_1

<Omega interface: tests>≡
    subroutine prc_omega_1 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_constants_t) :: data
        class(prc_core_driver_t), allocatable :: driver
        integer, parameter :: cdf = c_default_float
        integer, parameter :: ci = c_int
        real(cdf), dimension(4) :: par

```

```

real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i

write (u, "(A)")  "* Test output: prc_omega_1"
write (u, "(A)")  "* Purpose: create a simple process with OMega"
write (u, "(A)")  "*           build a library, link, load, and &
                    &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("omega1"))
call os_data%init ()

model_name = "QED"
allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false.)
end select
allocate (entry)
call entry%init (var_str ("omega1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"

```

```

write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active          = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes        = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of omega1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("omega1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID      = ", char (data%id)
write (u, "(1x,A,A)")  "model name        = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum          = '", data%md5sum, "'"
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in            = ", data%n_in
write (u, "(1x,A,I0)")  "n_out           = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv           = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel           = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col           = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin           = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf            = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
do i = 2, 16
    write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega1_a and initialize:"
write (u, "(A)")

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]
write (u, "(2x,A,F6.4)")  "ee      = ", par(1)
write (u, "(2x,A,F6.4)")  "me      = ", par(2)
write (u, "(2x,A,F6.4)")  "mmu     = ", par(3)
write (u, "(2x,A,F6.4)")  "mtau    = ", par(4)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

```

```

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf,-1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf,-1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

select type (driver)
type is (omega_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_1"

end subroutine prc_omega_1

```

Check prc_omega_t wrapper and options

The process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses and $e = 0.3$. We build the library using the high-level procedure `omega_make_process_component` and the “black box” `prc_omega_t` object. Two variants with different settings for restrictions and OpenMP.

For GNU make, `makeflags` is set to `-j1`. This eliminates a potential clash with a `-j<n>` flag if this test is called from a parallel make.

```

<Omega interface: execute tests>+≡
    call test (prc_omega_2, "prc_omega_2", &
        "OMega option passing", &
        u, results)

<Omega interface: test declarations>+≡
    public :: prc_omega_2

<Omega interface: tests>+≡
    subroutine prc_omega_2 (u)

```

```

integer, intent(in) :: u
type(process_library_t), target :: lib
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
type(string_t) :: model_name
class(model_data_t), pointer :: model
class(vars_t), pointer :: vars
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(string_t) :: restrictions
type(process_component_def_t), pointer :: config
type(prc_omega_t) :: prc1, prc2
type(process_constants_t) :: data
integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(:), allocatable :: par
real(cdf), dimension(0:3,4) :: p
complex(c_default_complex) :: amp
integer :: i
logical :: exist

write (u, "(A)")  "* Test output: prc_omega_2"
write (u, "(A)")  "* Purpose: create simple processes with OMega"
write (u, "(A)")  "*           use the prc_omega wrapper for this"
write (u, "(A)")  "*           and check OMega options"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with two entries, &
&different options."
write (u, "(A)")  "* (1) e- e+ -> e- e+  &
&(all diagrams, no OpenMP, report progress)"
write (u, "(A)")  "* (2) e- e+ -> e- e+  &
&(s-channel only, with OpenMP, report progress to file)"

call lib%init (var_str ("omega2"))
call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name, vars)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e-"), var_str ("e+")]
prt_out = prt_in
restrictions = "3+4~A"

allocate (entry)
call entry%init (var_str ("omega2_a"), &
model, n_in = 2, n_components = 2)

call omega_make_process_component (entry, 1, &
model_name, prt_in, prt_out, &
report_progress=.true.)
call omega_make_process_component (entry, 2, &
model_name, prt_in, prt_out, &

```

```

restrictions=restrictions, openmp_support=.true., &
extra_options=var_str ("-fusion:progress_file omega2.log"))

call lib%append (entry)

write (u, "(A)")
write (u, "(A)")  "* Remove left-over file"
write (u, "(A)")

call delete_file ("omega2.log")
inquire (file="omega2.log", exist=exist)
write (u, "(1x,A,L1)") "omega2.log exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Check extra output of OMega"
write (u, "(A)")

inquire (file="omega2.log", exist=exist)
write (u, "(1x,A,L1)") "omega2.log exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)") "is active                = ", &
lib%is_active ()
write (u, "(1x,A,I0)") "n_processes              = ", &
lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega2_a and initialize:"
write (u, "(A)")

call vars%set_rval (var_str ("ee"), 0.3_default)
call vars%set_rval (var_str ("me"), 0._default)
call vars%set_rval (var_str ("mmu"), 0._default)
call vars%set_rval (var_str ("mtau"), 0._default)
allocate (par (model%get_n_real ()))
call model%real_parameters_to_c_array (par)

write (u, "(2x,A,F6.4)") "ee   = ", par(1)
write (u, "(2x,A,F6.4)") "me   = ", par(2)
write (u, "(2x,A,F6.4)") "mmu  = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

```

```

call prc1%set_parameters (model)
call prc2%set_parameters (model)

write (u, "(A)")
write (u, "(A)")  "* Constants of omega2_a_i1:"
write (u, "(A)")

entry => lib%get_process_def_ptr (var_str ("omega2_a"))
config => entry%get_component_def_ptr (1)
call prc1%init (config%get_core_def_ptr (), &
               lib, var_str ("omega2_a"), 1)
call prc1%get_constants (data, 1)

write (u, "(1x,A,A)") "component ID      = ", &
      char (data%id)
write (u, "(1x,A,L1)") "openmp supported = ", &
      data%openmp_supported
write (u, "(1x,A,A,A)") "model name      = '", &
      char (data%model_name), "'"

write (u, "(A)")
write (u, "(A)")  "* Constants of omega2_a_i2:"
write (u, "(A)")

config => entry%get_component_def_ptr (2)
call prc2%init (config%get_core_def_ptr (), &
               lib, var_str ("omega2_a"), 2)
call prc2%get_constants (data, 1)

write (u, "(1x,A,A)") "component ID      = ", &
      char (data%id)
write (u, "(1x,A,L1)") "openmp supported = ", &
      data%openmp_supported
write (u, "(1x,A,A,A)") "model name      = '", &
      char (data%model_name), "'"

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
              1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
              1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
              1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
              1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
              ], [4,4])
do i = 1, 4
  write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

```



```

select type (driver => prc1%driver)
type is (omega_driver_t)
  call driver%new_event (p)
  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(2x,A,1x,E11.4)") "(1) |amp (1, 6, 1)| =", abs (amp)
end select

select type (driver => prc2%driver)
type is (omega_driver_t)
  call driver%new_event (p)
  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(2x,A,1x,E11.4)") "(2) |amp (1, 6, 1)| =", abs (amp)
end select

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
  1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
  1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
  1.0_cdf, sqrt(0.5_cdf), 0.0_cdf, sqrt(0.5_cdf), &
  1.0_cdf, -sqrt(0.5_cdf), 0.0_cdf, -sqrt(0.5_cdf) &
], [4,4])
do i = 1, 4
  write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver => prc1%driver)
type is (omega_driver_t)
  call driver%new_event (p)
  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(2x,A,1x,E11.4)") "(1) |amp (1, 6, 1)| =", abs (amp)
end select

select type (driver => prc2%driver)
type is (omega_driver_t)
  call driver%new_event (p)
  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(2x,A,1x,E11.4)") "(2) |amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()
call cleanup_model (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_2"

end subroutine prc_omega_2

```

Check helicity selection

The process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses. We call the matrix element several times to verify the switching off of irrelevant helicities.

```
(Omega interface: execute tests)+≡
    call test (prc_omega_3, "prc_omega_3", &
               "helicity selection", &
               u, results)

(Omega interface: test declarations)+≡
    public :: prc_omega_3

(Omega interface: tests)+≡
    subroutine prc_omega_3 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        class(model_data_t), pointer :: model
        class(vars_t), pointer :: vars => null ()
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_component_def_t), pointer :: config
        type(prc_omega_t) :: prc1
        type(process_constants_t) :: data
        integer, parameter :: cdf = c_default_float
        real(cdf), dimension(:), allocatable :: par
        real(cdf), dimension(0:3,4) :: p
        type(helicity_selection_t) :: helicity_selection
        integer :: i, h

        write (u, "(A)")  "* Test output: prc_omega_3"
        write (u, "(A)")  "*   Purpose: create simple process with OMega"
        write (u, "(A)")  "*               and check helicity selection"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library."
        write (u, "(A)")  "* (1) e- e+ -> e- e+   (all diagrams, no OpenMP)"

        call lib%init (var_str ("omega3"))
        call os_data%init ()

        model_name = "QED"
        model => null ()
        call prepare_model (model, model_name, vars)

        allocate (prt_in (2), prt_out (2))
        prt_in = [var_str ("e-"), var_str ("e+")]
        prt_out = prt_in

        allocate (entry)
        call entry%init (var_str ("omega3_a"), &
                        model, n_in = 2, n_components = 1)

        call omega_make_process_component (entry, 1, &
```

```

        model_name, prt_in, prt_out)
call lib%append (entry)

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active           = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes         = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega3_a and initialize:"
write (u, "(A)")

call vars%set_rval (var_str ("ee"), 0.3_default)
call vars%set_rval (var_str ("me"), 0._default)
call vars%set_rval (var_str ("mmu"), 0._default)
call vars%set_rval (var_str ("mtau"), 0._default)
allocate (par (model%get_n_real ()))
call model%real_parameters_to_c_array (par)

write (u, "(2x,A,F6.4)")  "ee   = ", par(1)
write (u, "(2x,A,F6.4)")  "me   = ", par(2)
write (u, "(2x,A,F6.4)")  "mmu  = ", par(3)
write (u, "(2x,A,F6.4)")  "mtau = ", par(4)

call prc1%set_parameters (model, helicity_selection=helicity_selection)

write (u, "(A)")
write (u, "(A)")  "* Helicity states of omega3_a_i1:"
write (u, "(A)")

entry => lib%get_process_def_ptr (var_str ("omega3_a"))
config => entry%get_component_def_ptr (1)
call prc1%init (config%get_core_def_ptr (), &
    lib, var_str ("omega3_a"), 1)
call prc1%get_constants (data, 1)

do i = 1, data%n_hel
    write (u, "(3x,I2,':',4(1x,I2))") i, data%hel_state(:,i)
end do

write (u, "(A)")

```

```

write (u, "(A)")  "* Initially allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
    write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Reset helicity selection (cutoff = 4)"
write (u, "(A)")

helicity_selection%active = .true.
helicity_selection%threshold = 1e10_default
helicity_selection%cutoff = 4
call helicity_selection%write (u)

call prc1%set_parameters (model, helicity_selection=helicity_selection)
call prc1%reset_helicity_selection ()

write (u, "(A)")
write (u, "(A)")  "* Allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
    write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute scattering matrix 5 times"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]

select type (driver => prc1%driver)

```

```

type is (omega_driver_t)
do i = 1, 5
  call driver%new_event (p)
  write (u, "(2x,I2)", advance = "no") i
  do h = 1, data%n_hel
    write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
  end do
  write (u, "(A)")
end do
end select

write (u, "(A)")
write (u, "(A)")  "* Reset helicity selection again"
write (u, "(A)")

call prc1%activate_parameters ()

write (u, "(A)")  "* Allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
  write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

call lib%final ()
call cleanup_model (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_3"

end subroutine prc_omega_3

```

QCD coupling

The process is $u\bar{u} \rightarrow d\bar{d}$ for vanishing masses. We compute the amplitude for a fixed configuration once, then reset α_s , then compute again.

For GNU make, makeflags is set to -j1. This eliminates a potential clash with a -j<n> flag if this test is called from a parallel make.

```

<Omega interface: execute tests>+≡
  call test (prc_omega_4, "prc_omega_4", &
    "update QCD alpha", &
    u, results)

```

```

<Omega interface: test declarations>+≡
  public :: prc_omega_4

```

```

<Omega interface: tests>+≡
  subroutine prc_omega_4 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib

```

```

class(prc_core_def_t), allocatable :: def
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
type(string_t) :: model_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(process_constants_t) :: data
class(prc_core_driver_t), allocatable :: driver
integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(8) :: par
real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i
real(cdf) :: alpha_s

write (u, "(A)")  "* Test output: prc_omega_4"
write (u, "(A)")  "* Purpose: create a QCD process with OMega"
write (u, "(A)")  "*           and check alpha_s dependence"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("prc_omega_4_lib"))
call os_data%init ()

model_name = "QCD"
allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("u"), var_str ("ubar")]
prt_out = [var_str ("d"), var_str ("dbar")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false.)
end select
allocate (entry)
call entry%init (var_str ("prc_omega_4_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"
write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

```

```

write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters:"
write (u, "(A)")

alpha_s = 0.1178_cdf

par = [alpha_s, &
       0._cdf, 0._cdf, 0._cdf, 0._cdf, 0._cdf, 173.1_cdf, 1.523_cdf]
write (u, "(2x,A,F8.4)")  "alpha_s = ", par(1)
write (u, "(2x,A,F8.4)")  "md      = ", par(2)
write (u, "(2x,A,F8.4)")  "mu      = ", par(3)
write (u, "(2x,A,F8.4)")  "ms      = ", par(4)
write (u, "(2x,A,F8.4)")  "mc      = ", par(5)
write (u, "(2x,A,F8.4)")  "mb      = ", par(6)
write (u, "(2x,A,F8.4)")  "mtop    = ", par(7)
write (u, "(2x,A,F8.4)")  "wtop    = ", par(8)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
              100.0_cdf, 0.0_cdf, 0.0_cdf, 100.0_cdf, &
              100.0_cdf, 0.0_cdf, 0.0_cdf, -100.0_cdf, &
              100.0_cdf, 100.0_cdf, 0.0_cdf, 0.0_cdf, &
              100.0_cdf, -100.0_cdf, 0.0_cdf, 0.0_cdf &
              ], [4,4])
do i = 1, 4
  write (u, "(2x,A,I0,A,4(1x,F7.1))")  "p", i, " =", p(:,i)
end do

call lib%connect_process (var_str ("prc_omega_4_p"), 1, data, driver)

select type (driver)
type is (omega_driver_t)
  call driver%init (par, 0)

  write (u, "(A)")
  write (u, "(A)")  "* Compute matrix element:"
  write (u, "(A)")

  call driver%new_event (p)

  call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
  write (u, "(1x,A,L1)")  "is_allowed (1, 6, 1) = ", flag

  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(1x,A,1x,E11.4)")  "|amp (1, 6, 1)| =", abs (amp)

```

```

write (u, "(A)")
write (u, "(A)")  "* Double alpha_s and compute matrix element again:"
write (u, "(A)")

call driver%update_alpha_s (2 * alpha_s)
call driver%new_event (p)

call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_4"

end subroutine prc_omega_4

```

Amplitude and QCD coupling

The same process as before. Here, we initialize with a running α_s coupling and compute twice with different scales. We use the high-level method `compute_amplitude`.

```

<Omega interface: execute tests>+≡
call test (prc_omega_5, "prc_omega_5", &
  "running QCD alpha", &
  u, results)

<Omega interface: test declarations>+≡
public :: prc_omega_5

<Omega interface: tests>+≡
subroutine prc_omega_5 (u)
  integer, intent(in) :: u
  type(process_library_t) :: lib
  class(prc_core_def_t), allocatable :: def
  type(process_component_def_t), pointer :: cdef_ptr
  class(prc_core_def_t), pointer :: def_ptr
  type(process_def_entry_t), pointer :: entry
  type(os_data_t) :: os_data
  class(model_data_t), pointer :: model
  type(string_t) :: model_name
  type(string_t), dimension(:), allocatable :: prt_in, prt_out
  type(qcd_t) :: qcd
  class(prc_core_t), allocatable :: core
  class(prc_core_state_t), allocatable :: core_state
  type(vector4_t), dimension(4) :: p
  complex(default) :: amp
  real(default) :: ren_scale
  real(default), allocatable :: alpha_qcd_forced

```



```

integer :: i

write (u, "(A)")  "* Test output: prc_omega_5"
write (u, "(A)")  "*   Purpose: create a QCD process with OMega"
write (u, "(A)")  "*               and check alpha_s dependence"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("prc_omega_5_lib"))
call os_data%init ()

model_name = "QCD"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("u"), var_str ("ubar")]
prt_out = [var_str ("d"), var_str ("dbar")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false.)
end select
allocate (entry)
call entry%init (var_str ("prc_omega_5_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"
write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")  "* Probe library API"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")
write (u, "(A)")  "* Set kinematics"
write (u, "(A)")

p(1) = vector4_moving (100._default, 100._default, 3)

```

```

p(2) = vector4_moving (100._default,-100._default, 3)
p(3) = vector4_moving (100._default, 100._default, 1)
p(4) = vector4_moving (100._default,-100._default, 1)
do i = 1, 4
    call vector4_write (p(i), u)
end do

write (u, "(A)")
write (u, "(A)")  "* Setup QCD data"
write (u, "(A)")

allocate (alpha_qcd_from_scale_t :: qcd%alpha)

write (u, "(A)")  "* Setup process core"
write (u, "(A)")

allocate (prc_omega_t :: core)
entry => lib%get_process_def_ptr (var_str ("prc_omega_5_p"))
cdef_ptr => entry%get_component_def_ptr (1)
def_ptr => cdef_ptr%get_core_def_ptr ()

select type (core)
type is (prc_omega_t)
    call core%allocate_workspace (core_state)
    call core%set_parameters (model, qcd = qcd)
    call core%init (def_ptr, lib, var_str ("prc_omega_5_p"), 1)
    call core%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element"
    write (u, "(A)")

    ren_scale = 100
    write (u, "(1x,A,F4.0)")  "renormalization scale = ", ren_scale

    amp = core%compute_amplitude &
        (1, p, 1, 6, 1, 100._default, ren_scale, alpha_qcd_forced)

    write (u, "(1x,A,1x,E11.4)")  "|amp (1, 6, 1)| =", abs (amp)

    write (u, "(A)")
    write (u, "(A)")  "* Modify renormalization scale and &
        &compute matrix element again"
    write (u, "(A)")

    ren_scale = 200
    write (u, "(1x,A,F4.0)")  "renormalization scale = ", ren_scale

    amp = core%compute_amplitude &
        (1, p, 1, 6, 1, 100._default, ren_scale, alpha_qcd_forced)

    write (u, "(1x,A,1x,E11.4)")  "|amp (1, 6, 1)| =", abs (amp)

    write (u, "(A)")

```

```

write (u, "(A)")  "* Set alpha(QCD) directly and &
                  &compute matrix element again"
write (u, "(A)")

allocate (alpha_qcd_forced, source = 0.1_default)
write (u, "(1x,A,F6.4)") "alpha_qcd = ", alpha_qcd_forced

amp = core%compute_amplitude &
      (1, p, 1, 6, 1, 100._default, ren_scale, alpha_qcd_forced)

write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)

end select

call lib%final ()
call cleanup_model (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_5"

end subroutine prc_omega_5

```

UFO model file support

Again, the process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses and $e = 0.3$. We build the library using the high-level procedure `omega_make_process_component` and the “black box” `prc_omega_t` object. OMega must be able to digest the specified UFO file and provide use with a fresh model file that can be read after producing the process code.

For GNU make, `makeflags` is set to `-j1`. This eliminates a potential clash with a `-j<n>` flag if this test is called from a parallel make.

```

<Omega interface: execute tests>+≡
call test (prc_omega_6, "prc_omega_6", &
          "OMega UFO support", &
          u, results)

```

```

<Omega interface: test declarations>+≡
public :: prc_omega_6

```

```

<Omega interface: tests>+≡
subroutine prc_omega_6 (u)
integer, intent(in) :: u
type(process_library_t), target :: lib
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
type(string_t) :: model_name
class(model_data_t), pointer :: model
class(vars_t), pointer :: vars
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(string_t) :: restrictions
type(process_component_def_t), pointer :: config
type(prc_omega_t) :: prc1, prc2
type(process_constants_t) :: data

```

```

integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(:), allocatable :: par
real(cdf), dimension(0:3,4) :: p
complex(c_default_complex) :: amp
integer :: i
logical :: exist

write (u, "(A)")  "* Test output: prc_omega_6"
write (u, "(A)")  "* Purpose: create simple process with OMega / UFO file"
write (u, "(A)")

call os_data%init ()

model_name = "SM"
model => null ()

os_data%whizard_modelpath_ufo = "../models/UFO"

write (u, "(A)")  "* Create process library entry"
write (u, "(A)")

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e-"), var_str ("e+")]
prt_out = prt_in
restrictions = "3+4~A"

allocate (entry)
call entry%init (var_str ("omega_6_a"), &
    model_name = model_name, n_in = 2, n_components = 1)

call omega_make_process_component (entry, 1, &
    model_name, prt_in, prt_out, &
    ufo=.true., ufo_path=os_data%whizard_modelpath_ufo, &
    report_progress=.true.)

call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%init (var_str ("omega_6"))
call lib%append (entry)

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

```

```

write (u, "(1x,A,L1)") "is active" = ", &
lib%is_active ()
write (u, "(1x,A,I0)") "n_processes" = ", &
lib%get_n_processes ()

call lib%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: prc_omega_6"

end subroutine prc_omega_6

```

Generate matrix element diagrams

The same process as before. No amplitude is computed here, instead we just generate Feynman (and color flow) diagrams, and check whether PS and PDF files have been generated. This test is only run if event analysis is possible.

```

<Omega interface: execute diags tests>≡
call test (prc_omega_diags_1, "prc_omega_diags_1", &
"generate Feynman diagrams", &
u, results)

<Omega interface: test declarations>+≡
public :: prc_omega_diags_1

<Omega interface: tests>+≡
subroutine prc_omega_diags_1 (u)
integer, intent(in) :: u
type(process_library_t) :: lib
class(prc_core_def_t), allocatable :: def
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
type(string_t) :: model_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(string_t) :: diags_file, pdf_file, ps_file
logical :: exist, exist_pdf, exist_ps
integer :: iostat, u_diags
character(128) :: buffer

write (u, "(A)") "* Test output: prc_omega_diags_1"
write (u, "(A)") "* Purpose: generate Feynman diagrams"
write (u, "(A)")

write (u, "(A)") "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("prc_omega_diags_1_lib"))
call os_data%init ()

model_name = "SM"

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("u"), var_str ("ubar")]
prt_out = [var_str ("d"), var_str ("dbar")]

```

```

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false., &
        diags = .true., diags_color = .true.)
end select
allocate (entry)
call entry%init (var_str ("prc_omega_diags_1_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"
write (u, "(A)")  "    and generate diagrams"
write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile &
    (os_data, force = .true., verbose = .false., testflag = .true.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")  "* Probe library API"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")  "* Check produced diagram files"
write (u, "(A)")

diags_file = "prc_omega_diags_1_p_i1_diags.tex"
ps_file = "prc_omega_diags_1_p_i1_diags.ps"
pdf_file = "prc_omega_diags_1_p_i1_diags.pdf"
inquire (file = char (diags_file), exist = exist)
if (exist) then
    u_diags = free_unit ()
    open (u_diags, file = char (diags_file), action = "read", status = "old")
    iostat = 0
    do while (iostat == 0)
        read (u_diags, "(A)", iostat = iostat) buffer
        if (iostat == 0) write (u, "(A)") trim (buffer)
    end do
    close (u_diags)
else
    write (u, "(A)")  "[Feynman diagrams LaTeX file is missing]"
end if
inquire (file = char (ps_file), exist = exist_ps)
if (exist_ps) then

```

```

        write (u, "(A)") "[Feynman diagrams Postscript file exists and is nonempty]"
    else
        write (u, "(A)") "[Feynman diagrams Postscript file is missing/non-regular]"
    end if
    inquire (file = char (pdf_file), exist = exist_pdf)
    if (exist_pdf) then
        write (u, "(A)") "[Feynman diagrams PDF file exists and is nonempty]"
    else
        write (u, "(A)") "[Feynman diagrams PDF file is missing/non-regular]"
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
    write (u, "(A)")

    call lib%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: prc_omega_diags_1"

end subroutine prc_omega_diags_1

```

17.5 External matrix elements (squared)

This defines an abstract framework that can handle matrix elements which are computed outside of WHIZARD. Such matrix elements typically (i) require extra code or libraries to be configured linked at execution time, and (ii) provide only plain or correlated squared matrix elements instead of amplitudes.

In particular, matrix-element libraries that conform to the BLHA standard belong to this class. They have their own (also abstract) extension of the abstract `prc_external_t` type introduced here. `prc_external_t`-type.

```

⟨prc_external.f90⟩≡
⟨File header⟩
module prc_external

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    ⟨Use strings⟩
    use constants
    use os_interface
    use lorentz
    use interactions
    use sm_qcd
    use sm_qed
    use variables, only: var_list_t

    use model_data
    use prclib_interfaces
    use prc_core_def
    use prc_core

```

```

    use sf_base
    use sf_pdf_builtin, only: pdf_builtin_t
    use sf_lhapdf, only: lhpdf_t

    <Standard module head>

    <Prc external: public>

    <Prc external: types>

    <Prc external: interfaces>

    interface
    <Prc external: sub interfaces>
    end interface

contains

    <Prc external: main procedures>

end module prc_external
<prc_external_sub.f90>≡
    <File header>

submodule (prc_external) prc_external_s

    <Use debug>
    use io_units
    use pdg_arrays, only: is_gluon, is_quark
    use system_defs, only: TAB
    use physics_defs, only: CF
    use diagnostics
    use prc_omega, only: omega_state_t

    implicit none

    <Prc external: parameters>

contains

    <Prc external: procedures>

end submodule prc_external_s

```

17.5.1 Handling of structure functions

External matrix elements do not have access to the structure functions stored in the evaluators. The current solution to this problem is to just apply them explicitly after the computation of the matrix element.

```

<Prc external: parameters>≡
    integer, parameter :: LEPTONS = 1

```



```

integer, parameter :: HADRONS = 2
<Prc external: types>≡
type :: sf_handler_t
integer :: initial_state_type = 0
integer :: n_sf = -1
real(default) :: val = one
contains
<Prc external: sf handler: TBP>
end type sf_handler_t

<Prc external: sf handler: TBP>≡
procedure :: init => sf_handler_init

<Prc external: sub interfaces>≡
module subroutine sf_handler_init (sf_handler, sf_chain)
class(sf_handler_t), intent(out) :: sf_handler
type(sf_chain_instance_t), intent(in) :: sf_chain
end subroutine sf_handler_init

<Prc external: procedures>≡
module subroutine sf_handler_init (sf_handler, sf_chain)
class(sf_handler_t), intent(out) :: sf_handler
type(sf_chain_instance_t), intent(in) :: sf_chain
integer :: i
sf_handler%n_sf = size (sf_chain%sf)
if (sf_handler%n_sf == 0) then
sf_handler%initial_state_type = LEPTONS
else
do i = 1, sf_handler%n_sf
select type (int => sf_chain%sf(i)%int)
type is (pdf_builtin_t)
sf_handler%initial_state_type = HADRONS
type is (lhpdf_t)
sf_handler%initial_state_type = HADRONS
class default
sf_handler%initial_state_type = LEPTONS
end select
end do
end if
end subroutine sf_handler_init

<Prc external: sf handler: TBP>+≡
procedure :: init_dummy => sf_handler_init_dummy

<Prc external: sub interfaces>+≡
module subroutine sf_handler_init_dummy (sf_handler)
class(sf_handler_t), intent(out) :: sf_handler
end subroutine sf_handler_init_dummy

<Prc external: procedures>+≡
module subroutine sf_handler_init_dummy (sf_handler)
class(sf_handler_t), intent(out) :: sf_handler
sf_handler%n_sf = 0
sf_handler%initial_state_type = LEPTONS
end subroutine sf_handler_init_dummy

```

```

<Prc external: sf handler: TBP>+≡
  procedure :: apply_structure_functions => &
    sf_handler_apply_structure_functions

<Prc external: sub interfaces>+≡
  module subroutine sf_handler_apply_structure_functions &
    (sf_handler, sf_chain, flavors)
    class(sf_handler_t), intent(inout) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in), dimension(2) :: flavors
  end subroutine sf_handler_apply_structure_functions

<Prc external: procedures>+≡
  module subroutine sf_handler_apply_structure_functions &
    (sf_handler, sf_chain, flavors)
    class(sf_handler_t), intent(inout) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in), dimension(2) :: flavors
    integer :: i
    real(default), dimension(:), allocatable :: f
    if (sf_handler%n_sf < 0) call msg_fatal ("sf_handler not initialized")
    sf_handler%val = one
    do i = 1, sf_handler%n_sf
      select case (sf_handler%initial_state_type)
      case (HADRONS)
        sf_handler%val = sf_handler%val * &
          sf_handler%get_pdf (sf_chain, i, flavors(i))
      case (LEPTONS)
        call sf_chain%get_matrix_elements (i, f)
        sf_handler%val = sf_handler%val * f(1)
      case default
        call msg_fatal ("sf_handler not initialized")
      end select
    end do
  end subroutine sf_handler_apply_structure_functions

<Prc external: sf handler: TBP>+≡
  procedure :: get_pdf => sf_handler_get_pdf

<Prc external: sub interfaces>+≡
  module function sf_handler_get_pdf &
    (sf_handler, sf_chain, i, flavor) result (f)
    real(default) :: f
    class(sf_handler_t), intent(in) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in) :: i, flavor
  end function sf_handler_get_pdf

<Prc external: procedures>+≡
  module function sf_handler_get_pdf &
    (sf_handler, sf_chain, i, flavor) result (f)
    real(default) :: f
    class(sf_handler_t), intent(in) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in) :: i, flavor
    integer :: k

```

```

real(default), dimension(:), allocatable :: ff
integer, parameter :: n_flv_light = 6

call sf_chain%get_matrix_elements (i, ff)

if (is_gluon (flavor)) then
  k = n_flv_light + 1
else if (is_quark (abs(flavor))) then
  k = n_flv_light + 1 + flavor
else
  call msg_fatal ("Not a colored particle")
end if

f = ff(k)
end function sf_handler_get_pdf

```

17.5.2 Abstract interface to external matrix elements

This process class allows us to factor out common necessities of processes that involve external code or libraries.

Workspace

This is the workspace that is available for external matrix elements.

```

<Prc external: public>≡
  public :: prc_external_state_t

<Prc external: types>+≡
  type, abstract, extends (prc_core_state_t) :: prc_external_state_t
    logical :: new_kinematics = .true.
    real(default) :: alpha_qcd = -1
    real(default) :: alpha_qed = -1
  contains
    <Prc external: external state: TBP>
  end type prc_external_state_t

<Prc external: external state: TBP>≡
  procedure :: reset_new_kinematics => prc_external_state_reset_new_kinematics

<Prc external: sub interfaces>+≡
  module subroutine prc_external_state_reset_new_kinematics (object)
    class(prc_external_state_t), intent(inout) :: object
  end subroutine prc_external_state_reset_new_kinematics

<Prc external: procedures>+≡
  module subroutine prc_external_state_reset_new_kinematics (object)
    class(prc_external_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine prc_external_state_reset_new_kinematics

```

Driver

We have to add two O'Mega-routines to the external matrix-element driver to ensure proper process setup. The problem is that during the setup of the real component, the particle and flavor data are taken from the Born component to set up the subtraction terms. However, the Born component expects this data to be obtained from the Omega code, accessed by the driver.

```
<Prc external: public>+≡
  public :: prc_external_driver_t

<Prc external: types>+≡
  type, abstract, extends (prc_core_driver_t) :: prc_external_driver_t
    procedure(omega_update_alpha_s), nopass, pointer :: &
      update_alpha_s => null ()
    procedure(omega_is_allowed), nopass, pointer :: &
      is_allowed => null ()
  end type prc_external_driver_t
```

Core

```
<Prc external: public>+≡
  public :: prc_external_t

<Prc external: types>+≡
  type, abstract, extends (prc_core_t) :: prc_external_t
    type(qcd_t) :: qcd
    type(qed_t) :: qed
    integer :: n_flv = 1
    real(default), dimension(:), allocatable :: par
    integer :: scheme = 0
    type(sf_handler_t) :: sf_handler
    real(default) :: maximum_accuracy = 10000.0
  contains
    <Prc external: prc external: TBP>
  end type prc_external_t
```

By definition, this class of process-core types require extra code.

```
<Prc external: prc external: TBP>≡
  procedure, nopass :: needs_external_code => &
    prc_external_needs_external_code

<Prc external: sub interfaces>+≡
  module function prc_external_needs_external_code () result (flag)
    logical :: flag
  end function prc_external_needs_external_code

<Prc external: procedures>+≡
  module function prc_external_needs_external_code () result (flag)
    logical :: flag
    flag = .true.
  end function prc_external_needs_external_code

<Prc external: prc external: TBP>+≡
  procedure :: get_n_flvs => prc_external_get_n_flvs
```

```

<Prc external: sub interfaces>+≡
  pure module function prc_external_get_n_flvs (object, i_flv) result (n)
    integer :: n
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
  end function prc_external_get_n_flvs

```

```

<Prc external: procedures>+≡
  pure module function prc_external_get_n_flvs (object, i_flv) result (n)
    integer :: n
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
    n = size (object%data%flv_state (:,i_flv))
  end function prc_external_get_n_flvs

```

```

<Prc external: prc external: TBP>+≡
  procedure :: get_flv_state => prc_external_get_flv_state

```

```

<Prc external: sub interfaces>+≡
  module function prc_external_get_flv_state (object, i_flv) result (flv)
    integer, dimension(:), allocatable :: flv
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
  end function prc_external_get_flv_state

```

```

<Prc external: procedures>+≡
  module function prc_external_get_flv_state (object, i_flv) result (flv)
    integer, dimension(:), allocatable :: flv
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
    allocate (flv (size (object%data%flv_state (:,i_flv))))
    flv = object%data%flv_state (:,i_flv)
  end function prc_external_get_flv_state

```

Return one single squared test matrix element. It is fixed to 1, therefore the integration output will be the phase space volume.

```

<Prc external: prc external: TBP>+≡
  procedure :: compute_sqme => prc_external_compute_sqme

```

```

<Prc external: sub interfaces>+≡
  module subroutine prc_external_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out) :: sqme
    logical, intent(out) :: bad_point
  end subroutine prc_external_compute_sqme

```

```

<Prc external: procedures>+≡
  module subroutine prc_external_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel

```

```

    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out) :: sqme
    logical, intent(out) :: bad_point
    sqme = one
    bad_point = .false.
end subroutine prc_external_compute_sqme

```

Return an array of 4 numbers corresponding to the BLHA output convention.
Used for testing.

```

<Prc external: prc external: TBP>+≡
    procedure :: compute_sqme_virt => prc_external_compute_sqme_virt

<Prc external: sub interfaces>+≡
    module subroutine prc_external_compute_sqme_virt (object, i_flg, i_hel, &
        p, ren_scale, es_scale, loop_method, sqme, bad_point)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_flg, i_hel
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: ren_scale, es_scale
        integer, intent(in) :: loop_method
        logical, intent(out) :: bad_point
        real(default), dimension(4), intent(out) :: sqme
    end subroutine prc_external_compute_sqme_virt

<Prc external: procedures>+≡
    module subroutine prc_external_compute_sqme_virt (object, i_flg, i_hel, &
        p, ren_scale, es_scale, loop_method, sqme, bad_point)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_flg, i_hel
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: ren_scale, es_scale
        integer, intent(in) :: loop_method
        logical, intent(out) :: bad_point
        real(default), dimension(4), intent(out) :: sqme
        if (debug_on) call msg_debug2 &
            (D_ME_METHODS, "prc_external_compute_sqme_virt")
        sqme(1) = 0.001_default
        sqme(2) = 0.001_default
        sqme(3) = 0.001_default
        sqme(4) = 0.0015_default
        bad_point = .false.
    end subroutine prc_external_compute_sqme_virt

```

Also return test output for color-correlated matrix elements. We only give a sensible result for the processes used in the functional tests, which have 2 -> 2 topology. All other processes will obtain a vanishing dummy color-correlation. This effectively switches off the subtraction contributions, reproducing the real phase-space volume.

```

<Prc external: prc external: TBP>+≡
    procedure :: compute_sqme_color_c => prc_external_compute_sqme_color_c

<Prc external: sub interfaces>+≡
    module subroutine prc_external_compute_sqme_color_c (object, i_flg, &

```

```

        i_hel, p, ren_scale, born_color_c, bad_point, born_out)
class(prc_external_t), intent(inout) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(inout), dimension(:, :) :: born_color_c
logical, intent(out) :: bad_point
real(default), intent(out), optional :: born_out
end subroutine prc_external_compute_sqme_color_c

<Prc external: procedures>+≡
module subroutine prc_external_compute_sqme_color_c (object, i_flv, &
    i_hel, p, ren_scale, born_color_c, bad_point, born_out)
class(prc_external_t), intent(inout) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(inout), dimension(:, :) :: born_color_c
logical, intent(out) :: bad_point
real(default), intent(out), optional :: born_out
if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_external_compute_sqme_color_c")
if (size(p) == 4) then
    if (present(born_out)) then
        born_out = 0.0015_default
        born_color_c = zero
        born_color_c(3,3) = - CF * born_out
        born_color_c(4,4) = - CF * born_out
        born_color_c(3,4) = CF * born_out
        born_color_c(4,3) = born_color_c(3,4)
        bad_point = .false.
    end if
else
    if (present(born_out)) born_out = zero
    born_color_c = zero
end if
end subroutine prc_external_compute_sqme_color_c

<Prc external: prc external: TBP>+≡
procedure :: compute_alpha_s => prc_external_compute_alpha_s

<Prc external: sub interfaces>+≡
module subroutine prc_external_compute_alpha_s &
    (object, core_state, ren_scale)
class(prc_external_t), intent(in) :: object
class(prc_external_state_t), intent(inout) :: core_state
real(default), intent(in) :: ren_scale
end subroutine prc_external_compute_alpha_s

<Prc external: procedures>+≡
module subroutine prc_external_compute_alpha_s &
    (object, core_state, ren_scale)
class(prc_external_t), intent(in) :: object
class(prc_external_state_t), intent(inout) :: core_state
real(default), intent(in) :: ren_scale
core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)

```

```
end subroutine prc_external_compute_alpha_s
```

```
<Prc external: prc external: TBP>+≡
```

```
procedure :: get_alpha_s => prc_external_get_alpha_s
```

```
<Prc external: sub interfaces>+≡
```

```
module function prc_external_get_alpha_s &
  (object, core_state) result (alpha_qcd)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(in), allocatable :: core_state
  real(default) :: alpha_qcd
end function prc_external_get_alpha_s
```

```
<Prc external: procedures>+≡
```

```
module function prc_external_get_alpha_s &
  (object, core_state) result (alpha_qcd)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(in), allocatable :: core_state
  real(default) :: alpha_qcd
  if (allocated (core_state)) then
    select type (core_state)
    class is (prc_external_state_t)
      alpha_qcd = core_state%alpha_qcd
    type is (omega_state_t)
      alpha_qcd = core_state%alpha_qcd
    class default
      alpha_qcd = zero
    end select
  else
    alpha_qcd = zero
  end if
end function prc_external_get_alpha_s
```

Getter for alpha_qed

```
<Prc external: prc external: TBP>+≡
```

```
procedure :: get_alpha_qed => prc_external_get_alpha_qed
```

```
<Prc external: sub interfaces>+≡
```

```
module function prc_external_get_alpha_qed &
  (object, core_state) result (alpha_qed)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(in), allocatable :: core_state
  real(default) :: alpha_qed
end function prc_external_get_alpha_qed
```

```
<Prc external: procedures>+≡
```

```
module function prc_external_get_alpha_qed &
  (object, core_state) result (alpha_qed)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(in), allocatable :: core_state
  real(default) :: alpha_qed
  if (allocated (core_state)) then
    select type (core_state)
    class is (prc_external_state_t)
      alpha_qed = core_state%alpha_qed
```



```

        type is (omega_state_t)
        alpha_qed = core_state%alpha_qed
    class default
        alpha_qed = zero
    end select
else
    alpha_qed = zero
end if
end function prc_external_get_alpha_qed

<Prc external: prc external: TBP>+≡
    procedure :: is_allowed => prc_external_is_allowed

<Prc external: sub interfaces>+≡
    module function prc_external_is_allowed &
        (object, i_term, f, h, c) result (flag)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
    end function prc_external_is_allowed

<Prc external: procedures>+≡
    module function prc_external_is_allowed &
        (object, i_term, f, h, c) result (flag)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
        logical(c_bool) :: cflag
        select type (driver => object%driver)
        class is (prc_external_driver_t)
            call driver%is_allowed (f, h, c, cflag)
            flag = cflag
        class default
            call msg_fatal &
                ("Driver does not fit to prc_external_t")
        end select
    end function prc_external_is_allowed

<Prc external: prc external: TBP>+≡
    procedure :: get_nflv => prc_external_get_nflv

<Prc external: sub interfaces>+≡
    module function prc_external_get_nflv (object) result (n_flg)
        class(prc_external_t), intent(in) :: object
        integer :: n_flg
    end function prc_external_get_nflv

<Prc external: procedures>+≡
    module function prc_external_get_nflv (object) result (n_flg)
        class(prc_external_t), intent(in) :: object
        integer :: n_flg
        n_flg = object%n_flg
    end function prc_external_get_nflv

```

```

<Prc external: prc external: TBP>+≡
    procedure :: compute_hard_kinematics => prc_external_compute_hard_kinematics

<Prc external: sub interfaces>+≡
    module subroutine prc_external_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(prc_external_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_external_compute_hard_kinematics

<Prc external: procedures>+≡
    module subroutine prc_external_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(prc_external_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        call int_hard%set_momenta (p_seed)
        if (allocated (core_state)) then
            select type (core_state)
                class is (prc_external_state_t); core_state%new_kinematics = .true.
            end select
        end if
    end subroutine prc_external_compute_hard_kinematics

<Prc external: prc external: TBP>+≡
    procedure :: compute_eff_kinematics => prc_external_compute_eff_kinematics

<Prc external: sub interfaces>+≡
    module subroutine prc_external_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_term
        type(interaction_t), intent(in) :: int_hard
        type(interaction_t), intent(inout) :: int_eff
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_external_compute_eff_kinematics

<Prc external: procedures>+≡
    module subroutine prc_external_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)
        class(prc_external_t), intent(in) :: object
        integer, intent(in) :: i_term
        type(interaction_t), intent(in) :: int_hard
        type(interaction_t), intent(inout) :: int_eff
        class(prc_core_state_t), intent(inout), allocatable :: core_state
    end subroutine prc_external_compute_eff_kinematics

Gfortran 7/8/9 bug, has to remain in the main module.
<Prc external: prc external: TBP>+≡
    procedure :: set_parameters => prc_external_set_parameters

```

```

<Prc external: main procedures>≡
subroutine prc_external_set_parameters (object, qcd, model)
  class(prc_external_t), intent(inout) :: object
  type(qcd_t), intent(in) :: qcd
  type(qed_t) :: qed
  class(model_data_t), intent(in), target, optional :: model
  object%qcd = qcd
  if (present (model)) then
    if (.not. allocated (object%par)) &
      allocate (object%par (model%get_n_real ()))
    call model%real_parameters_to_array (object%par)
    object%scheme = model%get_scheme_num ()
    if (associated (model%get_par_data_ptr (var_str ('alpha_em_i')))) then
      allocate (alpha_qed_fixed_t :: qed%alpha)
      select type (alpha => qed%alpha)
        type is (alpha_qed_fixed_t)
          alpha%val = one / model%get_real (var_str ('alpha_em_i'))
        end select
      end if
    object%qed = qed
  end if
end subroutine prc_external_set_parameters

<Prc external: prc external: TBP>+≡
procedure :: update_alpha_s => prc_external_update_alpha_s

<Prc external: sub interfaces>+≡
module subroutine prc_external_update_alpha_s (object, core_state, scale)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(inout), allocatable :: core_state
  real(default), intent(in) :: scale
end subroutine prc_external_update_alpha_s

<Prc external: procedures>+≡
module subroutine prc_external_update_alpha_s (object, core_state, scale)
  class(prc_external_t), intent(in) :: object
  class(prc_core_state_t), intent(inout), allocatable :: core_state
  real(default), intent(in) :: scale
  real(default) :: alpha_qcd
  if (allocated (object%qcd%alpha)) then
    alpha_qcd = object%qcd%alpha%get (scale)
    select type (driver => object%driver)
      class is (prc_external_driver_t)
        call driver%update_alpha_s (alpha_qcd)
      end select
    select type (core_state)
      class is (prc_external_state_t)
        core_state%alpha_qcd = alpha_qcd
      type is (omega_state_t)
        core_state%alpha_qcd = alpha_qcd
      end select
    end if
  end subroutine prc_external_update_alpha_s

```

```

<Prc external: prc external: TBP>+≡
    procedure :: init_sf_handler => prc_external_init_sf_handler

<Prc external: sub interfaces>+≡
    module subroutine prc_external_init_sf_handler (core, sf_chain)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
    end subroutine prc_external_init_sf_handler

<Prc external: procedures>+≡
    module subroutine prc_external_init_sf_handler (core, sf_chain)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
        if (allocated (sf_chain%sf)) then
            call core%sf_handler%init (sf_chain)
        else
            call core%sf_handler%init_dummy ()
        end if
    end subroutine prc_external_init_sf_handler

<Prc external: prc external: TBP>+≡
    procedure :: init_sf_handler_dummy => prc_external_init_sf_handler_dummy

<Prc external: sub interfaces>+≡
    module subroutine prc_external_init_sf_handler_dummy (core)
        class(prc_external_t), intent(inout) :: core
    end subroutine prc_external_init_sf_handler_dummy

<Prc external: procedures>+≡
    module subroutine prc_external_init_sf_handler_dummy (core)
        class(prc_external_t), intent(inout) :: core
        call core%sf_handler%init_dummy ()
    end subroutine prc_external_init_sf_handler_dummy

<Prc external: prc external: TBP>+≡
    procedure :: apply_structure_functions => &
        prc_external_apply_structure_functions

<Prc external: sub interfaces>+≡
    module subroutine prc_external_apply_structure_functions &
        (core, sf_chain, flavors)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
        integer, dimension(2), intent(in) :: flavors
    end subroutine prc_external_apply_structure_functions

<Prc external: procedures>+≡
    module subroutine prc_external_apply_structure_functions &
        (core, sf_chain, flavors)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
        integer, dimension(2), intent(in) :: flavors
        call core%sf_handler%apply_structure_functions (sf_chain, flavors)
    end subroutine prc_external_apply_structure_functions

```

```

<Prc external: prc external: TBP>+≡
    procedure :: get_sf_value => prc_external_get_sf_value

<Prc external: sub interfaces>+≡
    module function prc_external_get_sf_value (core) result (val)
        real(default) :: val
        class(prc_external_t), intent(in) :: core
    end function prc_external_get_sf_value

<Prc external: procedures>+≡
    module function prc_external_get_sf_value (core) result (val)
        real(default) :: val
        class(prc_external_t), intent(in) :: core
        val = core%sf_handler%val
    end function prc_external_get_sf_value

<Prc external: prc external: TBP>+≡
    procedure(prc_external_includes_polarization), deferred :: &
        includes_polarization

<Prc external: interfaces>≡
    abstract interface
        function prc_external_includes_polarization (object) result (polarized)
            import
            logical :: polarized
            class(prc_external_t), intent(in) :: object
        end function prc_external_includes_polarization
    end interface

```

Configuration

This is the abstract external matrix-element interface.

```

<Prc external: public>+≡
    public :: prc_external_def_t

<Prc external: types>+≡
    type, abstract, extends (prc_core_def_t) :: prc_external_def_t
        type(string_t) :: basename
    contains
        <Prc external: external def: TBP>
    end type prc_external_def_t

<Prc external: external def: TBP>≡
    procedure :: set_active_writer => prc_external_def_set_active_writer

<Prc external: sub interfaces>+≡
    module subroutine prc_external_def_set_active_writer (def, active)
        class(prc_external_def_t), intent(inout) :: def
        logical, intent(in) :: active
    end subroutine prc_external_def_set_active_writer

```

```

<Prc external: procedures>+≡
module subroutine prc_external_def_set_active_writer (def, active)
  class(prc_external_def_t), intent(inout) :: def
  logical, intent(in) :: active
  select type (writer => def%writer)
  class is (prc_external_writer_t)
    writer%active = active
  end select
end subroutine prc_external_def_set_active_writer

<Prc external: external def: TBP>+≡
procedure, nopass :: get_features => prc_external_def_get_features

<Prc external: sub interfaces>+≡
module subroutine prc_external_def_get_features (features)
  type(string_t), dimension(:), allocatable, intent(out) :: features
end subroutine prc_external_def_get_features

<Prc external: procedures>+≡
module subroutine prc_external_def_get_features (features)
  type(string_t), dimension(:), allocatable, intent(out) :: features
  allocate (features (6))
  features = [ &
    var_str ("init"), &
    var_str ("update_alpha_s"), &
    var_str ("reset_helicity_selection"), &
    var_str ("is_allowed"), &
    var_str ("new_event"), &
    var_str ("get_amplitude")]
end subroutine prc_external_def_get_features

<Prc external: external def: TBP>+≡
procedure :: connect => prc_external_def_connect
procedure :: omega_connect => prc_external_def_connect

<Prc external: sub interfaces>+≡
module subroutine prc_external_def_connect (def, lib_driver, i, proc_driver)
  class(prc_external_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
end subroutine prc_external_def_connect

<Prc external: procedures>+≡
module subroutine prc_external_def_connect (def, lib_driver, i, proc_driver)
  class(prc_external_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
  integer :: pid, fid
  type(c_funptr) :: fptr
  select type (proc_driver)
  class is (prc_external_driver_t)
    pid = i
    fid = 2

```

```

        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%update_alpha_s)
        fid = 4
        call lib_driver%get_fptr (pid, fid, fptr)
        call c_f_procpointer (fptr, proc_driver%is_allowed)
    end select
end subroutine prc_external_def_connect

```

```

<Prc external: external def: TBP>+≡
    procedure, nopass :: needs_code => prc_external_def_needs_code

```

```

<Prc external: sub interfaces>+≡
    module function prc_external_def_needs_code () result (flag)
        logical :: flag
    end function prc_external_def_needs_code

```

```

<Prc external: procedures>+≡
    module function prc_external_def_needs_code () result (flag)
        logical :: flag
        flag = .true.
    end function prc_external_def_needs_code

```

```

<Prc external: interfaces>+≡
    abstract interface
        subroutine omega_update_alpha_s (alpha_s) bind(C)
            import
            real(c_default_float), intent(in) :: alpha_s
        end subroutine omega_update_alpha_s
    end interface

    abstract interface
        subroutine omega_is_allowed (flv, hel, col, flag) bind(C)
            import
            integer(c_int), intent(in) :: flv, hel, col
            logical(c_bool), intent(out) :: flag
        end subroutine omega_is_allowed
    end interface

```

Writer

```

<Prc external: public>+≡
    public :: prc_external_writer_t

```

```

<Prc external: types>+≡
    type, abstract, extends (prc_writer_f_module_t) :: prc_external_writer_t
        type(string_t) :: model_name
        type(string_t) :: process_mode
        type(string_t) :: process_string
        type(string_t) :: restrictions
        integer :: n_in = 0
        integer :: n_out = 0
        logical :: active = .true.
        logical :: amp_triv = .true.

```

```

contains
  <Prc external: external writer: TBP>
end type prc_external_writer_t

<Prc external: external writer: TBP>≡
  procedure :: init => prc_external_writer_init
  procedure :: base_init => prc_external_writer_init

  <Prc external: sub interfaces>+≡
    pure module subroutine prc_external_writer_init &
      (writer, model_name, prt_in, prt_out, restrictions)
      class(prc_external_writer_t), intent(inout) :: writer
      type(string_t), intent(in) :: model_name
      type(string_t), dimension(:), intent(in) :: prt_in, prt_out
      type(string_t), intent(in), optional :: restrictions
    end subroutine prc_external_writer_init

  <Prc external: procedures>+≡
    pure module subroutine prc_external_writer_init &
      (writer, model_name, prt_in, prt_out, restrictions)
      class(prc_external_writer_t), intent(inout) :: writer
      type(string_t), intent(in) :: model_name
      type(string_t), dimension(:), intent(in) :: prt_in, prt_out
      type(string_t), intent(in), optional :: restrictions
      integer :: i
      writer%model_name = model_name
      if (present (restrictions)) then
        writer%restrictions = restrictions
      else
        writer%restrictions = ""
      end if
      writer%n_in = size (prt_in)
      writer%n_out = size (prt_out)
      select case (size (prt_in))
        case(1); writer%process_mode = " -decay"
        case(2); writer%process_mode = " -scatter"
      end select
      associate (s => writer%process_string)
        s = " '"
        do i = 1, size (prt_in)
          if (i > 1) s = s // " "
          s = s // prt_in(i)
        end do
        s = s // " ->"
        do i = 1, size (prt_out)
          s = s // " " // prt_out(i)
        end do
        s = s // "'"
      end associate
    end subroutine prc_external_writer_init

  <Prc external: external writer: TBP>+≡
    procedure, nopass :: get_module_name => prc_external_writer_get_module_name

```



```

<Prc external: sub interfaces>+≡
    module function prc_external_writer_get_module_name (id) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: id
    end function prc_external_writer_get_module_name

<Prc external: procedures>+≡
    module function prc_external_writer_get_module_name (id) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: id
        name = "opr_" // id
    end function prc_external_writer_get_module_name

<Prc external: external writer: TBP>+≡
    procedure :: write_wrapper => prc_external_writer_write_wrapper

<Prc external: sub interfaces>+≡
    module subroutine prc_external_writer_write_wrapper &
        (writer, unit, id, feature)
        class(prc_external_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
    end subroutine prc_external_writer_write_wrapper

<Prc external: procedures>+≡
    module subroutine prc_external_writer_write_wrapper &
        (writer, unit, id, feature)
        class(prc_external_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, *)
        select case (char (feature))
        case ("init")
            write (unit, "(9A)") "subroutine ", char (name), &
                " (par, scheme) bind(C)"
            write (unit, "(2x,9A)") "use iso_c_binding"
            write (unit, "(2x,9A)") "use kinds"
            write (unit, "(2x,9A)") "use opr_", char (id)
            write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
                &intent(in) :: par"
            write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
            if (c_default_float == default .and. c_int == kind (1)) then
                write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
            end if
            write (unit, "(9A)") "end subroutine ", char (name)
        case ("update_alpha_s")
            write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
            write (unit, "(2x,9A)") "use iso_c_binding"
            write (unit, "(2x,9A)") "use kinds"
            write (unit, "(2x,9A)") "use opr_", char (id)
            if (c_default_float == default) then
                write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
                    &:: alpha_s"
            end if
        end select
    end subroutine prc_external_writer_write_wrapper

```

```

        write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("reset_helicity_selection")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (threshold, cutoff) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
            &:: threshold"
        write (unit, "(2x,9A)") "integer(c_int), intent(in) :: cutoff"
        write (unit, "(2x,9A)") "call ", char (feature), &
            " (threshold, int (cutoff))"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("is_allowed")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, flag) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
    write (unit, "(2x,9A)") "flag = ", char (feature), &
        " (int (flv), int (hel), int (col))"
    write (unit, "(9A)") "end subroutine ", char (name)
case ("new_event")
    write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
            &intent(in) :: p"
        write (unit, "(2x,9A)") "call ", char (feature), " (p)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("get_amplitude")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, amp) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
        &:: amp"
    write (unit, "(2x,9A)") "amp = ", char (feature), &
        " (int (flv), int (hel), int (col))"
    write (unit, "(9A)") "end subroutine ", char (name)
end select

end subroutine prc_external_writer_write_wrapper

```

```

<Prc external: external writer: TBP>+≡
    procedure :: write_interface => prc_external_writer_write_interface

<Prc external: sub interfaces>+≡
    module subroutine prc_external_writer_write_interface &
        (writer, unit, id, feature)
        class(prc_external_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(string_t), intent(in) :: feature
    end subroutine prc_external_writer_write_interface

<Prc external: procedures>+≡
    module subroutine prc_external_writer_write_interface &
        (writer, unit, id, feature)
        class(prc_external_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(string_t), intent(in) :: feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, "(2x,9A)") "interface"
        select case (char (feature))
        case ("init")
            write (unit, "(5x,9A)") "subroutine ", char (name), &
                " (par, scheme) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
                &intent(in) :: par"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("update_alpha_s")
            write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("reset_helicity_selection")
            write (unit, "(5x,9A)") "subroutine ", char (name), " &
                &(threshold, cutoff) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: threshold"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: cutoff"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("is_allowed")
            write (unit, "(5x,9A)") "subroutine ", char (name), " &
                &(flv, hel, col, flag) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
            write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
            write (unit, "(5x,9A)") "end subroutine ", char (name)
        case ("new_event")
            write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
            write (unit, "(7x,9A)") "import"
            write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &

```

```

        &intent(in) :: p"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("get_amplitude")
    write (unit, "(5x,9A)") "subroutine ", char (name), " &
        &(flv, hel, col, amp) bind(C)"
    write (unit, "(7x,9A)") "import"
    write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
        &:: amp"
    write (unit, "(5x,9A)") "end subroutine ", char (name)
end select
write (unit, "(2x,9A)") "end interface"
end subroutine prc_external_writer_write_interface

```

Empty, but can be overridden.

```

<Prc external: external writer: TBP>+≡
    procedure :: write_source_code => prc_external_writer_write_source_code

<Prc external: sub interfaces>+≡
    module subroutine prc_external_writer_write_source_code (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine prc_external_writer_write_source_code

<Prc external: procedures>+≡
    module subroutine prc_external_writer_write_source_code (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        if (debug_on) call msg_debug (D_ME_METHODS, &
            "prc_external_writer_write_source_code (no-op)")
        !!! This is a dummy
    end subroutine prc_external_writer_write_source_code

```

Empty, but can be overridden.

```

<Prc external: external writer: TBP>+≡
    procedure :: before_compile => prc_external_writer_before_compile
    procedure :: after_compile => prc_external_writer_after_compile

<Prc external: sub interfaces>+≡
    module subroutine prc_external_writer_before_compile (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine prc_external_writer_before_compile
    module subroutine prc_external_writer_after_compile (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine prc_external_writer_after_compile

<Prc external: procedures>+≡
    module subroutine prc_external_writer_before_compile (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        if (debug_on) call msg_debug (D_ME_METHODS, &
            "prc_external_writer_before_compile (no-op)")
        !!! This is a dummy
    end subroutine prc_external_writer_before_compile

```

```

end subroutine prc_external_writer_before_compile

module subroutine prc_external_writer_after_compile (writer, id)
  class(prc_external_writer_t), intent(in) :: writer
  type(string_t), intent(in) :: id
  if (debug_on) call msg_debug (D_ME_METHODS, &
    "prc_external_writer_after_compile (no-op)")
  !!! This is a dummy
end subroutine prc_external_writer_after_compile

```

Standard Makefile, set up to call O'MEGA. Additionally, the O'MEGA output can be exploited for its data-management parts.

```

<Prc external: external writer: TBP>+≡
  procedure :: write_makefile_code => prc_external_writer_write_makefile_code
  procedure :: base_write_makefile_code => &
    prc_external_writer_write_makefile_code

<Prc external: sub interfaces>+≡
  module subroutine prc_external_writer_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)
    class(prc_external_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
  end subroutine prc_external_writer_write_makefile_code

<Prc external: procedures>+≡
  module subroutine prc_external_writer_write_makefile_code &
    (writer, unit, id, os_data, verbose, testflag)
    class(prc_external_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    type(string_t) :: omega_binary, omega_path
    type(string_t) :: restrictions_string, amp_triv_string
    omega_binary = "omega_" // writer%model_name // ".opt"
    omega_path = os_data%whizard_omega_binpath // "/" // omega_binary
    if (.not. verbose) omega_path = "@" // omega_path
    if (writer%restrictions /= "") then
      restrictions_string = " -cascade '" // writer%restrictions // "'"
    else
      restrictions_string = ""
    end if
    amp_triv_string = ""
    if (writer%amp_triv) amp_triv_string = " -target:amp_triv"
    write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") char (id), ".f90:"
    if (.not. verbose) then
      write (unit, "(5A)") TAB // '@echo " OMEGA ', trim (char (id)), '.f90"'
    end if
    write (unit, "(99A)") TAB, char (omega_path), &

```

```

" -o ", char (id), ".f90", &
" -target:whizard", char (amp_triv_string), &
" -target:parameter_module parameters_", char (writer%model_name), &
" -target:module opr_", char (id), &
" -target:md5sum '", writer%md5sum, "'", &
char (writer%process_mode), char (writer%process_string), &
char (restrictions_string)
write (unit, "(5A)") "clean-", char (id), ":"
write (unit, "(5A)") TAB, "rm -f ", char (id), ".f90"
write (unit, "(5A)") TAB, "rm -f opr_", char (id), ".mod"
write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
write (unit, "(5A)") "CLEAN_OBJECTS += opr_", char (id), ".mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " FC " "$@"
end if
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"

end subroutine prc_external_writer_write_makefile_code

```

```

<Prc external: external writer: TBP>+≡
    procedure, nopass:: get_procname => prc_external_writer_writer_get_procname

```

```

<Prc external: sub interfaces>+≡
    module function prc_external_writer_writer_get_procname &
        (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
    end function prc_external_writer_writer_get_procname

```

```

<Prc external: procedures>+≡
    module function prc_external_writer_writer_get_procname &
        (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
        select case (char (feature))
        case ("n_in"); name = "number_particles_in"
        case ("n_out"); name = "number_particles_out"
        case ("n_flv"); name = "number_flavor_states"
        case ("n_hel"); name = "number_spin_states"
        case ("n_col"); name = "number_color_flows"
        case ("n_cin"); name = "number_color_indices"
        case ("n_cf"); name = "number_color_factors"
        case ("flv_state"); name = "flavor_states"
        case ("hel_state"); name = "spin_states"
        case ("col_state"); name = "color_flows"
        case default
            name = feature
        end select
    end function prc_external_writer_writer_get_procname

```

17.5.3 external test

Writer

```
<Prc external: public>+≡
    public :: prc_external_test_writer_t

<Prc external: types>+≡
    type, extends (prc_external_writer_t) :: prc_external_test_writer_t
    contains
    <Prc external: external test writer: TBP>
    end type prc_external_test_writer_t

<Prc external: external test writer: TBP>≡
    procedure, nopass :: type_name => prc_external_test_writer_type_name

<Prc external: sub interfaces>+≡
    module function prc_external_test_writer_type_name () result (string)
        type(string_t) :: string
    end function prc_external_test_writer_type_name

<Prc external: procedures>+≡
    module function prc_external_test_writer_type_name () result (string)
        type(string_t) :: string
        string = "External matrix element dummy"
    end function prc_external_test_writer_type_name
```

Workspace

This looks pretty useless. Why don't we make `prc_external_state_t` nonabstract and remove this?

```
<Prc external: public>+≡
    public :: prc_external_test_state_t

<Prc external: types>+≡
    type, extends (prc_external_state_t) :: prc_external_test_state_t
    contains
    <Prc external: external test state: TBP>
    end type prc_external_test_state_t

<Prc external: external test state: TBP>≡
    procedure :: write => prc_external_test_state_write

<Prc external: sub interfaces>+≡
    module subroutine prc_external_test_state_write (object, unit)
        class(prc_external_test_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_external_test_state_write

<Prc external: procedures>+≡
    module subroutine prc_external_test_state_write (object, unit)
        class(prc_external_test_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_external_test_state_write
```

Driver

```
<Prc external: public>+≡
  public :: prc_external_test_driver_t

<Prc external: types>+≡
  type, extends (prc_external_driver_t) :: prc_external_test_driver_t
  contains
  <Prc external: external test driver: TBP>
  end type prc_external_test_driver_t

<Prc external: external test driver: TBP>≡
  procedure, nopass :: type_name => prc_external_test_driver_type_name

<Prc external: sub interfaces>+≡
  module function prc_external_test_driver_type_name () result (type)
    type(string_t) :: type
  end function prc_external_test_driver_type_name

<Prc external: procedures>+≡
  module function prc_external_test_driver_type_name () result (type)
    type(string_t) :: type
    type = "External matrix element dummy"
  end function prc_external_test_driver_type_name
```

Configuration

A external test definition.

```
<Prc external: public>+≡
  public :: prc_external_test_def_t

<Prc external: types>+≡
  type, extends (prc_external_def_t) :: prc_external_test_def_t
  contains
  <Prc external: external test def: TBP>
  end type prc_external_test_def_t

Gfortran 7/8/9 bug, has to remain in the main module.

<Prc external: external test def: TBP>≡
  procedure :: init => prc_external_test_def_init

<Prc external: main procedures>+≡
  subroutine prc_external_test_def_init (object, basename, model_name, &
    prt_in, prt_out)
    class(prc_external_test_def_t), intent(inout) :: object
    type(string_t), intent(in) :: basename, model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    object%basename = basename
    allocate (prc_external_test_writer_t :: object%writer)
    select type (writer => object%writer)
      type is (prc_external_test_writer_t)
        call writer%init (model_name, prt_in, prt_out)
      end select
  end subroutine prc_external_test_def_init
```



```

<Prc external: external test def: TBP>+≡
  procedure, nopass :: type_string => prc_external_test_def_type_string
<Prc external: sub interfaces>+≡
  module function prc_external_test_def_type_string () result (string)
    type(string_t) :: string
  end function prc_external_test_def_type_string
<Prc external: procedures>+≡
  module function prc_external_test_def_type_string () result (string)
    type(string_t) :: string
    string = "external test dummy"
  end function prc_external_test_def_type_string

```

```

<Prc external: external test def: TBP>+≡
  procedure :: write => prc_external_test_def_write
<Prc external: sub interfaces>+≡
  module subroutine prc_external_test_def_write (object, unit)
    class(prc_external_test_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_write
<Prc external: procedures>+≡
  module subroutine prc_external_test_def_write (object, unit)
    class(prc_external_test_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_write

```

```

<Prc external: external test def: TBP>+≡
  procedure :: read => prc_external_test_def_read
<Prc external: sub interfaces>+≡
  module subroutine prc_external_test_def_read (object, unit)
    class(prc_external_test_def_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_read
<Prc external: procedures>+≡
  module subroutine prc_external_test_def_read (object, unit)
    class(prc_external_test_def_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_read

```

Gfortran 7/8/9 bug, has to remain in the main module.

```

<Prc external: external test def: TBP>+≡
  procedure :: allocate_driver => prc_external_test_def_allocate_driver
<Prc external: main procedures>+≡
  subroutine prc_external_test_def_allocate_driver (object, driver, basename)
    class(prc_external_test_def_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    if (.not. allocated (driver)) &
      allocate (prc_external_test_driver_t :: driver)
  end subroutine prc_external_test_def_allocate_driver

```

Core

This external test just returns $|\mathcal{M}|^2 = 1$ and thus the result of the integration is the n-particle-phase-space volume.

```
<Prc external: public>+≡
    public :: prc_external_test_t

<Prc external: types>+≡
    type, extends (prc_external_t) :: prc_external_test_t
    contains
    <Prc external: prc test: TBP>
    end type prc_external_test_t

<Prc external: prc test: TBP>≡
    procedure :: write => prc_external_test_write

<Prc external: sub interfaces>+≡
    module subroutine prc_external_test_write (object, unit)
        class(prc_external_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_external_test_write

<Prc external: procedures>+≡
    module subroutine prc_external_test_write (object, unit)
        class(prc_external_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call msg_message ("Test external matrix elements")
    end subroutine prc_external_test_write

<Prc external: prc test: TBP>+≡
    procedure :: write_name => prc_external_test_write_name

<Prc external: sub interfaces>+≡
    module subroutine prc_external_test_write_name (object, unit)
        class(prc_external_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_external_test_write_name

<Prc external: procedures>+≡
    module subroutine prc_external_test_write_name (object, unit)
        class(prc_external_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u,"(1x,A)") "Core: external test"
    end subroutine prc_external_test_write_name

<Prc external: prc test: TBP>+≡
    procedure :: compute_amplitude => prc_external_test_compute_amplitude

<Prc external: sub interfaces>+≡
    module function prc_external_test_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
        core_state) result (amp)
        class(prc_external_test_t), intent(in) :: object
```

```

integer, intent(in) :: j
type(vector4_t), dimension(:), intent(in) :: p
integer, intent(in) :: f, h, c
real(default), intent(in) :: fac_scale, ren_scale
real(default), intent(in), allocatable :: alpha_qcd_forced
class(prc_core_state_t), intent(inout), allocatable, optional :: &
    core_state
complex(default) :: amp
end function prc_external_test_compute_amplitude

<Prc external: procedures>+≡
module function prc_external_test_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
    class(prc_external_test_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    complex(default) :: amp
    select type (core_state)
    class is (prc_external_test_state_t)
        core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)
    end select
    amp = 0.0
end function prc_external_test_compute_amplitude

Gfortran 7/8/9 bug, has to remain in the main module.

<Prc external: prc test: TBP>+≡
procedure :: allocate_workspace => prc_external_test_allocate_workspace

<Prc external: main procedures>+≡
subroutine prc_external_test_allocate_workspace (object, core_state)
    class(prc_external_test_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (prc_external_test_state_t :: core_state)
end subroutine prc_external_test_allocate_workspace

<Prc external: prc test: TBP>+≡
procedure :: includes_polarization => &
    prc_external_test_includes_polarization

<Prc external: sub interfaces>+≡
module function prc_external_test_includes_polarization &
    (object) result (polarized)
    logical :: polarized
    class(prc_external_test_t), intent(in) :: object
end function prc_external_test_includes_polarization

<Prc external: procedures>+≡
module function prc_external_test_includes_polarization &
    (object) result (polarized)
    logical :: polarized

```

```

        class(prc_external_test_t), intent(in) :: object
        polarized = .false.
    end function prc_external_test_includes_polarization

<Prc external: prc test: TBP>+≡
    procedure :: prepare_external_code => &
        prc_external_test_prepare_external_code

<Prc external: sub interfaces>+≡
    module subroutine prc_external_test_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_external_test_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
    end subroutine prc_external_test_prepare_external_code

<Prc external: procedures>+≡
    module subroutine prc_external_test_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_external_test_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
    end subroutine prc_external_test_prepare_external_code

```

17.5.4 Threshold

```

<prc_threshold.f90>≡
    <File header>
    module prc_threshold

        use, intrinsic :: iso_c_binding !NODEP!

        use kinds
        <Use strings>
        <Use debug>
        use physics_defs
        use diagnostics
        use os_interface
        use lorentz
        use interactions
        use model_data
        use variables, only: var_list_t
    end module prc_threshold

```

```

    use prclib_interfaces
    use process_libraries
    use prc_core_def
    use prc_core
    use prc_external

    <Standard module head>

    <Prc threshold: public>

    <Prc threshold: interfaces>

    <Prc threshold: types>

    interface
    <Prc threshold: sub interfaces>
    end interface

    contains

    <Prc threshold: main procedures>

    end module prc_threshold

<prc_threshold_sub.f90>≡
    <File header>

    submodule (prc_threshold) prc_threshold_s

        use constants
        use numeric_utils
        use string_utils, only: lower_case
        use io_units
        use system_defs, only: TAB
        use sm_qcd

        implicit none

    contains

    <Prc threshold: procedures>

    end submodule prc_threshold_s

```

Writer

```

    <Prc threshold: public>≡
        public :: threshold_writer_t

    <Prc threshold: types>≡
        type, extends (prc_external_writer_t) :: threshold_writer_t
            integer :: nlo_type
        contains
        <Prc threshold: threshold writer: TBP>

```

```

end type threshold_writer_t

<Prc threshold: threshold writer: TBP>≡
  procedure :: init => threshold_writer_init

<Prc threshold: sub interfaces>≡
  pure module subroutine threshold_writer_init &
    (writer, model_name, prt_in, prt_out, restrictions)
    class(threshold_writer_t), intent(inout) :: writer
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    type(string_t), intent(in), optional :: restrictions
  end subroutine threshold_writer_init

<Prc threshold: procedures>≡
  pure module subroutine threshold_writer_init &
    (writer, model_name, prt_in, prt_out, restrictions)
    class(threshold_writer_t), intent(inout) :: writer
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    type(string_t), intent(in), optional :: restrictions
    call writer%base_init (model_name, prt_in, prt_out, restrictions)
    writer%amp_triv = .false.
  end subroutine threshold_writer_init

<Prc threshold: threshold writer: TBP>+≡
  procedure :: write_makefile_extra => threshold_writer_write_makefile_extra

<Prc threshold: sub interfaces>+≡
  module subroutine threshold_writer_write_makefile_extra &
    (writer, unit, id, os_data, verbose, nlo_type)
    class(threshold_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    integer, intent(in) :: nlo_type
  end subroutine threshold_writer_write_makefile_extra

<Prc threshold: procedures>+≡
  module subroutine threshold_writer_write_makefile_extra &
    (writer, unit, id, os_data, verbose, nlo_type)
    class(threshold_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    integer, intent(in) :: nlo_type
    type(string_t) :: f90in, f90, lo, extra
    if (debug_on) call msg_debug &
      (D_ME_METHODS, "threshold_writer_write_makefile_extra")
    if (nlo_type /= BORN) then
      extra = "_" // component_status (nlo_type)
    else
      extra = var_str ("")

```

```

end if
f90 = id // "_threshold" // extra // ".f90"
f90in = f90 // ".in"
lo = id // "_threshold" // extra // ".lo"
write (unit, "(A)") "OBJECTS += " // char (lo)
write (unit, "(A)") char (f90in) // ":"
write (unit, "(A)") char (TAB // "if ! test -f " // f90in // &
      "; then cp " // os_data%whizard_sharepath // &
      "/SM_tt_threshold_data/threshold" // extra // ".f90 " // &
      f90in // "; fi")
write (unit, "(A)") char(f90) // ": " // char (f90in)
write (unit, "(A)") TAB // "sed 's/@ID@/" // char (id) // "/" " // &
      char (f90in) // " > " // char (f90)
write (unit, "(5A)") "CLEAN_SOURCES += ", char (f90)
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (f90in)
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_threshold.mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (lo)
write (unit, "(A)") char(lo) // ": " // char (f90) // " " // &
      char(id) // ".f90"
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
if (.not. verbose) then
  write (unit, "(5A)") TAB // '@echo " FC " $@"
end if
end subroutine threshold_writer_write_makefile_extra

```

<Prc threshold: threshold writer: TBP>+≡

```

procedure :: write_makefile_code => threshold_writer_write_makefile_code

```

<Prc threshold: sub interfaces>+≡

```

module subroutine threshold_writer_write_makefile_code &
  (writer, unit, id, os_data, verbose, testflag)
  class(threshold_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
end subroutine threshold_writer_write_makefile_code

```

<Prc threshold: procedures>+≡

```

module subroutine threshold_writer_write_makefile_code &
  (writer, unit, id, os_data, verbose, testflag)
  class(threshold_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
  if (debug_on) &
    call msg_debug (D_ME_METHODS, "threshold_writer_write_makefile_code")
  call writer%base_write_makefile_code &
    (unit, id, os_data, verbose, testflag = testflag)
  call writer%write_makefile_extra (unit, id, os_data, verbose, BORN)
  if (writer%nlo_type == NLO_VIRTUAL .and. writer%active) &
    call writer%write_makefile_extra (unit, id, os_data, verbose, writer%nlo_type)

```

```

end subroutine threshold_writer_write_makefile_code

<Prc threshold: threshold writer: TBP>+≡
  procedure, nopass :: type_name => threshold_writer_type_name

<Prc threshold: sub interfaces>+≡
  module function threshold_writer_type_name () result (string)
    type(string_t) :: string
  end function threshold_writer_type_name

<Prc threshold: procedures>+≡
  module function threshold_writer_type_name () result (string)
    type(string_t) :: string
    string = "Threshold"
  end function threshold_writer_type_name

```

Driver

```

<Prc threshold: public>+≡
  public :: threshold_set_process_mode

<Prc threshold: interfaces>≡
  interface
    subroutine threshold_set_process_mode (mode) bind(C)
      import
      integer(kind = c_int), intent(in) :: mode
    end subroutine threshold_set_process_mode
  end interface

<Prc threshold: public>+≡
  public :: threshold_get_amp_squared

<Prc threshold: interfaces>+≡
  interface
    subroutine threshold_get_amp_squared (amp2, p_ofs, p_ons, leg, n_tot, sel_hel_beam) bind(C)
      import
      real(c_default_float), intent(out) :: amp2
      real(c_default_float), dimension(0:3,*), intent(in) :: p_ofs
      real(c_default_float), dimension(0:3,*), intent(in) :: p_ons
      integer(kind = c_int) :: n_tot, leg, sel_hel_beam
    end subroutine threshold_get_amp_squared
  end interface

<Prc threshold: public>+≡
  public :: threshold_olp_eval2

<Prc threshold: interfaces>+≡
  interface
    subroutine threshold_olp_eval2 (i_flv, alpha_s_c, parray, mu_c, &
      sel_hel_beam, sqme_c, acc_c) bind(C)
      import
      integer(c_int), intent(in) :: i_flv
      real(c_default_float), intent(in) :: alpha_s_c

```



```

        real(c_default_float), dimension(0:3,*), intent(in) :: parray
        real(c_default_float), intent(in) :: mu_c
        integer, intent(in) :: sel_hel_beam
        real(c_default_float), dimension(4), intent(out) :: sqme_c
        real(c_default_float), intent(out) :: acc_c
    end subroutine threshold_olp_eval2
end interface

<Prc threshold: public>+≡
    public :: threshold_init

<Prc threshold: interfaces>+≡
    interface
        subroutine threshold_init (par, scheme) bind(C)
            import
            real(c_default_float), dimension(*), intent(in) :: par
            integer(c_int), intent(in) :: scheme
        end subroutine threshold_init
    end interface

<Prc threshold: public>+≡
    public :: threshold_start_openloops

<Prc threshold: interfaces>+≡
    interface
        subroutine threshold_start_openloops () bind(C)
            import
        end subroutine threshold_start_openloops
    end interface

<Prc threshold: public>+≡
    public :: threshold_driver_t

<Prc threshold: types>+≡
    type, extends (prc_external_driver_t) :: threshold_driver_t
        procedure(threshold_olp_eval2), nopass, pointer :: &
            olp_eval2 => null ()
        procedure(threshold_set_process_mode), nopass, pointer :: &
            set_process_mode => null ()
        procedure(threshold_get_amp_squared), nopass, pointer :: &
            get_amp_squared => null ()
        procedure(threshold_start_openloops), nopass, pointer :: &
            start_openloops => null ()
        procedure(threshold_init), nopass, pointer :: &
            init => null ()
        type(string_t) :: id
        integer :: nlo_type = BORN
    contains
        <Prc threshold: threshold driver: TBP>
    end type threshold_driver_t

<Prc threshold: threshold driver: TBP>≡
    procedure, nopass :: type_name => threshold_driver_type_name

```

```

<Prc threshold: sub interfaces>+≡
    module function threshold_driver_type_name () result (type)
        type(string_t) :: type
    end function threshold_driver_type_name

<Prc threshold: procedures>+≡
    module function threshold_driver_type_name () result (type)
        type(string_t) :: type
        type = "Threshold"
    end function threshold_driver_type_name

<Prc threshold: threshold driver: TBP>+≡
    procedure :: load => threshold_driver_load

<Prc threshold: sub interfaces>+≡
    module subroutine threshold_driver_load (threshold_driver, dlaccess)
        class(threshold_driver_t), intent(inout) :: threshold_driver
        type(dlaccess_t), intent(inout) :: dlaccess
    end subroutine threshold_driver_load

<Prc threshold: procedures>+≡
    module subroutine threshold_driver_load (threshold_driver, dlaccess)
        class(threshold_driver_t), intent(inout) :: threshold_driver
        type(dlaccess_t), intent(inout) :: dlaccess
        type(c_funptr) :: c_fptr
        type(string_t) :: lower_case_id
        if (debug_on) call msg_debug (D_ME_METHODS, "threshold_driver_load")
        lower_case_id = lower_case (threshold_driver%id)
        c_fptr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_set_process_mode")
        call c_f_procpointer (c_fptr, threshold_driver%set_process_mode)
        call check_for_error (lower_case_id // "_set_process_mode")
        c_fptr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_get_amp_squared")
        call c_f_procpointer (c_fptr, threshold_driver%get_amp_squared)
        call check_for_error (lower_case_id // "_get_amp_squared")
        c_fptr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_threshold_init")
        call c_f_procpointer (c_fptr, threshold_driver%init)
        call check_for_error (lower_case_id // "_threshold_init")
        select type (threshold_driver)
            type is (threshold_driver_t)
                if (threshold_driver%nlo_type == NLO_VIRTUAL) then
                    c_fptr = dlaccess_get_c_funptr &
                        (dlaccess, lower_case_id // "_start_openloops")
                    call c_f_procpointer (c_fptr, threshold_driver%start_openloops)
                    call check_for_error (lower_case_id // "_start_openloops")
                    c_fptr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_olp_eval2")
                    call c_f_procpointer (c_fptr, threshold_driver%olp_eval2)
                    call check_for_error (lower_case_id // "_olp_eval2")
                end if
            end select
        call msg_message ("Loaded extra threshold functions")
        contains
        subroutine check_for_error (function_name)
            type(string_t), intent(in) :: function_name
            if (dlaccess_has_error (dlaccess)) call msg_fatal &
                (char ("Loading of " // function_name // " failed!"))

```

```

        end subroutine check_for_error
    end subroutine threshold_driver_load

```

Configuration

```

<Prc threshold: public>+≡
    public :: threshold_def_t

<Prc threshold: types>+≡
    type, extends (prc_external_def_t) :: threshold_def_t
        integer :: nlo_type
    contains
    <Prc threshold: threshold def: TBP>
    end type threshold_def_t

Gfortran 7/8/9 bug: has to remain in the main module.

<Prc threshold: threshold def: TBP>≡
    procedure :: init => threshold_def_init

<Prc threshold: main procedures>≡
    subroutine threshold_def_init (object, basename, model_name, &
        prt_in, prt_out, nlo_type, restrictions)
        class(threshold_def_t), intent(inout) :: object
        type(string_t), intent(in) :: basename, model_name
        type(string_t), dimension(:), intent(in) :: prt_in, prt_out
        integer, intent(in) :: nlo_type
        type(string_t), intent(in), optional :: restrictions
        if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_init")
        object%basename = basename
        object%nlo_type = nlo_type
        allocate (threshold_writer_t :: object%writer)
        select type (writer => object%writer)
        type is (threshold_writer_t)
            call writer%init (model_name, prt_in, prt_out, restrictions)
            writer%nlo_type = nlo_type
        end select
    end subroutine threshold_def_init

<Prc threshold: threshold def: TBP>+≡
    procedure, nopass :: type_string => threshold_def_type_string

<Prc threshold: sub interfaces>+≡
    module function threshold_def_type_string () result (string)
        type(string_t) :: string
    end function threshold_def_type_string

<Prc threshold: procedures>+≡
    module function threshold_def_type_string () result (string)
        type(string_t) :: string
        string = "threshold computation"
    end function threshold_def_type_string

```

write and read could be put in the abstract version

```
<Prc threshold: threshold def: TBP>+≡  
  procedure :: write => threshold_def_write  
  
<Prc threshold: sub interfaces>+≡  
  module subroutine threshold_def_write (object, unit)  
    class(threshold_def_t), intent(in) :: object  
    integer, intent(in) :: unit  
  end subroutine threshold_def_write  
  
<Prc threshold: procedures>+≡  
  module subroutine threshold_def_write (object, unit)  
    class(threshold_def_t), intent(in) :: object  
    integer, intent(in) :: unit  
  end subroutine threshold_def_write
```

```
<Prc threshold: threshold def: TBP>+≡  
  procedure :: read => threshold_def_read  
  
<Prc threshold: sub interfaces>+≡  
  module subroutine threshold_def_read (object, unit)  
    class(threshold_def_t), intent(out) :: object  
    integer, intent(in) :: unit  
  end subroutine threshold_def_read  
  
<Prc threshold: procedures>+≡  
  module subroutine threshold_def_read (object, unit)  
    class(threshold_def_t), intent(out) :: object  
    integer, intent(in) :: unit  
  end subroutine threshold_def_read
```

Gfortran 7/8/9 bug: has to remain in the main module.

```
<Prc threshold: threshold def: TBP>+≡  
  procedure :: allocate_driver => threshold_def_allocate_driver  
  
<Prc threshold: main procedures>+≡  
  subroutine threshold_def_allocate_driver (object, driver, basename)  
    class(threshold_def_t), intent(in) :: object  
    class(prc_core_driver_t), intent(out), allocatable :: driver  
    type(string_t), intent(in) :: basename  
    if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_allocate_driver")  
    if (.not. allocated (driver)) allocate (threshold_driver_t :: driver)  
    select type (driver)  
    type is (threshold_driver_t)  
      driver%id = basename  
      driver%nlo_type = object%nlo_type  
    end select  
  end subroutine threshold_def_allocate_driver  
  
<Prc threshold: threshold def: TBP>+≡  
  procedure :: connect => threshold_def_connect
```

```

<Prc threshold: sub interfaces>+≡
    module subroutine threshold_def_connect (def, lib_driver, i, proc_driver)
        class(threshold_def_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
    end subroutine threshold_def_connect

<Prc threshold: procedures>+≡
    module subroutine threshold_def_connect (def, lib_driver, i, proc_driver)
        class(threshold_def_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
        type(dlaccess_t) :: dlaccess
        logical :: skip
        if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_connect")
        call def%omega_connect (lib_driver, i, proc_driver)
        select type (lib_driver)
            class is (prclib_driver_dynamic_t)
                dlaccess = lib_driver%dlaccess
            end select
        select type (proc_driver)
            class is (threshold_driver_t)
                select type (writer => def%writer)
                    type is (threshold_writer_t)
                        skip = writer%nlo_type == NLO_VIRTUAL .and. .not. writer%active
                        if (.not. skip) call proc_driver%load (dlaccess)
                    end select
                end select
            end select
        end subroutine threshold_def_connect

```

Core state

```

<Prc threshold: public>+≡
    public :: threshold_state_t

<Prc threshold: types>+≡
    type, extends (prc_external_state_t) :: threshold_state_t
    contains
    <Prc threshold: threshold state: TBP>
    end type threshold_state_t

<Prc threshold: threshold state: TBP>≡
    procedure :: write => threshold_state_write

<Prc threshold: sub interfaces>+≡
    module subroutine threshold_state_write (object, unit)
        class(threshold_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine threshold_state_write

<Prc threshold: procedures>+≡
    module subroutine threshold_state_write (object, unit)

```

```

        class(threshold_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine threshold_state_write

```

Core

```

<Prc threshold: public>+≡
    public :: prc_threshold_t

<Prc threshold: types>+≡
    type, extends (prc_external_t) :: prc_threshold_t
        real(default), dimension(:,:), allocatable :: parray_ofs
        real(default), dimension(:,:), allocatable :: parray_ons
        integer :: leg
        logical :: has_beam_pol = .false.
    contains
    <Prc threshold: prc threshold: TBP>
    end type prc_threshold_t

<Prc threshold: prc threshold: TBP>≡
    procedure :: write => prc_threshold_write

<Prc threshold: sub interfaces>+≡
    module subroutine prc_threshold_write (object, unit)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_threshold_write

<Prc threshold: procedures>+≡
    module subroutine prc_threshold_write (object, unit)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call msg_message ("Supply amplitudes squared for threshold computation")
    end subroutine prc_threshold_write

<Prc threshold: prc threshold: TBP>+≡
    procedure :: write_name => prc_threshold_write_name

<Prc threshold: sub interfaces>+≡
    module subroutine prc_threshold_write_name (object, unit)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_threshold_write_name

<Prc threshold: procedures>+≡
    module subroutine prc_threshold_write_name (object, unit)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u,"(1x,A)") "Core: Threshold"
    end subroutine prc_threshold_write_name

```

This core type has the beam polarization as an extra parameter.

```

<Prc threshold: prc threshold: TBP>+≡
    procedure :: set_beam_pol => prc_threshold_set_beam_pol

<Prc threshold: sub interfaces>+≡
    module subroutine prc_threshold_set_beam_pol (object, has_beam_pol)
        class(prc_threshold_t), intent(inout) :: object
        logical, intent(in), optional :: has_beam_pol
    end subroutine prc_threshold_set_beam_pol

<Prc threshold: procedures>+≡
    module subroutine prc_threshold_set_beam_pol (object, has_beam_pol)
        class(prc_threshold_t), intent(inout) :: object
        logical, intent(in), optional :: has_beam_pol
        if (present (has_beam_pol)) then
            object%has_beam_pol = has_beam_pol
        end if
    end subroutine prc_threshold_set_beam_pol

<Prc threshold: prc threshold: TBP>+≡
    procedure :: compute_amplitude => prc_threshold_compute_amplitude

<Prc threshold: sub interfaces>+≡
    module function prc_threshold_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
         core_state) result (amp)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in) :: j
        type(vector4_t), dimension(:), intent(in) :: p
        integer, intent(in) :: f, h, c
        real(default), intent(in) :: fac_scale, ren_scale
        real(default), intent(in), allocatable :: alpha_qcd_forced
        class(prc_core_state_t), intent(inout), allocatable, optional :: &
            core_state
        complex(default) :: amp
    end function prc_threshold_compute_amplitude

<Prc threshold: procedures>+≡
    module function prc_threshold_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
         core_state) result (amp)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in) :: j
        type(vector4_t), dimension(:), intent(in) :: p
        integer, intent(in) :: f, h, c
        real(default), intent(in) :: fac_scale, ren_scale
        real(default), intent(in), allocatable :: alpha_qcd_forced
        class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
        complex(default) :: amp
        select type (core_state)
        class is (prc_external_test_state_t)
            core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)
        end select
        amp = 0
    end function prc_threshold_compute_amplitude

```

Gfortran 7/8/9 bug: has to remain in the main module.

```
<Prc threshold: prc threshold: TBP>+≡
  procedure :: allocate_workspace => prc_threshold_allocate_workspace

<Prc threshold: main procedures>+≡
  subroutine prc_threshold_allocate_workspace (object, core_state)
    class(prc_threshold_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (threshold_state_t :: core_state)
  end subroutine prc_threshold_allocate_workspace

<Prc threshold: prc threshold: TBP>+≡
  procedure :: set_offshell_momenta => prc_threshold_set_offshell_momenta

<Prc threshold: sub interfaces>+≡
  module subroutine prc_threshold_set_offshell_momenta (object, p)
    class(prc_threshold_t), intent(inout) :: object
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine prc_threshold_set_offshell_momenta

<Prc threshold: procedures>+≡
  module subroutine prc_threshold_set_offshell_momenta (object, p)
    class(prc_threshold_t), intent(inout) :: object
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: i
    do i = 1, size(p)
      object%pararray_ofs(:,i) = p(i)%p
    end do
  end subroutine prc_threshold_set_offshell_momenta

<Prc threshold: prc threshold: TBP>+≡
  procedure :: set_onshell_momenta => prc_threshold_set_onshell_momenta

<Prc threshold: sub interfaces>+≡
  module subroutine prc_threshold_set_onshell_momenta (object, p)
    class(prc_threshold_t), intent(inout) :: object
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine prc_threshold_set_onshell_momenta

<Prc threshold: procedures>+≡
  module subroutine prc_threshold_set_onshell_momenta (object, p)
    class(prc_threshold_t), intent(inout) :: object
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: i
    do i = 1, size(p)
      object%pararray_ons(:,i) = p(i)%p
    end do
  end subroutine prc_threshold_set_onshell_momenta

<Prc threshold: prc threshold: TBP>+≡
  procedure :: set_leg => prc_threshold_set_leg

<Prc threshold: sub interfaces>+≡
  module subroutine prc_threshold_set_leg (object, leg)
    class(prc_threshold_t), intent(inout) :: object
    integer, intent(in) :: leg
  end subroutine prc_threshold_set_leg
```



```

<Prc threshold: procedures>+≡
module subroutine prc_threshold_set_leg (object, leg)
  class(prc_threshold_t), intent(inout) :: object
  integer, intent(in) :: leg
  object%leg = leg
end subroutine prc_threshold_set_leg

<Prc threshold: prc threshold: TBP>+≡
procedure :: set_process_mode => prc_threshold_set_process_mode

<Prc threshold: sub interfaces>+≡
module subroutine prc_threshold_set_process_mode (object, mode)
  class(prc_threshold_t), intent(in) :: object
  integer(kind = c_int), intent(in) :: mode
end subroutine prc_threshold_set_process_mode

<Prc threshold: procedures>+≡
module subroutine prc_threshold_set_process_mode (object, mode)
  class(prc_threshold_t), intent(in) :: object
  integer(kind = c_int), intent(in) :: mode
  select type (driver => object%driver)
  class is (threshold_driver_t)
    if (associated (driver%set_process_mode)) &
      call driver%set_process_mode (mode)
  end select
end subroutine prc_threshold_set_process_mode

<Prc threshold: prc threshold: TBP>+≡
procedure :: compute_sqme => prc_threshold_compute_sqme

<Prc threshold: sub interfaces>+≡
module subroutine prc_threshold_compute_sqme (object, i_flv, i_hel, p, &
  ren_scale, sqme, bad_point)
  class(prc_threshold_t), intent(in) :: object
  integer, intent(in) :: i_flv, i_hel
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: ren_scale
  real(default), intent(out) :: sqme
  logical, intent(out) :: bad_point
end subroutine prc_threshold_compute_sqme

<Prc threshold: procedures>+≡
module subroutine prc_threshold_compute_sqme (object, i_flv, i_hel, p, &
  ren_scale, sqme, bad_point)
  class(prc_threshold_t), intent(in) :: object
  integer, intent(in) :: i_flv, i_hel
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: ren_scale
  real(default), intent(out) :: sqme
  logical, intent(out) :: bad_point
  integer :: n_tot
  if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_threshold_compute_sqme")
  n_tot = size (p)
  select type (driver => object%driver)
  class is (threshold_driver_t)

```

```

        if (object%has_beam_pol) then
            call driver%get_amp_squared (sqme, object%pararray_ofs, &
                object%pararray_ons, object%leg, n_tot, i_flg - 1)
        else
            call driver%get_amp_squared (sqme, object%pararray_ofs, &
                object%pararray_ons, object%leg, n_tot, -1)
        end if
    end select
    bad_point = .false.
end subroutine prc_threshold_compute_sqme

```

<Prc threshold: prc threshold: TBP>+≡

```

    procedure :: compute_sqme_virt => prc_threshold_compute_sqme_virt

```

<Prc threshold: sub interfaces>+≡

```

    module subroutine prc_threshold_compute_sqme_virt (object, i_flg, i_hel, &
        p, ren_scale, es_scale, loop_method, sqme, bad_point)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in) :: i_flg, i_hel
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: ren_scale, es_scale
        integer, intent(in) :: loop_method
        real(default), dimension(4), intent(out) :: sqme
        real(c_default_float), dimension(:,:), allocatable, save :: pararray
        logical, intent(out) :: bad_point
    end subroutine prc_threshold_compute_sqme_virt

```

<Prc threshold: procedures>+≡

```

    module subroutine prc_threshold_compute_sqme_virt (object, i_flg, i_hel, &
        p, ren_scale, es_scale, loop_method, sqme, bad_point)
        class(prc_threshold_t), intent(in) :: object
        integer, intent(in) :: i_flg, i_hel
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: ren_scale, es_scale
        integer, intent(in) :: loop_method
        real(default), dimension(4), intent(out) :: sqme
        real(c_default_float), dimension(:,:), allocatable, save :: pararray
        logical, intent(out) :: bad_point
        integer :: n_tot, i
        real(default) :: mu
        real(c_default_float), dimension(4) :: sqme_c
        real(c_default_float) :: mu_c, acc_c, alpha_s_c
        integer(c_int) :: i_flg_c
        if (debug_on) call msgv_debug2 (D_ME_METHODS, "prc_threshold_compute_sqme_virt")
        n_tot = size (p)
        if (allocated (pararray)) then
            if (size(pararray) /= n_tot) deallocate (pararray)
        end if
        if (.not. allocated (pararray)) allocate (pararray (0:3, n_tot))
        forall (i = 1:n_tot) pararray(:,i) = p(i)%p

        if (vanishes (ren_scale)) then
            mu = sqrt (2* (p(1)*p(2)))
        else
            mu = ren_scale

```

```

end if
mu_c = mu
alpha_s_c = object%qcd%alpha%get (mu)
i_flv_c = i_flv
select type (driver => object%driver)
class is (threshold_driver_t)
  if (associated (driver%olp_eval2)) then
    if (object%has_beam_pol) then
      call driver%olp_eval2 (1, alpha_s_c, &
        parray, mu_c, i_flv_c - 1, sqme_c, acc_c)
    else
      call driver%olp_eval2 (i_flv_c, alpha_s_c, &
        parray, mu_c, -1, sqme_c, acc_c)
    end if
    bad_point = real(acc_c, kind=default) > object%maximum_accuracy
    sqme = sqme_c
  else
    sqme = 0._default
    bad_point = .true.
  end if
end select
end subroutine prc_threshold_compute_sqme_virt

```

<Prc threshold: prc threshold: TBP>+≡

```
procedure :: init => prc_threshold_init
```

<Prc threshold: sub interfaces>+≡

```

module subroutine prc_threshold_init (object, def, lib, id, i_component)
  class(prc_threshold_t), intent(inout) :: object
  class(prc_core_def_t), intent(in), target :: def
  type(process_library_t), intent(in), target :: lib
  type(string_t), intent(in) :: id
  integer, intent(in) :: i_component
end subroutine prc_threshold_init

```

<Prc threshold: procedures>+≡

```

module subroutine prc_threshold_init (object, def, lib, id, i_component)
  class(prc_threshold_t), intent(inout) :: object
  class(prc_core_def_t), intent(in), target :: def
  type(process_library_t), intent(in), target :: lib
  type(string_t), intent(in) :: id
  integer, intent(in) :: i_component
  integer :: n_tot
  call object%base_init (def, lib, id, i_component)
  n_tot = object%data%n_in + object%data%n_out
  allocate (object%parray_ofs (0:3,n_tot), object%parray_ons (0:3,n_tot))
  if (n_tot == 4) then
    call object%set_process_mode (PROC_MODE_TT)
  else
    call object%set_process_mode (PROC_MODE_WBWB)
  end if
  call object%activate_parameters ()
end subroutine prc_threshold_init

```

Activate the stored parameters by transferring them to the external matrix element.

```

(Prc threshold: prc threshold: TBP)+≡
    procedure :: activate_parameters => prc_threshold_activate_parameters

(Prc threshold: sub interfaces)+≡
    module subroutine prc_threshold_activate_parameters (object)
        class (prc_threshold_t), intent(inout) :: object
    end subroutine prc_threshold_activate_parameters

(Prc threshold: procedures)+≡
    module subroutine prc_threshold_activate_parameters (object)
        class (prc_threshold_t), intent(inout) :: object
        if (debug_on) &
            call msg_debug (D_ME_METHODS, "prc_threshold_activate_parameters")
        if (allocated (object%driver)) then
            if (allocated (object%par)) then
                select type (driver => object%driver)
                type is (threshold_driver_t)
                    if (associated (driver%init)) then
                        call driver%init (object%par, object%scheme)
                    end if
                end select
            else
                call msg_bug &
                    ("prc_threshold_activate: parameter set is not allocated")
            end if
        else
            call msg_bug ("prc_threshold_activate: driver is not allocated")
        end if
    end subroutine prc_threshold_activate_parameters

(Prc threshold: prc threshold: TBP)+≡
    procedure :: prepare_external_code => &
        prc_threshold_prepare_external_code

(Prc threshold: sub interfaces)+≡
    module subroutine prc_threshold_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_threshold_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
    end subroutine prc_threshold_prepare_external_code

(Prc threshold: procedures)+≡
    module subroutine prc_threshold_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_threshold_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list

```

```

type(os_data_t), intent(in) :: os_data
type(string_t), intent(in) :: libname
type(model_data_t), intent(in), target :: model
integer, intent(in) :: i_core
logical, intent(in) :: is_nlo
if (debug_on) call msg_debug (D_ME_METHODS, &
    "prc_threshold_prepare_external_code")
if (allocated (core%driver)) then
    select type (driver => core%driver)
    type is (threshold_driver_t)
        if (driver%nlo_type == NLO_VIRTUAL) call driver%start_openloops ()
    end select
else
    call msg_bug ("prc_threshold_prepare_external_code: " &
        // "driver is not allocated")
end if
end subroutine prc_threshold_prepare_external_code

```

<Prc threshold: prc threshold: TBP>+≡
 procedure :: includes_polarization => prc_threshold_includes_polarization

<Prc threshold: sub interfaces>+≡
 module function prc_threshold_includes_polarization &
 (object) result (polarized)
 logical :: polarized
 class(prc_threshold_t), intent(in) :: object
 end function prc_threshold_includes_polarization

<Prc threshold: procedures>+≡
 module function prc_threshold_includes_polarization &
 (object) result (polarized)
 logical :: polarized
 class(prc_threshold_t), intent(in) :: object
 polarized = object%has_beam_pol
 end function prc_threshold_includes_polarization

Chapter 18

Generic Event Handling

Event records allow the MC to communicate with the outside world. The event record should exhibit the observable contents of a physical event. We should be able to read and write events. The actual implementation of the event need not be defined yet, for that purpose.

We have the following basic modules:

event_base Abstract base type for event records. The base type contains a reference to a **particle_set_t** object as the event core, and it holds some data that we should always expect, such as the squared matrix element and event weight.

eio_data Transparent container for the metadata of an event sample.

eio_base Abstract base type for event-record input and output. The implementations of this base type represent specific event I/O formats.

These are the implementation modules:

eio_checkpoints Auxiliary output format. The only purpose is to provide screen diagnostics during event output.

eio_callback Auxiliary output format. The only purpose is to execute a callback procedure, so we have a hook for external access during event output.

eio_weights Print some event summary data, no details. The main use is for testing purposes.

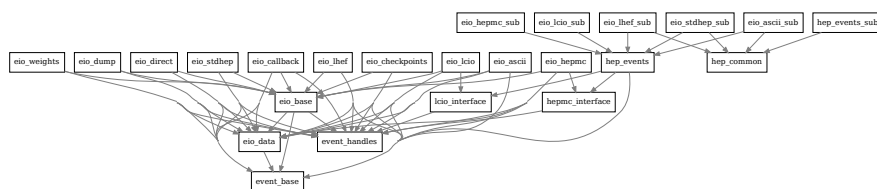


Figure 18.1: Module dependencies in **src/events**.

eio_dump Dump the contents of WHIZARD's `particle_set` internal record, using the `write` method of that record as-is. The main use is for testing purposes.

hep_common Implements traditional HEP common blocks that are (still) used by some of the event I/O formats below.

hepmc_interface Access particle objects of the HepMC package. Functional only if this package is linked. The interface is working both for HepMC2 and HepMC3.

lcio_interface Access objects of the LCIO package. Functional only if this package is linked.

hep_events Interface between the event record and the common blocks.

eio_ascii Collection of event output formats that write ASCII files.

eio_lhef LHEF for input and output.

eio_stdhep Support for the StdHEP format (binary, machine-independent).

eio_hepmc Support for the HepMC format (C++).

eio_lcio Support for the LCIO format (C++).

18.1 Generic Event Handling

We introduce events first in form of an abstract type, together with some utilities. Abstract events can be used by other modules, in particular event I/O, without introducing an explicit dependency on the event implementation.

```

<event_base.f90>≡
  <File header>

  module event_base

    <Use kinds>
    use kinds, only: i64
    <Use strings>
    use model_data
    use particles

    <Standard module head>

    <Event base: public>

    <Event base: parameters>

    <Event base: types>

    <Event base: interfaces>

    interface
    <Event base: sub interfaces>

```

```

        end interface

    end module event_base

    <event_base_sub.f90>≡
    <File header>

    submodule (event_base) event_base_s

        use io_units
        use string_utils, only: lower_case
        use diagnostics

        implicit none

    contains

    <Event base: procedures>

    end submodule event_base_s

```

18.1.1 generic event type

```

    <Event base: public>≡
        public :: generic_event_t

    <Event base: types>≡
        type, abstract :: generic_event_t
            !private
            logical :: particle_set_is_valid = .false.
            type(particle_set_t), pointer :: particle_set => null ()
            logical :: sqme_ref_known = .false.
            real(default) :: sqme_ref = 0
            logical :: sqme_prc_known = .false.
            real(default) :: sqme_prc = 0
            logical :: weight_ref_known = .false.
            real(default) :: weight_ref = 0
            logical :: weight_prc_known = .false.
            real(default) :: weight_prc = 0
            logical :: excess_prc_known = .false.
            real(default) :: excess_prc = 0
            logical :: n_dropped_known = .false.
            integer :: n_dropped = 0
            integer :: n_alt = 0
            logical :: sqme_alt_known = .false.
            real(default), dimension(:), allocatable :: sqme_alt
            logical :: weight_alt_known = .false.
            real(default), dimension(:), allocatable :: weight_alt
        contains
        <Event base: generic event: TBP>
    end type generic_event_t

```


18.1.2 Initialization

This determines the number of alternate weights and some values.

```
<Event base: generic event: TBP>≡
  procedure :: base_init => generic_event_init

<Event base: sub interfaces>≡
  module subroutine generic_event_init (event, n_alt)
    class(generic_event_t), intent(out) :: event
    integer, intent(in) :: n_alt
  end subroutine generic_event_init

<Event base: procedures>≡
  module subroutine generic_event_init (event, n_alt)
    class(generic_event_t), intent(out) :: event
    integer, intent(in) :: n_alt
    event%n_alt = n_alt
    allocate (event%sqme_alt (n_alt))
    allocate (event%weight_alt (n_alt))
  end subroutine generic_event_init
```

18.1.3 Access particle set

The particle set is the core of the event. We allow access to it via a pointer, and we maintain the information whether the particle set is valid, i.e., has been filled with meaningful data.

```
<Event base: generic event: TBP>+≡
  procedure :: has_valid_particle_set => generic_event_has_valid_particle_set
  procedure :: accept_particle_set => generic_event_accept_particle_set
  procedure :: discard_particle_set => generic_event_discard_particle_set

<Event base: sub interfaces>+≡
  module function generic_event_has_valid_particle_set (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_has_valid_particle_set

  module subroutine generic_event_accept_particle_set (event)
    class(generic_event_t), intent(inout) :: event
  end subroutine generic_event_accept_particle_set

  module subroutine generic_event_discard_particle_set (event)
    class(generic_event_t), intent(inout) :: event
  end subroutine generic_event_discard_particle_set

<Event base: procedures>+≡
  module function generic_event_has_valid_particle_set (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
    flag = event%particle_set_is_valid
  end function generic_event_has_valid_particle_set

  module subroutine generic_event_accept_particle_set (event)
    class(generic_event_t), intent(inout) :: event
```

```

        event%particle_set_is_valid = .true.
    end subroutine generic_event_accept_particle_set

    module subroutine generic_event_discard_particle_set (event)
        class(generic_event_t), intent(inout) :: event
        event%particle_set_is_valid = .false.
    end subroutine generic_event_discard_particle_set

```

These procedures deal with the particle set directly. Return the pointer:

```

(Event base: generic event: TBP)+≡
    procedure :: get_particle_set_ptr => generic_event_get_particle_set_ptr

(Event base: sub interfaces)+≡
    module function generic_event_get_particle_set_ptr (event) result (ptr)
        class(generic_event_t), intent(in) :: event
        type(particle_set_t), pointer :: ptr
    end function generic_event_get_particle_set_ptr

(Event base: procedures)+≡
    module function generic_event_get_particle_set_ptr (event) result (ptr)
        class(generic_event_t), intent(in) :: event
        type(particle_set_t), pointer :: ptr
        ptr => event%particle_set
    end function generic_event_get_particle_set_ptr

```

Let it point to some existing particle set:

```

(Event base: generic event: TBP)+≡
    procedure :: link_particle_set => generic_event_link_particle_set

(Event base: sub interfaces)+≡
    module subroutine generic_event_link_particle_set (event, particle_set)
        class(generic_event_t), intent(inout) :: event
        type(particle_set_t), intent(in), target :: particle_set
    end subroutine generic_event_link_particle_set

(Event base: procedures)+≡
    module subroutine generic_event_link_particle_set (event, particle_set)
        class(generic_event_t), intent(inout) :: event
        type(particle_set_t), intent(in), target :: particle_set
        event%particle_set => particle_set
        call event%accept_particle_set ()
    end subroutine generic_event_link_particle_set

```

18.1.4 Access sqme and weight

There are several incarnations: the current value, a reference value, alternate values.

```

(Event base: generic event: TBP)+≡
    procedure :: sqme_prc_is_known => generic_event_sqme_prc_is_known
    procedure :: sqme_ref_is_known => generic_event_sqme_ref_is_known
    procedure :: sqme_alt_is_known => generic_event_sqme_alt_is_known
    procedure :: weight_prc_is_known => generic_event_weight_prc_is_known
    procedure :: weight_ref_is_known => generic_event_weight_ref_is_known

```

```

procedure :: weight_alt_is_known => generic_event_weight_alt_is_known
procedure :: excess_prc_is_known => generic_event_excess_prc_is_known

(Event base: sub interfaces)+≡
  module function generic_event_sqme_prc_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_sqme_prc_is_known
  module function generic_event_sqme_ref_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_sqme_ref_is_known
  module function generic_event_sqme_alt_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_sqme_alt_is_known
  module function generic_event_weight_prc_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_weight_prc_is_known
  module function generic_event_weight_ref_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_weight_ref_is_known
  module function generic_event_weight_alt_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_weight_alt_is_known
  module function generic_event_excess_prc_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
  end function generic_event_excess_prc_is_known

(Event base: procedures)+≡
  module function generic_event_sqme_prc_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
    flag = event%sqme_prc_known
  end function generic_event_sqme_prc_is_known

  module function generic_event_sqme_ref_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
    flag = event%sqme_ref_known
  end function generic_event_sqme_ref_is_known

  module function generic_event_sqme_alt_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
    flag = event%sqme_alt_known
  end function generic_event_sqme_alt_is_known

  module function generic_event_weight_prc_is_known (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag

```

```

        flag = event%weight_prc_known
    end function generic_event_weight_prc_is_known

    module function generic_event_weight_ref_is_known (event) result (flag)
        class(generic_event_t), intent(in) :: event
        logical :: flag
        flag = event%weight_ref_known
    end function generic_event_weight_ref_is_known

    module function generic_event_weight_alt_is_known (event) result (flag)
        class(generic_event_t), intent(in) :: event
        logical :: flag
        flag = event%weight_alt_known
    end function generic_event_weight_alt_is_known

    module function generic_event_excess_prc_is_known (event) result (flag)
        class(generic_event_t), intent(in) :: event
        logical :: flag
        flag = event%excess_prc_known
    end function generic_event_excess_prc_is_known

    <Event base: generic event: TBP>+≡
        procedure :: get_n_alt => generic_event_get_n_alt

    <Event base: sub interfaces>+≡
        module function generic_event_get_n_alt (event) result (n)
            class(generic_event_t), intent(in) :: event
            integer :: n
            end function generic_event_get_n_alt

    <Event base: procedures>+≡
        module function generic_event_get_n_alt (event) result (n)
            class(generic_event_t), intent(in) :: event
            integer :: n
            n = event%n_alt
        end function generic_event_get_n_alt

    <Event base: generic event: TBP>+≡
        procedure :: get_sqme_prc => generic_event_get_sqme_prc
        procedure :: get_sqme_ref => generic_event_get_sqme_ref
        generic :: get_sqme_alt => &
            generic_event_get_sqme_alt_0, generic_event_get_sqme_alt_1
        procedure :: generic_event_get_sqme_alt_0
        procedure :: generic_event_get_sqme_alt_1
        procedure :: get_weight_prc => generic_event_get_weight_prc
        procedure :: get_weight_ref => generic_event_get_weight_ref
        generic :: get_weight_alt => &
            generic_event_get_weight_alt_0, generic_event_get_weight_alt_1
        procedure :: generic_event_get_weight_alt_0
        procedure :: generic_event_get_weight_alt_1
        procedure :: get_n_dropped => generic_event_get_n_dropped
        procedure :: get_excess_prc => generic_event_get_excess_prc

```

```

<Event base: sub interfaces>+≡
  module function generic_event_get_sqme_prc (event) result (sqme)
    class(generic_event_t), intent(in) :: event
    real(default) :: sqme
  end function generic_event_get_sqme_prc
  module function generic_event_get_sqme_ref (event) result (sqme)
    class(generic_event_t), intent(in) :: event
    real(default) :: sqme
  end function generic_event_get_sqme_ref
  module function generic_event_get_sqme_alt_0 (event, i) result (sqme)
    class(generic_event_t), intent(in) :: event
    integer, intent(in) :: i
    real(default) :: sqme
  end function generic_event_get_sqme_alt_0
  module function generic_event_get_sqme_alt_1 (event) result (sqme)
    class(generic_event_t), intent(in) :: event
    real(default), dimension(event%n_alt) :: sqme
  end function generic_event_get_sqme_alt_1
  module function generic_event_get_weight_prc (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default) :: weight
  end function generic_event_get_weight_prc
  module function generic_event_get_weight_ref (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default) :: weight
  end function generic_event_get_weight_ref
  module function generic_event_get_weight_alt_0 (event, i) result (weight)
    class(generic_event_t), intent(in) :: event
    integer, intent(in) :: i
    real(default) :: weight
  end function generic_event_get_weight_alt_0
  module function generic_event_get_weight_alt_1 (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default), dimension(event%n_alt) :: weight
  end function generic_event_get_weight_alt_1
  module function generic_event_get_excess_prc (event) result (excess)
    class(generic_event_t), intent(in) :: event
    real(default) :: excess
  end function generic_event_get_excess_prc
  module function generic_event_get_n_dropped (event) result (n_dropped)
    class(generic_event_t), intent(in) :: event
    integer :: n_dropped
  end function generic_event_get_n_dropped

<Event base: procedures>+≡
  module function generic_event_get_sqme_prc (event) result (sqme)
    class(generic_event_t), intent(in) :: event
    real(default) :: sqme
    if (event%sqme_prc_known) then
      sqme = event%sqme_prc
    else
      sqme = 0
    end if
  end function generic_event_get_sqme_prc

```

```

module function generic_event_get_sqme_ref (event) result (sqme)
  class(generic_event_t), intent(in) :: event
  real(default) :: sqme
  if (event%sqme_ref_known) then
    sqme = event%sqme_ref
  else
    sqme = 0
  end if
end function generic_event_get_sqme_ref

module function generic_event_get_sqme_alt_0 (event, i) result (sqme)
  class(generic_event_t), intent(in) :: event
  integer, intent(in) :: i
  real(default) :: sqme
  if (event%sqme_alt_known) then
    sqme = event%sqme_alt(i)
  else
    sqme = 0
  end if
end function generic_event_get_sqme_alt_0

module function generic_event_get_sqme_alt_1 (event) result (sqme)
  class(generic_event_t), intent(in) :: event
  real(default), dimension(event%n_alt) :: sqme
  sqme = event%sqme_alt
end function generic_event_get_sqme_alt_1

module function generic_event_get_weight_prc (event) result (weight)
  class(generic_event_t), intent(in) :: event
  real(default) :: weight
  if (event%weight_prc_known) then
    weight = event%weight_prc
  else
    weight = 0
  end if
end function generic_event_get_weight_prc

module function generic_event_get_weight_ref (event) result (weight)
  class(generic_event_t), intent(in) :: event
  real(default) :: weight
  if (event%weight_ref_known) then
    weight = event%weight_ref
  else
    weight = 0
  end if
end function generic_event_get_weight_ref

module function generic_event_get_weight_alt_0 (event, i) result (weight)
  class(generic_event_t), intent(in) :: event
  integer, intent(in) :: i
  real(default) :: weight
  if (event%weight_alt_known) then
    weight = event%weight_alt(i)
  else

```

```

        weight = 0
    end if
end function generic_event_get_weight_alt_0

module function generic_event_get_weight_alt_1 (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default), dimension(event%n_alt) :: weight
    weight = event%weight_alt
end function generic_event_get_weight_alt_1

module function generic_event_get_excess_prc (event) result (excess)
    class(generic_event_t), intent(in) :: event
    real(default) :: excess
    if (event%excess_prc_known) then
        excess = event%excess_prc
    else
        excess = 0
    end if
end function generic_event_get_excess_prc

module function generic_event_get_n_dropped (event) result (n_dropped)
    class(generic_event_t), intent(in) :: event
    integer :: n_dropped
    if (event%n_dropped_known) then
        n_dropped = event%n_dropped
    else
        n_dropped = 0
    end if
end function generic_event_get_n_dropped

```

(Event base: generic event: TBP)+≡

```

procedure :: set_sqme_prc => generic_event_set_sqme_prc
procedure :: set_sqme_ref => generic_event_set_sqme_ref
procedure :: set_sqme_alt => generic_event_set_sqme_alt
procedure :: set_weight_prc => generic_event_set_weight_prc
procedure :: set_weight_ref => generic_event_set_weight_ref
procedure :: set_weight_alt => generic_event_set_weight_alt
procedure :: set_excess_prc => generic_event_set_excess_prc
procedure :: set_n_dropped => generic_event_set_n_dropped

```

(Event base: sub interfaces)+≡

```

module subroutine generic_event_set_sqme_prc (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), intent(in) :: sqme
end subroutine generic_event_set_sqme_prc
module subroutine generic_event_set_sqme_ref (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), intent(in) :: sqme
end subroutine generic_event_set_sqme_ref
module subroutine generic_event_set_sqme_alt (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), dimension(:), intent(in) :: sqme
end subroutine generic_event_set_sqme_alt
module subroutine generic_event_set_weight_prc (event, weight)

```

```

        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: weight
    end subroutine generic_event_set_weight_prc
    module subroutine generic_event_set_weight_ref (event, weight)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: weight
    end subroutine generic_event_set_weight_ref
    module subroutine generic_event_set_weight_alt (event, weight)
        class(generic_event_t), intent(inout) :: event
        real(default), dimension(:), intent(in) :: weight
    end subroutine generic_event_set_weight_alt
    module subroutine generic_event_set_excess_prc (event, excess)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: excess
    end subroutine generic_event_set_excess_prc
    module subroutine generic_event_set_n_dropped (event, n_dropped)
        class(generic_event_t), intent(inout) :: event
        integer, intent(in) :: n_dropped
    end subroutine generic_event_set_n_dropped
    (Event base: procedures)+≡
    module subroutine generic_event_set_sqme_prc (event, sqme)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: sqme
        event%sqme_prc = sqme
        event%sqme_prc_known = .true.
    end subroutine generic_event_set_sqme_prc

    module subroutine generic_event_set_sqme_ref (event, sqme)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: sqme
        event%sqme_ref = sqme
        event%sqme_ref_known = .true.
    end subroutine generic_event_set_sqme_ref

    module subroutine generic_event_set_sqme_alt (event, sqme)
        class(generic_event_t), intent(inout) :: event
        real(default), dimension(:), intent(in) :: sqme
        event%sqme_alt = sqme
        event%sqme_alt_known = .true.
    end subroutine generic_event_set_sqme_alt

    module subroutine generic_event_set_weight_prc (event, weight)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: weight
        event%weight_prc = weight
        event%weight_prc_known = .true.
    end subroutine generic_event_set_weight_prc

    module subroutine generic_event_set_weight_ref (event, weight)
        class(generic_event_t), intent(inout) :: event
        real(default), intent(in) :: weight
        event%weight_ref = weight
        event%weight_ref_known = .true.
    end subroutine generic_event_set_weight_ref

```



```

module subroutine generic_event_set_weight_alt (event, weight)
  class(generic_event_t), intent(inout) :: event
  real(default), dimension(:), intent(in) :: weight
  event%weight_alt = weight
  event%weight_alt_known = .true.
end subroutine generic_event_set_weight_alt

module subroutine generic_event_set_excess_prc (event, excess)
  class(generic_event_t), intent(inout) :: event
  real(default), intent(in) :: excess
  event%excess_prc = excess
  event%excess_prc_known = .true.
end subroutine generic_event_set_excess_prc

module subroutine generic_event_set_n_dropped (event, n_dropped)
  class(generic_event_t), intent(inout) :: event
  integer, intent(in) :: n_dropped
  event%n_dropped = n_dropped
  event%n_dropped_known = .true.
end subroutine generic_event_set_n_dropped

```

Set the appropriate entry directly.

(Event base: generic event: TBP)+≡

```

procedure :: set => generic_event_set

```

(Event base: sub interfaces)+≡

```

module subroutine generic_event_set (event, &
  weight_ref, weight_prc, weight_alt, &
  excess_prc, n_dropped, &
  sqme_ref, sqme_prc, sqme_alt)
  class(generic_event_t), intent(inout) :: event
  real(default), intent(in), optional :: weight_ref, weight_prc
  real(default), intent(in), optional :: sqme_ref, sqme_prc
  real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
  real(default), intent(in), optional :: excess_prc
  integer, intent(in), optional :: n_dropped
end subroutine generic_event_set

```

(Event base: procedures)+≡

```

module subroutine generic_event_set (event, &
  weight_ref, weight_prc, weight_alt, &
  excess_prc, n_dropped, &
  sqme_ref, sqme_prc, sqme_alt)
  class(generic_event_t), intent(inout) :: event
  real(default), intent(in), optional :: weight_ref, weight_prc
  real(default), intent(in), optional :: sqme_ref, sqme_prc
  real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
  real(default), intent(in), optional :: excess_prc
  integer, intent(in), optional :: n_dropped
  if (present (sqme_prc)) then
    call event%set_sqme_prc (sqme_prc)
  end if
  if (present (sqme_ref)) then
    call event%set_sqme_ref (sqme_ref)
  end if
end subroutine generic_event_set

```

```

end if
if (present (sqme_alt)) then
  call event%set_sqme_alt (sqme_alt)
end if
if (present (weight_prc)) then
  call event%set_weight_prc (weight_prc)
end if
if (present (weight_ref)) then
  call event%set_weight_ref (weight_ref)
end if
if (present (weight_alt)) then
  call event%set_weight_alt (weight_alt)
end if
if (present (excess_prc)) then
  call event%set_excess_prc (excess_prc)
end if
if (present (n_dropped)) then
  call event%set_n_dropped (n_dropped)
end if
end subroutine generic_event_set

```

18.1.5 Pure Virtual Methods

These procedures can only be implemented in the concrete implementation.

Output (verbose, depending on parameters).

(Event base: generic event: TBP)+≡
 procedure (generic_event_write), deferred :: write

(Event base: interfaces)≡
 abstract interface
 subroutine generic_event_write (object, unit, &
 show_process, show_transforms, &
 show_decay, verbose, testflag)
 import
 class(generic_event_t), intent(in) :: object
 integer, intent(in), optional :: unit
 logical, intent(in), optional :: show_process
 logical, intent(in), optional :: show_transforms
 logical, intent(in), optional :: show_decay
 logical, intent(in), optional :: verbose
 logical, intent(in), optional :: testflag
 end subroutine generic_event_write
end interface

Generate an event, based on a selector index `i_mci`, and optionally on an extra set of random numbers `r`. For the main bunch of random numbers that the generator needs, the event object should contain its own generator.

(Event base: generic event: TBP)+≡
 procedure (generic_event_generate), deferred :: generate

(Event base: interfaces)+≡
 abstract interface

```

subroutine generic_event_generate (event, i_mci, r, i_nlo)
  import
  class(generic_event_t), intent(inout) :: event
  integer, intent(in) :: i_mci
  real(default), dimension(:), intent(in), optional :: r
  integer, intent(in), optional :: i_nlo
end subroutine generic_event_generate
end interface

```

Alternative : inject a particle set that is supposed to represent the hard process.
How this determines the event, is dependent on the event structure, therefore
this is a deferred method.

<Event base: generic event: TBP>+≡

```

  procedure (generic_event_set_hard_particle_set), deferred :: &
    set_hard_particle_set

```

<Event base: interfaces>+≡

```

  abstract interface
    subroutine generic_event_set_hard_particle_set (event, particle_set)
      import
      class(generic_event_t), intent(inout) :: event
      type(particle_set_t), intent(in) :: particle_set
    end subroutine generic_event_set_hard_particle_set
  end interface

```

Event index handlers.

<Event base: generic event: TBP>+≡

```

  procedure (generic_event_set_index), deferred :: set_index
  procedure (generic_event_handler), deferred :: reset_index
  procedure (generic_event_increment_index), deferred :: increment_index

```

<Event base: interfaces>+≡

```

  abstract interface
    subroutine generic_event_set_index (event, index)
      import
      class(generic_event_t), intent(inout) :: event
      integer, intent(in) :: index
    end subroutine generic_event_set_index
  end interface

```

```

  abstract interface
    subroutine generic_event_handler (event)
      import
      class(generic_event_t), intent(inout) :: event
    end subroutine generic_event_handler
  end interface

```

```

  abstract interface
    subroutine generic_event_increment_index (event, offset)
      import
      class(generic_event_t), intent(inout) :: event
      integer, intent(in), optional :: offset
    end subroutine generic_event_increment_index

```

```
end interface
```

Evaluate any expressions associated with the event. No argument needed.

(Event base: generic event: TBP)+≡

```
procedure (generic_event_handler), deferred :: evaluate_expressions
```

Select internal parameters

(Event base: generic event: TBP)+≡

```
procedure (generic_event_select), deferred :: select
```

(Event base: interfaces)+≡

```
abstract interface
```

```
subroutine generic_event_select (event, i_mci, i_term, channel)
```

```
import
```

```
class(generic_event_t), intent(inout) :: event
```

```
integer, intent(in) :: i_mci, i_term, channel
```

```
end subroutine generic_event_select
```

```
end interface
```

Return a pointer to the model for the currently active process.

(Event base: generic event: TBP)+≡

```
procedure (generic_event_get_model_ptr), deferred :: get_model_ptr
```

(Event base: interfaces)+≡

```
abstract interface
```

```
function generic_event_get_model_ptr (event) result (model)
```

```
import
```

```
class(generic_event_t), intent(in) :: event
```

```
class(model_data_t), pointer :: model
```

```
end function generic_event_get_model_ptr
```

```
end interface
```

Return data used by external event formats.

(Event base: generic event: TBP)+≡

```
procedure (generic_event_has_index), deferred :: has_index
```

```
procedure (generic_event_get_index), deferred :: get_index
```

```
procedure (generic_event_get_fac_scale), deferred :: get_fac_scale
```

```
procedure (generic_event_get_alpha_s), deferred :: get_alpha_s
```

```
procedure (generic_event_get_sqrts), deferred :: get_sqrts
```

```
procedure (generic_event_get_polarization), deferred :: get_polarization
```

```
procedure (generic_event_get_beam_file), deferred :: get_beam_file
```

```
procedure (generic_event_get_process_name), deferred :: &  
get_process_name
```

(Event base: interfaces)+≡

```
abstract interface
```

```
function generic_event_has_index (event) result (flag)
```

```
import
```

```
class(generic_event_t), intent(in) :: event
```

```
logical :: flag
```

```
end function generic_event_has_index
```

```
end interface
```

```
abstract interface
```

```

function generic_event_get_index (event) result (index)
  import
  class(generic_event_t), intent(in) :: event
  integer :: index
end function generic_event_get_index
end interface

abstract interface
  function generic_event_get_fac_scale (event) result (fac_scale)
  import
  class(generic_event_t), intent(in) :: event
  real(default) :: fac_scale
end function generic_event_get_fac_scale
end interface

abstract interface
  function generic_event_get_alpha_s (event) result (alpha_s)
  import
  class(generic_event_t), intent(in) :: event
  real(default) :: alpha_s
end function generic_event_get_alpha_s
end interface

abstract interface
  function generic_event_get_sqrts (event) result (sqrts)
  import
  class(generic_event_t), intent(in) :: event
  real(default) :: sqrts
end function generic_event_get_sqrts
end interface

abstract interface
  function generic_event_get_polarization (event) result (pol)
  import
  class(generic_event_t), intent(in) :: event
  real(default), dimension(:), allocatable :: pol
end function generic_event_get_polarization
end interface

abstract interface
  function generic_event_get_beam_file (event) result (file)
  import
  class(generic_event_t), intent(in) :: event
  type(string_t) :: file
end function generic_event_get_beam_file
end interface

abstract interface
  function generic_event_get_process_name (event) result (name)
  import
  class(generic_event_t), intent(in) :: event
  type(string_t) :: name
end function generic_event_get_process_name
end interface

```

Set data used by external event formats.

```

(Event base: generic event: TBP)+≡
  procedure (generic_event_set_alpha_qcd_forced), deferred :: &
    set_alpha_qcd_forced
  procedure (generic_event_set_scale_forced), deferred :: &
    set_scale_forced

(Event base: interfaces)+≡
  abstract interface
    subroutine generic_event_set_alpha_qcd_forced (event, alpha_qcd)
      import
      class(generic_event_t), intent(inout) :: event
      real(default), intent(in) :: alpha_qcd
    end subroutine generic_event_set_alpha_qcd_forced
  end interface

  abstract interface
    subroutine generic_event_set_scale_forced (event, scale)
      import
      class(generic_event_t), intent(inout) :: event
      real(default), intent(in) :: scale
    end subroutine generic_event_set_scale_forced
  end interface

```

18.1.6 Utilities

Applying this, current event contents are marked as incomplete but are not deleted. In particular, the initialization is kept.

```

(Event base: generic event: TBP)+≡
  procedure :: reset_contents => generic_event_reset_contents
  procedure :: base_reset_contents => generic_event_reset_contents

(Event base: sub interfaces)+≡
  module subroutine generic_event_reset_contents (event)
    class(generic_event_t), intent(inout) :: event
  end subroutine generic_event_reset_contents

(Event base: procedures)+≡
  module subroutine generic_event_reset_contents (event)
    class(generic_event_t), intent(inout) :: event
    call event%discard_particle_set ()
    event%sqme_ref_known = .false.
    event%sqme_prc_known = .false.
    event%sqme_alt_known = .false.
    event%weight_ref_known = .false.
    event%weight_prc_known = .false.
    event%weight_alt_known = .false.
    event%excess_prc_known = .false.
  end subroutine generic_event_reset_contents

```

Pacify particle set.

```

(Event base: generic event: TBP)+≡
    procedure :: pacify_particle_set => generic_event_pacify_particle_set

(Event base: sub interfaces)+≡
    module subroutine generic_event_pacify_particle_set (event)
        class(generic_event_t), intent(inout) :: event
    end subroutine generic_event_pacify_particle_set

(Event base: procedures)+≡
    module subroutine generic_event_pacify_particle_set (event)
        class(generic_event_t), intent(inout) :: event
        if (event%has_valid_particle_set ()) call pacify (event%particle_set)
    end subroutine generic_event_pacify_particle_set

```

18.1.7 Event normalization

The parameters for event normalization. For unweighted events, NORM_UNIT is intended as default, while for weighted events, it is NORM_SIGMA.

Note: the unit test for this is in eio_data_2 below.

```

(Event base: parameters)+≡
    integer, parameter, public :: NORM_UNDEFINED = 0
    integer, parameter, public :: NORM_UNIT = 1
    integer, parameter, public :: NORM_N_EVT = 2
    integer, parameter, public :: NORM_SIGMA = 3
    integer, parameter, public :: NORM_S_N = 4

These functions translate between the user representation and the internal one.

(Event base: public)+≡
    public :: event_normalization_mode
    public :: event_normalization_string

(Event base: sub interfaces)+≡
    module function event_normalization_mode (string, unweighted) result (mode)
        integer :: mode
        type(string_t), intent(in) :: string
        logical, intent(in) :: unweighted
    end function event_normalization_mode
    module function event_normalization_string (norm_mode) result (string)
        integer, intent(in) :: norm_mode
        type(string_t) :: string
    end function event_normalization_string

(Event base: procedures)+≡
    module function event_normalization_mode (string, unweighted) result (mode)
        integer :: mode
        type(string_t), intent(in) :: string
        logical, intent(in) :: unweighted
        select case (lower_case (char (string)))
        case ("auto")
            if (unweighted) then
                mode = NORM_UNIT
            else

```

```

        mode = NORM_SIGMA
    end if
case ("1")
    mode = NORM_UNIT
case ("1/n")
    mode = NORM_N_EVT
case ("sigma")
    mode = NORM_SIGMA
case ("sigma/n")
    mode = NORM_S_N
case default
    call msg_fatal ("Event normalization: unknown value '" &
        // char (string) // "'")
end select
end function event_normalization_mode

module function event_normalization_string (norm_mode) result (string)
    integer, intent(in) :: norm_mode
    type(string_t) :: string
    select case (norm_mode)
    case (NORM_UNDEFINED); string = "[undefined]"
    case (NORM_UNIT);      string = "'1'"
    case (NORM_N_EVT);     string = "'1/n'"
    case (NORM_SIGMA);     string = "'sigma'"
    case (NORM_S_N);       string = "'sigma/n'"
    case default;          string = "???"
    end select
end function event_normalization_string

```

We place this here as a generic helper, so we can update event weights whenever we need, not just in connection with an event sample data object.

```

(Event base: public)+≡
    public :: event_normalization_update

(Event base: sub interfaces)+≡
    module subroutine event_normalization_update &
        (weight, sigma, n, mode_new, mode_old)
        real(default), intent(inout) :: weight
        real(default), intent(in) :: sigma
        integer, intent(in) :: n
        integer, intent(in) :: mode_new, mode_old
    end subroutine event_normalization_update

(Event base: procedures)+≡
    module subroutine event_normalization_update &
        (weight, sigma, n, mode_new, mode_old)
        real(default), intent(inout) :: weight
        real(default), intent(in) :: sigma
        integer, intent(in) :: n
        integer, intent(in) :: mode_new, mode_old
        if (mode_new /= mode_old) then
            if (sigma > 0 .and. n > 0) then
                weight = weight / factor (mode_old) * factor (mode_new)
            else
                call msg_fatal ("Event normalization update: null sample")
            end if
        end if
    end subroutine event_normalization_update

```



```

        end if
    end if
contains
    function factor (mode)
        real(default) :: factor
        integer, intent(in) :: mode
        select case (mode)
            case (NORM_UNIT);    factor = 1._default
            case (NORM_N_EVT);    factor = 1._default / n
            case (NORM_SIGMA);    factor = sigma
            case (NORM_S_N);      factor = sigma / n
            case default
                call msg_fatal ("Event normalization update: undefined mode")
        end select
    end function factor
end subroutine event_normalization_update

```

18.1.8 Callback container

This derived type contains a callback procedure that can be executed during event I/O. The callback procedure is given the event object (with class `generic_event`) and an event index.

This is a simple wrapper. The object is abstract, so the the actual procedure is introduced by overriding the deferred one. We use the PASS attribute, so we may supplement runtime data in the callback object if desired.

```

<Event base: public>+≡
    public :: event_callback_t

<Event base: types>+≡
    type, abstract :: event_callback_t
    private
    contains
        procedure(event_callback_write), deferred :: write
        procedure(event_callback_proc), deferred :: proc
    end type event_callback_t

```

Identify the callback procedure in output

```

<Event base: interfaces>+≡
    abstract interface
        subroutine event_callback_write (event_callback, unit)
            import
            class(event_callback_t), intent(in) :: event_callback
            integer, intent(in), optional :: unit
        end subroutine event_callback_write
    end interface

```

This is the procedure interface.

```

<Event base: interfaces>+≡
    abstract interface
        subroutine event_callback_proc (event_callback, i, event)
            import

```

```

        class(event_callback_t), intent(in) :: event_callback
        integer(i64), intent(in) :: i
        class(generic_event_t), intent(in) :: event
    end subroutine event_callback_proc
end interface

```

A dummy implementation for testing and fallback.

```

<Event base: public>+≡
    public :: event_callback_nop_t

<Event base: types>+≡
    type, extends (event_callback_t) :: event_callback_nop_t
    private
    contains
        procedure :: write => event_callback_nop_write
        procedure :: proc => event_callback_nop
    end type event_callback_nop_t

<Event base: sub interfaces>+≡
    module subroutine event_callback_nop_write (event_callback, unit)
        class(event_callback_nop_t), intent(in) :: event_callback
        integer, intent(in), optional :: unit
    end subroutine event_callback_nop_write
    module subroutine event_callback_nop (event_callback, i, event)
        class(event_callback_nop_t), intent(in) :: event_callback
        integer(i64), intent(in) :: i
        class(generic_event_t), intent(in) :: event
    end subroutine event_callback_nop

<Event base: procedures>+≡
    module subroutine event_callback_nop_write (event_callback, unit)
        class(event_callback_nop_t), intent(in) :: event_callback
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "NOP"
    end subroutine event_callback_nop_write

    module subroutine event_callback_nop (event_callback, i, event)
        class(event_callback_nop_t), intent(in) :: event_callback
        integer(i64), intent(in) :: i
        class(generic_event_t), intent(in) :: event
    end subroutine event_callback_nop

```

18.2 Event Handle

This module defines an abstract base type that allows us to communicate any type of event record within the program. The concrete extensions are expected to consist of pointers, such as the C pointers for HepMC or LCIO events, so the communication object is a very light-weight one.

```

<event_handles.f90>≡

```

```

    <File header>

    module event_handles

    <Standard module head>

    <Event handle: public>

    <Event handle: types>

    end module event_handles

```

There is only one abstract type.

```

<Event handle: public>≡
    public :: event_handle_t

<Event handle: types>≡
    type, abstract :: event_handle_t
    end type event_handle_t

```

18.3 Event Sample Data

We define a simple and transparent container for (meta)data that are associated with an event sample.

```

<eio_data.f90>≡
    <File header>

    module eio_data

    <Use kinds>
    <Use strings>

    use event_base

    <Standard module head>

    <EIO data: public>

    <EIO data: types>

    interface
    <EIO data: sub interfaces>
    end interface

    end module eio_data

    <eio_data_sub.f90>≡
    <File header>

    submodule (eio_data) eio_data_s

    use io_units
    use numeric_utils

```

```

    use diagnostics

    implicit none

contains

    <EIO data: procedures>

end submodule eio_data_s

```

18.3.1 Event Sample Data

These are data that apply to an event sample as a whole. They are given in an easily portable form (no fancy structure) and are used for initializing event formats.

There are two MD5 sums here. `md5sum_proc` depends only on the definition of the contributing processes. A sample with matching checksum can be rescanned with modified model parameters, beam structure etc, to recalculate observables. `md5sum_config` includes all relevant data. Rescanning a sample with matching checksum will produce identical observables. (A third checksum might be added which depends on the event sample itself. This is not needed, so far.)

If alternate weights are part of the event sample (`n_alt` nonzero), there is a configuration MD5 sum for each of them.

```

<EIO data: public>≡
    public :: event_sample_data_t

<EIO data: types>≡
    type :: event_sample_data_t
        character(32) :: md5sum_prc = ""
        character(32) :: md5sum_cfg = ""
        logical :: unweighted = .true.
        logical :: negative_weights = .false.
        integer :: norm_mode = NORM_UNDEFINED
        integer :: n_beam = 0
        integer, dimension(2) :: pdg_beam = 0
        real(default), dimension(2) :: energy_beam = 0
        integer :: n_proc = 0
        integer :: n_evt = 0
        integer :: nlo_multiplier = 1
        integer :: split_n_evt = 0
        integer :: split_n_kbytes = 0
        integer :: split_index = 0
        real(default) :: total_cross_section = 0
        integer, dimension(:), allocatable :: proc_num_id
        integer :: n_alt = 0
        character(32), dimension(:), allocatable :: md5sum_alt
        real(default), dimension(:), allocatable :: cross_section
        real(default), dimension(:), allocatable :: error
    contains
        <EIO data: event sample data: TBP>
end type event_sample_data_t

```

Initialize: allocate for the number of processes

<EIO data: event sample data: TBP>≡

```
procedure :: init => event_sample_data_init
```

<EIO data: sub interfaces>≡

```
module subroutine event_sample_data_init (data, n_proc, n_alt)
  class(event_sample_data_t), intent(out) :: data
  integer, intent(in) :: n_proc
  integer, intent(in), optional :: n_alt
end subroutine event_sample_data_init
```

<EIO data: procedures>≡

```
module subroutine event_sample_data_init (data, n_proc, n_alt)
  class(event_sample_data_t), intent(out) :: data
  integer, intent(in) :: n_proc
  integer, intent(in), optional :: n_alt
  data%n_proc = n_proc
  allocate (data%proc_num_id (n_proc), source = 0)
  allocate (data%cross_section (n_proc), source = 0._default)
  allocate (data%error (n_proc), source = 0._default)
  if (present (n_alt)) then
    data%n_alt = n_alt
    allocate (data%md5sum_alt (n_alt))
    data%md5sum_alt = ""
  end if
end subroutine event_sample_data_init
```

Output.

<EIO data: event sample data: TBP>+≡

```
procedure :: write => event_sample_data_write
```

<EIO data: sub interfaces>+≡

```
module subroutine event_sample_data_write (data, unit)
  class(event_sample_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
end subroutine event_sample_data_write
```

<EIO data: procedures>+≡

```
module subroutine event_sample_data_write (data, unit)
  class(event_sample_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Event sample properties:"
  write (u, "(3x,A,A,A)") "MD5 sum (proc) = '", data%md5sum_prc, "'"
  write (u, "(3x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
  write (u, "(3x,A,L1)") "unweighted = ", data%unweighted
  write (u, "(3x,A,L1)") "negative weights = ", data%negative_weights
  write (u, "(3x,A,A)") "normalization = ", &
    char (event_normalization_string (data%norm_mode))
  write (u, "(3x,A,I0)") "number of beams = ", data%n_beam
  write (u, "(5x,A,2(1x,I19))") "PDG = ", &
    data%pdg_beam(:data%n_beam)
  write (u, "(5x,A,2(1x,ES19.12))") "Energy = ", &
```

```

        data%energy_beam(:data%n_beam)
    if (data%n_evt > 0) then
        write (u, "(3x,A,I0)") "number of events = ", data%n_evt
    end if
    if (.not. vanishes (data%total_cross_section)) then
        write (u, "(3x,A,ES19.12)") "total cross sec. = ", &
            data%total_cross_section
    end if
    write (u, "(3x,A,I0)") "num of processes = ", data%n_proc
    do i = 1, data%n_proc
        write (u, "(3x,A,I0)") "Process #", data%proc_num_id (i)
        select case (data%n_beam)
            case (1)
                write (u, "(5x,A,ES19.12)") "Width = ", data%cross_section(i)
            case (2)
                write (u, "(5x,A,ES19.12)") "CSec = ", data%cross_section(i)
        end select
        write (u, "(5x,A,ES19.12)") "Error = ", data%error(i)
    end do
    if (data%n_alt > 0) then
        write (u, "(3x,A,I0)") "num of alt wgt = ", data%n_alt
        do i = 1, data%n_alt
            write (u, "(5x,A,A,A,1x,I0)") "MD5 sum (cfg) = ', &
                data%md5sum_alt(i), "'", i
        end do
    end if
end subroutine event_sample_data_write

```

18.3.2 Unit tests

Test module, followed by the corresponding implementation module.

<eio_data_ut.f90>≡

<File header>

```

module eio_data_ut
    use unit_tests
    use eio_data_util

```

<Standard module head>

<EIO data: public test>

contains

<EIO data: test driver>

```

end module eio_data_ut

```

<eio_data_util.f90>≡

<File header>

```

module eio_data_util

```

```

    <Use kinds>
    <Use strings>
    use event_base

    use eio_data

    <Standard module head>

    <EIO data: test declarations>

contains

    <EIO data: tests>

end module eio_data_util

API: driver for the unit tests below.
<EIO data: public test>≡
    public :: eio_data_test
<EIO data: test driver>≡
    subroutine eio_data_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <EIO data: execute tests>
    end subroutine eio_data_test

```

Event Sample Data

Print the contents of a sample data block.

```

<EIO data: execute tests>≡
    call test (eio_data_1, "eio_data_1", &
        "event sample data", &
        u, results)
<EIO data: test declarations>≡
    public :: eio_data_1
<EIO data: tests>≡
    subroutine eio_data_1 (u)
        integer, intent(in) :: u
        type(event_sample_data_t) :: data

        write (u, "(A)")  "* Test output: eio_data_1"
        write (u, "(A)")  "* Purpose: display event sample data"
        write (u, "(A)")

        write (u, "(A)")  "* Decay process, one component"
        write (u, "(A)")

        call data%init (1, 1)
        data%n_beam = 1
        data%pdg_beam(1) = 25
        data%energy_beam(1) = 125
    end subroutine eio_data_1

```



```

write (u, "(A)")  "*"   Purpose:  handle event normalization"
write (u, "(A)")

write (u, "(A)")  "*" Normalization strings"
write (u, "(A)")

s = "auto"
unweighted = .true.
write (u, "(1x,A,1x,L1,1x,A)") char (s), unweighted, &
char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "AUTO"
unweighted = .false.
write (u, "(1x,A,1x,L1,1x,A)") char (s), unweighted, &
char (event_normalization_string &
(event_normalization_mode (s, unweighted)))

unweighted = .true.

s = "1"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "1/n"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "Sigma"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "sigma/N"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))

write (u, "(A)")
write (u, "(A)")  "*" Normalization update"
write (u, "(A)")

sigma = 5
n = 2

w0 = 1

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_UNIT)
write (u, "(2(F6.3))") w0, w

```

```

write (u, *)

w0 = 0.5

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w

write (u, *)

w0 = 5.0

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w

write (u, *)

w0 = 2.5

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_S_N)
write (u, "(2(F6.3))") w0, w

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_data_2"

```

```
end subroutine eio_data_2
```

18.4 Abstract I/O Handler

This module defines an abstract object for event I/O and the associated methods.

There are `output` and `input` methods which write or read a single event from/to the I/O stream, respectively. The I/O stream itself may be a file, a common block, or an externally linked structure, depending on the concrete implementation.

A `write` method prints the current content of the implementation-dependent event record in human-readable form.

The `init_in/init_out` and `final` prepare and finalize the I/O stream, respectively. There is also a `switch_inout` method which turns an input stream into an output stream where events can be appended.

Optionally, output files can be split in chunks of well-defined size. The `split_out` method takes care of this.

```
<eio_base.f90>≡
  <File header>

  module eio_base

    use kinds, only: i64
    <Use strings>
    use model_data
    use event_base
    use event_handles, only: event_handle_t
    use eio_data

    <Standard module head>

    <EIO base: public>

    <EIO base: types>

    <EIO base: interfaces>

    interface
    <EIO base: sub interfaces>
    end interface

  end module eio_base

<eio_base_sub.f90>≡
  <File header>

  submodule (eio_base) eio_base_s

    use io_units
    use diagnostics
```

```

        implicit none

contains

    <EIO base: procedures>

end submodule eio_base_s

```

18.4.1 Type

We can assume that most implementations will need the file extension as a fixed string and, if they support file splitting, the current file index.

The fallback model is useful for implementations that are able to read unknown files which may contain hadrons etc., not in the current hard-interaction model.

```

<EIO base: public>≡
    public :: eio_t

<EIO base: types>≡
    type, abstract :: eio_t
        type(string_t) :: sample
        type(string_t) :: extension
        type(string_t) :: filename
        logical :: has_file = .false.
        logical :: split = .false.
        integer :: split_n_evt = 0
        integer :: split_n_kbytes = 0
        integer :: split_index = 0
        integer :: split_count = 0
        class(model_data_t), pointer :: fallback_model => null ()
    contains
        <EIO base: eio: TBP>
    end type eio_t

```

Write to screen. If possible, this should display the contents of the current event, i.e., the last one that was written or read.

```

<EIO base: eio: TBP>≡
    procedure (eio_write), deferred :: write

<EIO base: interfaces>≡
    abstract interface
        subroutine eio_write (object, unit)
            import
            class(eio_t), intent(in) :: object
            integer, intent(in), optional :: unit
        end subroutine eio_write
    end interface

```

Finalize. This should write/read footer data and close input/output channels.

```

<EIO base: eio: TBP>+≡
    procedure (eio_final), deferred :: final

```

```

(EIO base: interfaces)+≡
  abstract interface
    subroutine eio_final (object)
      import
      class(eio_t), intent(inout) :: object
    end subroutine eio_final
  end interface

```

Determine splitting parameters from the event sample data.

```

(EIO base: eio: TBP)+≡
  procedure :: set_splitting => eio_set_splitting

(EIO base: sub interfaces)≡
  module subroutine eio_set_splitting (eio, data)
    class(eio_t), intent(inout) :: eio
    type(event_sample_data_t), intent(in) :: data
  end subroutine eio_set_splitting

(EIO base: procedures)≡
  module subroutine eio_set_splitting (eio, data)
    class(eio_t), intent(inout) :: eio
    type(event_sample_data_t), intent(in) :: data
    eio%split = data%split_n_evt > 0 .or. data%split_n_kbytes > 0
    if (eio%split) then
      eio%split_n_evt = data%split_n_evt
      eio%split_n_kbytes = data%split_n_kbytes
      eio%split_index = data%split_index
      eio%split_count = 0
    end if
  end subroutine eio_set_splitting

```

Update the byte count and check if it has increased. We use integer division to determine the number of `n_kbytes` blocks that are in the event file.

```

(EIO base: eio: TBP)+≡
  procedure :: update_split_count => eio_update_split_count

(EIO base: sub interfaces)+≡
  module subroutine eio_update_split_count (eio, increased)
    class(eio_t), intent(inout) :: eio
    logical, intent(out) :: increased
  end subroutine eio_update_split_count

(EIO base: procedures)+≡
  module subroutine eio_update_split_count (eio, increased)
    class(eio_t), intent(inout) :: eio
    logical, intent(out) :: increased
    integer :: split_count_old
    if (eio%split_n_kbytes > 0) then
      split_count_old = eio%split_count
      eio%split_count = eio%file_size_kbytes () / eio%split_n_kbytes
      increased = eio%split_count > split_count_old
    end if
  end subroutine eio_update_split_count

```

Generate a filename, taking a possible split index into account.

```

(EIO base: eio: TBP)+≡
    procedure :: set_filename => eio_set_filename

(EIO base: sub interfaces)+≡
    module subroutine eio_set_filename (eio)
        class(eio_t), intent(inout) :: eio
    end subroutine eio_set_filename

(EIO base: procedures)+≡
    module subroutine eio_set_filename (eio)
        class(eio_t), intent(inout) :: eio
        character(32) :: buffer
        if (eio%split) then
            write (buffer, "(I0,',')") eio%split_index
            eio%filename = eio%sample // "." // trim (buffer) // eio%extension
            eio%has_file = .true.
        else
            eio%filename = eio%sample // "." // eio%extension
            eio%has_file = .true.
        end if
    end subroutine eio_set_filename

```

Set the fallback model.

```

(EIO base: eio: TBP)+≡
    procedure :: set_fallback_model => eio_set_fallback_model

(EIO base: sub interfaces)+≡
    module subroutine eio_set_fallback_model (eio, model)
        class(eio_t), intent(inout) :: eio
        class(model_data_t), intent(in), target :: model
    end subroutine eio_set_fallback_model

(EIO base: procedures)+≡
    module subroutine eio_set_fallback_model (eio, model)
        class(eio_t), intent(inout) :: eio
        class(model_data_t), intent(in), target :: model
        eio%fallback_model => model
    end subroutine eio_set_fallback_model

```

Initialize for output. We provide process names. This should open an event file if appropriate and write header data. Some methods may require event sample data.

```

(EIO base: eio: TBP)+≡
    procedure (eio_init_out), deferred :: init_out

(EIO base: interfaces)+≡
    abstract interface
        subroutine eio_init_out (eio, sample, data, success, extension)
            import
            class(eio_t), intent(inout) :: eio
            type(string_t), intent(in) :: sample
            type(event_sample_data_t), intent(in), optional :: data
            logical, intent(out), optional :: success
            type(string_t), intent(in), optional :: extension

```

```

        end subroutine eio_init_out
    end interface

```

Initialize for input. We provide process names. This should open an event file if appropriate and read header data. The `md5sum` can be used to check the integrity of the configuration, it provides a checksum to compare with. In case the extension has changed the extension is also given as an argument.

The `data` argument is `intent(inout)`: we may read part of it and keep other parts and/or check them against the data in the file.

```

<EIO base: eio: TBP>+≡
    procedure (eio_init_in), deferred :: init_in

<EIO base: interfaces>+≡
    abstract interface
        subroutine eio_init_in (eio, sample, data, success, extension)
            import
            class(eio_t), intent(inout) :: eio
            type(string_t), intent(in) :: sample
            type(event_sample_data_t), intent(inout), optional :: data
            logical, intent(out), optional :: success
            type(string_t), intent(in), optional :: extension
        end subroutine eio_init_in
    end interface

```

Re-initialize for output. This should change the status of any event file from input to output and position it for appending new events.

```

<EIO base: eio: TBP>+≡
    procedure (eio_switch_inout), deferred :: switch_inout

<EIO base: interfaces>+≡
    abstract interface
        subroutine eio_switch_inout (eio, success)
            import
            class(eio_t), intent(inout) :: eio
            logical, intent(out), optional :: success
        end subroutine eio_switch_inout
    end interface

```

This is similar: split the output, i.e., close the current file and open a new one. The default implementation does nothing. For the feature to work, an implementation must override this.

```

<EIO base: eio: TBP>+≡
    procedure :: split_out => eio_split_out

<EIO base: sub interfaces>+≡
    module subroutine eio_split_out (eio)
        class(eio_t), intent(inout) :: eio
    end subroutine eio_split_out

<EIO base: procedures>+≡
    module subroutine eio_split_out (eio)
        class(eio_t), intent(inout) :: eio
    end subroutine eio_split_out

```

Determine the file size in kilobytes. More exactly, determine the size in units of 1024 storage units, as returned by the INQUIRE statement.

The implementation returns zero if there is no file. The `has_file` flag is set by the `set_filename` method, so we can be confident that the `inquire` call is meaningful. If this algorithm doesn't apply for a particular format, we still can override the procedure.

```

(EIO base: eio: TBP)+≡
    procedure :: file_size_kbytes => eio_file_size_kbytes

(EIO base: sub interfaces)+≡
    module function eio_file_size_kbytes (eio) result (kbytes)
        class(eio_t), intent(in) :: eio
        integer :: kbytes
    end function eio_file_size_kbytes

(EIO base: procedures)+≡
    module function eio_file_size_kbytes (eio) result (kbytes)
        class(eio_t), intent(in) :: eio
        integer :: kbytes
        integer(i64) :: bytes
        if (eio%has_file) then
            inquire (file = char (eio%filename), size = bytes)
            if (bytes > 0) then
                kbytes = bytes / 1024
            else
                kbytes = 0
            end if
        else
            kbytes = 0
        end if
    end function eio_file_size_kbytes

```

Output an event. All data can be taken from the `event` record. The index `i_prc` identifies the process among the processes that are contained in the current sample. The `reading` flag, if present, indicates that the event was read from file, not generated.

The `passed` flag tells us that this event has passed the selection criteria. Depending on the event format, we may choose to skip events that have not passed.

```

(EIO base: eio: TBP)+≡
    procedure (eio_output), deferred :: output

(EIO base: interfaces)+≡
    abstract interface
        subroutine eio_output &
            (eio, event, i_prc, reading, passed, pacify, event_handle)
        import
        class(eio_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_output
    end interface

```


Input an event. This should fill all event data that cannot be inferred from the associated process.

The input is broken down into two parts. First we read the `i_prc` index. So we know which process to expect in the subsequent event. If we have reached end of file, we also will know. Then, we read the event itself.

The parameter `iostat` is supposed to be set as the Fortran standard requires, negative for EOF and positive for error.

```

<EIO base: eio: TBP>+≡
  procedure (eio_input_i_prc), deferred :: input_i_prc
  procedure (eio_input_event), deferred :: input_event

<EIO base: interfaces>+≡
  abstract interface
    subroutine eio_input_i_prc (eio, i_prc, iostat)
      import
      class(eio_t), intent(inout) :: eio
      integer, intent(out) :: i_prc
      integer, intent(out) :: iostat
    end subroutine eio_input_i_prc
  end interface

  abstract interface
    subroutine eio_input_event (eio, event, iostat, event_handle)
      import
      class(eio_t), intent(inout) :: eio
      class(generic_event_t), intent(inout), target :: event
      integer, intent(out) :: iostat
      class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_input_event
  end interface

<EIO base: eio: TBP>+≡
  procedure (eio_skip), deferred :: skip

<EIO base: interfaces>+≡
  abstract interface
    subroutine eio_skip (eio, iostat)
      import
      class(eio_t), intent(inout) :: eio
      integer, intent(out) :: iostat
    end subroutine eio_skip
  end interface

```

18.4.2 Unit tests

Test module, followed by the corresponding implementation module.

```

(eio_base_ut.f90)≡
  <File header>

  module eio_base_ut

```

```

    use unit_tests
    use eio_base_ut

    <Standard module head>

    <EIO base: public test>

    <EIO base: public test auxiliary>

contains

    <EIO base: test driver>

end module eio_base_ut

<eio_base_ut.f90>≡
    <File header>

    module eio_base_ut

        <Use kinds>
        <Use strings>
        use io_units
        use lorentz
        use model_data
        use particles
        use event_base
        use event_handles, only: event_handle_t
        use eio_data

        use eio_base

        <Standard module head>

        <EIO base: public test auxiliary>

        <EIO base: test declarations>

        <EIO base: test types>

        <EIO base: test variables>

contains

        <EIO base: tests>

        <EIO base: test auxiliary>

    end module eio_base_ut
API: driver for the unit tests below.
<EIO base: public test>≡
    public :: eio_base_test
<EIO base: test driver>≡
    subroutine eio_base_test (u, results)

```

```

integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
<EIO base: execute tests>
end subroutine eio_base_test

```

The caller has to provide procedures that prepare and cleanup the test environment. They depend on modules that are not available here.

```

<EIO base: test types>≡
abstract interface
  subroutine eio_prepare_event (event, unweighted, n_alt, sample_norm)
    import
    class(generic_event_t), intent(inout), pointer :: event
    logical, intent(in), optional :: unweighted
    integer, intent(in), optional :: n_alt
    type(string_t), intent(in), optional :: sample_norm
  end subroutine eio_prepare_event
end interface

abstract interface
  subroutine eio_cleanup_event (event)
    import
    class(generic_event_t), intent(inout), pointer :: event
  end subroutine eio_cleanup_event
end interface

```

We store pointers to the test-environment handlers as module variables. This allows us to call them from the test routines themselves, which don't allow for extra arguments.

```

<EIO base: public test auxiliary>≡
public :: eio_prepare_test, eio_cleanup_test

<EIO base: test types>+≡
procedure(eio_prepare_event), pointer :: eio_prepare_test => null ()
procedure(eio_cleanup_event), pointer :: eio_cleanup_test => null ()

```

Similarly, for the fallback (hadron) model that some eio tests require:

```

<EIO base: test types>+≡
abstract interface
  subroutine eio_prepare_model (model)
    import
    class(model_data_t), intent(inout), pointer :: model
  end subroutine eio_prepare_model
end interface

abstract interface
  subroutine eio_cleanup_model (model)
    import
    class(model_data_t), intent(inout), target :: model
  end subroutine eio_cleanup_model
end interface

```

```

<EIO base: public test auxiliary>+≡
    public :: eio_prepare_fallback_model, eio_cleanup_fallback_model

<EIO base: test variables>≡
    procedure(eio_prepare_model), pointer :: eio_prepare_fallback_model => null ()
    procedure(eio_cleanup_model), pointer :: eio_cleanup_fallback_model => null ()

```

Test type for event I/O

The contents simulate the contents of an external file. We have the `sample` string as the file name and the array of momenta `event_p` as the list of events. The second index is the event index. The `event_i` component is the pointer to the current event, `event_n` is the total number of stored events.

```

<EIO base: test types>+≡
    type, extends (eio_t) :: eio_test_t
        integer :: event_n = 0
        integer :: event_i = 0
        integer :: i_prc = 0
        type(vector4_t), dimension(:,,:), allocatable :: event_p
    contains
        <EIO base: eio test: TBP>
    end type eio_test_t

```

Write to screen. Pretend that this is an actual event format.

```

<EIO base: eio test: TBP>≡
    procedure :: write => eio_test_write

<EIO base: test auxiliary>≡
    subroutine eio_test_write (object, unit)
        class(eio_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Test event stream"
        if (object%event_i /= 0) then
            write (u, "(1x,A,I0,A)") "Event #", object%event_i, ":"
            do i = 1, size (object%event_p, 1)
                call vector4_write (object%event_p(i, object%event_i), u)
            end do
        end if
    end subroutine eio_test_write

```

Finalizer. For the test case, we just reset the event count, but keep the stored “events”. For the real implementations, the events would be stored on an external medium, so we would delete the object contents.

```

<EIO base: eio test: TBP>+≡
    procedure :: final => eio_test_final

<EIO base: test auxiliary>+≡
    subroutine eio_test_final (object)
        class(eio_test_t), intent(inout) :: object
        object%event_i = 0
    end subroutine eio_test_final

```

```
end subroutine eio_test_final
```

Initialization: We store the process IDs and the energy from the beam-data object. We also allocate the momenta (i.e., the simulated event record) for a fixed maximum size of 10 events, 2 momenta each. There is only a single process.

```
<EIO base: eio test: TBP>+≡
  procedure :: init_out => eio_test_init_out

<EIO base: test auxiliary>+≡
  subroutine eio_test_init_out (eio, sample, data, success, extension)
    class(eio_test_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    eio%sample = sample
    eio%event_n = 0
    eio%event_i = 0
    allocate (eio%event_p (2, 10))
    if (present (success)) success = .true.
  end subroutine eio_test_init_out
```

Initialization for input. Nothing to do for the test type.

```
<EIO base: eio test: TBP>+≡
  procedure :: init_in => eio_test_init_in

<EIO base: test auxiliary>+≡
  subroutine eio_test_init_in (eio, sample, data, success, extension)
    class(eio_test_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(inout), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    if (present (success)) success = .true.
  end subroutine eio_test_init_in
```

Switch from output to input. Again, nothing to do for the test type.

```
<EIO base: eio test: TBP>+≡
  procedure :: switch_inout => eio_test_switch_inout

<EIO base: test auxiliary>+≡
  subroutine eio_test_switch_inout (eio, success)
    class(eio_test_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    if (present (success)) success = .true.
  end subroutine eio_test_switch_inout
```

Output. Increment the event counter and store the momenta of the current event.

```
<EIO base: eio test: TBP>+≡
  procedure :: output => eio_test_output
```

```

(EIO base: test auxiliary)+≡
  subroutine eio_test_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_test_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    integer, intent(in) :: i_prc
    type(particle_set_t), pointer :: pset
    type(particle_t) :: prt
    eio%event_n = eio%event_n + 1
    eio%event_i = eio%event_n
    eio%i_prc = i_prc
    pset => event%get_particle_set_ptr ()
    prt = pset%get_particle (3)
    eio%event_p(1, eio%event_i) = prt%get_momentum ()
    prt = pset%get_particle (4)
    eio%event_p(2, eio%event_i) = prt%get_momentum ()
  end subroutine eio_test_output

```

Input. Increment the event counter and retrieve the momenta of the current event. For the test case, we do not actually modify the current event.

```

(EIO base: eio test: TBP)+≡
  procedure :: input_i_prc => eio_test_input_i_prc
  procedure :: input_event => eio_test_input_event

(EIO base: test auxiliary)+≡
  subroutine eio_test_input_i_prc (eio, i_prc, iostat)
    class(eio_test_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    i_prc = eio%i_prc
    iostat = 0
  end subroutine eio_test_input_i_prc

  subroutine eio_test_input_event (eio, event, iostat, event_handle)
    class(eio_test_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    eio%event_i = eio%event_i + 1
    iostat = 0
  end subroutine eio_test_input_event

(EIO base: eio test: TBP)+≡
  procedure :: skip => eio_test_skip

(EIO base: test auxiliary)+≡
  subroutine eio_test_skip (eio, iostat)
    class(eio_test_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_test_skip

```

Test I/O methods

```
<EIO base: execute tests>≡
  call test (eio_base_1, "eio_base_1", &
    "read and write event contents", &
    u, results)

<EIO base: test declarations>≡
  public :: eio_base_1

<EIO base: tests>≡
  subroutine eio_base_1 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    class(eio_t), allocatable :: eio
    integer :: i_prc, iostat
    type(string_t) :: sample

    write (u, "(A)")  "* Test output: eio_base_1"
    write (u, "(A)")  "* Purpose: generate and read/write an event"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_test1"

    allocate (eio_test_t :: eio)

    call eio%init_out (sample)
    call event%generate (1, [0._default, 0._default])
    call eio%output (event, 42)
    call eio%write (u)
    call eio%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Re-read the event"
    write (u, "(A)")

    call eio%init_in (sample)
    call eio%input_i_prc (i_prc, iostat)
    call eio%input_event (event, iostat)
    call eio%write (u)
    write (u, "(A)")
    write (u, "(1x,A,I0)")  "i = ", i_prc

    write (u, "(A)")
    write (u, "(A)")  "* Generate and append another event"
    write (u, "(A)")

    call eio%switch_inout ()
```

```

call event%generate (1, [0._default, 0._default])
call eio%output (event, 5)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Re-read both events"
write (u, "(A)")

call eio%init_in (sample)
call eio%input_i_prc (i_prc, iostat)
call eio%input_event (event, iostat)
call eio%input_i_prc (i_prc, iostat)
call eio%input_event (event, iostat)
call eio%write (u)
write (u, "(A)")
write (u, "(1x,A,I0)")  "i = ", i_prc

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_base_1"

end subroutine eio_base_1

```

18.5 Direct Event Access

As a convenient application of the base type, we construct an event handler that allows us of setting and retrieving events just in the same way as an file I/O format, but directly dealing with particle data and momenta. This is an input and output format, but we do not care about counting events.

`<eio_direct.f90>`≡

<File header>

module eio_direct

<Use kinds>

<Use strings>

```

use lorentz, only: vector4_t
use particles, only: particle_set_t
use model_data, only: model_data_t
use event_base
use event_handles, only: event_handle_t
use eio_data
use eio_base

```



```

    <Standard module head>

    <EIO direct: public>

    <EIO direct: types>

    interface
    <EIO direct: sub interfaces>
    end interface

    end module eio_direct

(eio_direct_sub.f90)≡
    <File header>

    submodule (eio_direct) eio_direct_s

        use io_units
        use diagnostics
        use cputime

        implicit none

    contains

    <EIO direct: procedures>

    end submodule eio_direct_s

```

18.5.1 Type

```

    <EIO direct: public>≡
        public :: eio_direct_t

    <EIO direct: types>≡
        type, extends (eio_t) :: eio_direct_t
            private
            logical :: i_evt_set = .false.
            integer :: i_evt = 0
            integer :: i_prc = 0
            integer :: i_mci = 0
            integer :: i_term = 0
            integer :: channel = 0
            logical :: passed_set = .false.
            logical :: passed = .true.
            type(particle_set_t) :: pset
        contains
        <EIO direct: eio direct: TBP>
        end type eio_direct_t

```

18.5.2 Common Methods

Output.

```
<EIO direct: eio direct: TBP>≡
  procedure :: write => eio_direct_write

<EIO direct: sub interfaces>≡
  module subroutine eio_direct_write (object, unit)
    class(eio_direct_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine eio_direct_write

<EIO direct: procedures>≡
  module subroutine eio_direct_write (object, unit)
    class(eio_direct_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event direct access:"
    if (object%i_evt_set) then
      write (u, "(3x,A,1x,I0)") "i_evt =", object%i_evt
    else
      write (u, "(3x,A)") "i_evt = [undefined]"
    end if
    write (u, "(3x,A,1x,I0)") "i_prc =", object%i_prc
    write (u, "(3x,A,1x,I0)") "i_mci =", object%i_prc
    write (u, "(3x,A,1x,I0)") "i_term =", object%i_prc
    write (u, "(3x,A,1x,I0)") "channel =", object%i_prc
    if (object%passed_set) then
      write (u, "(3x,A,1x,L1)") "passed =", object%passed
    else
      write (u, "(3x,A)") "passed = [N/A]"
    end if
    call object%pset%write (u)
  end subroutine eio_direct_write
```

Finalizer: trivial.

```
<EIO direct: eio direct: TBP>+≡
  procedure :: final => eio_direct_final

<EIO direct: sub interfaces>+≡
  module subroutine eio_direct_final (object)
    class(eio_direct_t), intent(inout) :: object
  end subroutine eio_direct_final

<EIO direct: procedures>+≡
  module subroutine eio_direct_final (object)
    class(eio_direct_t), intent(inout) :: object
    call object%pset%final ()
  end subroutine eio_direct_final
```

Initialize for input and/or output, both are identical

```
<EIO direct: eio direct: TBP>+≡
  procedure :: init_out => eio_direct_init_out
```

```

<EIO direct: sub interfaces>+≡
    module subroutine eio_direct_init_out &
        (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_direct_init_out

<EIO direct: procedures>+≡
    module subroutine eio_direct_init_out &
        (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        if (present (success)) success = .true.
    end subroutine eio_direct_init_out

<EIO direct: eio direct: TBP>+≡
    procedure :: init_in => eio_direct_init_in

<EIO direct: sub interfaces>+≡
    module subroutine eio_direct_init_in &
        (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_direct_init_in

<EIO direct: procedures>+≡
    module subroutine eio_direct_init_in &
        (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        if (present (success)) success = .true.
    end subroutine eio_direct_init_in

```

Switch from input to output: no-op

```

<EIO direct: eio direct: TBP>+≡
    procedure :: switch_inout => eio_direct_switch_inout

<EIO direct: sub interfaces>+≡
    module subroutine eio_direct_switch_inout (eio, success)
        class(eio_direct_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_direct_switch_inout

```

```

<EIO direct: procedures>+≡
  module subroutine eio_direct_switch_inout (eio, success)
    class(eio_direct_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    if (present (success)) success = .true.
  end subroutine eio_direct_switch_inout

```

Output: transfer event contents from the `event` object to the `eio` object. Note that finalization of the particle set is not (yet) automatic.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: output => eio_direct_output

<EIO direct: sub interfaces>+≡
  module subroutine eio_direct_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_direct_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine eio_direct_output

```

```

<EIO direct: procedures>+≡
  module subroutine eio_direct_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_direct_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    type(particle_set_t), pointer :: pset_ptr
    call eio%pset%final ()
    if (event%has_index ()) then
      call eio%set_event_index (event%get_index ())
    else
      call eio%reset_event_index ()
    end if
    if (present (passed)) then
      eio%passed = passed
      eio%passed_set = .true.
    else
      eio%passed_set = .false.
    end if
    pset_ptr => event%get_particle_set_ptr ()
    if (associated (pset_ptr)) then
      eio%i_prc = i_prc
      eio%pset = pset_ptr
    end if
  end subroutine eio_direct_output

```

Input: transfer event contents from the `eio` object to the `event` object. The `i_prc` parameter has been stored inside the `eio` record before.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: input_i_prc => eio_direct_input_i_prc

```

```

        procedure :: input_event => eio_direct_input_event
    <EIO direct: sub interfaces>+≡
        module subroutine eio_direct_input_i_prc (eio, i_prc, iostat)
            class(eio_direct_t), intent(inout) :: eio
            integer, intent(out) :: i_prc
            integer, intent(out) :: iostat
        end subroutine eio_direct_input_i_prc
        module subroutine eio_direct_input_event (eio, event, iostat, event_handle)
            class(eio_direct_t), intent(inout) :: eio
            class(generic_event_t), intent(inout), target :: event
            integer, intent(out) :: iostat
            class(event_handle_t), intent(inout), optional :: event_handle
        end subroutine eio_direct_input_event
    <EIO direct: procedures>+≡
        module subroutine eio_direct_input_i_prc (eio, i_prc, iostat)
            class(eio_direct_t), intent(inout) :: eio
            integer, intent(out) :: i_prc
            integer, intent(out) :: iostat
            i_prc = eio%i_prc
            iostat = 0
        end subroutine eio_direct_input_i_prc

        module subroutine eio_direct_input_event (eio, event, iostat, event_handle)
            class(eio_direct_t), intent(inout) :: eio
            class(generic_event_t), intent(inout), target :: event
            integer, intent(out) :: iostat
            class(event_handle_t), intent(inout), optional :: event_handle
            call event%select (eio%i_mci, eio%i_term, eio%channel)
            if (eio%has_event_index ()) then
                call event%set_index (eio%get_event_index ())
            else
                call event%reset_index ()
            end if
            call event%set_hard_particle_set (eio%pset)
        end subroutine eio_direct_input_event

```

No-op.

```

    <EIO direct: eio direct: TBP>+≡
        procedure :: skip => eio_direct_skip
    <EIO direct: sub interfaces>+≡
        module subroutine eio_direct_skip (eio, iostat)
            class(eio_direct_t), intent(inout) :: eio
            integer, intent(out) :: iostat
        end subroutine eio_direct_skip
    <EIO direct: procedures>+≡
        module subroutine eio_direct_skip (eio, iostat)
            class(eio_direct_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            iostat = 0
        end subroutine eio_direct_skip

```

18.5.3 Retrieve individual contents

(EIO direct: eio direct: TBP)+≡

```

procedure :: has_event_index => eio_direct_has_event_index
procedure :: get_event_index => eio_direct_get_event_index
procedure :: passed_known => eio_direct_passed_known
procedure :: has_passed => eio_direct_has_passed
procedure :: get_n_in => eio_direct_get_n_in
procedure :: get_n_out => eio_direct_get_n_out
procedure :: get_n_tot => eio_direct_get_n_tot

```

(EIO direct: sub interfaces)+≡

```

module function eio_direct_has_event_index (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
end function eio_direct_has_event_index
module function eio_direct_get_event_index (eio) result (index)
  class(eio_direct_t), intent(in) :: eio
  integer :: index
end function eio_direct_get_event_index
module function eio_direct_passed_known (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
end function eio_direct_passed_known
module function eio_direct_has_passed (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
end function eio_direct_has_passed
module function eio_direct_get_n_in (eio) result (n_in)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_in
end function eio_direct_get_n_in
module function eio_direct_get_n_out (eio) result (n_out)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_out
end function eio_direct_get_n_out
module function eio_direct_get_n_tot (eio) result (n_tot)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_tot
end function eio_direct_get_n_tot

```

(EIO direct: procedures)+≡

```

module function eio_direct_has_event_index (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
  flag = eio%i_evt_set
end function eio_direct_has_event_index

module function eio_direct_get_event_index (eio) result (index)
  class(eio_direct_t), intent(in) :: eio
  integer :: index
  if (eio%has_event_index ()) then
    index = eio%i_evt
  else
    index = 0
  end if
end function eio_direct_get_event_index

```

```

end function eio_direct_get_event_index

module function eio_direct_passed_known (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
  flag = eio%passed_set
end function eio_direct_passed_known

module function eio_direct_has_passed (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
  if (eio%passed_known ()) then
    flag = eio%passed
  else
    flag = .true.
  end if
end function eio_direct_has_passed

module function eio_direct_get_n_in (eio) result (n_in)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_in
  n_in = eio%pset%get_n_in ()
end function eio_direct_get_n_in

module function eio_direct_get_n_out (eio) result (n_out)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_out
  n_out = eio%pset%get_n_out ()
end function eio_direct_get_n_out

module function eio_direct_get_n_tot (eio) result (n_tot)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_tot
  n_tot = eio%pset%get_n_tot ()
end function eio_direct_get_n_tot

```

All momenta as a single allocatable array.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: get_momentum_array => eio_direct_get_momentum_array

<EIO direct: sub interfaces>+≡
  module subroutine eio_direct_get_momentum_array (eio, p)
    class(eio_direct_t), intent(in) :: eio
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
  end subroutine eio_direct_get_momentum_array

<EIO direct: procedures>+≡
  module subroutine eio_direct_get_momentum_array (eio, p)
    class(eio_direct_t), intent(in) :: eio
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
    integer :: n
    n = eio%get_n_tot ()
    allocate (p (n))
    p(:) = eio%pset%get_momenta ()
  end subroutine eio_direct_get_momentum_array

```

18.5.4 Manual access

Build the contained particle set from scratch.

```
(EIO direct: eio direct: TBP)+≡
  procedure :: init_direct => eio_direct_init_direct

(EIO direct: sub interfaces)+≡
  module subroutine eio_direct_init_direct &
    (eio, n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
    class(eio_direct_t), intent(out) :: eio
    integer, intent(in) :: n_beam
    integer, intent(in) :: n_in
    integer, intent(in) :: n_rem
    integer, intent(in) :: n_vir
    integer, intent(in) :: n_out
    integer, dimension(:), intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
  end subroutine eio_direct_init_direct

(EIO direct: procedures)+≡
  module subroutine eio_direct_init_direct &
    (eio, n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
    class(eio_direct_t), intent(out) :: eio
    integer, intent(in) :: n_beam
    integer, intent(in) :: n_in
    integer, intent(in) :: n_rem
    integer, intent(in) :: n_vir
    integer, intent(in) :: n_out
    integer, dimension(:), intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
    call eio%pset%init_direct (n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
  end subroutine eio_direct_init_direct
```

Set/reset the event index, which is optional.

```
(EIO direct: eio direct: TBP)+≡
  procedure :: set_event_index => eio_direct_set_event_index
  procedure :: reset_event_index => eio_direct_reset_event_index

(EIO direct: sub interfaces)+≡
  module subroutine eio_direct_set_event_index (eio, index)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(in) :: index
  end subroutine eio_direct_set_event_index
  module subroutine eio_direct_reset_event_index (eio)
    class(eio_direct_t), intent(inout) :: eio
  end subroutine eio_direct_reset_event_index

(EIO direct: procedures)+≡
  module subroutine eio_direct_set_event_index (eio, index)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(in) :: index
    eio%i_evt = index
    eio%i_evt_set = .true.
```



```

end subroutine eio_direct_set_event_index

module subroutine eio_direct_reset_event_index (eio)
  class(eio_direct_t), intent(inout) :: eio
  eio%i_evt_set = .false.
end subroutine eio_direct_reset_event_index

```

Set the selection indices. This is supposed to select the `i_prc`, `i_mci`, `i_term`, and `channel` entries of the event where the momentum set has to be stored, respectively. The selection indices determine the process, MCI set, calculation term, and phase-space channel is to be used for recalculation. The index values must not be zero, even if the do not apply.

```

(EIO direct: eio direct: TBP)+≡
  procedure :: set_selection_indices => eio_direct_set_selection_indices

(EIO direct: sub interfaces)+≡
  module subroutine eio_direct_set_selection_indices &
    (eio, i_prc, i_mci, i_term, channel)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(in) :: i_prc
    integer, intent(in) :: i_mci
    integer, intent(in) :: i_term
    integer, intent(in) :: channel
  end subroutine eio_direct_set_selection_indices

(EIO direct: procedures)+≡
  module subroutine eio_direct_set_selection_indices &
    (eio, i_prc, i_mci, i_term, channel)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(in) :: i_prc
    integer, intent(in) :: i_mci
    integer, intent(in) :: i_term
    integer, intent(in) :: channel
    eio%i_prc = i_prc
    eio%i_mci = i_mci
    eio%i_term = i_term
    eio%channel = channel
  end subroutine eio_direct_set_selection_indices

```

Set momentum (or momenta – elemental).

```

(EIO direct: eio direct: TBP)+≡
  generic :: set_momentum => set_momentum_single
  generic :: set_momentum => set_momentum_all
  procedure :: set_momentum_single => eio_direct_set_momentum_single
  procedure :: set_momentum_all => eio_direct_set_momentum_all

(EIO direct: sub interfaces)+≡
  module subroutine eio_direct_set_momentum_single (eio, i, p, p2, on_shell)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    real(default), intent(in), optional :: p2
    logical, intent(in), optional :: on_shell
  end subroutine eio_direct_set_momentum_single

```

```

module subroutine eio_direct_set_momentum_all (eio, p, p2, on_shell)
  class(eio_direct_t), intent(inout) :: eio
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), dimension(:), intent(in), optional :: p2
  logical, intent(in), optional :: on_shell
end subroutine eio_direct_set_momentum_all

<EIO direct: procedures>+≡
module subroutine eio_direct_set_momentum_single (eio, i, p, p2, on_shell)
  class(eio_direct_t), intent(inout) :: eio
  integer, intent(in) :: i
  type(vector4_t), intent(in) :: p
  real(default), intent(in), optional :: p2
  logical, intent(in), optional :: on_shell
  call eio%pset%set_momentum (i, p, p2, on_shell)
end subroutine eio_direct_set_momentum_single

module subroutine eio_direct_set_momentum_all (eio, p, p2, on_shell)
  class(eio_direct_t), intent(inout) :: eio
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), dimension(:), intent(in), optional :: p2
  logical, intent(in), optional :: on_shell
  call eio%pset%set_momentum (p, p2, on_shell)
end subroutine eio_direct_set_momentum_all

```

18.5.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_direct_ut.f90>≡
  <File header>

  module eio_direct_ut
    use unit_tests
    use eio_direct_util

    <Standard module head>

    <EIO direct: public test>

    contains

    <EIO direct: test driver>

  end module eio_direct_ut

<eio_direct_util.f90>≡
  <File header>

  module eio_direct_util

    <Use kinds>
    <Use strings>
    use lorentz, only: vector4_t

```

```

    use model_data, only: model_data_t
    use event_base
    use eio_data
    use eio_base

    use eio_direct

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO direct: test declarations>

    contains

    <EIO direct: tests>

    end module eio_direct_util
API: driver for the unit tests below.
    <EIO direct: public test>≡
        public :: eio_direct_test
    <EIO direct: test driver>≡
        subroutine eio_direct_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO direct: execute tests>
        end subroutine eio_direct_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

    <EIO direct: execute tests>≡
        call test (eio_direct_1, "eio_direct_1", &
            "read and write event contents", &
            u, results)
    <EIO direct: test declarations>≡
        public :: eio_direct_1
    <EIO direct: tests>≡
        subroutine eio_direct_1 (u)
            integer, intent(in) :: u
            class(generic_event_t), pointer :: event
            class(eio_t), allocatable :: eio
            type(event_sample_data_t) :: data
            type(string_t) :: sample
            type(vector4_t), dimension(:), allocatable :: p
            class(model_data_t), pointer :: model
            integer :: i, n_events, iostat, i_prc

            write (u, "(A)")  "*" Test output: eio_direct_1"
            write (u, "(A)")  "*" Purpose: generate and read/write an event"
            write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")
write (u, "(A)")  "* Initial state"
write (u, "(A)")

allocate (eio_direct_t :: eio)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract an empty event"
write (u, "(A)")

call eio%output (event, 1)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Retrieve contents"
write (u, "(A)")

select type (eio)
class is (eio_direct_t)
  if (eio%has_event_index ()) write (u, "(A,1x,I0)") "index =", eio%get_event_index ()
  if (eio%passed_known ()) write (u, "(A,1x,L1)") "passed =", eio%has_passed ()
  write (u, "(A,1x,I0)") "n_in =", eio%get_n_in ()
  write (u, "(A,1x,I0)") "n_out =", eio%get_n_out ()
end select

write (u, "(A)")
write (u, "(A)")  "* Generate and extract an event"
write (u, "(A)")

call event%generate (1, [0._default, 0._default])
call event%set_index (42)
model => event%get_model_ptr ()

sample = ""
call eio%init_out (sample)
call eio%output (event, 1, passed = .true.)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Retrieve contents"
write (u, "(A)")

select type (eio)
class is (eio_direct_t)
  if (eio%has_event_index ()) write (u, "(A,1x,I0)") "index =", eio%get_event_index ()
  if (eio%passed_known ()) write (u, "(A,1x,L1)") "passed =", eio%has_passed ()
  write (u, "(A,1x,I0)") "n_in =", eio%get_n_in ()
  write (u, "(A,1x,I0)") "n_out =", eio%get_n_out ()

```

```

end select

select type (eio)
class is (eio_direct_t)
  call eio%get_momentum_array (p)
  if (allocated (p)) then
    write (u, "(A)") "p[3] ="
    call p(3)%write (u)
  end if
end select

write (u, "(A)")
write (u, "(A)")  "* Re-create an eio event record: initialization"
write (u, "(A)")

call eio%final ()

select type (eio)
class is (eio_direct_t)
  call eio%init_direct ( &
    n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 2, &
    pdg = [25, 25, 25, 25], model = model)
  call eio%set_event_index (42)
  call eio%set_selection_indices (1, 1, 1, 1)
  call eio%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Re-create an eio event record: &
  &set momenta, interchanged"
write (u, "(A)")

select type (eio)
class is (eio_direct_t)
  call eio%set_momentum (p([1,2,4,3]), on_shell=.true.)
  call eio%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* 'read' i_prc"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(1x,A,1x,I0)") "i_prc =", i_prc
write (u, "(1x,A,1x,I0)") "iostat =", iostat

write (u, "(A)")
write (u, "(A)")  "* 'read' (fill) event"
write (u, "(A)")

call eio%input_event (event, iostat)
write (u, "(1x,A,1x,I0)") "iostat =", iostat
write (u, "(A)")

```

```

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_direct_1"

end subroutine eio_direct_1

```

18.6 Event Generation Checkpoints

This is an output-only format. Its only use is to write screen messages every n events, to inform the user about progress.

```

<eio_checkpoints.f90>≡
  <File header>

  module eio_checkpoints

    <Use strings>
    use cputime
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO checkpoints: public>

    <EIO checkpoints: types>

    interface
    <EIO checkpoints: sub interfaces>
    end interface

  end module eio_checkpoints

<eio_checkpoints_sub.f90>≡
  <File header>

  submodule (eio_checkpoints) eio_checkpoints_s

    use io_units
    use diagnostics

    implicit none

```

```

    <EIO checkpoints: parameters>

contains

    <EIO checkpoints: procedures>

end submodule eio_checkpoints_s

```

18.6.1 Type

```

<EIO checkpoints: public>≡
    public :: eio_checkpoints_t

<EIO checkpoints: types>≡
    type, extends (eio_t) :: eio_checkpoints_t
        logical :: active = .false.
        logical :: running = .false.
        integer :: val = 0
        integer :: n_events = 0
        integer :: n_read = 0
        integer :: i_evt = 0
        logical :: blank = .false.
        type(timer_t) :: timer
    contains
        <EIO checkpoints: eio checkpoints: TBP>
    end type eio_checkpoints_t

```

18.6.2 Specific Methods

Set parameters that are specifically used for checkpointing.

```

<EIO checkpoints: eio checkpoints: TBP>≡
    procedure :: set_parameters => eio_checkpoints_set_parameters

<EIO checkpoints: sub interfaces>≡
    module subroutine eio_checkpoints_set_parameters (eio, checkpoint, blank)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(in) :: checkpoint
        logical, intent(in), optional :: blank
    end subroutine eio_checkpoints_set_parameters

<EIO checkpoints: procedures>≡
    module subroutine eio_checkpoints_set_parameters (eio, checkpoint, blank)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(in) :: checkpoint
        logical, intent(in), optional :: blank
        eio%val = checkpoint
        if (present (blank)) eio%blank = blank
    end subroutine eio_checkpoints_set_parameters

```

18.6.3 Common Methods

Output. This is not the actual event format, but a readable account of the current status.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: write => eio_checkpoints_write

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_write (object, unit)
        class(eio_checkpoints_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_checkpoints_write

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_write (object, unit)
        class(eio_checkpoints_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%active) then
            write (u, "(1x,A)") "Event-sample checkpoints: active"
            write (u, "(3x,A,I0)") "interval = ", object%val
            write (u, "(3x,A,I0)") "n_events = ", object%n_events
            write (u, "(3x,A,I0)") "n_read = ", object%n_read
            write (u, "(3x,A,I0)") "n_current = ", object%i_evt
            write (u, "(3x,A,L1)") "blanking = ", object%blank
            call object%timer%write (u)
        else
            write (u, "(1x,A)") "Event-sample checkpoints: off"
        end if
    end subroutine eio_checkpoints_write
```

Finalizer: trivial.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: final => eio_checkpoints_final

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_final (object)
        class(eio_checkpoints_t), intent(inout) :: object
    end subroutine eio_checkpoints_final

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_final (object)
        class(eio_checkpoints_t), intent(inout) :: object
        object%active = .false.
    end subroutine eio_checkpoints_final
```

Activate checkpointing for event generation or writing.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: init_out => eio_checkpoints_init_out

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_init_out &
        (eio, sample, data, success, extension)
        class(eio_checkpoints_t), intent(inout) :: eio
```



```

        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_checkpoints_init_out

```

(EIO checkpoints: procedures)+≡

```

module subroutine eio_checkpoints_init_out &
    (eio, sample, data, success, extension)
class(eio_checkpoints_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(in), optional :: data
logical, intent(out), optional :: success
if (present (data)) then
    if (eio%val > 0) then
        eio%active = .true.
        eio%i_evt = 0
        eio%n_read = 0
        eio%n_events = data%n_evt * data%nlo_multiplier
    end if
end if
if (present (success)) success = .true.
end subroutine eio_checkpoints_init_out

```

No checkpointing for event reading.

(EIO checkpoints: eio checkpoints: TBP)+≡

```

procedure :: init_in => eio_checkpoints_init_in

```

(EIO checkpoints: sub interfaces)+≡

```

module subroutine eio_checkpoints_init_in &
    (eio, sample, data, success, extension)
class(eio_checkpoints_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
end subroutine eio_checkpoints_init_in

```

(EIO checkpoints: procedures)+≡

```

module subroutine eio_checkpoints_init_in &
    (eio, sample, data, success, extension)
class(eio_checkpoints_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
call msg_bug ("Event checkpoints: event input not supported")
if (present (success)) success = .false.
end subroutine eio_checkpoints_init_in

```

Switch from input to output: also not supported.

(EIO checkpoints: eio checkpoints: TBP)+≡

```

procedure :: switch_inout => eio_checkpoints_switch_inout

```

```

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_switch_inout (eio, success)
        class(eio_checkpoints_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_checkpoints_switch_inout

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_switch_inout (eio, success)
        class(eio_checkpoints_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("Event checkpoints: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_checkpoints_switch_inout

```

Checkpoints: display progress for the current event, if applicable.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: output => eio_checkpoints_output

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_checkpoints_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_checkpoints_output

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_checkpoints_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        logical :: rd
        rd = .false.; if (present (reading)) rd = reading
        if (eio%active) then
            if (.not. eio%running) call eio%startup ()
            if (eio%running) then
                eio%i_evt = eio%i_evt + 1
                if (rd) then
                    eio%n_read = eio%n_read + 1
                else if (mod (eio%i_evt, eio%val) == 0) then
                    call eio%message (eio%blank)
                end if
                if (eio%i_evt == eio%n_events) call eio%shutdown ()
            end if
        end if
    end subroutine eio_checkpoints_output

```

When the first event is called, we have to initialize the screen output.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: startup => eio_checkpoints_startup

```

```

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_startup (eio)
        class(eio_checkpoints_t), intent(inout) :: eio
    end subroutine eio_checkpoints_startup

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_startup (eio)
        class(eio_checkpoints_t), intent(inout) :: eio
        if (eio%active .and. eio%i_evt < eio%n_events) then
            call msg_message ("")
            call msg_message (checkpoint_bar)
            call msg_message (checkpoint_head)
            call msg_message (checkpoint_bar)
            write (msg_buffer, checkpoint_fmt) 0., 0, eio%n_events - eio%i_evt, "???"
            call msg_message ()
            eio%running = .true.
            call eio%timer%start ()
        end if
    end subroutine eio_checkpoints_startup

```

This message is printed at every checkpoint.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: message => eio_checkpoints_message

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_message (eio, testflag)
        class(eio_checkpoints_t), intent(inout) :: eio
        logical, intent(in), optional :: testflag
    end subroutine eio_checkpoints_message

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_message (eio, testflag)
        class(eio_checkpoints_t), intent(inout) :: eio
        logical, intent(in), optional :: testflag
        real :: t
        type(time_t) :: time_remaining
        type(string_t) :: time_string
        call eio%timer%stop ()
        t = eio%timer
        call eio%timer%restart ()
        time_remaining = &
            nint (t / (eio%i_evt - eio%n_read) * (eio%n_events - eio%i_evt))
        time_string = time_remaining%to_string_ms (blank = testflag)
        write (msg_buffer, checkpoint_fmt) &
            100 * ((eio%i_evt - eio%n_read) / real (eio%n_events - eio%n_read)), &
            eio%i_evt - eio%n_read, &
            eio%n_events - eio%i_evt, &
            char (time_string)
        call msg_message ()
    end subroutine eio_checkpoints_message

```

When the last event is called, wrap up.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: shutdown => eio_checkpoints_shutdown

```

```

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_shutdown (eio)
        class(eio_checkpoints_t), intent(inout) :: eio
    end subroutine eio_checkpoints_shutdown

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_shutdown (eio)
        class(eio_checkpoints_t), intent(inout) :: eio
        if (mod (eio%i_evt, eio%val) /= 0) then
            write (msg_buffer, checkpoint_fmt) &
                100., eio%i_evt - eio%n_read, 0, "0m:00s"
            call msg_message ()
        end if
        call msg_message (checkpoint_bar)
        call msg_message ("")
        eio%running = .false.
    end subroutine eio_checkpoints_shutdown

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: input_i_prc => eio_checkpoints_input_i_prc
    procedure :: input_event => eio_checkpoints_input_event

<EIO checkpoints: sub interfaces>+≡
    module subroutine eio_checkpoints_input_i_prc (eio, i_prc, iostat)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
    end subroutine eio_checkpoints_input_i_prc
    module subroutine eio_checkpoints_input_event &
        (eio, event, iostat, event_handle)
        class(eio_checkpoints_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_checkpoints_input_event

<EIO checkpoints: procedures>+≡
    module subroutine eio_checkpoints_input_i_prc (eio, i_prc, iostat)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        call msg_bug ("Event checkpoints: event input not supported")
        i_prc = 0
        iostat = 1
    end subroutine eio_checkpoints_input_i_prc

    module subroutine eio_checkpoints_input_event &
        (eio, event, iostat, event_handle)
        class(eio_checkpoints_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        call msg_bug ("Event checkpoints: event input not supported")
        iostat = 1
    end subroutine eio_checkpoints_input_event

```

```

⟨EIO checkpoints: eio checkpoints: TBP⟩+≡
    procedure :: skip => eio_checkpoints_skip

⟨EIO checkpoints: sub interfaces⟩+≡
    module subroutine eio_checkpoints_skip (eio, iostat)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(out) :: iostat
    end subroutine eio_checkpoints_skip

⟨EIO checkpoints: procedures⟩+≡
    module subroutine eio_checkpoints_skip (eio, iostat)
        class(eio_checkpoints_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        iostat = 0
    end subroutine eio_checkpoints_skip

```

18.6.4 Message header

```

⟨EIO checkpoints: parameters⟩≡
    character(*), parameter :: &
        checkpoint_head = "| % complete | events generated | events remaining &
        &| time remaining"
    character(*), parameter :: &
        checkpoint_bar = "|=====|&
        &=====|"
    character(*), parameter :: &
        checkpoint_fmt = "(' ',F5.1,T16,I9,T35,I9,T58,A)"

```

18.6.5 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨eio_checkpoints_ut.f90⟩≡
    ⟨File header⟩

    module eio_checkpoints_ut
        use unit_tests
        use eio_checkpoints_util

    ⟨Standard module head⟩

    ⟨EIO checkpoints: public test⟩

    contains

    ⟨EIO checkpoints: test driver⟩

    end module eio_checkpoints_ut

⟨eio_checkpoints_util.f90⟩≡
    ⟨File header⟩

    module eio_checkpoints_util

```

```

    <Use kinds>
    <Use strings>
    use event_base
    use eio_data
    use eio_base

    use eio_checkpoints

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO checkpoints: test declarations>

    contains

    <EIO checkpoints: tests>

    end module eio_checkpoints_utl
API: driver for the unit tests below.
    <EIO checkpoints: public test>≡
        public :: eio_checkpoints_test
    <EIO checkpoints: test driver>≡
        subroutine eio_checkpoints_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO checkpoints: execute tests>
        end subroutine eio_checkpoints_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

    <EIO checkpoints: execute tests>≡
        call test (eio_checkpoints_1, "eio_checkpoints_1", &
            "read and write event contents", &
            u, results)
    <EIO checkpoints: test declarations>≡
        public :: eio_checkpoints_1
    <EIO checkpoints: tests>≡
        subroutine eio_checkpoints_1 (u)
            integer, intent(in) :: u
            class(generic_event_t), pointer :: event
            class(eio_t), allocatable :: eio
            type(event_sample_data_t) :: data
            type(string_t) :: sample
            integer :: i, n_events

            write (u, "(A)")  "* Test output: eio_checkpoints_1"
            write (u, "(A)")  "* Purpose: generate a number of events &
                &with screen output"
            write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event)

write (u, "(A)")
write (u, "(A)")  "* Generate events"
write (u, "(A)")

sample = "eio_checkpoints_1"

allocate (eio_checkpoints_t :: eio)

n_events = 10
call data%init (1, 0)
data%n_evt = n_events

select type (eio)
type is (eio_checkpoints_t)
  call eio%set_parameters (checkpoint = 4)
end select

call eio%init_out (sample, data)

do i = 1, n_events
  call event%generate (1, [0._default, 0._default])
  call eio%output (event, i_prc = 0)
end do

write (u, "(A)")  "* Checkpointing status"
write (u, "(A)")

call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_checkpoints_1"

end subroutine eio_checkpoints_1

```

18.7 Event Generation Callback

This is an output-only format. Its only use is to write screen messages every n events, to inform the user about progress.

`<eio_callback.f90>`≡
<File header>

```

module eio_callback

    use kinds, only: i64
    <Use strings>
    use cputime
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO callback: public>

    <EIO callback: types>

    interface
    <EIO callback: sub interfaces>
    end interface

end module eio_callback
<eio_callback_sub.f90>≡
<File header>

submodule (eio_callback) eio_callback_s

    use io_units
    use diagnostics

    implicit none

contains

    <EIO callback: procedures>

end submodule eio_callback_s

```

18.7.1 Type

```

<EIO callback: public>≡
    public :: eio_callback_t

<EIO callback: types>≡
    type, extends (eio_t) :: eio_callback_t
        class(event_callback_t), allocatable :: callback
        integer(i64) :: i_evt = 0
        integer :: i_interval = 0
        integer :: n_interval = 0
    !     type(timer_t) :: timer
    contains
    <EIO callback: eio callback: TBP>
end type eio_callback_t

```


18.7.2 Specific Methods

Set parameters that are specifically used for callback: the procedure and the number of events to wait until the procedure is called (again).

```
<EIO callback: eio callback: TBP>≡
    procedure :: set_parameters => eio_callback_set_parameters

<EIO callback: sub interfaces>≡
    module subroutine eio_callback_set_parameters &
        (eio, callback, count_interval)
        class(eio_callback_t), intent(inout) :: eio
        class(event_callback_t), intent(in) :: callback
        integer, intent(in) :: count_interval
    end subroutine eio_callback_set_parameters

<EIO callback: procedures>≡
    module subroutine eio_callback_set_parameters &
        (eio, callback, count_interval)
        class(eio_callback_t), intent(inout) :: eio
        class(event_callback_t), intent(in) :: callback
        integer, intent(in) :: count_interval
        allocate (eio%callback, source = callback)
        eio%n_interval = count_interval
    end subroutine eio_callback_set_parameters
```

18.7.3 Common Methods

Output. This is not the actual event format, but a readable account of the current status.

```
<EIO callback: eio callback: TBP>+≡
    procedure :: write => eio_callback_write

<EIO callback: sub interfaces>+≡
    module subroutine eio_callback_write (object, unit)
        class(eio_callback_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_callback_write

<EIO callback: procedures>+≡
    module subroutine eio_callback_write (object, unit)
        class(eio_callback_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event-sample callback:"
        write (u, "(3x,A,I0)") "interval = ", object%n_interval
        write (u, "(3x,A,I0)") "evt count = ", object%i_evt
        ! call object%timer%write (u)
    end subroutine eio_callback_write
```

Finalizer: trivial.

```
<EIO callback: eio callback: TBP>+≡  
  procedure :: final => eio_callback_final  
  
<EIO callback: sub interfaces>+≡  
  module subroutine eio_callback_final (object)  
    class(eio_callback_t), intent(inout) :: object  
  end subroutine eio_callback_final  
  
<EIO callback: procedures>+≡  
  module subroutine eio_callback_final (object)  
    class(eio_callback_t), intent(inout) :: object  
  end subroutine eio_callback_final
```

Activate checkpointing for event generation or writing.

```
<EIO callback: eio callback: TBP>+≡  
  procedure :: init_out => eio_callback_init_out  
  
<EIO callback: sub interfaces>+≡  
  module subroutine eio_callback_init_out &  
    (eio, sample, data, success, extension)  
    class(eio_callback_t), intent(inout) :: eio  
    type(string_t), intent(in) :: sample  
    type(string_t), intent(in), optional :: extension  
    type(event_sample_data_t), intent(in), optional :: data  
    logical, intent(out), optional :: success  
  end subroutine eio_callback_init_out  
  
<EIO callback: procedures>+≡  
  module subroutine eio_callback_init_out &  
    (eio, sample, data, success, extension)  
    class(eio_callback_t), intent(inout) :: eio  
    type(string_t), intent(in) :: sample  
    type(string_t), intent(in), optional :: extension  
    type(event_sample_data_t), intent(in), optional :: data  
    logical, intent(out), optional :: success  
    eio%i_evt = 0  
    eio%i_interval = 0  
    if (present (success)) success = .true.  
  end subroutine eio_callback_init_out
```

No callback for event reading.

```
<EIO callback: eio callback: TBP>+≡  
  procedure :: init_in => eio_callback_init_in  
  
<EIO callback: sub interfaces>+≡  
  module subroutine eio_callback_init_in &  
    (eio, sample, data, success, extension)  
    class(eio_callback_t), intent(inout) :: eio  
    type(string_t), intent(in) :: sample  
    type(string_t), intent(in), optional :: extension  
    type(event_sample_data_t), intent(inout), optional :: data  
    logical, intent(out), optional :: success  
  end subroutine eio_callback_init_in
```

```

<EIO callback: procedures>+≡
  module subroutine eio_callback_init_in &
    (eio, sample, data, success, extension)
    class(eio_callback_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(inout), optional :: data
    logical, intent(out), optional :: success
    call msg_bug ("Event callback: event input not supported")
    if (present (success)) success = .false.
  end subroutine eio_callback_init_in

```

Switch from input to output: also not supported.

```

<EIO callback: eio callback: TBP>+≡
  procedure :: switch_inout => eio_callback_switch_inout

<EIO callback: sub interfaces>+≡
  module subroutine eio_callback_switch_inout (eio, success)
    class(eio_callback_t), intent(inout) :: eio
    logical, intent(out), optional :: success
  end subroutine eio_callback_switch_inout

<EIO callback: procedures>+≡
  module subroutine eio_callback_switch_inout (eio, success)
    class(eio_callback_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    call msg_bug ("Event callback: in-out switch not supported")
    if (present (success)) success = .false.
  end subroutine eio_callback_switch_inout

```

The actual callback. First increment counters, then call the procedure if the counter hits the interval.

```

<EIO callback: eio callback: TBP>+≡
  procedure :: output => eio_callback_output

<EIO callback: sub interfaces>+≡
  module subroutine eio_callback_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_callback_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine eio_callback_output

<EIO callback: procedures>+≡
  module subroutine eio_callback_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_callback_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    eio%i_evt = eio%i_evt + 1
    if (eio%n_interval > 0) then

```

```

        eio%i_interval = eio%i_interval + 1
        if (eio%i_interval >= eio%n_interval) then
            call eio%callback%proc (eio%i_evt, event)
            eio%i_interval = 0
        end if
    end if
end if
end subroutine eio_callback_output

```

No input.

<EIO callback: eio callback: TBP>+≡

```

    procedure :: input_i_prc => eio_callback_input_i_prc
    procedure :: input_event => eio_callback_input_event

```

<EIO callback: sub interfaces>+≡

```

    module subroutine eio_callback_input_i_prc (eio, i_prc, iostat)
        class(eio_callback_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
    end subroutine eio_callback_input_i_prc
    module subroutine eio_callback_input_event &
        (eio, event, iostat, event_handle)
        class(eio_callback_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_callback_input_event

```

<EIO callback: procedures>+≡

```

    module subroutine eio_callback_input_i_prc (eio, i_prc, iostat)
        class(eio_callback_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        call msg_bug ("Event callback: event input not supported")
        i_prc = 0
        iostat = 1
    end subroutine eio_callback_input_i_prc

    module subroutine eio_callback_input_event &
        (eio, event, iostat, event_handle)
        class(eio_callback_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        call msg_bug ("Event callback: event input not supported")
        iostat = 1
    end subroutine eio_callback_input_event

```

<EIO callback: eio callback: TBP>+≡

```

    procedure :: skip => eio_callback_skip

```

<EIO callback: sub interfaces>+≡

```

    module subroutine eio_callback_skip (eio, iostat)
        class(eio_callback_t), intent(inout) :: eio
        integer, intent(out) :: iostat
    end subroutine eio_callback_skip

```

```

<EIO callback: procedures>+≡
  module subroutine eio_callback_skip (eio, iostat)
    class(eio_callback_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_callback_skip

```

18.8 Event Weight Output

This is an output-only format. For each event, we print the indices that identify process, process part (MCI group), and term. As numerical information we print the squared matrix element (trace) and the event weight.

```

<eio_weights.f90>≡
  <File header>

  module eio_weights

    <Use kinds>
    <Use strings>
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO weights: public>

    <EIO weights: types>

    interface
    <EIO weights: sub interfaces>
    end interface

  end module eio_weights

<eio_weights_sub.f90>≡
  <File header>

  submodule (eio_weights) eio_weights_s

    use io_units
    use diagnostics

    implicit none

  contains

    <EIO weights: procedures>

  end submodule eio_weights_s

```

18.8.1 Type

```
<EIO weights: public>≡
    public :: eio_weights_t
<EIO weights: types>≡
    type, extends (eio_t) :: eio_weights_t
        logical :: writing = .false.
        integer :: unit = 0
        logical :: pacify = .false.
    contains
        <EIO weights: eio weights: TBP>
    end type eio_weights_t
```

18.8.2 Specific Methods

Set pacify flags.

```
<EIO weights: eio weights: TBP>≡
    procedure :: set_parameters => eio_weights_set_parameters
<EIO weights: sub interfaces>≡
    module subroutine eio_weights_set_parameters (eio, pacify)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(in), optional :: pacify
    end subroutine eio_weights_set_parameters
<EIO weights: procedures>≡
    module subroutine eio_weights_set_parameters (eio, pacify)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(in), optional :: pacify
        if (present (pacify)) eio%pacify = pacify
        eio%extension = "weights.dat"
    end subroutine eio_weights_set_parameters
```

18.8.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```
<EIO weights: eio weights: TBP>+≡
    procedure :: write => eio_weights_write
<EIO weights: sub interfaces>+≡
    module subroutine eio_weights_write (object, unit)
        class(eio_weights_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_weights_write
<EIO weights: procedures>+≡
    module subroutine eio_weights_write (object, unit)
        class(eio_weights_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
```

```

write (u, "(1x,A)") "Weight stream:"
if (object%writing) then
  write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
  write (u, "(3x,A,L1)") "Reduced I/O prec. = ", object%pacify
else
  write (u, "(3x,A)") "[closed]"
end if
end subroutine eio_weights_write

```

Finalizer: close any open file.

```

<EIO weights: eio weights: TBP>+≡
  procedure :: final => eio_weights_final

<EIO weights: sub interfaces>+≡
  module subroutine eio_weights_final (object)
    class(eio_weights_t), intent(inout) :: object
  end subroutine eio_weights_final

<EIO weights: procedures>+≡
  module subroutine eio_weights_final (object)
    class(eio_weights_t), intent(inout) :: object
    if (object%writing) then
      write (msg_buffer, "(A,A,A)") "Events: closing weight stream file '", &
        char (object%filename), "'"
      call msg_message ()
      close (object%unit)
      object%writing = .false.
    end if
  end subroutine eio_weights_final

```

Initialize event writing.

```

<EIO weights: eio weights: TBP>+≡
  procedure :: init_out => eio_weights_init_out

<EIO weights: sub interfaces>+≡
  module subroutine eio_weights_init_out &
    (eio, sample, data, success, extension)
    class(eio_weights_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
  end subroutine eio_weights_init_out

<EIO weights: procedures>+≡
  module subroutine eio_weights_init_out &
    (eio, sample, data, success, extension)
    class(eio_weights_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    if (present(extension)) then
      eio%extension = extension
    else

```

```

        eio%extension = "weights.dat"
    end if
    eio%filename = sample // "." // eio%extension
    eio%unit = free_unit ()
    write (msg_buffer, "(A,A,A)") "Events: writing to weight stream file '", &
        char (eio%filename), "'"
    call msg_message ()
    eio%writing = .true.
    open (eio%unit, file = char (eio%filename), &
        action = "write", status = "replace")
    if (present (success)) success = .true.
end subroutine eio_weights_init_out

```

Initialize event reading.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: init_in => eio_weights_init_in

<EIO weights: sub interfaces>+≡
    module subroutine eio_weights_init_in &
        (eio, sample, data, success, extension)
        class(eio_weights_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_weights_init_in

<EIO weights: procedures>+≡
    module subroutine eio_weights_init_in &
        (eio, sample, data, success, extension)
        class(eio_weights_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("Weight stream: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_weights_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: switch_inout => eio_weights_switch_inout

<EIO weights: sub interfaces>+≡
    module subroutine eio_weights_switch_inout (eio, success)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_weights_switch_inout

<EIO weights: procedures>+≡
    module subroutine eio_weights_switch_inout (eio, success)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("Weight stream: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_weights_switch_inout

```



```
end subroutine eio_weights_switch_inout
```

Output an event. Write first the event indices, then weight and two values of the squared matrix element: `sqme_ref` is the value stored in the event record, and `sqme_prc` is the one stored in the process instance. (They can differ: when recalculating, the former is read from file and the latter is the result of the new calculation.)

For the alternative entries, the `sqme` value is always obtained by a new calculation, and thus qualifies as `sqme_prc`.

Don't write the file if the `passed` flag is set and false.

(EIO weights: eio weights: TBP)+≡

```
procedure :: output => eio_weights_output
```

(EIO weights: sub interfaces)+≡

```
module subroutine eio_weights_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_weights_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
end subroutine eio_weights_output
```

(EIO weights: procedures)+≡

```
module subroutine eio_weights_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_weights_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  integer :: n_alt, i
  real(default) :: weight, sqme_ref, sqme_prc
  logical :: evt_pacify, evt_passed
  evt_pacify = eio%pacify; if (present (pacify)) evt_pacify = pacify
  evt_passed = .true.; if (present (passed)) evt_passed = passed
  if (eio%writing) then
    if (evt_passed) then
      weight = event%get_weight_prc ()
      sqme_ref = event%get_sqme_ref ()
      sqme_prc = event%get_sqme_prc ()
      n_alt = event%get_n_alt ()
1      format (IO,3(1x,ES17.10),3(1x,I0))
2      format (IO,3(1x,ES15.8),3(1x,I0))
      if (evt_pacify) then
        write (eio%unit, 2) 0, weight, sqme_prc, sqme_ref, &
          i_prc
      else
        write (eio%unit, 1) 0, weight, sqme_prc, sqme_ref, &
          i_prc
      end if
    do i = 1, n_alt
      weight = event%get_weight_alt(i)
      sqme_prc = event%get_sqme_alt(i)
    end do
  end if
```

```

        if (evt_pacify) then
            write (eio%unit, 2) i, weight, sqme_prc
        else
            write (eio%unit, 1) i, weight, sqme_prc
        end if
    end do
end if
else
    call eio%write ()
    call msg_fatal ("Weight stream file is not open for writing")
end if
end subroutine eio_weights_output

```

Input an event.

(EIO weights: eio weights: TBP)+≡

```

procedure :: input_i_prc => eio_weights_input_i_prc
procedure :: input_event => eio_weights_input_event

```

(EIO weights: sub interfaces)+≡

```

module subroutine eio_weights_input_i_prc (eio, i_prc, iostat)
    class(eio_weights_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
end subroutine eio_weights_input_i_prc
module subroutine eio_weights_input_event &
    (eio, event, iostat, event_handle)
    class(eio_weights_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
end subroutine eio_weights_input_event

```

(EIO weights: procedures)+≡

```

module subroutine eio_weights_input_i_prc (eio, i_prc, iostat)
    class(eio_weights_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    call msg_bug ("Weight stream: event input not supported")
    i_prc = 0
    iostat = 1
end subroutine eio_weights_input_i_prc

module subroutine eio_weights_input_event &
    (eio, event, iostat, event_handle)
    class(eio_weights_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    call msg_bug ("Weight stream: event input not supported")
    iostat = 1
end subroutine eio_weights_input_event

```

(EIO weights: eio weights: TBP)+≡

```

procedure :: skip => eio_weights_skip

```

```

<EIO weights: sub interfaces>+≡
    module subroutine eio_weights_skip (eio, iostat)
        class(eio_weights_t), intent(inout) :: eio
        integer, intent(out) :: iostat
    end subroutine eio_weights_skip

```

```

<EIO weights: procedures>+≡
    module subroutine eio_weights_skip (eio, iostat)
        class(eio_weights_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        iostat = 0
    end subroutine eio_weights_skip

```

18.8.4 Unit tests

Test module, followed by the corresponding implementation module.

```

(eio_weights_ut.f90)≡
    <File header>

```

```

    module eio_weights_ut
        use unit_tests
        use eio_weights_uti

```

```

    <Standard module head>

```

```

    <EIO weights: public test>

```

```

    contains

```

```

    <EIO weights: test driver>

```

```

    end module eio_weights_ut

```

```

(eio_weights_uti.f90)≡
    <File header>

```

```

    module eio_weights_uti

```

```

    <Use kinds>

```

```

    <Use strings>

```

```

        use io_units
        use event_base
        use eio_data
        use eio_base

```

```

        use eio_weights

```

```

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

```

```

    <Standard module head>

```

```

    <EIO weights: test declarations>

```

contains

<EIO weights: tests>

end module eio_weights_util

API: driver for the unit tests below.

<EIO weights: public test>≡

public :: eio_weights_test

<EIO weights: test driver>≡

subroutine eio_weights_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<EIO weights: execute tests>

end subroutine eio_weights_test

Simple event

We test the implementation of all I/O methods.

<EIO weights: execute tests>≡

call test (eio_weights_1, "eio_weights_1", &
"read and write event contents", &
u, results)

<EIO weights: test declarations>≡

public :: eio_weights_1

<EIO weights: tests>≡

subroutine eio_weights_1 (u)

integer, intent(in) :: u

class(generic_event_t), pointer :: event

class(eio_t), allocatable :: eio

type(string_t) :: sample

integer :: u_file

character(80) :: buffer

write (u, "(A)") "* Test output: eio_weights_1"

write (u, "(A)") "* Purpose: generate an event and write weight to file"

write (u, "(A)")

write (u, "(A)") "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")

write (u, "(A)") "* Generate and write an event"

write (u, "(A)")

sample = "eio_weights_1"

allocate (eio_weights_t :: eio)

call eio%init_out (sample)

call event%generate (1, [0._default, 0._default])

```

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents: &
    &(weight, sqme(evt), sqme(prc), i_prc)"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_weights_1.weights.dat", &
    action = "read", status = "old")
read (u_file, "(A)") buffer
write (u, "(A)") trim (buffer)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_weights_1"
end subroutine eio_weights_1

```

Multiple weights

Event with several weight entries set.

```

<EIO weights: execute tests>+≡
    call test (eio_weights_2, "eio_weights_2", &
        "multiple weights", &
        u, results)

<EIO weights: test declarations>+≡
    public :: eio_weights_2

<EIO weights: tests>+≡
    subroutine eio_weights_2 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, i
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_weights_2"
        write (u, "(A)")  "*   Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false., n_alt = 2)

```

```

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_weights_2"

allocate (eio_weights_t :: eio)

call eio%init_out (sample)
select type (eio)
type is (eio_weights_t)
  call eio%set_parameters (pacify = .true.)
end select
call event%generate (1, [0._default, 0._default])
call event%set (sqme_alt = [2._default, 3._default])
call event%set (weight_alt = &
  [2 * event%get_weight_prc (), 3 * event%get_weight_prc ()])

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents: &
  &(weight, sqme(evt), sqme(prc), i_prc)"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_weights_2.weights.dat", &
  action = "read", status = "old")
do i = 1, 3
  read (u_file, "(A)") buffer
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_weights_2"

end subroutine eio_weights_2

```

Multiple events

Events with passed flag switched on/off.

(EIO weights: execute tests)+≡

```

call test (eio_weights_3, "eio_weights_3", &
  "check passed-flag", &
  u, results)

```

```

<EIO weights: test declarations>+=
    public :: eio_weights_3

<EIO weights: tests>+=
    subroutine eio_weights_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_weights_3"
        write (u, "(A)")  "* Purpose: generate three events and write to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write events"
        write (u, "(A)")

        sample = "eio_weights_3"

        allocate (eio_weights_t :: eio)
        select type (eio)
        type is (eio_weights_t)
            call eio%set_parameters (pacify = .true.)
        end select

        call eio%init_out (sample)

        call event%generate (1, [0._default, 0._default])
        call eio%output (event, i_prc = 1)

        call event%generate (1, [0.1_default, 0._default])
        call eio%output (event, i_prc = 1, passed = .false.)

        call event%generate (1, [0.2_default, 0._default])
        call eio%output (event, i_prc = 1, passed = .true.)

        call eio%write (u)
        call eio%final ()

        write (u, "(A)")
        write (u, "(A)")  "* File contents: &
            &(weight, sqme(evt), sqme(prc), i_prc), should be just two entries"
        write (u, "(A)")

        u_file = free_unit ()
        open (u_file, file = "eio_weights_3.weights.dat", &
            action = "read", status = "old")
    do

```

```

        read (u_file, "(A)", iostat=iostat) buffer
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_weights_3"
end subroutine eio_weights_3

```

18.9 Event Dump Output

This is an output-only format. We simply dump the contents of the `particle_set`, using the `write` method of that type. The event-format options are the options of that procedure.

```

⟨eio_dump.f90⟩≡
  ⟨File header⟩

  module eio_dump

    use, intrinsic :: iso_fortran_env, only: output_unit

    use kinds, only: i64
    ⟨Use strings⟩
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    ⟨Standard module head⟩

    ⟨EIO dump: public⟩

    ⟨EIO dump: types⟩

    interface
    ⟨EIO dump: sub interfaces⟩
    end interface

  end module eio_dump

⟨eio_dump_sub.f90⟩≡
  ⟨File header⟩

  submodule (eio_dump) eio_dump_s

    use io_units

```



```

    use diagnostics
    use format_utils, only: write_separator
    use format_utils, only: pac_fmt
    use format_defs, only: FMT_16, FMT_19

    implicit none

contains

    <EIO dump: procedures>

end submodule eio_dump_s

```

18.9.1 Type

```

<EIO dump: public>≡
    public :: eio_dump_t

<EIO dump: types>≡
    type, extends (eio_t) :: eio_dump_t
        integer(i64) :: count = 0
        integer :: unit = 0
        logical :: writing = .false.
        logical :: screen = .false.
        logical :: pacify = .false.
        logical :: weights = .false.
        logical :: compressed = .false.
        logical :: summary = .false.
    contains
        <EIO dump: eio dump: TBP>
    end type eio_dump_t

```

18.9.2 Specific Methods

Set control parameters. We may provide a `unit` for input or output; this will be taken if the sample file name is empty. In that case, the unit is assumed to be open and will be kept open; no messages will be issued.

```

<EIO dump: eio dump: TBP>≡
    procedure :: set_parameters => eio_dump_set_parameters

<EIO dump: sub interfaces>≡
    module subroutine eio_dump_set_parameters (eio, extension, &
        pacify, weights, compressed, summary, screen, unit)
        class(eio_dump_t), intent(inout) :: eio
        type(string_t), intent(in), optional :: extension
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: weights
        logical, intent(in), optional :: compressed
        logical, intent(in), optional :: summary
        logical, intent(in), optional :: screen
        integer, intent(in), optional :: unit
    end subroutine eio_dump_set_parameters

```

```

<EIO dump: procedures>≡
module subroutine eio_dump_set_parameters (eio, extension, &
    pacify, weights, compressed, summary, screen, unit)
    class(eio_dump_t), intent(inout) :: eio
    type(string_t), intent(in), optional :: extension
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: weights
    logical, intent(in), optional :: compressed
    logical, intent(in), optional :: summary
    logical, intent(in), optional :: screen
    integer, intent(in), optional :: unit
    if (present (pacify)) eio%pacify = pacify
    if (present (weights)) eio%weights = weights
    if (present (compressed)) eio%compressed = compressed
    if (present (summary)) eio%summary = summary
    if (present (screen)) eio%screen = screen
    if (present (unit)) eio%unit = unit
    eio%extension = "pset.dat"
    if (present (extension)) eio%extension = extension
end subroutine eio_dump_set_parameters

```

18.9.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO dump: eio dump: TBP>+≡
    procedure :: write => eio_dump_write

<EIO dump: sub interfaces>+≡
    module subroutine eio_dump_write (object, unit)
        class(eio_dump_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_dump_write

<EIO dump: procedures>+≡
module subroutine eio_dump_write (object, unit)
    class(eio_dump_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Dump event stream:"
    if (object%writing) then
        write (u, "(3x,A,L1)") "Screen output      = ", object%screen
        write (u, "(3x,A,A,A)") "Writing to file  = '", char (object%filename), "'"
        write (u, "(3x,A,L1)") "Reduced I/O prec. = ", object%pacify
        write (u, "(3x,A,L1)") "Show weights/sqme = ", object%weights
        write (u, "(3x,A,L1)") "Compressed       = ", object%compressed
        write (u, "(3x,A,L1)") "Summary          = ", object%summary
    else
        write (u, "(3x,A)") "[closed]"
    end if
end subroutine eio_dump_write

```

Finalizer: close any open file.

```
(EIO dump: eio dump: TBP)+≡
    procedure :: final => eio_dump_final

(EIO dump: sub interfaces)+≡
    module subroutine eio_dump_final (object)
        class(eio_dump_t), intent(inout) :: object
    end subroutine eio_dump_final

(EIO dump: procedures)+≡
    module subroutine eio_dump_final (object)
        class(eio_dump_t), intent(inout) :: object
        if (object%screen) then
            write (msg_buffer, "(A,A,A)") "Events: display complete"
            call msg_message ()
            object%screen = .false.
        end if
        if (object%writing) then
            if (object%filename /= "") then
                write (msg_buffer, "(A,A,A)") "Events: closing event dump file '", &
                    char (object%filename), "'"
                call msg_message ()
                close (object%unit)
            end if
            object%writing = .false.
        end if
    end subroutine eio_dump_final
```

Initialize event writing.

```
(EIO dump: eio dump: TBP)+≡
    procedure :: init_out => eio_dump_init_out

(EIO dump: sub interfaces)+≡
    module subroutine eio_dump_init_out &
        (eio, sample, data, success, extension)
        class(eio_dump_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_dump_init_out

(EIO dump: procedures)+≡
    module subroutine eio_dump_init_out &
        (eio, sample, data, success, extension)
        class(eio_dump_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        if (present(extension)) then
            eio%extension = extension
        else
            eio%extension = "pset.dat"
        end if
```

```

if (sample == "" .and. eio%unit /= 0) then
    eio%filename = ""
    eio%writing = .true.
else if (sample /= "") then
    eio%filename = sample // "." // eio%extension
    eio%unit = free_unit ()
    write (msg_buffer, "(A,A,A)") "Events: writing to event dump file '", &
        char (eio%filename), "'"
    call msg_message ()
    eio%writing = .true.
    open (eio%unit, file = char (eio%filename), &
        action = "write", status = "replace")
end if
if (eio%screen) then
    write (msg_buffer, "(A,A,A)") "Events: display on standard output"
    call msg_message ()
end if
eio%count = 0
if (present (success)) success = .true.
end subroutine eio_dump_init_out

```

Initialize event reading.

(EIO dump: eio dump: TBP)+≡

```

procedure :: init_in => eio_dump_init_in

```

(EIO dump: sub interfaces)+≡

```

module subroutine eio_dump_init_in &
    (eio, sample, data, success, extension)
class(eio_dump_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
end subroutine eio_dump_init_in

```

(EIO dump: procedures)+≡

```

module subroutine eio_dump_init_in &
    (eio, sample, data, success, extension)
class(eio_dump_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
call msg_bug ("Event dump: event input not supported")
if (present (success)) success = .false.
end subroutine eio_dump_init_in

```

Switch from input to output: reopen the file for reading.

(EIO dump: eio dump: TBP)+≡

```

procedure :: switch_inout => eio_dump_switch_inout

```

(EIO dump: sub interfaces)+≡

```

module subroutine eio_dump_switch_inout (eio, success)
class(eio_dump_t), intent(inout) :: eio

```

```

        logical, intent(out), optional :: success
    end subroutine eio_dump_switch_inout

<EIO dump: procedures>+=
module subroutine eio_dump_switch_inout (eio, success)
    class(eio_dump_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    call msg_bug ("Event dump: in-out switch not supported")
    if (present (success)) success = .false.
end subroutine eio_dump_switch_inout

Output an event. Delegate the output call to the write method of the current
particle set, if valid. Output both to file (if defined) and to screen (if requested).

<EIO dump: eio dump: TBP>+=
    procedure :: output => eio_dump_output

<EIO dump: sub interfaces>+=
    module subroutine eio_dump_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_dump_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_dump_output

<EIO dump: procedures>+=
module subroutine eio_dump_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_dump_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    character(len=7) :: fmt
    eio%count = eio%count + 1
    if (present (pacify)) then
        call pac_fmt (fmt, FMT_19, FMT_16, pacify)
    else
        call pac_fmt (fmt, FMT_19, FMT_16, eio%pacify)
    end if
    if (eio%writing) call dump (eio%unit)
    if (eio%screen) then
        call dump (output_unit)
        if (logfile_unit () > 0) call dump (logfile_unit ())
    end if
contains
    subroutine dump (u)
        integer, intent(in) :: u
        integer :: i
        call write_separator (u, 2)
        write (u, "(1x,A,I0)", advance="no") "Event"
        if (event%has_index ()) then
            write (u, "(1x,'#',I0)") event%get_index ()
        else

```

```

        write (u, *)
    end if
    call write_separator (u, 2)
    write (u, "(1x,A,1x,I0)" "count =", eio%count
    if (present (passed)) then
        write (u, "(1x,A,1x,L1)" "passed =", passed
    else
        write (u, "(1x,A)" "passed = [N/A]"
    end if
    write (u, "(1x,A,1x,I0)" "prc id =", i_prc
    if (eio%weights) then
        call write_separator (u)
        if (event%sqme_ref_known) then
            write (u, "(1x,A," // fmt // ")") "sqme (ref) = ", &
                event%sqme_ref
        else
            write (u, "(1x,A)" "sqme (ref) = [undefined]"
        end if
        if (event%sqme_prc_known) then
            write (u, "(1x,A," // fmt // ")") "sqme (prc) = ", &
                event%sqme_prc
        else
            write (u, "(1x,A)" "sqme (prc) = [undefined]"
        end if
        if (event%weight_ref_known) then
            write (u, "(1x,A," // fmt // ")") "weight (ref) = ", &
                event%weight_ref
        else
            write (u, "(1x,A)" "weight (ref) = [undefined]"
        end if
        if (event%weight_prc_known) then
            write (u, "(1x,A," // fmt // ")") "weight (prc) = ", &
                event%weight_prc
        else
            write (u, "(1x,A)" "weight (prc) = [undefined]"
        end if
        if (event%excess_prc_known) then
            write (u, "(1x,A," // fmt // ")") "excess (prc) = ", &
                event%excess_prc
        else
            write (u, "(1x,A)" "excess (prc) = [undefined]"
        end if
        do i = 1, event%n_alt
            if (event%sqme_ref_known) then
                write (u, "(1x,A,I0,A," // fmt // ")") "sqme (", i, ") = ", &
                    event%sqme_prc
            else
                write (u, "(1x,A,I0,A)" "sqme (", i, ") = [undefined]"
            end if
            if (event%weight_prc_known) then
                write (u, "(1x,A,I0,A," // fmt // ")") "weight (", i, ") = ", &
                    event%weight_prc
            else
                write (u, "(1x,A,I0,A)" "weight (", i, ") = [undefined]"
            end if
        end do
    end if
end if

```

```

        end if
    end do
end if
call write_separator (u)
if (event%particle_set_is_valid) then
    call event%particle_set%write (unit = u, &
        summary = eio%summary, compressed = eio%compressed, &
        testflag = eio%pacify)
else
    write (u, "(1x,A)") "Particle set: [invalid]"
end if
end subroutine dump
end subroutine eio_dump_output

```

Input an event.

(EIO dump: eio dump: TBP)+≡

```

procedure :: input_i_prc => eio_dump_input_i_prc
procedure :: input_event => eio_dump_input_event

```

(EIO dump: sub interfaces)+≡

```

module subroutine eio_dump_input_i_prc (eio, i_prc, iostat)
    class(eio_dump_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
end subroutine eio_dump_input_i_prc
module subroutine eio_dump_input_event &
    (eio, event, iostat, event_handle)
    class(eio_dump_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
end subroutine eio_dump_input_event

```

(EIO dump: procedures)+≡

```

module subroutine eio_dump_input_i_prc (eio, i_prc, iostat)
    class(eio_dump_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    call msg_bug ("Dump stream: event input not supported")
    i_prc = 0
    iostat = 1
end subroutine eio_dump_input_i_prc

module subroutine eio_dump_input_event &
    (eio, event, iostat, event_handle)
    class(eio_dump_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    call msg_bug ("Dump stream: event input not supported")
    iostat = 1
end subroutine eio_dump_input_event

```

(EIO dump: eio dump: TBP)+≡

```

        procedure :: skip => eio_dump_skip
    <EIO dump: sub interfaces>+≡
        module subroutine eio_dump_skip (eio, iostat)
            class(eio_dump_t), intent(inout) :: eio
            integer, intent(out) :: iostat
        end subroutine eio_dump_skip
    <EIO dump: procedures>+≡
        module subroutine eio_dump_skip (eio, iostat)
            class(eio_dump_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            iostat = 0
        end subroutine eio_dump_skip

```

18.9.4 Unit tests

Test module, followed by the corresponding implementation module.

```

    <eio_dump_ut.f90>≡
    <File header>

    module eio_dump_ut
        use unit_tests
        use eio_dump_util

    <Standard module head>

    <EIO dump: public test>

    contains

    <EIO dump: test driver>

    end module eio_dump_ut
    <eio_dump_util.f90>≡
    <File header>

    module eio_dump_util

    <Use kinds>
    <Use strings>
        use io_units
        use event_base
        use eio_data
        use eio_base

        use eio_dump

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO dump: test declarations>

```


contains

<EIO dump: tests>

end module eio_dump_util

API: driver for the unit tests below.

<EIO dump: public test>≡

public :: eio_dump_test

<EIO dump: test driver>≡

subroutine eio_dump_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<EIO dump: execute tests>

end subroutine eio_dump_test

Test I/O methods

We test the implementation of all I/O methods.

<EIO dump: execute tests>≡

call test (eio_dump_1, "eio_dump_1", &
"write event contents", &
u, results)

<EIO dump: test declarations>≡

public :: eio_dump_1

<EIO dump: tests>≡

subroutine eio_dump_1 (u)

integer, intent(in) :: u

class(generic_event_t), pointer :: event

class(eio_t), allocatable :: eio

integer :: i_prc

integer :: u_file

write (u, "(A)") "* Test output: eio_dump_1"

write (u, "(A)") "* Purpose: generate events and write essentials to output"

write (u, "(A)")

write (u, "(A)") "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")

write (u, "(A)") "* Generate and write three events (two passed)"

write (u, "(A)")

allocate (eio_dump_t :: eio)

select type (eio)

type is (eio_dump_t)

call eio%set_parameters (unit = u, weights = .true., pacify = .true.)

end select

```

i_prc = 42

call eio%init_out (var_str (""))

call event%generate (1, [0._default, 0._default])
call eio%output (event, i_prc = i_prc)

call event%generate (1, [0.1_default, 0._default])
call event%set_index (99)
call eio%output (event, i_prc = i_prc, passed = .false.)

call event%generate (1, [0.2_default, 0._default])
call event%increment_index ()
call eio%output (event, i_prc = i_prc, passed = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of eio_dump object"
write (u, "(A)")

call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

select type (eio)
type is (eio_dump_t)
    eio%writing = .false.
end select
call eio%final ()

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_dump_1"
end subroutine eio_dump_1

```

18.10 ASCII File Formats

Here, we implement several ASCII file formats. It is possible to switch between them using flags.

```

⟨eio_ascii.f90⟩≡
  ⟨File header⟩

module eio_ascii

  ⟨Use strings⟩
  use event_base
  use event_handles, only: event_handle_t
  use eio_data
  use eio_base

```

```

    <Standard module head>

    <EIO ascii: public>

    <EIO ascii: types>

    interface
    <EIO ascii: sub interfaces>
    end interface

    end module eio_ascii

    <eio_ascii_sub.f90>≡
    <File header>

    submodule (eio_ascii) eio_ascii_s

        use io_units
        use diagnostics
        use hep_common
        use hep_events

        implicit none

    contains

    <EIO ascii: procedures>

    end submodule eio_ascii_s

```

18.10.1 Type

```

    <EIO ascii: public>≡
    public :: eio_ascii_t

    <EIO ascii: types>≡
    type, abstract, extends (eio_t) :: eio_ascii_t
        logical :: writing = .false.
        integer :: unit = 0
        logical :: keep_beams = .false.
        logical :: keep_remnants = .true.
        logical :: ensure_order = .false.
    contains
    <EIO ascii: eio_ascii: TBP>
    end type eio_ascii_t

    <EIO ascii: public>+≡
    public :: eio_ascii_ascii_t

    <EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_ascii_t
    end type eio_ascii_ascii_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_athena_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_athena_t
  end type eio_ascii_athena_t

```

The debug format has a few options that can be controlled by Sindarin variables.

```

<EIO ascii: public>+≡
  public :: eio_ascii_debug_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_debug_t
    logical :: show_process = .true.
    logical :: show_transforms = .true.
    logical :: show_decay = .true.
    logical :: verbose = .true.
  end type eio_ascii_debug_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_hepevt_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_hepevt_t
  end type eio_ascii_hepevt_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_hepevt_verb_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_hepevt_verb_t
  end type eio_ascii_hepevt_verb_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_lha_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_lha_t
  end type eio_ascii_lha_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_lha_verb_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_lha_verb_t
  end type eio_ascii_lha_verb_t

```

```

<EIO ascii: public>+≡
  public :: eio_ascii_long_t

<EIO ascii: types>+≡
  type, extends (eio_ascii_t) :: eio_ascii_long_t
  end type eio_ascii_long_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_mokka_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_mokka_t
    end type eio_ascii_mokka_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_short_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_short_t
    end type eio_ascii_short_t

```

18.10.2 Specific Methods

Set parameters that are specifically used with ASCII file formats. In particular, this is the file extension.

```

<EIO ascii: eio ascii: TBP>≡
    procedure :: set_parameters => eio_ascii_set_parameters

<EIO ascii: sub interfaces>≡
    module subroutine eio_ascii_set_parameters (eio, &
        keep_beams, keep_remnants, ensure_order, extension, &
        show_process, show_transforms, show_decay, verbose)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: ensure_order
        type(string_t), intent(in), optional :: extension
        logical, intent(in), optional :: show_process, show_transforms, show_decay
        logical, intent(in), optional :: verbose
    end subroutine eio_ascii_set_parameters

<EIO ascii: procedures>≡
    module subroutine eio_ascii_set_parameters (eio, &
        keep_beams, keep_remnants, ensure_order, extension, &
        show_process, show_transforms, show_decay, verbose)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: ensure_order
        type(string_t), intent(in), optional :: extension
        logical, intent(in), optional :: show_process, show_transforms, show_decay
        logical, intent(in), optional :: verbose
        if (present (keep_beams)) eio%keep_beams = keep_beams
        if (present (keep_remnants)) eio%keep_remnants = keep_remnants
        if (present (ensure_order)) eio%ensure_order = ensure_order
        if (present (extension)) then
            eio%extension = extension
        else
            select type (eio)
            type is (eio_ascii_ascii_t)
                eio%extension = "evt"

```

```

        type is (eio_ascii_athena_t)
            eio%extension = "athena.evt"
        type is (eio_ascii_debug_t)
            eio%extension = "debug"
        type is (eio_ascii_hepevt_t)
            eio%extension = "hepevt"
        type is (eio_ascii_hepevt_verb_t)
            eio%extension = "hepevt.verb"
        type is (eio_ascii_lha_t)
            eio%extension = "lha"
        type is (eio_ascii_lha_verb_t)
            eio%extension = "lha.verb"
        type is (eio_ascii_long_t)
            eio%extension = "long.evt"
        type is (eio_ascii_mokka_t)
            eio%extension = "mokka.evt"
        type is (eio_ascii_short_t)
            eio%extension = "short.evt"
    end select
end if
select type (eio)
type is (eio_ascii_debug_t)
    if (present (show_process)) eio%show_process = show_process
    if (present (show_transforms)) eio%show_transforms = show_transforms
    if (present (show_decay)) eio%show_decay = show_decay
    if (present (verbose)) eio%verbose = verbose
end select
end subroutine eio_ascii_set_parameters

```

18.10.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: write => eio_ascii_write

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_write (object, unit)
        class(eio_ascii_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_ascii_write

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_write (object, unit)
        class(eio_ascii_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        select type (object)
        type is (eio_ascii_ascii_t)
            write (u, "(1x,A)") "ASCII event stream (default format):"
        type is (eio_ascii_athena_t)
            write (u, "(1x,A)") "ASCII event stream (ATHENA format):"

```

```

type is (eio_ascii_debug_t)
  write (u, "(1x,A)") "ASCII event stream (Debugging format):"
type is (eio_ascii_hepevt_t)
  write (u, "(1x,A)") "ASCII event stream (HEPEVT format):"
type is (eio_ascii_hepevt_verb_t)
  write (u, "(1x,A)") "ASCII event stream (verbose HEPEVT format):"
type is (eio_ascii_lha_t)
  write (u, "(1x,A)") "ASCII event stream (LHA format):"
type is (eio_ascii_lha_verb_t)
  write (u, "(1x,A)") "ASCII event stream (verbose LHA format):"
type is (eio_ascii_long_t)
  write (u, "(1x,A)") "ASCII event stream (long format):"
type is (eio_ascii_mokka_t)
  write (u, "(1x,A)") "ASCII event stream (MOKKA format):"
type is (eio_ascii_short_t)
  write (u, "(1x,A)") "ASCII event stream (short format):"
end select
if (object%writing) then
  write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
else
  write (u, "(3x,A)") "[closed]"
end if
write (u, "(3x,A,L1)") "Keep beams      = ", object%keep_beams
write (u, "(3x,A,L1)") "Keep remnants   = ", object%keep_remnants
select type (object)
type is (eio_ascii_debug_t)
  write (u, "(3x,A,L1)") "Show process     = ", object%show_process
  write (u, "(3x,A,L1)") "Show transforms  = ", object%show_transforms
  write (u, "(3x,A,L1)") "Show decay tree  = ", object%show_decay
  write (u, "(3x,A,L1)") "Verbose output   = ", object%verbose
end select
end subroutine eio_ascii_write

```

Finalizer: close any open file.

```

<EIO ascii: eio ascii: TBP>+≡
  procedure :: final => eio_ascii_final

<EIO ascii: sub interfaces>+≡
  module subroutine eio_ascii_final (object)
    class(eio_ascii_t), intent(inout) :: object
  end subroutine eio_ascii_final

```

```

<EIO ascii: procedures>+≡
  module subroutine eio_ascii_final (object)
    class(eio_ascii_t), intent(inout) :: object
    if (object%writing) then
      write (msg_buffer, "(A,A,A)") "Events: closing ASCII file '", &
        char (object%filename), "'"
      call msg_message ()
      close (object%unit)
      object%writing = .false.
    end if
  end subroutine eio_ascii_final

```

Initialize event writing.

Check weight normalization. This applies to all ASCII-type files that use the HEPUP common block. We can't allow normalization conventions that are not covered by the HEPUP definition.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: init_out => eio_ascii_init_out

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_init_out &
        (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_ascii_init_out

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_init_out &
        (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        logical :: is_width
        integer :: i
        if (.not. present (data)) &
            call msg_bug ("ASCII initialization: missing data")
        is_width = data%n_beam == 1
        eio%sample = sample
        call eio%check_normalization (data)
        call eio%set_splitting (data)
        call eio%set_filename ()
        eio%unit = free_unit ()
        write (msg_buffer, "(A,A,A)") "Events: writing to ASCII file '", &
            char (eio%filename), "'"
        call msg_message ()
        eio%writing = .true.
        open (eio%unit, file = char (eio%filename), &
            action = "write", status = "replace")
        select type (eio)
        type is (eio_ascii_lha_t)
            call heprup_init( &
                data%pdg_beam, &
                data%energy_beam, &
                n_processes = data%n_proc, &
                unweighted = data%unweighted, &
                negative_weights = data%negative_weights)
            do i = 1, data%n_proc
                call heprup_set_process_parameters (i = i, &
                    process_id = data%proc_num_id(i), &
                    cross_section = data%cross_section(i), &
                    error = data%error(i), &
                    is_width = is_width)
            end do
        end select
    end module

```



```

end do
call heprup_write_ascii (eio%unit)
type is (eio_ascii_lha_verb_t)
call heprup_init( &
    data%pdg_beam, &
    data%energy_beam, &
    n_processes = data%n_proc, &
    unweighted = data%unweighted, &
    negative_weights = data%negative_weights)
do i = 1, data%n_proc
    call heprup_set_process_parameters (i = i, &
        process_id = data%proc_num_id(i), &
        cross_section = data%cross_section(i), &
        error = data%error(i), &
        is_width = is_width)
end do
call heprup_write_verbos (eio%unit)
end select
if (present (success)) success = .true.
end subroutine eio_ascii_init_out

```

Some event properties do not go well with some output formats. In particular, many formats require unweighted events.

(EIO ascii: eio ascii: TBP)+≡

```

procedure :: check_normalization => eio_ascii_check_normalization

```

(EIO ascii: sub interfaces)+≡

```

module subroutine eio_ascii_check_normalization (eio, data)
    class(eio_ascii_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
end subroutine eio_ascii_check_normalization

```

(EIO ascii: procedures)+≡

```

module subroutine eio_ascii_check_normalization (eio, data)
    class(eio_ascii_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
    if (data%unweighted) then
    else
        select type (eio)
        type is (eio_ascii_athena_t); call msg_fatal &
            ("Event output (Athena format): events must be unweighted.")
        type is (eio_ascii_hepevt_t); call msg_fatal &
            ("Event output (HEPEVT format): events must be unweighted.")
        type is (eio_ascii_hepevt_verb_t); call msg_fatal &
            ("Event output (HEPEVT format): events must be unweighted.")
        end select
        select case (data%norm_mode)
        case (NORM_SIGMA)
        case default
            select type (eio)
            type is (eio_ascii_lha_t)
            call msg_fatal &
                ("Event output (LHA): normalization for weighted events &
                &must be 'sigma'")
            type is (eio_ascii_lha_verb_t)

```

```

        call msg_fatal &
            ("Event output (LHA): normalization for weighted events &
            &must be 'sigma'")
    end select
end select
end if
end subroutine eio_ascii_check_normalization

```

Initialize event reading.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: init_in => eio_ascii_init_in

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_init_in &
        (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_ascii_init_in

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_init_in &
        (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("ASCII: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_ascii_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: switch_inout => eio_ascii_switch_inout

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_switch_inout (eio, success)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_ascii_switch_inout

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_switch_inout (eio, success)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("ASCII: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_ascii_switch_inout

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common block contents are still intact.)

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: split_out => eio_ascii_split_out

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_split_out (eio)
        class(eio_ascii_t), intent(inout) :: eio
    end subroutine eio_ascii_split_out

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_split_out (eio)
        class(eio_ascii_t), intent(inout) :: eio
        if (eio%split) then
            eio%split_index = eio%split_index + 1
            call eio%set_filename ()
            write (msg_buffer, "(A,A,A)") "Events: writing to ASCII file '", &
                char (eio%filename), "'"
            call msg_message ()
            close (eio%unit)
            open (eio%unit, file = char (eio%filename), &
                action = "write", status = "replace")
            select type (eio)
            type is (eio_ascii_lha_t)
                call heprup_write_ascii (eio%unit)
            type is (eio_ascii_lha_verb_t)
                call heprup_write_verbos (eio%unit)
            end select
        end if
    end subroutine eio_ascii_split_out

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

Events that did not pass the selection are skipped. The exceptions are the `ascii` and `debug` formats. These are the formats that contain the `passed` flag in their output, and should be most useful for debugging purposes.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: output => eio_ascii_output

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_ascii_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_ascii_output

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_ascii_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event

```

```

integer, intent(in) :: i_prc
logical, intent(in), optional :: reading, passed, pacify
class(event_handle_t), intent(inout), optional :: event_handle
if (present (passed)) then
    if (.not. passed) then
        select type (eio)
            type is (eio_ascii_debug_t)
            type is (eio_ascii_ascii_t)
            class default
                return
            end select
        end if
    end if
    if (eio%writing) then
        select type (eio)
            type is (eio_ascii_lha_t)
                call hepeup_from_event (event, &
                    process_index = i_prc, &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants)
                call hepeup_write_lha (eio%unit)
            type is (eio_ascii_lha_verb_t)
                call hepeup_from_event (event, &
                    process_index = i_prc, &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants)
                call hepeup_write_verbose (eio%unit)
            type is (eio_ascii_ascii_t)
                call event%write (eio%unit, &
                    show_process = .false., &
                    show_transforms = .false., &
                    show_decay = .false., &
                    verbose = .false., testflag = pacify)
            type is (eio_ascii_athena_t)
                call hepevt_from_event (event, &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants, &
                    ensure_order = eio%ensure_order)
                call hepevt_write_athena (eio%unit)
            type is (eio_ascii_debug_t)
                call event%write (eio%unit, &
                    show_process = eio%show_process, &
                    show_transforms = eio%show_transforms, &
                    show_decay = eio%show_decay, &
                    verbose = eio%verbose, &
                    testflag = pacify)
            type is (eio_ascii_hepevt_t)
                call hepevt_from_event (event, &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants, &
                    ensure_order = eio%ensure_order)
                call hepevt_write_hepevt (eio%unit)
            type is (eio_ascii_hepevt_verb_t)
                call hepevt_from_event (event, &

```

```

        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants, &
        ensure_order = eio%ensure_order)
    call hepevt_write_verbose (eio%unit)
type is (eio_ascii_long_t)
    call hepevt_from_event (event, &
        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants, &
        ensure_order = eio%ensure_order)
    call hepevt_write_ascii (eio%unit, .true.)
type is (eio_ascii_mokka_t)
    call hepevt_from_event (event, &
        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants, &
        ensure_order = eio%ensure_order)
    call hepevt_write_mokka (eio%unit)
type is (eio_ascii_short_t)
    call hepevt_from_event (event, &
        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants, &
        ensure_order = eio%ensure_order)
    call hepevt_write_ascii (eio%unit, .false.)
end select
else
    call eio%write ()
    call msg_fatal ("ASCII file is not open for writing")
end if
end subroutine eio_ascii_output

```

Input an event.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: input_i_prc => eio_ascii_input_i_prc
    procedure :: input_event => eio_ascii_input_event

<EIO ascii: sub interfaces>+≡
    module subroutine eio_ascii_input_i_prc (eio, i_prc, iostat)
        class(eio_ascii_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
    end subroutine eio_ascii_input_i_prc
    module subroutine eio_ascii_input_event &
        (eio, event, iostat, event_handle)
        class(eio_ascii_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_ascii_input_event

<EIO ascii: procedures>+≡
    module subroutine eio_ascii_input_i_prc (eio, i_prc, iostat)
        class(eio_ascii_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        call msg_bug ("ASCII: event input not supported")
        i_prc = 0
    end subroutine eio_ascii_input_i_prc

```

```

        iostat = 1
    end subroutine eio_ascii_input_i_prc

    module subroutine eio_ascii_input_event &
        (eio, event, iostat, event_handle)
        class(eio_ascii_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        call msg_bug ("ASCII: event input not supported")
        iostat = 1
    end subroutine eio_ascii_input_event

    <EIO ascii: eio ascii: TBP>+≡
        procedure :: skip => eio_ascii_skip

    <EIO ascii: sub interfaces>+≡
        module subroutine eio_ascii_skip (eio, iostat)
            class(eio_ascii_t), intent(inout) :: eio
            integer, intent(out) :: iostat
        end subroutine eio_ascii_skip

    <EIO ascii: procedures>+≡
        module subroutine eio_ascii_skip (eio, iostat)
            class(eio_ascii_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            iostat = 0
        end subroutine eio_ascii_skip

```

18.10.4 Unit tests

Test module, followed by the corresponding implementation module.

```

    <eio_ascii_ut.f90>≡
        <File header>

        module eio_ascii_ut
            use unit_tests
            use eio_ascii_uti

            <Standard module head>

            <EIO ascii: public test>

            contains

            <EIO ascii: test driver>

        end module eio_ascii_ut

    <eio_ascii_uti.f90>≡
        <File header>

        module eio_ascii_uti

```

```

    <Use kinds>
    <Use strings>
    use io_units
    use lorentz
    use model_data
    use event_base
    use particles
    use eio_data
    use eio_base

    use eio_ascii

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO ascii: test declarations>

    contains

    <EIO ascii: tests>

    end module eio_ascii_ut
API: driver for the unit tests below.
    <EIO ascii: public test>≡
    public :: eio_ascii_test
    <EIO ascii: test driver>≡
    subroutine eio_ascii_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <EIO ascii: execute tests>
    end subroutine eio_ascii_test

```

Test I/O methods

We test the implementation of all I/O methods, method `ascii`:

```

    <EIO ascii: execute tests>≡
    call test (eio_ascii_1, "eio_ascii_1", &
    "read and write event contents, format [ascii]", &
    u, results)
    <EIO ascii: test declarations>≡
    public :: eio_ascii_1
    <EIO ascii: tests>≡
    subroutine eio_ascii_1 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat

```

```

character(80) :: buffer

write (u, "(A)")  "* Test output: eio_ascii_1"
write (u, "(A)")  "* Purpose: generate an event in ASCII ascii format"
write (u, "(A)")  "*           and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_1"

allocate (eio_ascii_ascii_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (42)
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do

```



```

close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_ascii_t :: eio)

select type (eio)
type is (eio_ascii_ascii_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_1"

end subroutine eio_ascii_1

```

We test the implementation of all I/O methods, method `athena`:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_2, "eio_ascii_2", &
    "read and write event contents, format [athena]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_2

<EIO ascii: tests>+≡
  subroutine eio_ascii_2 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_ascii_2"
    write (u, "(A)")  "*   Purpose: generate an event in ASCII athena format"
    write (u, "(A)")  "*           and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%n_evt = 1

```

```

data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_2"

allocate (eio_ascii_athena_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (42)
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char(sample // ".athena.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_athena_t :: eio)

select type (eio)
type is (eio_ascii_athena_t)
  call eio%set_parameters (keep_beams = .true.)
end select

```

```

call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_2"

end subroutine eio_ascii_2

```

We test the implementation of all I/O methods, method `debug`:

```

<EIO ascii: execute tests>+≡
call test (eio_ascii_3, "eio_ascii_3", &
  "read and write event contents, format [debug]", &
  u, results)

<EIO ascii: test declarations>+≡
public :: eio_ascii_3

<EIO ascii: tests>+≡
subroutine eio_ascii_3 (u)
  integer, intent(in) :: u
  class(generic_event_t), pointer :: event
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  type(string_t) :: sample
  integer :: u_file, iostat
  character(80) :: buffer

  write (u, "(A)")  "* Test output: eio_ascii_3"
  write (u, "(A)")  "* Purpose: generate an event in ASCII debug format"
  write (u, "(A)")  "* and write weight to file"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize test process"

  call eio_prepare_test (event, unweighted = .false.)

  call data%init (1)
  data%n_evt = 1
  data%n_beam = 2
  data%pdg_beam = 25
  data%energy_beam = 500
  data%proc_num_id = [42]
  data%cross_section(1) = 100
  data%error(1) = 1
  data%total_cross_section = sum (data%cross_section)

  write (u, "(A)")
  write (u, "(A)")  "* Generate and write an event"
  write (u, "(A)")

  sample = "eio_ascii_3"

```

```

allocate (eio_ascii_debug_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".debug"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_debug_t :: eio)

select type (eio)
type is (eio_ascii_debug_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_3"

end subroutine eio_ascii_3

```

We test the implementation of all I/O methods, method `hepevt`:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_4, "eio_ascii_4", &
    "read and write event contents, format [hepevt]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_4

<EIO ascii: tests>+≡
  subroutine eio_ascii_4 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_ascii_4"
    write (u, "(A)")  "* Purpose: generate an event in ASCII hepevt format"
    write (u, "(A)")  "* and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%n_evt = 1
    data%n_beam = 2
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    data%cross_section(1) = 100
    data%error(1) = 1
    data%total_cross_section = sum (data%cross_section)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_ascii_4"

    allocate (eio_ascii_hepevt_t :: eio)

    select type (eio)
    class is (eio_ascii_t); call eio%set_parameters ()
    end select
    call eio%init_out (sample, data)
    call event%generate (1, [0._default, 0._default])
    call event%increment_index ()
    call event%evaluate_expressions ()

    call eio%output (event, i_prc = 1)
    call eio%write (u)

```

```

call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepevt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_hepevt_t :: eio)

select type (eio)
type is (eio_ascii_hepevt_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_4"

end subroutine eio_ascii_4

```

We test the implementation of all I/O methods, method `lha` (old LHA):

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_5, "eio_ascii_5", &
    "read and write event contents, format [lha]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_5

<EIO ascii: tests>+≡
  subroutine eio_ascii_5 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio

```

```

type(string_t) :: sample
integer :: u_file, iostat
character(80) :: buffer

write (u, "(A)")  "* Test output: eio_ascii_5"
write (u, "(A)")  "* Purpose: generate an event in ASCII LHA format"
write (u, "(A)")  "*           and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_5"

allocate (eio_ascii_lha_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lha"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit

```

```

        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Reset data"
    write (u, "(A)")

    deallocate (eio)
    allocate (eio_ascii_lha_t :: eio)

    select type (eio)
    type is (eio_ascii_lha_t)
        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_5"

end subroutine eio_ascii_5

```

We test the implementation of all I/O methods, method long:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_6, "eio_ascii_6", &
        "read and write event contents, format [long]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_6

<EIO ascii: tests>+≡
    subroutine eio_ascii_6 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_6"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII long format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

```



```

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_6"

allocate (eio_ascii_long_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".long.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_long_t :: eio)

select type (eio)
type is (eio_ascii_long_t)

```

```

        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_6"

end subroutine eio_ascii_6

```

We test the implementation of all I/O methods, method mokka:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_7, "eio_ascii_7", &
        "read and write event contents, format [mokka]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_7

<EIO ascii: tests>+≡
    subroutine eio_ascii_7 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_7"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII mokka format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

```

```

sample = "eio_ascii_7"

allocate (eio_ascii_mokka_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".mokka.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_mokka_t :: eio)

select type (eio)
type is (eio_ascii_mokka_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_7"

end subroutine eio_ascii_7

```

We test the implementation of all I/O methods, method **short**:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_8, "eio_ascii_8", &
        "read and write event contents, format [short]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_8

<EIO ascii: tests>+≡
    subroutine eio_ascii_8 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_8"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII short format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_ascii_8"

        allocate (eio_ascii_short_t :: eio)

        select type (eio)
            class is (eio_ascii_t); call eio%set_parameters ()
        end select
        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%increment_index ()
        call event%evaluate_expressions ()

```

```

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".short.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_short_t :: eio)

select type (eio)
type is (eio_ascii_short_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_8"

end subroutine eio_ascii_8

```

We test the implementation of all I/O methods, method `lha` (old LHA) in verbose version:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_9, "eio_ascii_9", &
    "read and write event contents, format [lha_verb]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_9

<EIO ascii: tests>+≡
  subroutine eio_ascii_9 (u)
    integer, intent(in) :: u

```

```

class(generic_event_t), pointer :: event
type(event_sample_data_t) :: data
class(eio_t), allocatable :: eio
type(string_t) :: sample
integer :: u_file, iostat
character(80) :: buffer

write (u, "(A)")  "* Test output: eio_ascii_9"
write (u, "(A)")  "*   Purpose: generate an event in ASCII LHA verbose format"
write (u, "(A)")  "*           and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_9"

allocate (eio_ascii_lha_verb_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lha.verb"), &
      action = "read", status = "old")
do

```

```

        read (u_file, "(A)", iostat = iostat) buffer
        if (buffer(1:21) == " <generator_version>") buffer = "[...]"
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Reset data"
    write (u, "(A)")

    deallocate (eio)
    allocate (eio_ascii_lha_verb_t :: eio)

    select type (eio)
    type is (eio_ascii_lha_verb_t)
        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_9"

end subroutine eio_ascii_9

```

We test the implementation of all I/O methods, method `hepevt_verb`:

(EIO ascii: execute tests)+≡

```

    call test (eio_ascii_10, "eio_ascii_10", &
        "read and write event contents, format [hepevt_verb]", &
        u, results)

```

(EIO ascii: test declarations)+≡

```

    public :: eio_ascii_10

```

(EIO ascii: tests)+≡

```

subroutine eio_ascii_10 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_ascii_10"
    write (u, "(A)")  "*   Purpose: generate an event in ASCII hepevt verbose format"
    write (u, "(A)")  "*           and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

```

```

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_10"

allocate (eio_ascii_hepevt_verb_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepevt.verb"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_hepevt_verb_t :: eio)

```



```

select type (eio)
type is (eio_ascii_hepevt_verb_t)
    call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_10"

end subroutine eio_ascii_10

```

We test the implementation of all I/O methods, method mokka:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_11, "eio_ascii_11", &
        "read and write event contents, format [mokka], tiny value", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_11

<EIO ascii: tests>+≡
    subroutine eio_ascii_11 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(particle_set_t), pointer :: pset
        type(vector4_t) :: pnew
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(128) :: buffer
        real(default), parameter :: tval = 1.e-111_default

        write (u, "(A)")  "* Test output: eio_ascii_11"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII mokka format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")  "*           with low-value cutoff"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
    end subroutine eio_ascii_11

```

```

data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_11"

allocate (eio_ascii_mokka_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

! Manipulate values in the event record
pset => event%get_particle_set_ptr ()
call pset%set_momentum (3, &
    vector4_moving (-tval, vector3_moving ([-tval, -tval, -tval])), &
    -tval**2)
call pset%set_momentum (4, &
    vector4_moving (tval, vector3_moving ([tval, tval, tval])), &
    tval**2)

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".mokka.evt"), &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:21) == " <generator_version>") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")

```

```

write (u, "(A)")  "* Test output end: eio_ascii_11"

end subroutine eio_ascii_11

```

18.11 HEP Common Blocks

Long ago, to transfer data between programs one had to set up a common block and link both programs as libraries to the main executable. The HEP community standardizes several of those common blocks.

The modern way of data exchange uses data files with standard formats. However, the LHEF standard data format derives from a common block (actually, two).

WHIZARD used to support those common blocks, and LHEF was implemented via writing/reading blocks. We still keep this convention, but intend to eliminate common blocks (or any other static storage) from the workflow in the future. This will gain flexibility towards concurrent running of program images.

We encapsulate everything here in a module. The module holds the variables which are part of the common block. To access the common block variables, we just have to `use` this module. (They are nevertheless in the common block, since external software may access it in this way.)

Note: This code is taken essentially unchanged from WHIZARD 2.1 and does not (yet) provide unit tests.

```

(hep_common.f90)≡
  <File header>

  module hep_common

    <Use kinds>
    use kinds, only: double
    use constants
    <Use strings>
    <Use debug>
    use lorentz
    use polarizations
    use model_data
    use particles

    <Standard module head>

    <HEP common: public>

    <HEP common: interfaces>

    <HEP common: parameters>

    <HEP common: variables>

    <HEP common: common blocks>

    interface

```

```

    <HEP common: sub interfaces>
    end interface

end module hep_common

<hep_common_sub.f90>≡
<File header>

submodule (hep_common) hep_common_s

    use io_units
    use diagnostics
    use numeric_utils
    use format_utils, only: refmt_tiny
    use physics_defs, only: pb_per_fb
    use physics_defs, only: HADRON_REMNANT
    use physics_defs, only: HADRON_REMNANT_SINGLET
    use physics_defs, only: HADRON_REMNANT_TRIPLET
    use physics_defs, only: HADRON_REMNANT_OCTET
    use xml
    use flavors
    use colors
    use subevents, only: PRT_BEAM, PRT_INCOMING, PRT_OUTGOING
    use subevents, only: PRT_UNDEFINED
    use subevents, only: PRT_VIRTUAL, PRT_RESONANT, PRT_BEAM_REMNANT

    implicit none

contains

    <HEP common: procedures>

end submodule hep_common_s

```

18.11.1 Event characteristics

The maximal number of particles in an event record.

```

<HEP common: parameters>≡
    integer, parameter, public :: MAXNUP = 500

```

The number of particles in this event.

```

<HEP common: variables>≡
    integer, public :: NUP

```

The process ID for this event.

```

<HEP common: variables>+≡
    integer, public :: IDPRUP

```

The weight of this event (± 1 for unweighted events).

```

<HEP common: variables>+≡
    double precision, public :: XWGTUP

```

The factorization scale that is used for PDF calculation (-1 if undefined).

```

<HEP common: variables>+≡
    double precision, public :: SCALUP

```

The QED and QCD couplings α used for this event (-1 if undefined).

```
<HEP common: variables>+≡  
  double precision, public :: AQEDUP  
  double precision, public :: AQCDUP
```

18.11.2 Particle characteristics

The PDG code:

```
<HEP common: variables>+≡  
  integer, dimension(MAXNUP), public :: IDUP
```

The status code. Incoming: -1 , outgoing: $+1$. Intermediate t-channel propagator: -2 (currently not used by WHIZARD). Intermediate resonance whose mass should be preserved: 2 . Intermediate resonance for documentation: 3 (currently not used). Beam particles: -9 .

```
<HEP common: variables>+≡  
  integer, dimension(MAXNUP), public :: ISTUP
```

Index of first and last mother.

```
<HEP common: variables>+≡  
  integer, dimension(2,MAXNUP), public :: MOTHUP
```

Color line index of the color and anticolor entry for the particle. The standard recommends using large numbers; we start from $\text{MAXNUP}+1$.

```
<HEP common: variables>+≡  
  integer, dimension(2,MAXNUP), public :: ICOLUP
```

Momentum, energy, and invariant mass: (p_x, p_y, p_z, E, M) . For space-like particles, M is the negative square root of the absolute value of the invariant mass.

```
<HEP common: variables>+≡  
  double precision, dimension(5,MAXNUP), public :: PUP
```

Invariant lifetime (distance) from production to decay in mm.

```
<HEP common: variables>+≡  
  double precision, dimension(MAXNUP), public :: VTIMUP
```

Cosine of the angle between the spin-vector and a particle and the 3-momentum of its mother, given in the lab frame. If undefined/unpolarized: 9 .

```
<HEP common: variables>+≡  
  double precision, dimension(MAXNUP), public :: SPINUP
```

18.11.3 The HEPRUP common block

This common block is filled once per run.

Run characteristics

The maximal number of different processes.

```
<HEP common: parameters>+≡  
  integer, parameter, public :: MAXPUP = 100
```

The beam PDG codes.

```
<HEP common: variables>+≡  
  integer, dimension(2), public :: IDBMUP
```

The beam energies in GeV.

```
<HEP common: variables>+≡  
    double precision, dimension(2), public :: EBMUP
```

The PDF group and set for the two beams. (Undefined: use -1; LHAPDF: use group = 0).

```
<HEP common: variables>+≡  
    integer, dimension(2), public :: PDFGUP  
    integer, dimension(2), public :: PDFSUP
```

The (re)weighting model. 1: events are weighted, the shower generator (SHG) selects processes according to the maximum weight (in pb) and unweights events. 2: events are weighted, the SHG selects processes according to their cross section (in pb) and unweights events. 3: events are unweighted and simply run through the SHG. 4: events are weighted, and the SHG keeps the weight. Negative numbers: negative weights are allowed (and are reweighted to ± 1 by the SHG, if allowed).

WHIZARD only supports modes 3 and 4, as the SHG is not given control over process selection. This is consistent with writing events to file, for offline showering.

```
<HEP common: variables>+≡  
    integer, public :: IDWTUP
```

The number of different processes.

```
<HEP common: variables>+≡  
    integer, public :: NPRUP
```

Process characteristics

Cross section and error in pb. (Cross section is needed only for IDWTUP = 2, so here both values are given for informational purposes only.)

```
<HEP common: variables>+≡  
    double precision, dimension(MAXPUP), public :: XSECUP  
    double precision, dimension(MAXPUP), public :: XERRUP
```

Maximum weight, i.e., the maximum value that XWGTUP can take. Also unused for the supported weighting models. It is ± 1 for unweighted events.

```
<HEP common: variables>+≡  
    double precision, dimension(MAXPUP), public :: XMAXUP
```

Internal ID of the selected process, matches IDPRUP below.

```
<HEP common: variables>+≡  
    integer, dimension(MAXPUP), public :: LPRUP
```

The common block

```
<HEP common: common blocks>≡  
    common /HEPRUP/ &  
        IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP, &  
        XSECUP, XERRUP, XMAXUP, LPRUP  
    save /HEPRUP/
```

Fill the run characteristics of the common block. The initialization sets the beam properties, number of processes, and weighting model.

```

<HEP common: public>≡
    public :: heprup_init

<HEP common: sub interfaces>≡
    module subroutine heprup_init &
        (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)
        integer, dimension(2), intent(in) :: beam_pdg
        real(default), dimension(2), intent(in) :: beam_energy
        integer, intent(in) :: n_processes
        logical, intent(in) :: unweighted
        logical, intent(in) :: negative_weights
    end subroutine heprup_init

<HEP common: procedures>≡
    module subroutine heprup_init &
        (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)
        integer, dimension(2), intent(in) :: beam_pdg
        real(default), dimension(2), intent(in) :: beam_energy
        integer, intent(in) :: n_processes
        logical, intent(in) :: unweighted
        logical, intent(in) :: negative_weights
        IDBMUP = beam_pdg
        EBMUP = beam_energy
        PDFGUP = -1
        PDFSUP = -1
        if (unweighted) then
            IDWTUP = 3
        else
            IDWTUP = 4
        end if
        if (negative_weights) IDWTUP = - IDWTUP
        NPRUP = n_processes
    end subroutine heprup_init

```

The HEPRUP (event) common block is needed for the interface to the shower. Filling of it is triggered by some output file formats. If these are not present, the common block is filled with some dummy information. Be generous with the number of processes in HEPRUP so that PYTHIA only rarely needs to be reinitialized in case events with higher process ids are generated.

```

<HEP common: public>+≡
    public :: assure_heprup

<HEP common: sub interfaces>+≡
    module subroutine assure_heprup (pset)
        type(particle_set_t), intent(in) :: pset
    end subroutine assure_heprup

<HEP common: procedures>+≡
    module subroutine assure_heprup (pset)
        type(particle_set_t), intent(in) :: pset
        integer :: i, num_id
        integer, parameter :: min_processes = 10
        num_id = 1

```

```

if (LPRUP (num_id) /= 0) return
call heprup_init ( &
    [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()] , &
    [pset%prt(1)%p%p(0), pset%prt(2)%p%p(0)], &
    num_id, .false., .false.)
do i = 1, (num_id / min_processes + 1) * min_processes
    call heprup_set_process_parameters (i = i, process_id = &
        i, cross_section = 1._default, error = 1._default)
end do
end subroutine assure_heprup

```

Read in the LHE file opened in unit u and add the final particles to the `particle_set`, the outgoing particles of the existing `particle_set` are compared to the particles that are read in. When they are equal in flavor and momenta, they are erased and their mother-daughter relations are transferred to the existing particles.

```

<HEP common: public>+≡
    public :: combine_lhef_with_particle_set

<HEP common: sub interfaces>+≡
    module subroutine combine_lhef_with_particle_set &
        (particle_set, u, model_in, model_hadrons)
        type(particle_set_t), intent(inout) :: particle_set
        integer, intent(in) :: u
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
    end subroutine combine_lhef_with_particle_set

<HEP common: procedures>+≡
    module subroutine combine_lhef_with_particle_set &
        (particle_set, u, model_in, model_hadrons)
        type(particle_set_t), intent(inout) :: particle_set
        integer, intent(in) :: u
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
        type(flavor_t) :: flv
        type(color_t) :: col
        class(model_data_t), pointer :: model
        type(particle_t), dimension(:), allocatable :: prt_tmp, prt
        integer :: i, j
        type(vector4_t) :: mom, d_mom
        integer, PARAMETER :: MAXLEN=200
        character(len=maxlen) :: string
        integer :: ibeg, n_tot, n_entries
        integer, dimension(:), allocatable :: relations, mothers, tbd
        INTEGER :: NUP, IDPRUP, IDUP, ISTUP
        real(kind=double) :: XWGTUP, SCALUP, AQEDUP, AQCDUP, VTIMUP, SPINUP
        integer :: MOTHUP(1:2), ICOLUP(1:2)
        real(kind=double) :: PUP(1:5)
        real(kind=default) :: pup_dum(1:5)
        character(len=5) :: buffer
        character(len=6) :: strfmt
        logical :: not_found
        logical :: debug_lhef = .false.

```



```

STRFMT='(A000)'
WRITE (STRFMT(3:5),'(I3)') MAXLEN

if (debug_lhef) call particle_set%write ()

rewind (u)

do
  read (u,*, END=501, ERR=502) STRING
  IBEG = 0
  do
    if (signal_is_pending ()) return
    IBEG = IBEG + 1
    ! Allow indentation.
    IF (STRING (IBEG:IBEG) .EQ. ' ' .and. IBEG < MAXLEN-6) cycle
    exit
  end do
  IF (string(IBEG:IBEG+6) /= '<event>' .and. &
      string(IBEG:IBEG+6) /= '<event ') cycle
  exit
end do
!!! Read first line of event info -> number of entries
read (u, *, END=503, ERR=504) NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
n_tot = particle_set%get_n_tot ()
allocate (prt_tmp (1:n_tot+NUP))
allocate (relations (1:NUP), mothers (1:NUP), tbd(1:NUP))
do i = 1, n_tot
  if (signal_is_pending ()) return
  prt_tmp (i) = particle_set%get_particle (i)
end do
!!! transfer particles from lhef to particle_set
!!!...Read NUP subsequent lines with information on each particle.
n_entries = 1
mothers = 0
relations = 0
PARTICLE_LOOP: do I = 1, NUP
  read (u,*, END=200, ERR=505) IDUP, ISTUP, MOTHUP(1), MOTHUP(2), &
    ICOLUP(1), ICOLUP(2), (PUP (J),J=1,5), VTIMUP, SPINUP
  if (model_in%test_field (IDUP)) then
    model => model_in
  else if (model_hadrons%test_field (IDUP)) then
    model => model_hadrons
  else
    write (buffer, "(I5)") IDUP
    call msg_error ("Parton " // buffer // &
        " found neither in given model file nor in SM_hadrons")
    return
  end if
  if (debug_lhef) then
    print *, "IDUP, ISTUP, MOTHUP, PUP = ", IDUP, ISTUP, MOTHUP(1), &
      MOTHUP(2), PUP
  end if
  call flv%init (IDUP, model)
  if (IABS(IDUP) == 2212 .or. IABS(IDUP) == 2112) then

```

```

! PYTHIA sometimes sets color indices for protons and neutrons (?)
ICOLUP (1) = 0
ICOLUP (2) = 0
end if
call col%init_col_acl (ICOLUP (1), ICOLUP (2))
!!! Settings for unpolarized particles
! particle_set%prt (oldsize+i)%hel = ??
! particle_set%prt (oldsize+i)%pol = ??
if (MOTHUP(1) /= 0) then
  mothers(i) = MOTHUP(1)
end if
pup_dum = PUP
if (pup_dum(4) < 1E-10_default) cycle
mom = vector4_moving (pup_dum (4), &
  vector3_moving ([pup_dum (1), pup_dum (2), pup_dum (3)]))
not_found = .true.
SCAN_PARTICLES: do j = 1, n_tot
  d_mom = prt_tmp(j)%get_momentum ()
  if (all (nearly_equal &
    (mom%p, d_mom%p, abs_smallness = 1.E-4_default)) .and. &
    (prt_tmp(j)%get_pdg () == IDUP)) then
    if (.not. prt_tmp(j)%get_status () == PRT_BEAM .or. &
      .not. prt_tmp(j)%get_status () == PRT_BEAM_REMNANT) &
      relations(i) = j
    not_found = .false.
  end if
end do SCAN_PARTICLES
if (not_found) then
  if (debug_lhef) &
    print *, "Not found: adding particle"
  call prt_tmp(n_tot+n_entries)%set_flavor (flv)
  call prt_tmp(n_tot+n_entries)%set_color (col)
  call prt_tmp(n_tot+n_entries)%set_momentum (mom)
  if (MOTHUP(1) /= 0) then
    if (relations(MOTHUP(1)) /= 0) then
      call prt_tmp(n_tot+n_entries)%set_parents &
        ([relations(MOTHUP(1))])
      call prt_tmp(relations(MOTHUP(1)))%add_child (n_tot+n_entries)
      if (prt_tmp(relations(MOTHUP(1)))%get_status () &
        == PRT_OUTGOING) &
        call prt_tmp(relations(MOTHUP(1)))%reset_status &
          (PRT_VIRTUAL)
    end if
  end if
  call prt_tmp(n_tot+n_entries)%set_status (PRT_OUTGOING)
  if (debug_lhef) call prt_tmp(n_tot+n_entries)%write ()
  n_entries = n_entries + 1
end if
end do PARTICLE_LOOP
do i = 1, n_tot
  if (prt_tmp(i)%get_status () == PRT_OUTGOING .and. &
    prt_tmp(i)%get_n_children () /= 0) then
    call prt_tmp(i)%reset_status (PRT_VIRTUAL)
  end if
end do

```

```

end do

allocate (prt (1:n_tot+n_entries-1))
prt = prt_tmp (1:n_tot+n_entries-1)
! transfer to particle_set
call particle_set%replace (prt)
deallocate (prt, prt_tmp)

if (debug_lhef) then
  call particle_set%write ()
  print *, "combine_lhef_with_particle_set"
  ! stop
end if

200 continue
return

501 write(*,*) "READING LHEF failed 501"
return
502 write(*,*) "READING LHEF failed 502"
return
503 write(*,*) "READING LHEF failed 503"
return
504 write(*,*) "READING LHEF failed 504"
return
505 write(*,*) "READING LHEF failed 505"
return
end subroutine combine_lhef_with_particle_set

<HEP common: public>+≡
  public :: w2p_write_lhef_event

<HEP common: sub interfaces>+≡
  module subroutine w2p_write_lhef_event (unit)
    integer, intent(in) :: unit
  end subroutine w2p_write_lhef_event

<HEP common: procedures>+≡
  module subroutine w2p_write_lhef_event (unit)
    integer, intent(in) :: unit
    type(xml_tag_t), allocatable :: tag_lhef, tag_head, tag_init, &
      tag_event, tag_gen_n, tag_gen_v
    if (debug_on) call msg_debug (D_EVENTS, "w2p_write_lhef_event")
    allocate (tag_lhef, tag_head, tag_init, tag_event, &
      tag_gen_n, tag_gen_v)
    call tag_lhef%init (var_str ("LesHouchesEvents"), &
      [xml_attribute (var_str ("version"), var_str ("1.0"))], .true.)
    call tag_head%init (var_str ("header"), .true.)
    call tag_init%init (var_str ("init"), .true.)
    call tag_event%init (var_str ("event"), .true.)
    call tag_gen_n%init (var_str ("generator_name"), .true.)
    call tag_gen_v%init (var_str ("generator_version"), .true.)
    call tag_lhef%write (unit); write (unit, *)
    call tag_head%write (unit); write (unit, *)
    write (unit, "(2x)", advance = "no")

```

```

call tag_gen_n%write (var_str ("WHIZARD"), unit)
write (unit, *)
write (unit, "(2x)", advance = "no")
call tag_gen_v%write (var_str ("Version"), unit)
write (unit, *)
call tag_head%close (unit); write (unit, *)
call tag_init%write (unit); write (unit, *)
call heprup_write_lhef (unit)
call tag_init%close (unit); write (unit, *)
call tag_event%write (unit); write (unit, *)
call hepeup_write_lhef (unit)
call tag_event%close (unit); write (unit, *)
call tag_lhef%close (unit); write (unit, *)
deallocate (tag_lhef, tag_head, tag_init, tag_event, &
            tag_gen_n, tag_gen_v)
end subroutine w2p_write_lhef_event

```

Extract parameters from the common block. We leave it to the caller to specify which parameters it actually needs.

PDFGUP and PDFSUP are not extracted. IDWTUP=1,2 are not supported by WHIZARD, but correspond to weighted events.

```

<HEP common: public>+≡
public :: heprup_get_run_parameters

<HEP common: sub interfaces>+≡
module subroutine heprup_get_run_parameters &
    (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)
    integer, dimension(2), intent(out), optional :: beam_pdg
    real(default), dimension(2), intent(out), optional :: beam_energy
    integer, intent(out), optional :: n_processes
    logical, intent(out), optional :: unweighted
    logical, intent(out), optional :: negative_weights
end subroutine heprup_get_run_parameters

<HEP common: procedures>+≡
module subroutine heprup_get_run_parameters &
    (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)
    integer, dimension(2), intent(out), optional :: beam_pdg
    real(default), dimension(2), intent(out), optional :: beam_energy
    integer, intent(out), optional :: n_processes
    logical, intent(out), optional :: unweighted
    logical, intent(out), optional :: negative_weights
    if (present (beam_pdg)) beam_pdg = IDBMUP
    if (present (beam_energy)) beam_energy = EBMUP
    if (present (n_processes)) n_processes = NPRUP
    if (present (unweighted)) then
        select case (abs (IDWTUP))
            case (3)
                unweighted = .true.
            case (4)
                unweighted = .false.
            case (1,2) !!! not supported by WHIZARD
                unweighted = .false.
            case default

```

```

        call msg_fatal ("HEPRUP: unsupported IDWTUP value")
    end select
end if
if (present (negative_weights)) then
    negative_weights = IDWTUP < 0
end if
end subroutine heprup_get_run_parameters

```

Specify PDF set info. Since we support only LHAPDF, the group entry is zero.

```

<HEP common: public>+≡
    public :: heprup_set_lhapdf_id

<HEP common: sub interfaces>+≡
    module subroutine heprup_set_lhapdf_id (i_beam, pdf_id)
        integer, intent(in) :: i_beam, pdf_id
    end subroutine heprup_set_lhapdf_id

<HEP common: procedures>+≡
    module subroutine heprup_set_lhapdf_id (i_beam, pdf_id)
        integer, intent(in) :: i_beam, pdf_id
        PDFGUP(i_beam) = 0
        PDFSUP(i_beam) = pdf_id
    end subroutine heprup_set_lhapdf_id

```

Fill the characteristics for a particular process. Only the process ID is mandatory. Note that WHIZARD computes cross sections in fb, so we have to rescale to pb. The maximum weight is meaningless for unweighted events.

```

<HEP common: public>+≡
    public :: heprup_set_process_parameters

<HEP common: sub interfaces>+≡
    module subroutine heprup_set_process_parameters &
        (i, process_id, cross_section, error, max_weight, is_width)
        integer, intent(in) :: i, process_id
        real(default), intent(in), optional :: cross_section, error, max_weight
        logical, intent(in), optional :: is_width
    end subroutine heprup_set_process_parameters

<HEP common: procedures>+≡
    module subroutine heprup_set_process_parameters &
        (i, process_id, cross_section, error, max_weight, is_width)
        integer, intent(in) :: i, process_id
        real(default), intent(in), optional :: cross_section, error, max_weight
        logical, intent(in), optional :: is_width
        logical :: is_w
        is_w = .false.
        if (present (is_width)) is_w = is_width
        LPRUP(i) = process_id
        if (present (cross_section)) then
            if (is_w) then
                XSECUP(i) = cross_section
            else
                XSECUP(i) = cross_section * pb_per_fb
            end if
        else

```

```

        XSECUP(i) = 0
    end if
    if (present (error)) then
        if (is_w) then
            XERRUP(i) = error
        else
            XERRUP(i) = error * pb_per_fb
        end if
    else
        XERRUP(i) = 0
    end if
    select case (IDWTUP)
    case (3); XMAXUP(i) = 1
    case (4)
        if (present (max_weight)) then
            if (is_w) then
                XMAXUP(i) = max_weight
            else
                XMAXUP(i) = max_weight * pb_per_fb
            end if
        else
            XMAXUP(i) = 0
        end if
    end select
end subroutine heprup_set_process_parameters

```

Extract the process parameters, as far as needed.

(HEP common: public)+≡

```
public :: heprup_get_process_parameters
```

(HEP common: sub interfaces)+≡

```

module subroutine heprup_get_process_parameters &
    (i, process_id, cross_section, error, max_weight, is_width)
    integer, intent(in) :: i
    integer, intent(out), optional :: process_id
    real(default), intent(out), optional :: cross_section, error, max_weight
    logical, intent(in), optional :: is_width
end subroutine heprup_get_process_parameters

```

(HEP common: procedures)+≡

```

module subroutine heprup_get_process_parameters &
    (i, process_id, cross_section, error, max_weight, is_width)
    integer, intent(in) :: i
    integer, intent(out), optional :: process_id
    real(default), intent(out), optional :: cross_section, error, max_weight
    logical, intent(in), optional :: is_width
    logical :: is_w
    is_w = .false.
    if (present (is_width)) is_w = is_width
    if (present (process_id)) process_id = LPRUP(i)
    if (present (cross_section)) then
        if (is_w) then
            cross_section = XSECUP(i)
        else
            cross_section = XSECUP(i) / pb_per_fb
        end if
    end if
end subroutine heprup_get_process_parameters

```

```

        end if
    end if
    if (present (error)) then
        if (is_w) then
            error = XERRUP(i)
        else
            error = XERRUP(i) / pb_per_fb
        end if
    end if
    if (present (max_weight)) then
        select case (IDWTUP)
        case (3)
            max_weight = 1
        case (4)
            max_weight = XMAXUP(i) / pb_per_fb
        case (1,2)    !!! not supported by WHIZARD
            max_weight = 0
        case default
            call msg_fatal ("HEPRUP: unsupported IDWTUP value")
        end select
    end if
end subroutine heprup_get_process_parameters

```

18.11.4 Run parameter output (verbose)

This is a verbose output of the HEPRUP block.

```

<HEP common: public>+≡
    public :: heprup_write_verbose

<HEP common: sub interfaces>+≡
    module subroutine heprup_write_verbose (unit)
        integer, intent(in), optional :: unit
    end subroutine heprup_write_verbose

<HEP common: procedures>+≡
    module subroutine heprup_write_verbose (unit)
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(A)") "HEPRUP Common Block"
        write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "IDBMUP", IDBMUP, &
            "PDG code of beams"
        write (u, "(3x,A6,' = ',G12.5,1x,G12.5,8x,A)") "EBMUP ", EBMUP, &
            "Energy of beams in GeV"
        write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "PDFGUP", PDFGUP, &
            "PDF author group [-1 = undefined]"
        write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "PDFSUP", PDFSUP, &
            "PDF set ID [-1 = undefined]"
        write (u, "(3x,A6,' = ',I9,3x,1x,9x,3x,8x,A)") "IDWTUP", IDWTUP, &
            "LHA code for event weight mode"
        write (u, "(3x,A6,' = ',I9,3x,1x,9x,3x,8x,A)") "NPRUP ", NPRUP, &
            "Number of user subprocesses"
        do i = 1, NPRUP

```

```

write (u, "(1x,A,I0)") "Subprocess #", i
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XSECUP", XSECUP(i), &
"Cross section in pb"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XERRUP", XERRUP(i), &
"Cross section error in pb"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XMAXUP", XMAXUP(i), &
"Maximum event weight (cf. IDWTUP)"
write (u, "(3x,A6,' = ',I9,3x,1x,12x,8x,A)") "LPRUP ", LPRUP(i), &
"Subprocess ID"
end do
end subroutine heprup_write_verbose

```

18.11.5 Run parameter output (other formats)

This routine writes the initialization block according to the LHEF standard. It uses the current contents of the HEPRUP block.

```

<HEP common: public>+≡
public :: heprup_write_lhef

<HEP common: sub interfaces>+≡
module subroutine heprup_write_lhef (unit)
integer, intent(in), optional :: unit
end subroutine heprup_write_lhef

<HEP common: procedures>+≡
module subroutine heprup_write_lhef (unit)
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(2(1x,I0),2(1x,ES17.10),6(1x,I0))") &
IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
do i = 1, NPRUP
write (u, "(3(1x,ES17.10),1x,I0)") &
XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
end do
end subroutine heprup_write_lhef

```

This routine is a complete dummy at the moment. It uses the current contents of the HEPRUP block. At the end, it should depend on certain input flags for the different ASCII event formats.

```

<HEP common: public>+≡
public :: heprup_write_ascii

<HEP common: sub interfaces>+≡
module subroutine heprup_write_ascii (unit)
integer, intent(in), optional :: unit
end subroutine heprup_write_ascii

<HEP common: procedures>+≡
module subroutine heprup_write_ascii (unit)
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return

```



```

write (u, "(2(1x,I0),2(1x,ES17.10),6(1x,I0))") &
      IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
do i = 1, NPRUP
  write (u, "(3(1x,ES17.10),1x,I0)") &
        XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
end do
end subroutine heprup_write_ascii

```

Run parameter input (LHEF)

In a LHEF file, the parameters are written in correct order on separate lines, but we should not count on the precise format. List-directed input should just work.

```

<HEP common: public>+≡
  public :: heprup_read_lhef

<HEP common: sub interfaces>+≡
  module subroutine heprup_read_lhef (u)
    integer, intent(in) :: u
  end subroutine heprup_read_lhef

<HEP common: procedures>+≡
  module subroutine heprup_read_lhef (u)
    integer, intent(in) :: u
    integer :: i
    read (u, *) &
      IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
    do i = 1, NPRUP
      read (u, *) &
        XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
    end do
  end subroutine heprup_read_lhef

```

18.11.6 The HEPEUP common block

```

<HEP common: common blocks>+≡
  common /HEPEUP/ &
    NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP, &
    IDUP, ISTUP, MOTHUP, ICOLUP, PUP, VTIMUP, SPINUP
  save /HEPEUP/

```

Initialization

Fill the event characteristics of the common block. The initialization sets only the number of particles and initializes the rest with default values. The other routine sets the optional parameters.

```

<HEP common: public>+≡
  public :: hepeup_init
  public :: hepeup_set_event_parameters

```

```

<HEP common: sub interfaces>+≡
  module subroutine hepeup_init (n_tot)
    integer, intent(in) :: n_tot
  end subroutine hepeup_init
  module subroutine hepeup_set_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(in), optional :: proc_id
    real(default), intent(in), optional :: &
      weight, scale, alpha_qed, alpha_qcd
  end subroutine hepeup_set_event_parameters

<HEP common: procedures>+≡
  module subroutine hepeup_init (n_tot)
    integer, intent(in) :: n_tot
    NUP = n_tot
    IDPRUP = 0
    XWGTUP = 1
    SCALUP = -1
    AQEDUP = -1
    AQCDUP = -1
  end subroutine hepeup_init

  module subroutine hepeup_set_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(in), optional :: proc_id
    real(default), intent(in), optional :: &
      weight, scale, alpha_qed, alpha_qcd
    if (present (proc_id)) IDPRUP = proc_id
    if (present (weight)) XWGTUP = weight
    if (present (scale)) SCALUP = scale
    if (present (alpha_qed)) AQEDUP = alpha_qed
    if (present (alpha_qcd)) AQCDUP = alpha_qcd
  end subroutine hepeup_set_event_parameters

```

Extract event information. The caller determines the parameters.

```

<HEP common: public>+≡
  public :: hepeup_get_event_parameters

<HEP common: sub interfaces>+≡
  module subroutine hepeup_get_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(out), optional :: proc_id
    real(default), intent(out), optional :: &
      weight, scale, alpha_qed, alpha_qcd
  end subroutine hepeup_get_event_parameters

<HEP common: procedures>+≡
  module subroutine hepeup_get_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(out), optional :: proc_id
    real(default), intent(out), optional :: &
      weight, scale, alpha_qed, alpha_qcd
    if (present (proc_id)) proc_id = IDPRUP
    if (present (weight)) weight = XWGTUP
    if (present (scale)) scale = SCALUP

```

```

        if (present (alpha_qed)) alpha_qed = AQEDUP
        if (present (alpha_qcd)) alpha_qcd = AQCDUP
    end subroutine hepeup_get_event_parameters

```

Particle data

Below we need the particle status codes which are actually defined in the `subevents` module.

Set the entry for a specific particle. All parameters are set with the exception of lifetime and spin, where default values are stored.

```

<HEP common: public>+≡
    public :: hepeup_set_particle

<HEP common: sub interfaces>+≡
    module subroutine hepeup_set_particle (i, pdg, status, parent, col, p, m2)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        type(vector4_t), intent(in) :: p
        integer, dimension(2), intent(in) :: col
        real(default), intent(in) :: m2
    end subroutine hepeup_set_particle

<HEP common: procedures>+≡
    module subroutine hepeup_set_particle (i, pdg, status, parent, col, p, m2)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        type(vector4_t), intent(in) :: p
        integer, dimension(2), intent(in) :: col
        real(default), intent(in) :: m2
        if (i > MAXNUP) then
            call msg_error (arr=[ &
                var_str ("Too many particles in HEPEUP common block. " // &
                    "If this happened "), &
                var_str ("during event output, your events will be " // &
                    "invalid; please consider "), &
                var_str ("switching to a modern event format like HEPMC. " // &
                    "If you are not "), &
                var_str ("using an old, HEPEUP based format and " // &
                    "nevertheless get this error,"), &
                var_str ("please notify the WHIZARD developers,") ])
            return
        end if
        IDUP(i) = pdg
        select case (status)
        case (PRT_BEAM);           ISTUP(i) = -9
        case (PRT_INCOMING);       ISTUP(i) = -1
        case (PRT_BEAM_REMNANT);   ISTUP(i) = 3
        case (PRT_OUTGOING);       ISTUP(i) = 1
        case (PRT_RESONANT);       ISTUP(i) = 2
        case (PRT_VIRTUAL);        ISTUP(i) = 3
        case default;              ISTUP(i) = 0
    end subroutine

```

```

end select
select case (size (parent))
case (0);      MOTHUP(:,i) = 0
case (1);      MOTHUP(1,i) = parent(1); MOTHUP(2,i) = 0
case default;  MOTHUP(:,i) = [ parent(1), parent(size (parent)) ]
end select
if (col(1) > 0) then
    ICOLUP(1,i) = 500 + col(1)
else
    ICOLUP(1,i) = 0
end if
if (col(2) > 0) then
    ICOLUP(2,i) = 500 + col(2)
else
    ICOLUP(2,i) = 0
end if
PUP(1:3,i) = refmt_tiny (vector3_get_components (space_part (p)))
PUP(4,i) = refmt_tiny (energy (p))
PUP(5,i) = refmt_tiny (sign (sqrt (abs (m2))), m2))
VTIMUP(i) = 0
SPINUP(i) = 9
end subroutine hepeup_set_particle

```

Set the lifetime, actually $c\tau$ measured in mm, where τ is the invariant lifetime.

```

<HEP common: public>+≡
    public :: hepeup_set_particle_lifetime

<HEP common: sub interfaces>+≡
    module subroutine hepeup_set_particle_lifetime (i, lifetime)
        integer, intent(in) :: i
        real(default), intent(in) :: lifetime
    end subroutine hepeup_set_particle_lifetime

<HEP common: procedures>+≡
    module subroutine hepeup_set_particle_lifetime (i, lifetime)
        integer, intent(in) :: i
        real(default), intent(in) :: lifetime
        VTIMUP(i) = lifetime
    end subroutine hepeup_set_particle_lifetime

```

Set the particle spin entry. We need the cosine of the angle of the spin axis with respect to the three-momentum of the parent particle.

If the particle has a full polarization density matrix given, we need the particle momentum and polarization as well as the mother-particle momentum. The polarization is transformed into a spin vector (which is sensible only for spin-1/2 or massless particles), which then is transformed into the lab frame (by a rotation of the 3-axis to the particle momentum axis). Finally, we compute the scalar product of this vector with the mother-particle three-momentum.

This puts severe restrictions on the applicability of this definition, and Lorentz invariance is lost. Unfortunately, the Les Houches Accord requires this computation.

```

<HEP common: public>+≡
    public :: hepeup_set_particle_spin

```

```

<HEP common: interfaces>≡
  interface hepeup_set_particle_spin
    module procedure hepeup_set_particle_spin_pol
  end interface

<HEP common: sub interfaces>+≡
  module subroutine hepeup_set_particle_spin_pol (i, p, pol, p_mother)
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    type(polarization_t), intent(in) :: pol
    type(vector4_t), intent(in) :: p_mother
  end subroutine hepeup_set_particle_spin_pol

<HEP common: procedures>+≡
  module subroutine hepeup_set_particle_spin_pol (i, p, pol, p_mother)
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    type(polarization_t), intent(in) :: pol
    type(vector4_t), intent(in) :: p_mother
    type(vector3_t) :: s3, p3
    type(vector4_t) :: s4
    s3 = vector3_moving (pol%get_axis ())
    p3 = space_part (p)
    s4 = rotation_to_2nd (3, p3) * vector4_moving (0._default, s3)
    SPINUP(i) = enclosed_angle_ct (s4, p_mother)
  end subroutine hepeup_set_particle_spin_pol

```

Extract particle data. The caller decides which ones to retrieve.

Status codes: beam remnants share the status code with virtual particles. However, for the purpose of WHIZARD we should identify them. We use the PDG code for this.

```

<HEP common: public>+≡
  public :: hepeup_get_particle

<HEP common: sub interfaces>+≡
  module subroutine hepeup_get_particle (i, pdg, status, parent, col, p, m2)
    integer, intent(in) :: i
    integer, intent(out), optional :: pdg, status
    integer, dimension(:), intent(out), optional :: parent
    type(vector4_t), intent(out), optional :: p
    integer, dimension(2), intent(out), optional :: col
    real(default), dimension(5,MAXNUP) :: pup_def
    real(default), intent(out), optional :: m2
  end subroutine hepeup_get_particle

<HEP common: procedures>+≡
  module subroutine hepeup_get_particle (i, pdg, status, parent, col, p, m2)
    integer, intent(in) :: i
    integer, intent(out), optional :: pdg, status
    integer, dimension(:), intent(out), optional :: parent
    type(vector4_t), intent(out), optional :: p
    integer, dimension(2), intent(out), optional :: col
    real(default), dimension(5,MAXNUP) :: pup_def
    real(default), intent(out), optional :: m2
    if (present (pdg)) pdg = IDUP(i)
  end subroutine hepeup_get_particle

```

```

if (present (status)) then
  select case (ISTUP(i))
    case (-9); status = PRT_BEAM
    case (-1); status = PRT_INCOMING
    case (1); status = PRT_OUTGOING
    case (2); status = PRT_RESONANT
    case (3);
      select case (abs (IDUP(i)))
        case (HADRON_REMNANT, HADRON_REMNANT_SINGLET, &
              HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET)
          status = PRT_BEAM_REMNANT
        case default
          status = PRT_VIRTUAL
      end select
    case default
      status = PRT_UNDEFINED
  end select
end if
if (present (parent)) then
  select case (size (parent))
    case (0)
    case (1); parent(1) = MOTHUP(1,i)
    case (2); parent = MOTHUP(:,i)
  end select
end if
if (present (col)) then
  col = ICOLUP(:,i)
end if
if (present (p)) then
  pup_def = PUP
  p = vector4_moving (pup_def(4,i), vector3_moving (pup_def(1:3,i)))
end if
if (present (m2)) then
  m2 = sign (PUP(5,i) ** 2, PUP(5,i))
end if
end subroutine hepeup_get_particle

```

18.11.7 The HEPEVT and HEPEV4 common block

For the LEP Monte Carlos, a standard common block has been proposed in AKV89. We strongly recommend its use. (The description is an abbreviated transcription of AKV89, Vol. 3, pp. 327-330).

NMXHEP is the maximum number of entries:

```

<HEP common: variables>+≡
integer, parameter :: NMXHEP = 4000

```

NEVHEP is normally the event number, but may take special values as follows:

0 the program does not keep track of event numbers. -1 a special initialization record. -2 a special final record.

```

<HEP common: variables>+≡
integer :: NEVHEP

```

NHEP holds the number of entries for this event.

```
<HEP common: variables>+≡
integer, public :: NHEP
```

The entry ISTHEP(N) gives the status code for the Nth entry, with the following semantics: 0 a null entry. 1 an existing entry, which has not decayed or fragmented. 2 a decayed or fragmented entry, which is retained for event history information. 3 documentation line. 4- 10 reserved for future standards. 11-200 at the disposal of each model builder. 201- at the disposal of users.

```
<HEP common: variables>+≡
integer, dimension(NMXHEP), public :: ISTHEP
```

The Particle Data Group has proposed standard particle codes, which are to be stored in IDHEP(N).

```
<HEP common: variables>+≡
integer, dimension(NMXHEP), public :: IDHEP
```

JMOHEP(1,N) points to the mother of the Nth entry, if any. It is set to zero for initial entries. JMOHEP(2,N) points to the second mother, if any.

```
<HEP common: variables>+≡
integer, dimension(2, NMXHEP), public :: JMOHEP
```

JDAHEP(1,N) and JDAHEP(2,N) point to the first and last daughter of the Nth entry, if any. These are zero for entries which have not yet decayed. The other daughters are stored in between these two.

```
<HEP common: variables>+≡
integer, dimension(2, NMXHEP), public :: JDAHEP
```

In PHEP we store the momentum of the particle, more specifically this means that PHEP(1,N), PHEP(2,N), and PHEP(3,N) contain the momentum in the x , y , and z direction (as defined by the machine people), measured in GeV/c. PHEP(4,N) contains the energy in GeV and PHEP(5,N) the mass in GeV/ c^2 . The latter may be negative for spacelike partons.

```
<HEP common: variables>+≡
double precision, dimension(5, NMXHEP), public :: PHEP
```

Finally VHEP is the place to store the position of the production vertex. VHEP(1,N), VHEP(2,N), and VHEP(3,N) contain the x , y , and z coordinate (as defined by the machine people), measured in mm. VHEP(4,N) contains the production time in mm/c.

```
<HEP common: variables>+≡
double precision, dimension(4, NMXHEP) :: VHEP
```

As an amendment to the proposed standard common block HEPEVT, we also have a polarisation common block HEPSPN, as described in AKV89. SHEP(1,N), SHEP(2,N), and SHEP(3,N) give the x , y , and z component of the spinvector s of a fermion in the fermions restframe.

Furthermore, we add the polarization of the corresponding outgoing particles:

```
<HEP common: variables>+≡
    integer, dimension(NMXHEP) :: hepevt_pol
```

By this variable the identity of the current process is given, defined via the LPRUP codes.

```
<HEP common: variables>+≡
    integer, public :: idruplh
```

This is the event weight, i.e. the cross section divided by the total number of generated events for the output of the parton shower programs.

```
<HEP common: variables>+≡
    double precision, public :: eventweightlh
```

There are the values for the electromagnetic and the strong coupling constants, α_{em} and α_s .

```
<HEP common: variables>+≡
    double precision, public :: alphaqedlh, alphaqcdlh
```

This is the squared scale Q of the event.

```
<HEP common: variables>+≡
    double precision, dimension(10), public :: scalelh
```

Finally, these variables contain the spin information and the color/anticolor flow of the particles.

```
<HEP common: variables>+≡
    double precision, dimension (3,NMXHEP), public :: spinlh
    integer, dimension (2,NMXHEP), public :: icolorflowlh
```

By convention, SHEP(4,N) is always 1. All this is taken from StdHep 4.06 manual and written using Fortran90 conventions.

```
<HEP common: common blocks>+≡
    common /HEPEVT/ &
        NEVHEP, NHEP, ISTHEP, IDHEP, &
        JMOHEP, JDAHEP, PHEP, VHEP
    save /HEPEVT/
```

Here we store HEPEVT parameters of the WHIZARD 1 realization which are not part of the HEPEVT common block.

```
<HEP common: variables>+≡
    integer :: hepevt_n_out, hepevt_n_remnants

<HEP common: variables>+≡
    double precision :: hepevt_weight, hepevt_function_value
    double precision :: hepevt_function_ratio
```


The HEPEV4 common block is an extension of the HEPEVT common block to allow for partonic colored events, including especially the color flow etc.

```
<HEP common: common blocks>+≡
common /HEPEV4/ &
    eventweightlh, alphaqedlh, alphaqcdlh, scalelh, &
    spinlh, icolorflowlh, idruplh
save /HEPEV4/
```

Filling HEPEVT: If the event count is not provided, set NEVHEP to zero. If the event count is -1 or -2, the record corresponds to initialization and finalization, and the event is irrelevant.

Note that the event count may be larger than 2^{31} (2 GEvents). In that case, cut off the upper bits since NEVHEP is probably limited to default integer.

For the HEPEV4 common block, it is unclear why the `scalelh` variable is 10-dimensional. We choose to only set the first value of the array.

```
<HEP common: public>+≡
public :: hepevt_init
public :: hepevt_set_event_parameters

<HEP common: sub interfaces>+≡
module subroutine hepevt_init (n_tot, n_out)
    integer, intent(in) :: n_tot, n_out
end subroutine hepevt_init
module subroutine hepevt_set_event_parameters &
    (proc_id, weight, function_value, function_ratio, &
    alpha_qcd, alpha_qed, scale, i_evt)
    integer, intent(in), optional :: proc_id
    integer, intent(in), optional :: i_evt
    real(default), intent(in), optional :: weight, function_value, &
    function_ratio, alpha_qcd, alpha_qed, scale
end subroutine hepevt_set_event_parameters

<HEP common: procedures>+≡
module subroutine hepevt_init (n_tot, n_out)
    integer, intent(in) :: n_tot, n_out
    NHEP = n_tot
    NEVHEP = 0
    idruplh = 0
    hepevt_n_out = n_out
    hepevt_n_remnants = 0
    hepevt_weight = 1
    eventweightlh = 1
    hepevt_function_value = 0
    hepevt_function_ratio = 1
    alphaqcdlh = -1
    alphaqedlh = -1
    scalelh = -1
end subroutine hepevt_init

module subroutine hepevt_set_event_parameters &
    (proc_id, weight, function_value, function_ratio, &
    alpha_qcd, alpha_qed, scale, i_evt)
    integer, intent(in), optional :: proc_id
    integer, intent(in), optional :: i_evt
```

```

real(default), intent(in), optional :: weight, function_value, &
    function_ratio, alpha_qcd, alpha_qed, scale
if (present (proc_id)) idruplh = proc_id
if (present (i_evt)) NEVHEP = i_evt
if (present (weight)) then
    hepevt_weight = weight
    eventweightlh = weight
end if
if (present (function_value)) hepevt_function_value = &
    function_value
if (present (function_ratio)) hepevt_function_ratio = &
    function_ratio
if (present (alpha_qcd)) alphaqcdlh = alpha_qcd
if (present (alpha_qed)) alphaqedlh = alpha_qed
if (present (scale)) scalelh(1) = scale
if (present (i_evt)) NEVHEP = i_evt
end subroutine hepevt_set_event_parameters

```

Set the entry for a specific particle. All parameters are set with the exception of lifetime and spin, where default values are stored.

```

<HEP common: public>+≡
    public :: hepevt_set_particle

<HEP common: sub interfaces>+≡
    module subroutine hepevt_set_particle &
        (i, pdg, status, parent, child, p, m2, hel, vtx, &
         col, pol_status, pol, fill_hepev4)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        integer, dimension(:), intent(in) :: child
        logical, intent(in), optional :: fill_hepev4
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: m2
        integer, dimension(2), intent(in) :: col
        integer, intent(in) :: pol_status
        integer, intent(in) :: hel
        type(polarization_t), intent(in), optional :: pol
        type(vector4_t), intent(in) :: vtx
    end subroutine hepevt_set_particle

<HEP common: procedures>+≡
    module subroutine hepevt_set_particle &
        (i, pdg, status, parent, child, p, m2, hel, vtx, &
         col, pol_status, pol, fill_hepev4)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        integer, dimension(:), intent(in) :: child
        logical, intent(in), optional :: fill_hepev4
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: m2
        integer, dimension(2), intent(in) :: col
        integer, intent(in) :: pol_status
        integer, intent(in) :: hel

```

```

type(polarization_t), intent(in), optional :: pol
type(vector4_t), intent(in) :: vtx
logical :: hepev4
hepev4 = .false.; if (present (fill_hepev4)) hepev4 = fill_hepev4
IDHEP(i) = pdg
select case (status)
  case (PRT_BEAM);      ISTHEP(i) = 2
  case (PRT_INCOMING);  ISTHEP(i) = 2
  case (PRT_OUTGOING);  ISTHEP(i) = 1
  case (PRT_VIRTUAL);   ISTHEP(i) = 2
  case (PRT_RESONANT);  ISTHEP(i) = 2
  case default;         ISTHEP(i) = 0
end select
select case (size (parent))
case (0);      JMOHEP(:,i) = 0
case (1);      JMOHEP(1,i) = parent(1); JMOHEP(2,i) = 0
case default;  JMOHEP(:,i) = [ parent(1), parent(size (parent)) ]
end select
select case (size (child))
case (0);      JDAHEP(:,i) = 0
case (1);      JDAHEP(:,i) = child(1)
case default;  JDAHEP(:,i) = [ child(1), child(size (child)) ]
end select
PHEP(1:3,i) = refmt_tiny (vector3_get_components (space_part (p)))
PHEP(4,i) = refmt_tiny (energy (p))
PHEP(5,i) = refmt_tiny (sign (sqrt (abs (m2))), m2))
VHEP(1:3,i) = vtx%p(1:3)
VHEP(4,i) = vtx%p(0)
hepevt_pol(i) = hel
if (hepev4) then
  if (col(1) > 0) then
    icolorflowlh(1,i) = 500 + col(1)
  else
    icolorflowlh(1,i) = 0
  end if
  if (col(2) > 0) then
    icolorflowlh(2,i) = 500 + col(2)
  else
    icolorflowlh(2,i) = 0
  end if
  if (present (pol) .and. &
    pol_status == PRT_GENERIC_POLARIZATION) then
    if (pol%is_polarized ()) &
      spinlh(:,i) = pol%get_axis ()
  else
    spinlh(:,i) = zero
    spinlh(3,i) = hel
  end if
end if
end subroutine hepevt_set_particle

```

18.11.8 Event output

This is a verbose output of the HEPEVT block.

```
<HEP common: public>+≡
    public :: hepevt_write_verbose

<HEP common: sub interfaces>+≡
    module subroutine hepevt_write_verbose (unit)
        integer, intent(in), optional :: unit
    end subroutine hepevt_write_verbose

<HEP common: procedures>+≡
    module subroutine hepevt_write_verbose (unit)
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(A)") "HEPEVT Common Block"
        write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NEVHEP", NEVHEP, &
            "Event number"
        write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NHEP ", NHEP, &
            "Number of particles in event"
        do i = 1, NHEP
            write (u, "(1x,A,I0)") "Particle #", i
            write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)", advance="no") &
                "ISTHEP", ISTHEP(i), "Status code: "
            select case (ISTHEP(i))
            case ( 0); write (u, "(A)") "null entry"
            case ( 1); write (u, "(A)") "outgoing"
            case ( 2); write (u, "(A)") "decayed"
            case ( 3); write (u, "(A)") "documentation"
            case (4:10); write (u, "(A)") "[unspecified]"
            case (11:200); write (u, "(A)") "[model-specific]"
            case (201:); write (u, "(A)") "[user-defined]"
            case default; write (u, "(A)") "[undefined]"
            end select
            write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDHEP ", IDHEP(i), &
                "PDG code of particle"
            write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "JMOHEP", JMOHEP(:,i), &
                "Index of first/second mother"
            write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "JDAHEP", JDAHEP(:,i), &
                "Index of first/last daughter"
            write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "PHEP12", &
                PHEP(1:2,i), "Transversal momentum (x/y) in GeV"
            write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP3 ", PHEP(3,i), &
                "Longitudinal momentum (z) in GeV"
            write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP4 ", PHEP(4,i), &
                "Energy in GeV"
            write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP5 ", PHEP(5,i), &
                "Invariant mass in GeV"
            write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "VHEP12", VHEP(1:2,i), &
                "Transversal displacement (xy) in mm"
            write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VHEP3 ", VHEP(3,i), &
                "Longitudinal displacement (z) in mm"
            write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VHEP4 ", VHEP(4,i), &
                "Production time in mm"
```

```

end do
end subroutine hepevt_write_verbose

```

This is a verbose output of the HEPEUP block.

```

<HEP common: public>+≡
public :: hepeup_write_verbose

<HEP common: sub interfaces>+≡
module subroutine hepeup_write_verbose (unit)
integer, intent(in), optional :: unit
end subroutine hepeup_write_verbose

<HEP common: procedures>+≡
module subroutine hepeup_write_verbose (unit)
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(A)") "HEPEUP Common Block"
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NUP ", NUP, &
"Number of particles in event"
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDPRUP", IDPRUP, &
"Subprocess ID"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "XWGTUP", XWGTUP, &
"Event weight"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "SCALUP", SCALUP, &
"Event energy scale in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "AQEDUP", AQEDUP, &
"QED coupling [-1 = undefined]"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "AQCDUP", AQCDUP, &
"QCD coupling [-1 = undefined]"
do i = 1, NUP
write (u, "(1x,A,I0)") "Particle #", i
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDUP ", IDUP(i), &
"PDG code of particle"
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)", advance="no") &
"ISTUP ", ISTUP(i), "Status code: "
select case (ISTUP(i))
case (-1); write (u, "(A)") "incoming"
case ( 1); write (u, "(A)") "outgoing"
case (-2); write (u, "(A)") "spacelike"
case ( 2); write (u, "(A)") "resonance"
case ( 3); write (u, "(A)") "resonance (doc)"
case (-9); write (u, "(A)") "beam"
case default; write (u, "(A)") "[undefined]"
end select
write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "MOTHUP", MOTHUP(:,i), &
"Index of first/last mother"
write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "ICOLUP", ICOLUP(:,i), &
"Color/anticolor flow index"
write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "PUP1/2", PUP(1:2,i), &
"Transversal momentum (x/y) in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP3 ", PUP(3,i), &
"Longitudinal momentum (z) in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP4 ", PUP(4,i), &
"Energy in GeV"

```

```

        write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP5  ", PUP(5,i), &
            "Invariant mass in GeV"
        write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VTIMUP", VTIMUP(i), &
            "Invariant lifetime in mm"
        write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "SPINUP", SPINUP(i), &
            "cos(spin angle) [9 = undefined]"
    end do
end subroutine hepeup_write_verbose

```

18.11.9 Event output in various formats

This routine writes event output according to the LHEF standard. It uses the current contents of the HEPEUP block.

```

<HEP common: public>+=
    public :: hepeup_write_lhef
    public :: hepeup_write_lha

<HEP common: sub interfaces>+=
    module subroutine hepeup_write_lhef (unit)
        integer, intent(in), optional :: unit
    end subroutine hepeup_write_lhef
    module subroutine hepeup_write_lha (unit)
        integer, intent(in), optional :: unit
    end subroutine hepeup_write_lha

<HEP common: procedures>+=
    module subroutine hepeup_write_lhef (unit)
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        if (debug_on) call msg_debug (D_EVENTS, "hepeup_write_lhef")
        if (debug_on) call msg_debug2 (D_EVENTS, "ID IST MOTH ICOL P VTIM SPIN")
        write (u, "(2(1x,I0),4(1x,ES17.10))") &
            NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
        do i = 1, NUP
            write (u, "(6(1x,I0),7(1x,ES17.10))") &
                IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
                    PUP(:,i), VTIMUP(i), SPINUP(i)
            if (debug2_active (D_EVENTS)) then
                write (msg_buffer, "(6(1x,I0),7(1x,ES17.10))") &
                    IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
                        PUP(:,i), VTIMUP(i), SPINUP(i)
                call msg_message ()
            end if
        end do
    end subroutine hepeup_write_lhef

    module subroutine hepeup_write_lha (unit)
        integer, intent(in), optional :: unit
        integer :: u, i
        integer, dimension(MAXNUP) :: spin_up
        spin_up = int(SPINUP)
        u = given_output_unit (unit); if (u < 0) return

```

```

write (u, "(2(1x,I5),1x,ES17.10,3(1x,ES13.6))") &
    NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
write (u, "(500(1x,I5))") IDUP(:NUP)
write (u, "(500(1x,I5))") MOTHUP(1,:NUP)
write (u, "(500(1x,I5))") MOTHUP(2,:NUP)
write (u, "(500(1x,I5))") ICOLUP(1,:NUP)
write (u, "(500(1x,I5))") ICOLUP(2,:NUP)
write (u, "(500(1x,I5))") ISTUP(:NUP)
write (u, "(500(1x,I5))") spin_up(:NUP)
do i = 1, NUP
    write (u, "(1x,I5,4(1x,ES17.10))") i, PUP([ 4,1,2,3 ], i)
end do

end subroutine hepeup_write_lha

```

This routine writes event output according to the HEPEVT standard. It uses the current contents of the HEPEVT block and some additional parameters according to the standard in WHIZARD 1. For the long ASCII format, the value of the sample function (i.e. the product of squared matrix element, structure functions and phase space factor is printed out). The option of reweighting matrix elements with respect to some reference cross section is not implemented in WHIZARD 2 for this event format, therefore the second entry in the long ASCII format (the function ratio) is always one. The ATHENA format is an implementation of the HEPEVT format that is readable by the ATLAS ATHENA software framework. It is very similar to the WHIZARD 1 HEPEVT format, except that it contains an event counter, a particle counter inside the event, and has the HEPEVT ISTHEP status before the PDG code. The MOKKA format is a special ASCII format that contains the information to be parsed to the MOKKA LC fast simulation software.

```

<HEP common: public>+≡
public :: hepevt_write_hepevt
public :: hepevt_write_ascii
public :: hepevt_write_athena
public :: hepevt_write_mokka

<HEP common: sub interfaces>+≡
module subroutine hepevt_write_hepevt (unit)
    integer, intent(in), optional :: unit
end subroutine hepevt_write_hepevt
module subroutine hepevt_write_ascii (unit, long)
    integer, intent(in), optional :: unit
    logical, intent(in) :: long
end subroutine hepevt_write_ascii
module subroutine hepevt_write_athena (unit)
    integer, intent(in), optional :: unit
end subroutine hepevt_write_athena
module subroutine hepevt_write_mokka (unit)
    integer, intent(in), optional :: unit
end subroutine hepevt_write_mokka

<HEP common: procedures>+≡
module subroutine hepevt_write_hepevt (unit)
    integer, intent(in), optional :: unit

```

```

integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
do i = 1, NHEP
    write (u, "(7(1x,I0))") &
        ISTHEP(i), IDHEP(i), JMOHEP(:,i), JDAHEP(:,i), hepevt_pol(i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
    write (u, "(5(1x,ES17.10))") VHEP(:,i), 0.d0
end do
end subroutine hepevt_write_hepevt

module subroutine hepevt_write_ascii (unit, long)
integer, intent(in), optional :: unit
logical, intent(in) :: long
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
do i = 1, NHEP
    if (ISTHEP(i) /= 1) cycle
    write (u, "(2(1x,I0))") IDHEP(i), hepevt_pol(i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
end do
if (long) then
    write (u, "(2(1x,ES17.10))") &
        hepevt_function_value, hepevt_function_ratio
end if
end subroutine hepevt_write_ascii

module subroutine hepevt_write_athena (unit)
integer, intent(in), optional :: unit
integer :: u, i, num_event
num_event = 0
u = given_output_unit (unit); if (u < 0) return
write (u, "(2(1x,I0))") NEVHEP, NHEP
do i = 1, NHEP
    write (u, "(7(1x,I0))") &
        i, ISTHEP(i), IDHEP(i), JMOHEP(:,i), JDAHEP(:,i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
    write (u, "(5(1x,ES17.10))") VHEP(1:4,i)
end do
end subroutine hepevt_write_athena

module subroutine hepevt_write_mokka (unit)
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
do i = 1, NHEP
    write (u, "(4(1x,I0),4(1x,ES17.10))") &
        ISTHEP(i), IDHEP(i), JDAHEP(1,i), JDAHEP(2,i), &
        PHEP(1:3,i), PHEP(5,i)
end do
end subroutine hepevt_write_mokka

```



```

end do
end subroutine hepevt_write_mokka

```

18.11.10 Event input in various formats

This routine writes event output according to the LHEF standard. It uses the current contents of the HEPEUP block.

```

<HEP common: public>+≡
public :: hepeup_read_lhef

<HEP common: sub interfaces>+≡
module subroutine hepeup_read_lhef (u)
  integer, intent(in) :: u
end subroutine hepeup_read_lhef

<HEP common: procedures>+≡
module subroutine hepeup_read_lhef (u)
  integer, intent(in) :: u
  integer :: i
  read (u, *) &
    NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
  do i = 1, NUP
    read (u, *) &
      IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
        PUP(:,i), VTIMUP(i), SPINUP(i)
  end do
end subroutine hepeup_read_lhef

```

18.11.11 Data Transfer: particle sets

The WHIZARD format for handling particle data in events is `particle_set_t`. We have to interface this to the common blocks.

We first create a new particle set that contains only the particles that are supported by the LHEF format. These are: beam, incoming, resonant, outgoing. We drop particles with unknown, virtual or beam-remnant status.

From this set we fill the common block. Event information such as process ID and weight is not transferred here; this has to be done by the caller. The spin information is set only if the particle has a unique mother, and if its polarization is fully defined.

We use this routine also to hand over information to Pythia which lets Tauola access SPINUP. Tauola expects in SPINUP the helicity and not the LHA convention. We switch to this mode with `tauola_convention`.

```

<HEP common: public>+≡
public :: hepeup_from_particle_set

<HEP common: sub interfaces>+≡
module subroutine hepeup_from_particle_set (pset_in, &
  keep_beams, keep_remnants, tauola_convention)
  type(particle_set_t), intent(in) :: pset_in
  type(particle_set_t), target :: pset
  logical, intent(in), optional :: keep_beams

```

```

        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: tauola_convention
    end subroutine hepeup_from_particle_set

    (HEP common: procedures)+≡
    module subroutine hepeup_from_particle_set (pset_in, &
        keep_beams, keep_remnants, tauola_convention)
        type(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), target :: pset
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: tauola_convention
        integer :: i, n_parents, status, n_tot
        integer, dimension(1) :: i_mother
        logical :: kr, tc
        kr = .true.; if (present (keep_remnants)) kr = keep_remnants
        tc = .false.; if (present (tauola_convention)) tc = tauola_convention
        call pset_in%filter_particles (pset, real_parents = .true. , &
            keep_beams = keep_beams, keep_virtuals = .false.)
        n_tot = pset%get_n_tot ()
        call hepeup_init (n_tot)
        do i = 1, n_tot
            associate (prt => pset%prt(i))
                status = prt%get_status ()
                if (kr .and. status == PRT_BEAM_REMNANT &
                    .and. prt%get_n_children () == 0) &
                    status = PRT_OUTGOING
                call hepeup_set_particle (i, &
                    prt%get_pdg (), &
                    status, &
                    prt%get_parents (), &
                    prt%get_color (), &
                    prt%get_momentum (), &
                    prt%get_p2 ())
                n_parents = prt%get_n_parents ()
                call hepeup_set_particle_lifetime (i, &
                    prt%get_lifetime ())
                if (.not. tc) then
                    if (n_parents == 1) then
                        i_mother = prt%get_parents ()
                        select case (prt%get_polarization_status ())
                        case (PRT_GENERIC_POLARIZATION)
                            call hepeup_set_particle_spin (i, &
                                prt%get_momentum (), &
                                prt%get_polarization (), &
                                pset%prt(i_mother(1))%get_momentum ())
                        end select
                    end if
                else
                    select case (prt%get_polarization_status ())
                    case (PRT_DEFINITE_HELICITY)
                        SPINUP(i) = prt%get_helicity()
                    end select
                end if
            end associate
        end do
    end module

```

```

end do
end subroutine hepeup_from_particle_set

```

Input. The particle set should be allocated properly, but we replace the particle contents.

If there are no beam particles in the event, we try to reconstruct beam particles and beam remnants. We assume for simplicity that the beam particles, if any, are the first two particles. If they are absent, the first two particles should be the incoming partons.

```

<HEP common: public>+≡
public :: hepeup_to_particle_set

<HEP common: sub interfaces>+≡
module subroutine hepeup_to_particle_set &
    (particle_set, recover_beams, model, alt_model)
    type(particle_set_t), intent(inout), target :: particle_set
    logical, intent(in), optional :: recover_beams
    class(model_data_t), intent(in), target :: model, alt_model
end subroutine hepeup_to_particle_set

<HEP common: procedures>+≡
module subroutine hepeup_to_particle_set &
    (particle_set, recover_beams, model, alt_model)
    type(particle_set_t), intent(inout), target :: particle_set
    logical, intent(in), optional :: recover_beams
    class(model_data_t), intent(in), target :: model, alt_model
    type(particle_t), dimension(:), allocatable :: prt
    integer, dimension(2) :: parent
    integer, dimension(:), allocatable :: child
    integer :: i, j, k, pdg, status
    type(flavor_t) :: flv
    type(color_t) :: col
    integer, dimension(2) :: c
    type(vector4_t) :: p
    real(default) :: p2
    logical :: reconstruct
    integer :: off
    if (present (recover_beams)) then
        reconstruct = recover_beams .and. .not. all (ISTUP(1:2) == PRT_BEAM)
    else
        reconstruct = .false.
    end if
    if (reconstruct) then
        off = 4
    else
        off = 0
    end if
    allocate (prt (NUP + off), child (NUP + off))
    do i = 1, NUP
        k = i + off
        call hepeup_get_particle (i, pdg, status, col = c, p = p, m2 = p2)
        call flv%init (pdg, model, alt_model)
        call prt(k)%set_flavor (flv)
        call prt(k)%reset_status (status)
    end do
end module hepeup_to_particle_set

```

```

      call col%init (c)
      call prt(k)%set_color (col)
      call prt(k)%set_momentum (p, p2)
      where (MOTHUP(:,i) /= 0)
        parent = MOTHUP(:,i) + off
      elsewhere
        parent = 0
      end where
      call prt(k)%set_parents (parent)
      child = [(j, j = 1 + off, NUP + off)]
      where (MOTHUP(1,:NUP) /= i .and. MOTHUP(2,:NUP) /= i) child = 0
      call prt(k)%set_children (child)
    end do
    if (reconstruct) then
      do k = 1, 2
        call prt(k)%reset_status (PRT_BEAM)
        call prt(k)%set_children ([k+2,k+4])
      end do
      do k = 3, 4
        call prt(k)%reset_status (PRT_BEAM_REMNANT)
        call prt(k)%set_parents ([k-2])
      end do
      do k = 5, 6
        call prt(k)%set_parents ([k-4])
      end do
    end if
    call particle_set%replace (prt)
  end subroutine hepeup_to_particle_set

```

The HEPEVT common block is quite similar, but does contain less information, e.g. no color flows (it was LEP time). The spin information is set only if the particle has a unique mother, and if its polarization is fully defined.

```

<HEP common: public>+≡
  public :: hepevt_from_particle_set

<HEP common: sub interfaces>+≡
  module subroutine hepevt_from_particle_set &
    (particle_set, keep_beams, keep_remnants, ensure_order, fill_hepev4)
    type(particle_set_t), intent(in) :: particle_set
    type(particle_set_t), target :: pset_hepevt, pset_tmp
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    logical, intent(in), optional :: ensure_order
    logical, intent(in), optional :: fill_hepev4
  end subroutine hepevt_from_particle_set

<HEP common: procedures>+≡
  module subroutine hepevt_from_particle_set &
    (particle_set, keep_beams, keep_remnants, ensure_order, fill_hepev4)
    type(particle_set_t), intent(in) :: particle_set
    type(particle_set_t), target :: pset_hepevt, pset_tmp
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    logical, intent(in), optional :: ensure_order

```

```

logical, intent(in), optional :: fill_hepev4
integer :: i, status, n_tot
logical :: activate_remnants, ensure
activate_remnants = .true.
if (present (keep_remnants)) activate_remnants = keep_remnants
ensure = .false.
if (present (ensure_order)) ensure = ensure_order
call particle_set%filter_particles (pset_tmp, real_parents = .true., &
    keep_virtuals = .false., keep_beams = keep_beams)
if (ensure) then
    call pset_tmp%to_hepevt_form (pset_hepevt)
else
    pset_hepevt = pset_tmp
end if
n_tot = pset_hepevt%get_n_tot ()
call hepevt_init (n_tot, pset_hepevt%get_n_out ())
do i = 1, n_tot
    associate (prt => pset_hepevt%prt(i))
        status = prt%get_status ()
        if (activate_remnants &
            .and. status == PRT_BEAM_REMNANT &
            .and. prt%get_n_children () == 0) &
            status = PRT_OUTGOING
        select case (prt%get_polarization_status ())
        case (PRT_GENERIC_POLARIZATION)
            call hepevt_set_particle (i, &
                prt%get_pdg (), status, &
                prt%get_parents (), &
                prt%get_children (), &
                prt%get_momentum (), &
                prt%get_p2 (), &
                prt%get_helicity (), &
                prt%get_vertex (), &
                prt%get_color (), &
                prt%get_polarization_status (), &
                pol = prt%get_polarization (), &
                fill_hepev4 = fill_hepev4)
        case default
            call hepevt_set_particle (i, &
                prt%get_pdg (), status, &
                prt%get_parents (), &
                prt%get_children (), &
                prt%get_momentum (), &
                prt%get_p2 (), &
                prt%get_helicity (), &
                prt%get_vertex (), &
                prt%get_color (), &
                prt%get_polarization_status (), &
                fill_hepev4 = fill_hepev4)
        end select
    end associate
end do
call pset_hepevt%final ()
end subroutine hepevt_from_particle_set

```

18.12 HepMC events

This section provides the interface to the HepMC C++ library for handling Monte-Carlo events.

Each C++ class of HepMC that we use is mirrored by a Fortran type, which contains as its only component the C pointer to the C++ object.

Each C++ method of HepMC that we use has a C wrapper function. This function takes a pointer to the host object as its first argument. Further arguments are either C pointers, or in the case of simple types (integer, real), interoperable C/Fortran objects.

The C wrapper functions have explicit interfaces in the Fortran module. They are called by Fortran wrapper procedures. These are treated as methods of the corresponding Fortran type.

```
<hepmc_interface.f90>≡  
  <File header>  
  
  module hepmc_interface  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use kinds>  
    <Use strings>  
    use lorentz  
    use flavors  
    use colors  
    use helicities  
    use polarizations  
    use event_handles, only: event_handle_t  
  
    <Standard module head>  
  
    <HepMC interface: public>  
  
    <HepMC interface: types>  
  
    <HepMC interface: parameters>  
  
    <HepMC interface: interfaces>  
  
    interface  
    <HepMC interface: sub interfaces>  
    end interface  
  
  end module hepmc_interface  
  
<hepmc_interface_sub.f90>≡  
  <File header>  
  
  submodule (hepmc_interface) hepmc_interface_s
```

```

    use constants, only: PI
    use physics_defs, only: pb_per_fb
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE
    use diagnostics

    implicit none

contains

    <HepMC interface: procedures>

end submodule hepmc_interface_s

```

18.12.1 Interface check

This function can be called in order to verify that we are using the actual HepMC library, and not the dummy version.

```

<HepMC interface: interfaces>≡
    interface
        logical(c_bool) function hepmc_available () bind(C)
        import
        end function hepmc_available
    end interface

<HepMC interface: public>≡
    public :: hepmc_is_available

<HepMC interface: sub interfaces>≡
    module function hepmc_is_available () result (flag)
        logical :: flag
    end function hepmc_is_available

<HepMC interface: procedures>≡
    module function hepmc_is_available () result (flag)
        logical :: flag
        flag = hepmc_available ()
    end function hepmc_is_available

```

18.12.2 FourVector

The C version of four-vectors is often transferred by value, and the associated procedures are all inlined. The wrapper needs to transfer by reference, so we create FourVector objects on the heap which have to be deleted explicitly. The input is a `vector4_t` or `vector3_t` object from the `lorentz` module.

```

<HepMC interface: public>+≡
    public :: hepmc_four_vector_t

<HepMC interface: types>≡
    type :: hepmc_four_vector_t
    private
    type(c_ptr) :: obj

```

```
end type hepmc_four_vector_t
```

In the C constructor, the zero-component (fourth argument) is optional; if missing, it is set to zero. The Fortran version has initializer form and takes either a three-vector or a four-vector. A further version extracts the four-vector from a HepMC particle object.

```
<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_four_vector_xyz (x, y, z) bind(C)
    import
    real(c_double), value :: x, y, z
    end function new_four_vector_xyz
  end interface
  interface
    type(c_ptr) function new_four_vector_xyzt (x, y, z, t) bind(C)
    import
    real(c_double), value :: x, y, z, t
    end function new_four_vector_xyzt
  end interface

<HepMC interface: public>+≡
  public :: hepmc_four_vector_init

<HepMC interface: interfaces>+≡
  interface hepmc_four_vector_init
    module procedure hepmc_four_vector_init_v4
    module procedure hepmc_four_vector_init_v3
    module procedure hepmc_four_vector_init_hepmc_prt
  end interface

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_four_vector_init_v4 (pp, p)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(vector4_t), intent(in) :: p
  end subroutine hepmc_four_vector_init_v4
  module subroutine hepmc_four_vector_init_v3 (pp, p)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(vector3_t), intent(in) :: p
  end subroutine hepmc_four_vector_init_v3
  module subroutine hepmc_four_vector_init_hepmc_prt (pp, prt)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(hepmc_particle_t), intent(in) :: prt
  end subroutine hepmc_four_vector_init_hepmc_prt

<HepMC interface: procedures>+≡
  module subroutine hepmc_four_vector_init_v4 (pp, p)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(vector4_t), intent(in) :: p
    real(default), dimension(0:3) :: pa
    pa = vector4_get_components (p)
    pp%obj = new_four_vector_xyzt &
      (real (pa(1), c_double), &
       real (pa(2), c_double), &
       real (pa(3), c_double), &
       real (pa(0), c_double))
```



```

end subroutine hepmc_four_vector_init_v4

module subroutine hepmc_four_vector_init_v3 (pp, p)
  type(hepmc_four_vector_t), intent(out) :: pp
  type(vector3_t), intent(in) :: p
  real(default), dimension(3) :: pa
  pa = vector3_get_components (p)
  pp%obj = new_four_vector_xyz &
    (real (pa(1), c_double), &
     real (pa(2), c_double), &
     real (pa(3), c_double))
end subroutine hepmc_four_vector_init_v3

module subroutine hepmc_four_vector_init_hepmc_prt (pp, prt)
  type(hepmc_four_vector_t), intent(out) :: pp
  type(hepmc_particle_t), intent(in) :: prt
  pp%obj = gen_particle_momentum (prt%obj)
end subroutine hepmc_four_vector_init_hepmc_prt

```

Here, the destructor is explicitly needed.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine four_vector_delete (p_obj) bind(C)
      import
      type(c_ptr), value :: p_obj
    end subroutine four_vector_delete
  end interface

<HepMC interface: public>+≡
  public :: hepmc_four_vector_final

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_four_vector_final (p)
    type(hepmc_four_vector_t), intent(inout) :: p
  end subroutine hepmc_four_vector_final

<HepMC interface: procedures>+≡
  module subroutine hepmc_four_vector_final (p)
    type(hepmc_four_vector_t), intent(inout) :: p
    call four_vector_delete (p%obj)
  end subroutine hepmc_four_vector_final

```

Convert to a Lorentz vector.

```

<HepMC interface: interfaces>+≡
  interface
    function four_vector_px (p_obj) result (px) bind(C)
      import
      real(c_double) :: px
      type(c_ptr), value :: p_obj
    end function four_vector_px
  end interface
  interface
    function four_vector_py (p_obj) result (py) bind(C)
      import

```

```

        real(c_double) :: py
        type(c_ptr), value :: p_obj
    end function four_vector_py
end interface
interface
    function four_vector_pz (p_obj) result (pz) bind(C)
        import
        real(c_double) :: pz
        type(c_ptr), value :: p_obj
    end function four_vector_pz
end interface
interface
    function four_vector_e (p_obj) result (e) bind(C)
        import
        real(c_double) :: e
        type(c_ptr), value :: p_obj
    end function four_vector_e
end interface
<HepMC interface: public>+≡
    public :: hepmc_four_vector_to_vector4
<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_four_vector_to_vector4 (pp, p)
        type(hepmc_four_vector_t), intent(in) :: pp
        type(vector4_t), intent(out) :: p
    end subroutine hepmc_four_vector_to_vector4
<HepMC interface: procedures>+≡
    module subroutine hepmc_four_vector_to_vector4 (pp, p)
        type(hepmc_four_vector_t), intent(in) :: pp
        type(vector4_t), intent(out) :: p
        real(default) :: E
        real(default), dimension(3) :: p3
        E = four_vector_e (pp%obj)
        p3(1) = four_vector_px (pp%obj)
        p3(2) = four_vector_py (pp%obj)
        p3(3) = four_vector_pz (pp%obj)
        p = vector4_moving (E, vector3_moving (p3))
    end subroutine hepmc_four_vector_to_vector4

```

18.12.3 Polarization

Polarization objects are temporarily used for assigning particle polarization. We add a flag `polarized`. If this is false, the polarization is not set and should not be transferred to `hepmc_particle` objects.

```

<HepMC interface: public>+≡
    public :: hepmc_polarization_t
<HepMC interface: types>+≡
    type :: hepmc_polarization_t
        private
        logical :: polarized = .false.
        type(c_ptr) :: obj

```

```
end type hepmc_polarization_t
```

Constructor. The C wrapper takes polar and azimuthal angle as arguments. The Fortran version allows for either a complete polarization density matrix, or for a definite (diagonal) helicity.

HepMC does not allow to specify the degree of polarization, therefore we have to map it to either 0 or 1. We choose 0 for polarization less than 0.5 and 1 for polarization greater than 0.5. Even this simplification works only for spin-1/2 and for massless particles; massive vector bosons cannot be treated this way. In particular, zero helicity is always translated as unpolarized.

For massive vector bosons, we arbitrarily choose the convention that the longitudinal (zero) helicity state is mapped to the theta angle $\pi/2$. This works under the condition that helicity is projected onto one of the basis states.

```
<HepMC interface: interfaces>+≡
```

```
interface
  type(c_ptr) function new_polarization (theta, phi) bind(C)
  import
    real(c_double), value :: theta, phi
  end function new_polarization
end interface
```

```
<HepMC interface: public>+≡
```

```
public :: hepmc_polarization_init
```

```
<HepMC interface: interfaces>+≡
```

```
interface hepmc_polarization_init
  module procedure hepmc_polarization_init_pol
  module procedure hepmc_polarization_init_hel
  module procedure hepmc_polarization_init_int
end interface
```

```
<HepMC interface: sub interfaces>+≡
```

```
module subroutine hepmc_polarization_init_pol (hpol, pol)
  type(hepmc_polarization_t), intent(out) :: hpol
  type(polarization_t), intent(in) :: pol
end subroutine hepmc_polarization_init_pol
module subroutine hepmc_polarization_init_hel (hpol, hel)
  type(hepmc_polarization_t), intent(out) :: hpol
  type(helicity_t), intent(in) :: hel
end subroutine hepmc_polarization_init_hel
module subroutine hepmc_polarization_init_int (hpol, hel)
  type(hepmc_polarization_t), intent(out) :: hpol
  integer, intent(in) :: hel
end subroutine hepmc_polarization_init_int
```

```
<HepMC interface: procedures>+≡
```

```
module subroutine hepmc_polarization_init_pol (hpol, pol)
  type(hepmc_polarization_t), intent(out) :: hpol
  type(polarization_t), intent(in) :: pol
  real(default) :: r, theta, phi
  if (pol%is_polarized ()) then
    call pol%to_angles (r, theta, phi)
    if (r >= 0.5) then
      hpol%polarized = .true.
      hpol%obj = new_polarization &
```

```

        (real (theta, c_double), real (phi, c_double))
    end if
end if
end subroutine hepmc_polarization_init_pol

module subroutine hepmc_polarization_init_hel (hpol, hel)
    type(hepmc_polarization_t), intent(out) :: hpol
    type(helicity_t), intent(in) :: hel
    integer, dimension(2) :: h
    if (hel%is_defined ()) then
        h = hel%to_pair ()
        select case (h(1))
            case (1:)
                hpol%polarized = .true.
                hpol%obj = new_polarization (0._c_double, 0._c_double)
            case (:-1)
                hpol%polarized = .true.
                hpol%obj = new_polarization (real (pi, c_double), 0._c_double)
            case (0)
                hpol%polarized = .true.
                hpol%obj = new_polarization (real (pi/2, c_double), 0._c_double)
        end select
    end if
end subroutine hepmc_polarization_init_hel

module subroutine hepmc_polarization_init_int (hpol, hel)
    type(hepmc_polarization_t), intent(out) :: hpol
    integer, intent(in) :: hel
    select case (hel)
        case (1:)
            hpol%polarized = .true.
            hpol%obj = new_polarization (0._c_double, 0._c_double)
        case (:-1)
            hpol%polarized = .true.
            hpol%obj = new_polarization (real (pi, c_double), 0._c_double)
        case (0)
            hpol%polarized = .true.
            hpol%obj = new_polarization (real (pi/2, c_double), 0._c_double)
    end select
end subroutine hepmc_polarization_init_int

```

Destructor. The C object is deallocated only if the polarized flag is set.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine polarization_delete (pol_obj) bind(C)
            import
            type(c_ptr), value :: pol_obj
        end subroutine polarization_delete
    end interface

<HepMC interface: public>+≡
    public :: hepmc_polarization_final

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_polarization_final (hpol)

```

```

        type(hepmc_polarization_t), intent(inout) :: hpol
    end subroutine hepmc_polarization_final
<HepMC interface: procedures>+≡
    module subroutine hepmc_polarization_final (hpol)
        type(hepmc_polarization_t), intent(inout) :: hpol
        if (hpol%polarized) call polarization_delete (hpol%obj)
    end subroutine hepmc_polarization_final

```

Recover polarization from HepMC polarization object (with the abovementioned deficiencies).

```

<HepMC interface: interfaces>+≡
    interface
        function polarization_theta (pol_obj) result (theta) bind(C)
            import
            real(c_double) :: theta
            type(c_ptr), value :: pol_obj
        end function polarization_theta
    end interface
    interface
        function polarization_phi (pol_obj) result (phi) bind(C)
            import
            real(c_double) :: phi
            type(c_ptr), value :: pol_obj
        end function polarization_phi
    end interface
<HepMC interface: public>+≡
    public :: hepmc_polarization_to_pol
<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_polarization_to_pol (hpol, flv, pol)
        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(polarization_t), intent(out) :: pol
    end subroutine hepmc_polarization_to_pol
<HepMC interface: procedures>+≡
    module subroutine hepmc_polarization_to_pol (hpol, flv, pol)
        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(polarization_t), intent(out) :: pol
        real(default) :: theta, phi
        theta = polarization_theta (hpol%obj)
        phi = polarization_phi (hpol%obj)
        call pol%init_angles (flv, 1._default, theta, phi)
    end subroutine hepmc_polarization_to_pol

```

Recover helicity. Here, ϕ is ignored and only the sign of $\cos \theta$ is relevant, mapped to positive/negative helicity.

```

<HepMC interface: public>+≡
    public :: hepmc_polarization_to_hel
<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_polarization_to_hel (hpol, flv, hel)

```

```

        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(out) :: hel
    end subroutine hepmc_polarization_to_hel

<HepMC interface: procedures>+≡
    module subroutine hepmc_polarization_to_hel (hpol, flv, hel)
        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(out) :: hel
        real(default) :: theta
        integer :: hmax
        theta = polarization_theta (hpol%obj)
        hmax = flv%get_spin_type () / 2
        call hel%init (sign (hmax, nint (cos (theta))))
    end subroutine hepmc_polarization_to_hel

```

18.12.4 GenParticle

Particle objects have the obvious meaning.

```

<HepMC interface: public>+≡
    public :: hepmc_particle_t

<HepMC interface: types>+≡
    type :: hepmc_particle_t
    private
    type(c_ptr) :: obj
    end type hepmc_particle_t

```

Constructor. The C version takes a FourVector object, which in the Fortran wrapper is created on the fly from a `vector4` Lorentz vector.

No destructor is needed as long as all particles are entered into vertex containers.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function new_gen_particle (prt_obj, pdg_id, status) bind(C)
            import
            type(c_ptr), value :: prt_obj
            integer(c_int), value :: pdg_id, status
        end function new_gen_particle
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_init

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_particle_init (prt, p, pdg, status)
        type(hepmc_particle_t), intent(out) :: prt
        type(vector4_t), intent(in) :: p
        integer, intent(in) :: pdg, status
    end subroutine hepmc_particle_init

```

<HepMC interface: procedures>+≡

```

module subroutine hepmc_particle_init (prt, p, pdg, status)
  type(hepmc_particle_t), intent(out) :: prt
  type(vector4_t), intent(in) :: p
  integer, intent(in) :: pdg, status
  type(hepmc_four_vector_t) :: pp
  call hepmc_four_vector_init (pp, p)
  prt%obj = new_gen_particle (pp%obj, int (pdg, c_int), int (status, c_int))
  call hepmc_four_vector_final (pp)
end subroutine hepmc_particle_init

```

Set the particle color flow.

<HepMC interface: interfaces>+≡

```

interface
  subroutine gen_particle_set_flow (prt_obj, code_index, code) bind(C)
    import
    type(c_ptr), value :: prt_obj
    integer(c_int), value :: code_index, code
  end subroutine gen_particle_set_flow
end interface

```

Set the particle color. Either from a color_t object or directly from a pair of integers.

<HepMC interface: interfaces>+≡

```

interface hepmc_particle_set_color
  module procedure hepmc_particle_set_color_col
  module procedure hepmc_particle_set_color_int
end interface hepmc_particle_set_color

```

<HepMC interface: public>+≡

```

public :: hepmc_particle_set_color

```

<HepMC interface: sub interfaces>+≡

```

module subroutine hepmc_particle_set_color_col (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt
  type(color_t), intent(in) :: col
end subroutine hepmc_particle_set_color_col
module subroutine hepmc_particle_set_color_int (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt
  integer, dimension(2), intent(in) :: col
end subroutine hepmc_particle_set_color_int

```

<HepMC interface: procedures>+≡

```

module subroutine hepmc_particle_set_color_col (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt
  type(color_t), intent(in) :: col
  integer(c_int) :: c
  c = col%get_col ()
  if (c /= 0) call gen_particle_set_flow (prt%obj, 1_c_int, c)
  c = col%get_acl ()
  if (c /= 0) call gen_particle_set_flow (prt%obj, 2_c_int, c)
end subroutine hepmc_particle_set_color_col

module subroutine hepmc_particle_set_color_int (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt

```

```

integer, dimension(2), intent(in) :: col
integer(c_int) :: c
c = col(1)
if (c /= 0) call gen_particle_set_flow (prt%obj, 1_c_int, c)
c = col(2)
if (c /= 0) call gen_particle_set_flow (prt%obj, 2_c_int, c)
end subroutine hepmc_particle_set_color_int

```

Set the particle polarization. For the restrictions on particle polarization in HepMC, see above `hepmc_polarization_init`.

<HepMC interface: interfaces>+≡

```

interface
  subroutine gen_particle_set_polarization (prt_obj, pol_obj) bind(C)
    import
    type(c_ptr), value :: prt_obj, pol_obj
  end subroutine gen_particle_set_polarization
end interface

```

<HepMC interface: public>+≡

```

public :: hepmc_particle_set_polarization

```

<HepMC interface: interfaces>+≡

```

interface hepmc_particle_set_polarization
  module procedure hepmc_particle_set_polarization_pol
  module procedure hepmc_particle_set_polarization_hel
  module procedure hepmc_particle_set_polarization_int
end interface

```

<HepMC interface: sub interfaces>+≡

```

module subroutine hepmc_particle_set_polarization_pol (prt, pol)
  type(hepmc_particle_t), intent(inout) :: prt
  type(polarization_t), intent(in) :: pol
end subroutine hepmc_particle_set_polarization_pol
module subroutine hepmc_particle_set_polarization_hel (prt, hel)
  type(hepmc_particle_t), intent(inout) :: prt
  type(helicity_t), intent(in) :: hel
end subroutine hepmc_particle_set_polarization_hel
module subroutine hepmc_particle_set_polarization_int (prt, hel)
  type(hepmc_particle_t), intent(inout) :: prt
  integer, intent(in) :: hel
end subroutine hepmc_particle_set_polarization_int

```

<HepMC interface: procedures>+≡

```

module subroutine hepmc_particle_set_polarization_pol (prt, pol)
  type(hepmc_particle_t), intent(inout) :: prt
  type(polarization_t), intent(in) :: pol
  type(hepmc_polarization_t) :: hpol
  call hepmc_polarization_init (hpol, pol)
  if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
  call hepmc_polarization_final (hpol)
end subroutine hepmc_particle_set_polarization_pol

```

```

module subroutine hepmc_particle_set_polarization_hel (prt, hel)
  type(hepmc_particle_t), intent(inout) :: prt
  type(helicity_t), intent(in) :: hel
  type(hepmc_polarization_t) :: hpol

```



```

    call hepmc_polarization_init (hpol, hel)
    if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
    call hepmc_polarization_final (hpol)
end subroutine hepmc_particle_set_polarization_hel

module subroutine hepmc_particle_set_polarization_int (prt, hel)
    type(hepmc_particle_t), intent(inout) :: prt
    integer, intent(in) :: hel
    type(hepmc_polarization_t) :: hpol
    call hepmc_polarization_init (hpol, hel)
    if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
    call hepmc_polarization_final (hpol)
end subroutine hepmc_particle_set_polarization_int

```

Return the HepMC barcode (unique integer ID) of the particle.

```

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_barcode (prt_obj) result (barcode) bind(C)
            import
            integer(c_int) :: barcode
            type(c_ptr), value :: prt_obj
        end function gen_particle_barcode
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_barcode

<HepMC interface: sub interfaces>+≡
    module function hepmc_particle_get_barcode (prt) result (barcode)
        integer :: barcode
        type(hepmc_particle_t), intent(in) :: prt
    end function hepmc_particle_get_barcode

<HepMC interface: procedures>+≡
    module function hepmc_particle_get_barcode (prt) result (barcode)
        integer :: barcode
        type(hepmc_particle_t), intent(in) :: prt
        barcode = gen_particle_barcode (prt%obj)
    end function hepmc_particle_get_barcode

```

Return the four-vector component of the particle object as a `vector4_t` Lorentz vector.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function gen_particle_momentum (prt_obj) bind(C)
            import
            type(c_ptr), value :: prt_obj
        end function gen_particle_momentum
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_momentum

<HepMC interface: sub interfaces>+≡
    module function hepmc_particle_get_momentum (prt) result (p)

```

```

        type(vector4_t) :: p
        type(hepmc_particle_t), intent(in) :: prt
    end function hepmc_particle_get_momentum

<HepMC interface: procedures>+≡
    module function hepmc_particle_get_momentum (prt) result (p)
        type(vector4_t) :: p
        type(hepmc_particle_t), intent(in) :: prt
        type(hepmc_four_vector_t) :: pp
        call hepmc_four_vector_init (pp, prt)
        call hepmc_four_vector_to_vector4 (pp, p)
        call hepmc_four_vector_final (pp)
    end function hepmc_particle_get_momentum

```

Return the invariant mass squared of the particle object. HepMC stores the signed invariant mass (no squaring).

```

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_generated_mass (prt_obj) result (mass) bind(C)
            import
            real(c_double) :: mass
            type(c_ptr), value :: prt_obj
        end function gen_particle_generated_mass
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_mass_squared

<HepMC interface: sub interfaces>+≡
    module function hepmc_particle_get_mass_squared (prt) result (m2)
        real(default) :: m2
        type(hepmc_particle_t), intent(in) :: prt
    end function hepmc_particle_get_mass_squared

<HepMC interface: procedures>+≡
    module function hepmc_particle_get_mass_squared (prt) result (m2)
        real(default) :: m2
        type(hepmc_particle_t), intent(in) :: prt
        real(default) :: m
        m = gen_particle_generated_mass (prt%obj)
        m2 = sign (m**2, m)
    end function hepmc_particle_get_mass_squared

```

Return the PDG ID:

```

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_pdg_id (prt_obj) result (pdg_id) bind(C)
            import
            integer(c_int) :: pdg_id
            type(c_ptr), value :: prt_obj
        end function gen_particle_pdg_id
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_pdg

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_get_pdg (prt) result (pdg)
    integer :: pdg
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_pdg

```

```

<HepMC interface: procedures>+≡
  module function hepmc_particle_get_pdg (prt) result (pdg)
    integer :: pdg
    type(hepmc_particle_t), intent(in) :: prt
    pdg = gen_particle_pdg_id (prt%obj)
  end function hepmc_particle_get_pdg

```

Return the status code:

```

<HepMC interface: interfaces>+≡
  interface
    function gen_particle_status (prt_obj) result (status) bind(C)
      import
      integer(c_int) :: status
      type(c_ptr), value :: prt_obj
    end function gen_particle_status
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_particle_get_status

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_get_status (prt) result (status)
    integer :: status
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_status

```

```

<HepMC interface: procedures>+≡
  module function hepmc_particle_get_status (prt) result (status)
    integer :: status
    type(hepmc_particle_t), intent(in) :: prt
    status = gen_particle_status (prt%obj)
  end function hepmc_particle_get_status

```

```

<HepMC interface: interfaces>+≡
  interface
    function gen_particle_is_beam (prt_obj) result (is_beam) bind(C)
      import
      logical(c_bool) :: is_beam
      type(c_ptr), value :: prt_obj
    end function gen_particle_is_beam
  end interface

```

Determine whether a particle is a beam particle.

```

<HepMC interface: public>+≡
  public :: hepmc_particle_is_beam

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_is_beam (prt) result (is_beam)
    logical :: is_beam
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_is_beam

```

```

<HepMC interface: procedures>+≡
  module function hepmc_particle_is_beam (prt) result (is_beam)
    logical :: is_beam
    type(hepmc_particle_t), intent(in) :: prt
    is_beam = gen_particle_is_beam (prt%obj)
  end function hepmc_particle_is_beam

```

Return the production/decay vertex (as a pointer, no finalization necessary).

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function gen_particle_production_vertex (prt_obj) bind(C)
      import
      type(c_ptr), value :: prt_obj
    end function gen_particle_production_vertex
  end interface
  interface
    type(c_ptr) function gen_particle_end_vertex (prt_obj) bind(C)
      import
      type(c_ptr), value :: prt_obj
    end function gen_particle_end_vertex
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_particle_get_production_vertex
  public :: hepmc_particle_get_decay_vertex

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_get_production_vertex (prt) result (v)
    type(hepmc_vertex_t) :: v
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_production_vertex
  module function hepmc_particle_get_decay_vertex (prt) result (v)
    type(hepmc_vertex_t) :: v
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_decay_vertex

```

```

<HepMC interface: procedures>+≡
  module function hepmc_particle_get_production_vertex (prt) result (v)
    type(hepmc_vertex_t) :: v
    type(hepmc_particle_t), intent(in) :: prt
    v%obj = gen_particle_production_vertex (prt%obj)
  end function hepmc_particle_get_production_vertex

  module function hepmc_particle_get_decay_vertex (prt) result (v)
    type(hepmc_vertex_t) :: v
    type(hepmc_particle_t), intent(in) :: prt
    v%obj = gen_particle_end_vertex (prt%obj)
  end function hepmc_particle_get_decay_vertex

```

Convenience function: Return the array of parent particles for a given HepMC particle. The contents are HepMC barcodes that still have to be mapped to the particle indices.

```

<HepMC interface: public>+≡
  public :: hepmc_particle_get_parent_barcodes
  public :: hepmc_particle_get_child_barcodes

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_get_parent_barcodes &
    (prt) result (parent_barcode)
    type(hepmc_particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: parent_barcode
  end function hepmc_particle_get_parent_barcodes
  module function hepmc_particle_get_child_barcodes &
    (prt) result (child_barcode)
    type(hepmc_particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: child_barcode
  end function hepmc_particle_get_child_barcodes

<HepMC interface: procedures>+≡
  module function hepmc_particle_get_parent_barcodes &
    (prt) result (parent_barcode)
    type(hepmc_particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: parent_barcode
    type(hepmc_vertex_t) :: v
    type(hepmc_vertex_particle_in_iterator_t) :: it
    integer :: i
    v = hepmc_particle_get_production_vertex (prt)
    if (hepmc_vertex_is_valid (v)) then
      allocate (parent_barcode (hepmc_vertex_get_n_in (v)))
      if (size (parent_barcode) /= 0) then
        if (HEPMC2_AVAILABLE) then
          call hepmc_vertex_particle_in_iterator_init (it, v)
          do i = 1, size (parent_barcode)
            parent_barcode(i) = hepmc_particle_get_barcode &
              (hepmc_vertex_particle_in_iterator_get (it))
            call hepmc_vertex_particle_in_iterator_advance (it)
          end do
          call hepmc_vertex_particle_in_iterator_final (it)
        else if (HEPMC3_AVAILABLE) then
          do i = 1, size (parent_barcode)
            parent_barcode(i) = hepmc_particle_get_barcode &
              (hepmc_vertex_get_nth_particle_in (v, i))
          end do
        end if
      end if
    end if
  else
    allocate (parent_barcode (0))
  end if
end function hepmc_particle_get_parent_barcodes

  module function hepmc_particle_get_child_barcodes &
    (prt) result (child_barcode)
    type(hepmc_particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: child_barcode
    type(hepmc_vertex_t) :: v
    type(hepmc_vertex_particle_out_iterator_t) :: it
    integer :: i
    v = hepmc_particle_get_decay_vertex (prt)
    if (hepmc_vertex_is_valid (v)) then
      allocate (child_barcode (hepmc_vertex_get_n_out (v)))
      if (size (child_barcode) /= 0) then

```

```

    if (HEPMC2_AVAILABLE) then
        call hePMC_vertex_particle_out_iterator_init (it, v)
        do i = 1, size (child_barcode)
            child_barcode(i) = hePMC_particle_get_barcode &
                (hePMC_vertex_particle_out_iterator_get (it))
            call hePMC_vertex_particle_out_iterator_advance (it)
        end do
        call hePMC_vertex_particle_out_iterator_final (it)
    else if (HEPMC3_AVAILABLE) then
        do i = 1, size (child_barcode)
            child_barcode(i) = hePMC_particle_get_barcode &
                (hePMC_vertex_get_nth_particle_out (v, i))
        end do
    end if
end if
else
    allocate (child_barcode (0))
end if
end function hePMC_particle_get_child_barcodes

```

Return the polarization (assuming that the particle is completely polarized).
 Note that the generated polarization object needs finalization.

(HepMC interface: interfaces)+≡

```

interface
    type(c_ptr) function gen_particle_polarization (prt_obj) bind(C)
    import
    type(c_ptr), value :: prt_obj
    end function gen_particle_polarization
end interface

```

(HepMC interface: public)+≡

```

public :: hePMC_particle_get_polarization

```

(HepMC interface: sub interfaces)+≡

```

module function hePMC_particle_get_polarization (prt) result (pol)
    type(hePMC_polarization_t) :: pol
    type(hePMC_particle_t), intent(in) :: prt
end function hePMC_particle_get_polarization

```

(HepMC interface: procedures)+≡

```

module function hePMC_particle_get_polarization (prt) result (pol)
    type(hePMC_polarization_t) :: pol
    type(hePMC_particle_t), intent(in) :: prt
    pol%obj = gen_particle_polarization (prt%obj)
end function hePMC_particle_get_polarization

```

Return the particle color as a two-dimensional array (color, anticolor).

(HepMC interface: interfaces)+≡

```

interface
    function gen_particle_flow (prt_obj, code_index) result (code) bind(C)
    import
    integer(c_int) :: code
    type(c_ptr), value :: prt_obj
    integer(c_int), value :: code_index

```

```

        end function gen_particle_flow
    end interface

    <HepMC interface: public>+≡
        public :: hepmc_particle_get_color

    <HepMC interface: sub interfaces>+≡
        module function hepmc_particle_get_color (prt) result (col)
            integer, dimension(2) :: col
            type(hepmc_particle_t), intent(in) :: prt
        end function hepmc_particle_get_color

    <HepMC interface: procedures>+≡
        module function hepmc_particle_get_color (prt) result (col)
            integer, dimension(2) :: col
            type(hepmc_particle_t), intent(in) :: prt
            col(1) = gen_particle_flow (prt%obj, 1)
            col(2) = - gen_particle_flow (prt%obj, 2)
        end function hepmc_particle_get_color

    <HepMC interface: interfaces>+≡
        interface
            function gen_vertex_pos_x (v_obj) result (x) bind(C)
                import
                type(c_ptr), value :: v_obj
                real(c_double) :: x
            end function gen_vertex_pos_x
        end interface
        interface
            function gen_vertex_pos_y (v_obj) result (y) bind(C)
                import
                type(c_ptr), value :: v_obj
                real(c_double) :: y
            end function gen_vertex_pos_y
        end interface
        interface
            function gen_vertex_pos_z (v_obj) result (z) bind(C)
                import
                type(c_ptr), value :: v_obj
                real(c_double) :: z
            end function gen_vertex_pos_z
        end interface
        interface
            function gen_vertex_time (v_obj) result (t) bind(C)
                import
                type(c_ptr), value :: v_obj
                real(c_double) :: t
            end function gen_vertex_time
        end interface

    <HepMC interface: public>+≡
        public :: hepmc_vertex_to_vertex

    <HepMC interface: sub interfaces>+≡
        module function hepmc_vertex_to_vertex (vtx) result (v)
            type(hepmc_vertex_t), intent(in) :: vtx

```

```

        type(vector4_t) :: v
    end function hepmc_vertex_to_vertex

<HepMC interface: procedures>+≡
module function hepmc_vertex_to_vertex (vtx) result (v)
    type(hepmc_vertex_t), intent(in) :: vtx
    type(vector4_t) :: v
    real(default) :: t, vx, vy, vz
    if (hepmc_vertex_is_valid (vtx)) then
        t = gen_vertex_time (vtx%obj)
        vx = gen_vertex_pos_x (vtx%obj)
        vy = gen_vertex_pos_y (vtx%obj)
        vz = gen_vertex_pos_z (vtx%obj)
        v = vector4_moving (t, &
            vector3_moving ([vx, vy, vz]))
    end if
end function hepmc_vertex_to_vertex

```

18.12.5 GenVertex

Vertices are made of particles (incoming and outgoing).

```

<HepMC interface: public>+≡
    public :: hepmc_vertex_t

<HepMC interface: types>+≡
    type :: hepmc_vertex_t
    private
    type(c_ptr) :: obj
end type hepmc_vertex_t

```

Constructor. Two versions, one plain, one with the position in space and time (measured in mm) as argument. The Fortran version has initializer form, and the vertex position is an optional argument.

A destructor is unnecessary as long as all vertices are entered into an event container.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function new_gen_vertex () bind(C)
            import
        end function new_gen_vertex
    end interface
    interface
        type(c_ptr) function new_gen_vertex_pos (prt_obj) bind(C)
            import
            type(c_ptr), value :: prt_obj
        end function new_gen_vertex_pos
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_init

```



```

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_vertex_init (v, x)
    type(hepmc_vertex_t), intent(out) :: v
    type(vector4_t), intent(in), optional :: x
  end subroutine hepmc_vertex_init

```

```

<HepMC interface: procedures>+≡
  module subroutine hepmc_vertex_init (v, x)
    type(hepmc_vertex_t), intent(out) :: v
    type(vector4_t), intent(in), optional :: x
    type(hepmc_four_vector_t) :: pos
    if (present (x)) then
      call hepmc_four_vector_init (pos, x)
      v%obj = new_gen_vertex_pos (pos%obj)
      call hepmc_four_vector_final (pos)
    else
      v%obj = new_gen_vertex ()
    end if
  end subroutine hepmc_vertex_init

```

Return true if the vertex pointer is non-null:

```

<HepMC interface: interfaces>+≡
  interface
    function gen_vertex_is_valid (v_obj) result (flag) bind(C)
      import
      logical(c_bool) :: flag
      type(c_ptr), value :: v_obj
    end function gen_vertex_is_valid
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_vertex_is_valid

```

```

<HepMC interface: sub interfaces>+≡
  module function hepmc_vertex_is_valid (v) result (flag)
    logical :: flag
    type(hepmc_vertex_t), intent(in) :: v
  end function hepmc_vertex_is_valid

```

```

<HepMC interface: procedures>+≡
  module function hepmc_vertex_is_valid (v) result (flag)
    logical :: flag
    type(hepmc_vertex_t), intent(in) :: v
    flag = gen_vertex_is_valid (v%obj)
  end function hepmc_vertex_is_valid

```

Add a particle to a vertex, incoming or outgoing.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_vertex_add_particle_in (v_obj, prt_obj) bind(C)
      import
      type(c_ptr), value :: v_obj, prt_obj
    end subroutine gen_vertex_add_particle_in
  end interface
  interface

```

```

        subroutine gen_vertex_add_particle_out (v_obj, prt_obj) bind(C)
            import
            type(c_ptr), value :: v_obj, prt_obj
        end subroutine gen_vertex_add_particle_out
    end interface

    <HepMC interface: public>+≡
        public :: hepmc_vertex_add_particle_in
        public :: hepmc_vertex_add_particle_out

    <HepMC interface: sub interfaces>+≡
        module subroutine hepmc_vertex_add_particle_in (v, prt)
            type(hepmc_vertex_t), intent(inout) :: v
            type(hepmc_particle_t), intent(in) :: prt
        end subroutine hepmc_vertex_add_particle_in
        module subroutine hepmc_vertex_add_particle_out (v, prt)
            type(hepmc_vertex_t), intent(inout) :: v
            type(hepmc_particle_t), intent(in) :: prt
        end subroutine hepmc_vertex_add_particle_out

    <HepMC interface: procedures>+≡
        module subroutine hepmc_vertex_add_particle_in (v, prt)
            type(hepmc_vertex_t), intent(inout) :: v
            type(hepmc_particle_t), intent(in) :: prt
            call gen_vertex_add_particle_in (v%obj, prt%obj)
        end subroutine hepmc_vertex_add_particle_in

        module subroutine hepmc_vertex_add_particle_out (v, prt)
            type(hepmc_vertex_t), intent(inout) :: v
            type(hepmc_particle_t), intent(in) :: prt
            call gen_vertex_add_particle_out (v%obj, prt%obj)
        end subroutine hepmc_vertex_add_particle_out

    Return the number of incoming/outgoing particles.

    <HepMC interface: interfaces>+≡
        interface
            function gen_vertex_particles_in_size (v_obj) result (size) bind(C)
                import
                integer(c_int) :: size
                type(c_ptr), value :: v_obj
            end function gen_vertex_particles_in_size
        end interface
        interface
            function gen_vertex_particles_out_size (v_obj) result (size) bind(C)
                import
                integer(c_int) :: size
                type(c_ptr), value :: v_obj
            end function gen_vertex_particles_out_size
        end interface
        interface
            function gen_particle_get_n_parents (p_obj) result (size) bind(C)
                import
                integer(c_int) :: size
                type(c_ptr), value :: p_obj
            end function gen_particle_get_n_parents

```

```

end interface
interface
    function gen_particle_get_n_children (p_obj) result (size) bind(C)
        import
        integer(c_int) :: size
        type(c_ptr), value :: p_obj
    end function gen_particle_get_n_children
end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_get_n_in
    public :: hepmc_vertex_get_n_out
    public :: hepmc_particle_get_parents
    public :: hepmc_particle_get_children

<HepMC interface: sub interfaces>+≡
    module function hepmc_vertex_get_n_in (v) result (n_in)
        integer :: n_in
        type(hepmc_vertex_t), intent(in) :: v
    end function hepmc_vertex_get_n_in
    module function hepmc_vertex_get_n_out (v) result (n_out)
        integer :: n_out
        type(hepmc_vertex_t), intent(in) :: v
    end function hepmc_vertex_get_n_out
    module function hepmc_particle_get_parents (p) result (n_p)
        integer :: n_p
        type(hepmc_particle_t), intent(in) :: p
    end function hepmc_particle_get_parents
    module function hepmc_particle_get_children (p) result (n_ch)
        integer :: n_ch
        type(hepmc_particle_t), intent(in) :: p
    end function hepmc_particle_get_children

<HepMC interface: procedures>+≡
    module function hepmc_vertex_get_n_in (v) result (n_in)
        integer :: n_in
        type(hepmc_vertex_t), intent(in) :: v
        n_in = gen_vertex_particles_in_size (v%obj)
    end function hepmc_vertex_get_n_in

    module function hepmc_vertex_get_n_out (v) result (n_out)
        integer :: n_out
        type(hepmc_vertex_t), intent(in) :: v
        n_out = gen_vertex_particles_out_size (v%obj)
    end function hepmc_vertex_get_n_out

    module function hepmc_particle_get_parents (p) result (n_p)
        integer :: n_p
        type(hepmc_particle_t), intent(in) :: p
        n_p = gen_particle_get_n_parents (p%obj)
    end function hepmc_particle_get_parents

    module function hepmc_particle_get_children (p) result (n_ch)
        integer :: n_ch
        type(hepmc_particle_t), intent(in) :: p
        n_ch = gen_particle_get_n_children (p%obj)
    end function hepmc_particle_get_children

```

```
end function hepmc_particle_get_children
```

Return the number of parents/children.

```

<HepMC interface: public>+≡
  public :: hepmc_particle_get_n_parents
  public :: hepmc_particle_get_n_children

<HepMC interface: sub interfaces>+≡
  module function hepmc_particle_get_n_parents (prt) result (n_parents)
    integer :: n_parents
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_n_parents
  module function hepmc_particle_get_n_children (prt) result (n_children)
    integer :: n_children
    type(hepmc_particle_t), intent(in) :: prt
  end function hepmc_particle_get_n_children

<HepMC interface: procedures>+≡
  module function hepmc_particle_get_n_parents (prt) result (n_parents)
    integer :: n_parents
    type(hepmc_particle_t), intent(in) :: prt
    type(hepmc_vertex_t) :: v
    if (HEPMC2_AVAILABLE) then
      v = hepmc_particle_get_production_vertex (prt)
      if (hepmc_vertex_is_valid (v)) then
        n_parents = hepmc_vertex_get_n_in (v)
      else
        n_parents = 0
      end if
    else if (HEPMC3_AVAILABLE) then
      n_parents = hepmc_particle_get_parents (prt)
    end if
  end function hepmc_particle_get_n_parents

  module function hepmc_particle_get_n_children (prt) result (n_children)
    integer :: n_children
    type(hepmc_particle_t), intent(in) :: prt
    type(hepmc_vertex_t) :: v
    if (HEPMC2_AVAILABLE) then
      v = hepmc_particle_get_decay_vertex (prt)
      if (hepmc_vertex_is_valid (v)) then
        n_children = hepmc_vertex_get_n_out (v)
      else
        n_children = 0
      end if
    else if (HEPMC3_AVAILABLE) then
      n_children = hepmc_particle_get_children (prt)
    end if
  end function hepmc_particle_get_n_children

```

18.12.6 Vertex-particle-in iterator

This iterator iterates over all incoming particles in an vertex. We store a pointer to the vertex in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

```
<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_t

<HepMC interface: types>+≡
    type :: hepmc_vertex_particle_in_iterator_t
    private
        type(c_ptr) :: obj
        type(c_ptr) :: v_obj
    end type hepmc_vertex_particle_in_iterator_t
```

Constructor. The iterator is initialized at the first particle in the vertex.

```
<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function &
            new_vertex_particles_in_const_iterator (v_obj) bind(C)
        import
            type(c_ptr), value :: v_obj
        end function new_vertex_particles_in_const_iterator
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_init

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_in_iterator_init (it, v)
        type(hepmc_vertex_particle_in_iterator_t), intent(out) :: it
        type(hepmc_vertex_t), intent(in) :: v
    end subroutine hepmc_vertex_particle_in_iterator_init

<HepMC interface: procedures>+≡
    module subroutine hepmc_vertex_particle_in_iterator_init (it, v)
        type(hepmc_vertex_particle_in_iterator_t), intent(out) :: it
        type(hepmc_vertex_t), intent(in) :: v
        it%obj = new_vertex_particles_in_const_iterator (v%obj)
        it%v_obj = v%obj
    end subroutine hepmc_vertex_particle_in_iterator_init
```

Destructor. Necessary because the iterator is allocated on the heap.

```
<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_delete (it_obj) bind(C)
        import
            type(c_ptr), value :: it_obj
        end subroutine vertex_particles_in_const_iterator_delete
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_final
```

```

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_in_iterator_final (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
    end subroutine hepmc_vertex_particle_in_iterator_final
<HepMC interface: procedures>+≡
    module subroutine hepmc_vertex_particle_in_iterator_final (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_delete (it%obj)
    end subroutine hepmc_vertex_particle_in_iterator_final

```

Increment

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_advance (it_obj) bind(C)
            import
            type(c_ptr), value :: it_obj
        end subroutine vertex_particles_in_const_iterator_advance
    end interface
<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_advance
<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_in_iterator_advance (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
    end subroutine hepmc_vertex_particle_in_iterator_advance
<HepMC interface: procedures>+≡
    module subroutine hepmc_vertex_particle_in_iterator_advance (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_advance (it%obj)
    end subroutine hepmc_vertex_particle_in_iterator_advance

```

Reset to the beginning

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_reset &
            (it_obj, v_obj) bind(C)
            import
            type(c_ptr), value :: it_obj, v_obj
        end subroutine vertex_particles_in_const_iterator_reset
    end interface
<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_reset
<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_in_iterator_reset (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
    end subroutine hepmc_vertex_particle_in_iterator_reset
<HepMC interface: procedures>+≡
    module subroutine hepmc_vertex_particle_in_iterator_reset (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_reset (it%obj, it%v_obj)
    end subroutine hepmc_vertex_particle_in_iterator_reset

```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
  interface
    function vertex_particles_in_const_iterator_is_valid &
      (it_obj, v_obj) result (flag) bind(C)
    import
      logical(c_bool) :: flag
      type(c_ptr), value :: it_obj, v_obj
    end function vertex_particles_in_const_iterator_is_valid
  end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_in_iterator_is_valid

<HepMC interface: sub interfaces>+≡
  module function hepmc_vertex_particle_in_iterator_is_valid &
    (it) result (flag)
    logical :: flag
    type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
  end function hepmc_vertex_particle_in_iterator_is_valid

<HepMC interface: procedures>+≡
  module function hepmc_vertex_particle_in_iterator_is_valid &
    (it) result (flag)
    logical :: flag
    type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
    flag = vertex_particles_in_const_iterator_is_valid (it%obj, it%v_obj)
  end function hepmc_vertex_particle_in_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function &
      vertex_particles_in_const_iterator_get (it_obj) bind(C)
    import
      type(c_ptr), value :: it_obj
    end function vertex_particles_in_const_iterator_get
  end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_in_iterator_get

<HepMC interface: sub interfaces>+≡
  module function hepmc_vertex_particle_in_iterator_get (it) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
  end function hepmc_vertex_particle_in_iterator_get

<HepMC interface: procedures>+≡
  module function hepmc_vertex_particle_in_iterator_get (it) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
    prt%obj = vertex_particles_in_const_iterator_get (it%obj)
  end function hepmc_vertex_particle_in_iterator_get

```

```

<HepMC interface: interfaces>+≡
interface
  type(c_ptr) function vertex_get_nth_particle_in (vtx_obj, n) bind(C)
  import
    type(c_ptr), value :: vtx_obj
    integer(c_int), value :: n
  end function vertex_get_nth_particle_in
end interface
interface
  type(c_ptr) function vertex_get_nth_particle_out (vtx_obj, n) bind(C)
  import
    type(c_ptr), value :: vtx_obj
    integer(c_int), value :: n
  end function vertex_get_nth_particle_out
end interface

<HepMC interface: public>+≡
public :: hepmc_vertex_get_nth_particle_in
public :: hepmc_vertex_get_nth_particle_out

<HepMC interface: sub interfaces>+≡
module function hepmc_vertex_get_nth_particle_in (vtx, n) result (prt)
  type(hepmc_particle_t) :: prt
  type(hepmc_vertex_t), intent(in) :: vtx
  integer, intent(in) :: n
end function hepmc_vertex_get_nth_particle_in
module function hepmc_vertex_get_nth_particle_out (vtx, n) result (prt)
  type(hepmc_particle_t) :: prt
  type(hepmc_vertex_t), intent(in) :: vtx
  integer, intent(in) :: n
end function hepmc_vertex_get_nth_particle_out

<HepMC interface: procedures>+≡
module function hepmc_vertex_get_nth_particle_in (vtx, n) result (prt)
  type(hepmc_particle_t) :: prt
  type(hepmc_vertex_t), intent(in) :: vtx
  integer, intent(in) :: n
  integer(c_int) :: nth
  nth = n
  prt%obj = vertex_get_nth_particle_in (vtx%obj, nth)
end function hepmc_vertex_get_nth_particle_in

module function hepmc_vertex_get_nth_particle_out (vtx, n) result (prt)
  type(hepmc_particle_t) :: prt
  type(hepmc_vertex_t), intent(in) :: vtx
  integer, intent(in) :: n
  integer(c_int) :: nth
  nth = n
  prt%obj = vertex_get_nth_particle_out (vtx%obj, nth)
end function hepmc_vertex_get_nth_particle_out

```

18.12.7 Vertex-particle-out iterator

This iterator iterates over all incoming particles in an vertex. We store a pointer to the vertex in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

```

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_out_iterator_t

<HepMC interface: types>+≡
    type :: hepmc_vertex_particle_out_iterator_t
    private
    type(c_ptr) :: obj
    type(c_ptr) :: v_obj
    end type hepmc_vertex_particle_out_iterator_t

```

Constructor. The iterator is initialized at the first particle in the vertex.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function &
            new_vertex_particles_out_const_iterator (v_obj) bind(C)
        import
        type(c_ptr), value :: v_obj
        end function new_vertex_particles_out_const_iterator
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_out_iterator_init

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_out_iterator_init (it, v)
        type(hepmc_vertex_particle_out_iterator_t), intent(out) :: it
        type(hepmc_vertex_t), intent(in) :: v
    end subroutine hepmc_vertex_particle_out_iterator_init

<HepMC interface: procedures>+≡
    module subroutine hepmc_vertex_particle_out_iterator_init (it, v)
        type(hepmc_vertex_particle_out_iterator_t), intent(out) :: it
        type(hepmc_vertex_t), intent(in) :: v
        it%obj = new_vertex_particles_out_const_iterator (v%obj)
        it%v_obj = v%obj
    end subroutine hepmc_vertex_particle_out_iterator_init

```

Destructor. Necessary because the iterator is allocated on the heap.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_out_const_iterator_delete (it_obj) bind(C)
        import
        type(c_ptr), value :: it_obj
        end subroutine vertex_particles_out_const_iterator_delete
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_out_iterator_final

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_vertex_particle_out_iterator_final (it)
        type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
    end subroutine hepmc_vertex_particle_out_iterator_final

```

```

<HepMC interface: procedures>+≡
  module subroutine hepmc_vertex_particle_out_iterator_final (it)
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
    call vertex_particles_out_const_iterator_delete (it%obj)
  end subroutine hepmc_vertex_particle_out_iterator_final

```

Increment

```

<HepMC interface: interfaces>+≡
  interface
    subroutine vertex_particles_out_const_iterator_advance (it_obj) bind(C)
      import
      type(c_ptr), value :: it_obj
    end subroutine vertex_particles_out_const_iterator_advance
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_out_iterator_advance

```

```

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_vertex_particle_out_iterator_advance (it)
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
  end subroutine hepmc_vertex_particle_out_iterator_advance

```

```

<HepMC interface: procedures>+≡
  module subroutine hepmc_vertex_particle_out_iterator_advance (it)
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
    call vertex_particles_out_const_iterator_advance (it%obj)
  end subroutine hepmc_vertex_particle_out_iterator_advance

```

Reset to the beginning

```

<HepMC interface: interfaces>+≡
  interface
    subroutine vertex_particles_out_const_iterator_reset &
      (it_obj, v_obj) bind(C)
      import
      type(c_ptr), value :: it_obj, v_obj
    end subroutine vertex_particles_out_const_iterator_reset
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_out_iterator_reset

```

```

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_vertex_particle_out_iterator_reset (it)
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
  end subroutine hepmc_vertex_particle_out_iterator_reset

```

```

<HepMC interface: procedures>+≡
  module subroutine hepmc_vertex_particle_out_iterator_reset (it)
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it
    call vertex_particles_out_const_iterator_reset (it%obj, it%v_obj)
  end subroutine hepmc_vertex_particle_out_iterator_reset

```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
  interface
    function vertex_particles_out_const_iterator_is_valid &
      (it_obj, v_obj) result (flag) bind(C)
    import
      logical(c_bool) :: flag
      type(c_ptr), value :: it_obj, v_obj
    end function vertex_particles_out_const_iterator_is_valid
  end interface

<HepMC interface: public>+≡
  public :: hepvc_vertex_particle_out_iterator_is_valid

<HepMC interface: sub interfaces>+≡
  module function hepvc_vertex_particle_out_iterator_is_valid &
    (it) result (flag)
    logical :: flag
    type(hepvc_vertex_particle_out_iterator_t), intent(in) :: it
  end function hepvc_vertex_particle_out_iterator_is_valid

<HepMC interface: procedures>+≡
  module function hepvc_vertex_particle_out_iterator_is_valid &
    (it) result (flag)
    logical :: flag
    type(hepvc_vertex_particle_out_iterator_t), intent(in) :: it
    flag = vertex_particles_out_const_iterator_is_valid (it%obj, it%v_obj)
  end function hepvc_vertex_particle_out_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function &
      vertex_particles_out_const_iterator_get (it_obj) bind(C)
    import
      type(c_ptr), value :: it_obj
    end function vertex_particles_out_const_iterator_get
  end interface

<HepMC interface: public>+≡
  public :: hepvc_vertex_particle_out_iterator_get

<HepMC interface: sub interfaces>+≡
  module function hepvc_vertex_particle_out_iterator_get (it) result (prt)
    type(hepvc_particle_t) :: prt
    type(hepvc_vertex_particle_out_iterator_t), intent(in) :: it
  end function hepvc_vertex_particle_out_iterator_get

<HepMC interface: procedures>+≡
  module function hepvc_vertex_particle_out_iterator_get (it) result (prt)
    type(hepvc_particle_t) :: prt
    type(hepvc_vertex_particle_out_iterator_t), intent(in) :: it
    prt%obj = vertex_particles_out_const_iterator_get (it%obj)
  end function hepvc_vertex_particle_out_iterator_get

```

18.12.8 GenEvent

The main object of HepMC is a GenEvent. The object is filled by GenVertex objects, which in turn contain GenParticle objects.

This is an extension of the abstract `event_handle_t`, so we can use the according communicator features.

```
<HepMC interface: public>+≡
    public :: hepmc_event_t

<HepMC interface: types>+≡
    type, extends (event_handle_t) :: hepmc_event_t
    private
        type(c_ptr) :: obj = c_null_ptr
    end type hepmc_event_t
```

Constructor. Arguments are process ID (integer) and event ID (integer).

The Fortran version has initializer form.

```
<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function new_gen_event (proc_id, event_id) bind(C)
            import
                integer(c_int), value :: proc_id, event_id
        end function new_gen_event
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_init

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_init (evt, proc_id, event_id)
        type(hepmc_event_t), intent(out) :: evt
        integer, intent(in), optional :: proc_id, event_id
    end subroutine hepmc_event_init

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_init (evt, proc_id, event_id)
        type(hepmc_event_t), intent(out) :: evt
        integer, intent(in), optional :: proc_id, event_id
        integer(c_int) :: pid, eid
        pid = 0; if (present (proc_id)) pid = proc_id
        eid = 0; if (present (event_id)) eid = event_id
        evt%obj = new_gen_event (pid, eid)
    end subroutine hepmc_event_init
```

Destructor.

```
<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_delete (evt_obj) bind(C)
            import
                type(c_ptr), value :: evt_obj
        end subroutine gen_event_delete
    end interface
```

Finalize: use the HepMC destructor. Also nullify the pointer explicitly, to be on the safe side.

```

<HepMC interface: public>+≡
    public :: hepmc_event_final

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_final (evt)
        type(hepmc_event_t), intent(inout) :: evt
    end subroutine hepmc_event_final

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_final (evt)
        type(hepmc_event_t), intent(inout) :: evt
        if (c_associated (evt%obj)) then
            call gen_event_delete (evt%obj)
            evt%obj = c_null_ptr
        end if
    end subroutine hepmc_event_final

```

Nullify: do not call the destructor, just nullify the C pointer. There should be another pointer associated with the object.

```

<HepMC interface: public>+≡
    public :: hepmc_event_nullify

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_nullify (evt)
        type(hepmc_event_t), intent(inout) :: evt
    end subroutine hepmc_event_nullify

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_nullify (evt)
        type(hepmc_event_t), intent(inout) :: evt
        evt%obj = c_null_ptr
    end subroutine hepmc_event_nullify

```

Return the actual object as a C pointer. For use in the native C++ interface only.

```

<HepMC interface: public>+≡
    public :: hepmc_event_get_c_ptr

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_get_c_ptr (evt) result (p)
        type(hepmc_event_t), intent(in) :: evt
        type(c_ptr) :: p
    end function hepmc_event_get_c_ptr

<HepMC interface: procedures>+≡
    module function hepmc_event_get_c_ptr (evt) result (p)
        type(hepmc_event_t), intent(in) :: evt
        type(c_ptr) :: p
        p = evt%obj
    end function hepmc_event_get_c_ptr

```

Screen output. Printing to file is possible in principle (using a C++ output channel), by allowing an argument. Printing to an open Fortran unit is obviously not possible.

```
<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_print (evt_obj) bind(C)
      import
      type(c_ptr), value :: evt_obj
    end subroutine gen_event_print
  end interface
```

```
<HepMC interface: public>+≡
  public :: hepmc_event_print
```

```
<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_print (evt)
    type(hepmc_event_t), intent(in) :: evt
  end subroutine hepmc_event_print
```

```
<HepMC interface: procedures>+≡
  module subroutine hepmc_event_print (evt)
    type(hepmc_event_t), intent(in) :: evt
    call gen_event_print (evt%obj)
  end subroutine hepmc_event_print
```

Get the event number.

```
<HepMC interface: interfaces>+≡
  interface
    integer(c_int) function gen_event_event_number (evt_obj) bind(C)
      use iso_c_binding !NODEP!
      type(c_ptr), value :: evt_obj
    end function gen_event_event_number
  end interface
```

```
<HepMC interface: public>+≡
  public :: hepmc_event_get_event_index
```

```
<HepMC interface: sub interfaces>+≡
  module function hepmc_event_get_event_index (evt) result (i_proc)
    integer :: i_proc
    type(hepmc_event_t), intent(in) :: evt
  end function hepmc_event_get_event_index
```

```
<HepMC interface: procedures>+≡
  module function hepmc_event_get_event_index (evt) result (i_proc)
    integer :: i_proc
    type(hepmc_event_t), intent(in) :: evt
    i_proc = gen_event_event_number (evt%obj)
  end function hepmc_event_get_event_index
```

```
<HepMC interface: interfaces>+≡
  interface
    integer(c_int) function gen_event_get_n_particles &
      (evt_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
```

```

        end function gen_event_get_n_particles
    end interface
    interface
        integer(c_int) function gen_event_get_n_beams &
            (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
    end function gen_event_get_n_beams
    end interface

    <HepMC interface: public>+≡
    public :: hepmc_event_get_n_particles
    public :: hepmc_event_get_n_beams

    <HepMC interface: sub interfaces>+≡
    module function hepmc_event_get_n_particles (evt) result (n_tot)
        integer :: n_tot
        type(hepmc_event_t), intent(in) :: evt
    end function hepmc_event_get_n_particles
    module function hepmc_event_get_n_beams (evt) result (n_tot)
        integer :: n_tot
        type(hepmc_event_t), intent(in) :: evt
    end function hepmc_event_get_n_beams

    <HepMC interface: procedures>+≡
    module function hepmc_event_get_n_particles (evt) result (n_tot)
        integer :: n_tot
        type(hepmc_event_t), intent(in) :: evt
        n_tot = gen_event_get_n_particles (evt%obj)
    end function hepmc_event_get_n_particles

    module function hepmc_event_get_n_beams (evt) result (n_tot)
        integer :: n_tot
        type(hepmc_event_t), intent(in) :: evt
        n_tot = gen_event_get_n_beams (evt%obj)
    end function hepmc_event_get_n_beams

    Set the numeric signal process ID

    <HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_set_signal_process_id (evt_obj, proc_id) bind(C)
        import
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: proc_id
    end subroutine gen_event_set_signal_process_id
    end interface

    <HepMC interface: public>+≡
    public :: hepmc_event_set_process_id

    <HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_set_process_id (evt, proc)
        type(hepmc_event_t), intent(in) :: evt
        integer, intent(in) :: proc
    end subroutine hepmc_event_set_process_id

```

```

<HepMC interface: procedures>+≡
module subroutine hepmc_event_set_process_id (evt, proc)
  type(hepmc_event_t), intent(in) :: evt
  integer, intent(in) :: proc
  integer(c_int) :: i_proc
  i_proc = proc
  call gen_event_set_signal_process_id (evt%obj, i_proc)
end subroutine hepmc_event_set_process_id

```

Get the numeric signal process ID

```

<HepMC interface: interfaces>+≡
interface
  integer(c_int) function gen_event_signal_process_id (evt_obj) bind(C)
  import
  type(c_ptr), value :: evt_obj
end function gen_event_signal_process_id
end interface

```

```

<HepMC interface: public>+≡
public :: hepmc_event_get_process_id

```

```

<HepMC interface: sub interfaces>+≡
module function hepmc_event_get_process_id (evt) result (i_proc)
  integer :: i_proc
  type(hepmc_event_t), intent(in) :: evt
end function hepmc_event_get_process_id

```

```

<HepMC interface: procedures>+≡
module function hepmc_event_get_process_id (evt) result (i_proc)
  integer :: i_proc
  type(hepmc_event_t), intent(in) :: evt
  i_proc = gen_event_signal_process_id (evt%obj)
end function hepmc_event_get_process_id

```

Set the event energy scale

```

<HepMC interface: interfaces>+≡
interface
  subroutine gen_event_set_event_scale (evt_obj, scale) bind(C)
  import
  type(c_ptr), value :: evt_obj
  real(c_double), value :: scale
end subroutine gen_event_set_event_scale
end interface

```

```

<HepMC interface: public>+≡
public :: hepmc_event_set_scale

```

```

<HepMC interface: sub interfaces>+≡
module subroutine hepmc_event_set_scale (evt, scale)
  type(hepmc_event_t), intent(in) :: evt
  real(default), intent(in) :: scale
end subroutine hepmc_event_set_scale

```

```

<HepMC interface: procedures>+≡
module subroutine hepmc_event_set_scale (evt, scale)
  type(hepmc_event_t), intent(in) :: evt

```



```

    real(default), intent(in) :: scale
    real(c_double) :: cscale
    cscale = scale
    call gen_event_set_event_scale (evt%obj, cscale)
end subroutine hepmc_event_set_scale

```

Get the event energy scale

```

<HepMC interface: interfaces>+≡
    interface
        real(c_double) function gen_event_event_scale (evt_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
        end function gen_event_event_scale
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_get_scale

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_get_scale (evt) result (scale)
        real(default) :: scale
        type(hepmc_event_t), intent(in) :: evt
    end function hepmc_event_get_scale

<HepMC interface: procedures>+≡
    module function hepmc_event_get_scale (evt) result (scale)
        real(default) :: scale
        type(hepmc_event_t), intent(in) :: evt
        scale = gen_event_event_scale (evt%obj)
    end function hepmc_event_get_scale

```

Set the value of α_{QCD} .

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_set_alpha_qcd (evt_obj, a) bind(C)
            import
            type(c_ptr), value :: evt_obj
            real(c_double), value :: a
        end subroutine gen_event_set_alpha_qcd
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_set_alpha_qcd

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_set_alpha_qcd (evt, alpha)
        type(hepmc_event_t), intent(in) :: evt
        real(default), intent(in) :: alpha
    end subroutine hepmc_event_set_alpha_qcd

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_set_alpha_qcd (evt, alpha)
        type(hepmc_event_t), intent(in) :: evt
        real(default), intent(in) :: alpha
        real(c_double) :: a
        a = alpha
    end subroutine hepmc_event_set_alpha_qcd

```

```

        call gen_event_set_alpha_qcd (evt%obj, a)
    end subroutine hepmc_event_set_alpha_qcd

```

Get the value of α_{QCD} .

```

<HepMC interface: interfaces>+≡
    interface
        real(c_double) function gen_event_alpha_qcd (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
        end function gen_event_alpha_qcd
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_get_alpha_qcd

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_get_alpha_qcd (evt) result (alpha)
        real(default) :: alpha
        type(hepmc_event_t), intent(in) :: evt
    end function hepmc_event_get_alpha_qcd

<HepMC interface: procedures>+≡
    module function hepmc_event_get_alpha_qcd (evt) result (alpha)
        real(default) :: alpha
        type(hepmc_event_t), intent(in) :: evt
        alpha = gen_event_alpha_qcd (evt%obj)
    end function hepmc_event_get_alpha_qcd

```

Set the value of α_{QED} .

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_set_alpha_qed (evt_obj, a) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: a
        end subroutine gen_event_set_alpha_qed
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_set_alpha_qed

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_set_alpha_qed (evt, alpha)
        type(hepmc_event_t), intent(in) :: evt
        real(default), intent(in) :: alpha
    end subroutine hepmc_event_set_alpha_qed

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_set_alpha_qed (evt, alpha)
        type(hepmc_event_t), intent(in) :: evt
        real(default), intent(in) :: alpha
        real(c_double) :: a
        a = alpha
        call gen_event_set_alpha_qed (evt%obj, a)
    end subroutine hepmc_event_set_alpha_qed

```

Get the value of α_{QED} .

```

<HepMC interface: interfaces>+≡
  interface
    real(c_double) function gen_event_alpha_qed (evt_obj) bind(C)
      import
      type(c_ptr), value :: evt_obj
    end function gen_event_alpha_qed
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_get_alpha_qed

<HepMC interface: sub interfaces>+≡
  module function hepmc_event_get_alpha_qed (evt) result (alpha)
    real(default) :: alpha
    type(hepmc_event_t), intent(in) :: evt
  end function hepmc_event_get_alpha_qed

<HepMC interface: procedures>+≡
  module function hepmc_event_get_alpha_qed (evt) result (alpha)
    real(default) :: alpha
    type(hepmc_event_t), intent(in) :: evt
    alpha = gen_event_alpha_qed (evt%obj)
  end function hepmc_event_get_alpha_qed

```

Clear a weight value to the end of the weight container.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_clear_weights (evt_obj) bind(C)
      use iso_c_binding !NODEP!
      type(c_ptr), value :: evt_obj
    end subroutine gen_event_clear_weights
  end interface

```

The HepMC weights are measured in pb.

```

<HepMC interface: parameters>≡
  integer, parameter, public :: HEPMC3_MODE_HEPMC2 = 1
  integer, parameter, public :: HEPMC3_MODE_HEPMC3 = 2
  integer, parameter, public :: HEPMC3_MODE_ROOT = 3
  integer, parameter, public :: HEPMC3_MODE_ROOTTREE = 4
  integer, parameter, public :: HEPMC3_MODE_HEPEVT = 5

<HepMC interface: public>+≡
  public :: hepmc_event_clear_weights

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_clear_weights (evt)
    type(hepmc_event_t), intent(in) :: evt
  end subroutine hepmc_event_clear_weights

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_clear_weights (evt)
    type(hepmc_event_t), intent(in) :: evt
    call gen_event_clear_weights (evt%obj)
  end subroutine hepmc_event_clear_weights

```

Add a weight value to the end of the weight container.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_add_weight (evt_obj, w) bind(C)
      use iso_c_binding !NODEP!
      type(c_ptr), value :: evt_obj
      real(c_double), value :: w
    end subroutine gen_event_add_weight
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_add_weight

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_add_weight (evt, weight, rescale)
    type(hepmc_event_t), intent(in) :: evt
    real(default), intent(in) :: weight
    logical, intent(in) :: rescale
  end subroutine hepmc_event_add_weight

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_add_weight (evt, weight, rescale)
    type(hepmc_event_t), intent(in) :: evt
    real(default), intent(in) :: weight
    logical, intent(in) :: rescale
    real(c_double) :: w
    if (rescale) then
      w = weight * pb_per_fb
    else
      w = weight
    end if
    call gen_event_add_weight (evt%obj, w)
  end subroutine hepmc_event_add_weight

```

Get the size of the weight container (the number of valid elements).

```

<HepMC interface: interfaces>+≡
  interface
    integer(c_int) function gen_event_weights_size (evt_obj) bind(C)
      use iso_c_binding !NODEP!
      type(c_ptr), value :: evt_obj
    end function gen_event_weights_size
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_get_weights_size

<HepMC interface: sub interfaces>+≡
  module function hepmc_event_get_weights_size (evt) result (n)
    integer :: n
    type(hepmc_event_t), intent(in) :: evt
  end function hepmc_event_get_weights_size

<HepMC interface: procedures>+≡
  module function hepmc_event_get_weights_size (evt) result (n)
    integer :: n
    type(hepmc_event_t), intent(in) :: evt

```

```

    n = gen_event_weights_size (evt%obj)
end function hepmc_event_get_weights_size

```

Get the value of the weight with index i. (Count from 1, while C counts from zero.)

```

<HepMC interface: interfaces>+≡
interface
    real(c_double) function gen_event_weight (evt_obj, i) bind(C)
    use iso_c_binding !NODEP!
    type(c_ptr), value :: evt_obj
    integer(c_int), value :: i
    end function gen_event_weight
end interface

<HepMC interface: public>+≡
public :: hepmc_event_get_weight

<HepMC interface: sub interfaces>+≡
module function hepmc_event_get_weight (evt, index, rescale) result (weight)
    real(default) :: weight
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: index
    logical, intent(in) :: rescale
end function hepmc_event_get_weight

<HepMC interface: procedures>+≡
module function hepmc_event_get_weight (evt, index, rescale) result (weight)
    real(default) :: weight
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: index
    logical, intent(in) :: rescale
    integer(c_int) :: i
    i = index - 1
    if (rescale) then
        weight = gen_event_weight (evt%obj, i) / pb_per_fb
    else
        weight = gen_event_weight (evt%obj, i)
    end if
end function hepmc_event_get_weight

```

Add a vertex to the event container.

```

<HepMC interface: interfaces>+≡
interface
    subroutine gen_event_add_vertex (evt_obj, v_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
    type(c_ptr), value :: v_obj
    end subroutine gen_event_add_vertex
end interface

<HepMC interface: public>+≡
public :: hepmc_event_add_vertex

<HepMC interface: sub interfaces>+≡
module subroutine hepmc_event_add_vertex (evt, v)

```

```

        type(hepmc_event_t), intent(inout) :: evt
        type(hepmc_vertex_t), intent(in) :: v
    end subroutine hepmc_event_add_vertex

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_add_vertex (evt, v)
        type(hepmc_event_t), intent(inout) :: evt
        type(hepmc_vertex_t), intent(in) :: v
        call gen_event_add_vertex (evt%obj, v%obj)
    end subroutine hepmc_event_add_vertex

```

Mark a particular vertex as the signal process (hard interaction).

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_set_signal_process_vertex (evt_obj, v_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
            type(c_ptr), value :: v_obj
        end subroutine gen_event_set_signal_process_vertex
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_set_signal_process_vertex

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_set_signal_process_vertex (evt, v)
        type(hepmc_event_t), intent(inout) :: evt
        type(hepmc_vertex_t), intent(in) :: v
    end subroutine hepmc_event_set_signal_process_vertex

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_set_signal_process_vertex (evt, v)
        type(hepmc_event_t), intent(inout) :: evt
        type(hepmc_vertex_t), intent(in) :: v
        call gen_event_set_signal_process_vertex (evt%obj, v%obj)
    end subroutine hepmc_event_set_signal_process_vertex

```

Return the the signal process (hard interaction).

```

<HepMC interface: interfaces>+≡
    interface
        function gen_event_get_signal_process_vertex (evt_obj) &
            result (v_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
            type(c_ptr) :: v_obj
        end function gen_event_get_signal_process_vertex
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_get_signal_process_vertex

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_get_signal_process_vertex (evt) result (v)
        type(hepmc_event_t), intent(in) :: evt
        type(hepmc_vertex_t) :: v
    end function hepmc_event_get_signal_process_vertex

```

```

<HepMC interface: procedures>+≡
module function hepmc_event_get_signal_process_vertex (evt) result (v)
  type(hepmc_event_t), intent(in) :: evt
  type(hepmc_vertex_t) :: v
  v%obj = gen_event_get_signal_process_vertex (evt%obj)
end function hepmc_event_get_signal_process_vertex

```

Set the beam particles explicitly.

```

<HepMC interface: public>+≡
  public :: hepmc_event_set_beam_particles

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_set_beam_particles (evt, prt1, prt2)
    type(hepmc_event_t), intent(inout) :: evt
    type(hepmc_particle_t), intent(in) :: prt1, prt2
    logical(c_bool) :: flag
  end subroutine hepmc_event_set_beam_particles

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_set_beam_particles (evt, prt1, prt2)
    type(hepmc_event_t), intent(inout) :: evt
    type(hepmc_particle_t), intent(in) :: prt1, prt2
    logical(c_bool) :: flag
    flag = gen_event_set_beam_particles (evt%obj, prt1%obj, prt2%obj)
  end subroutine hepmc_event_set_beam_particles

```

The C function returns a boolean which we do not use.

```

<HepMC interface: interfaces>+≡
  interface
    logical(c_bool) function gen_event_set_beam_particles &
      (evt_obj, prt1_obj, prt2_obj) bind(C)
  import
    type(c_ptr), value :: evt_obj, prt1_obj, prt2_obj
  end function gen_event_set_beam_particles
end interface

```

Set the cross section and error explicitly. Note that HepMC uses pb, while WHIZARD uses fb.

```

<HepMC interface: public>+≡
  public :: hepmc_event_set_cross_section

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_set_cross_section (evt, xsec, xsec_err)
    type(hepmc_event_t), intent(inout) :: evt
    real(default), intent(in) :: xsec, xsec_err
  end subroutine hepmc_event_set_cross_section

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_set_cross_section (evt, xsec, xsec_err)
    type(hepmc_event_t), intent(inout) :: evt
    real(default), intent(in) :: xsec, xsec_err
    call gen_event_set_cross_section &
      (evt%obj, &
       real (xsec * 1e-3_default, c_double), &

```

```

        real (xsec_err * 1e-3_default, c_double))
    end subroutine hepmc_event_set_cross_section

```

The C function returns a boolean which we do not use.

(HepMC interface: interfaces)+≡

```

interface
    subroutine gen_event_set_cross_section (evt_obj, xs, xs_err) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: xs, xs_err
    end subroutine gen_event_set_cross_section
end interface

```

18.12.9 Event-particle iterator

This iterator iterates over all particles in an event. We store a pointer to the event in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

(HepMC interface: public)+≡

```

    public :: hepmc_event_particle_iterator_t

```

(HepMC interface: types)+≡

```

    type :: hepmc_event_particle_iterator_t
    private
    type(c_ptr) :: obj
    type(c_ptr) :: evt_obj
    end type hepmc_event_particle_iterator_t

```

Constructor. The iterator is initialized at the first particle in the event.

(HepMC interface: interfaces)+≡

```

interface
    type(c_ptr) function new_event_particle_const_iterator (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
    end function new_event_particle_const_iterator
end interface

```

(HepMC interface: public)+≡

```

    public :: hepmc_event_particle_iterator_init

```

(HepMC interface: sub interfaces)+≡

```

module subroutine hepmc_event_particle_iterator_init (it, evt)
    type(hepmc_event_particle_iterator_t), intent(out) :: it
    type(hepmc_event_t), intent(in) :: evt
    end subroutine hepmc_event_particle_iterator_init

```

(HepMC interface: procedures)+≡

```

module subroutine hepmc_event_particle_iterator_init (it, evt)
    type(hepmc_event_particle_iterator_t), intent(out) :: it
    type(hepmc_event_t), intent(in) :: evt
    it%obj = new_event_particle_const_iterator (evt%obj)
    it%evt_obj = evt%obj
    end subroutine hepmc_event_particle_iterator_init

```


Destructor. Necessary because the iterator is allocated on the heap.

```
<HepMC interface: interfaces>+≡
  interface
    subroutine event_particle_const_iterator_delete (it_obj) bind(C)
    import
      type(c_ptr), value :: it_obj
    end subroutine event_particle_const_iterator_delete
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_particle_iterator_final

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_particle_iterator_final (it)
    type(hepmc_event_particle_iterator_t), intent(inout) :: it
  end subroutine hepmc_event_particle_iterator_final

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_particle_iterator_final (it)
    type(hepmc_event_particle_iterator_t), intent(inout) :: it
    call event_particle_const_iterator_delete (it%obj)
  end subroutine hepmc_event_particle_iterator_final
```

Increment

```
<HepMC interface: interfaces>+≡
  interface
    subroutine event_particle_const_iterator_advance (it_obj) bind(C)
    import
      type(c_ptr), value :: it_obj
    end subroutine event_particle_const_iterator_advance
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_particle_iterator_advance

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_event_particle_iterator_advance (it)
    type(hepmc_event_particle_iterator_t), intent(inout) :: it
  end subroutine hepmc_event_particle_iterator_advance

<HepMC interface: procedures>+≡
  module subroutine hepmc_event_particle_iterator_advance (it)
    type(hepmc_event_particle_iterator_t), intent(inout) :: it
    call event_particle_const_iterator_advance (it%obj)
  end subroutine hepmc_event_particle_iterator_advance
```

Reset to the beginning

```
<HepMC interface: interfaces>+≡
  interface
    subroutine event_particle_const_iterator_reset (it_obj, evt_obj) bind(C)
    import
      type(c_ptr), value :: it_obj, evt_obj
    end subroutine event_particle_const_iterator_reset
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_particle_iterator_reset
```

```

<HepMC interface: sub interfaces>+≡
    module subroutine hepmc_event_particle_iterator_reset (it)
        type(hepmc_event_particle_iterator_t), intent(inout) :: it
    end subroutine hepmc_event_particle_iterator_reset

<HepMC interface: procedures>+≡
    module subroutine hepmc_event_particle_iterator_reset (it)
        type(hepmc_event_particle_iterator_t), intent(inout) :: it
        call event_particle_const_iterator_reset (it%obj, it%evt_obj)
    end subroutine hepmc_event_particle_iterator_reset

```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
    interface
        function event_particle_const_iterator_is_valid &
            (it_obj, evt_obj) result (flag) bind(C)
        import
        logical(c_bool) :: flag
        type(c_ptr), value :: it_obj, evt_obj
    end function event_particle_const_iterator_is_valid
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_particle_iterator_is_valid

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_particle_iterator_is_valid (it) result (flag)
        logical :: flag
        type(hepmc_event_particle_iterator_t), intent(in) :: it
    end function hepmc_event_particle_iterator_is_valid

<HepMC interface: procedures>+≡
    module function hepmc_event_particle_iterator_is_valid (it) result (flag)
        logical :: flag
        type(hepmc_event_particle_iterator_t), intent(in) :: it
        flag = event_particle_const_iterator_is_valid (it%obj, it%evt_obj)
    end function hepmc_event_particle_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function event_particle_const_iterator_get (it_obj) bind(C)
        import
        type(c_ptr), value :: it_obj
    end function event_particle_const_iterator_get
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_particle_iterator_get

<HepMC interface: sub interfaces>+≡
    module function hepmc_event_particle_iterator_get (it) result (prt)
        type(hepmc_particle_t) :: prt
        type(hepmc_event_particle_iterator_t), intent(in) :: it
    end function hepmc_event_particle_iterator_get

```

```

<HepMC interface: procedures>+≡
  module function hepmc_event_particle_iterator_get (it) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_event_particle_iterator_t), intent(in) :: it
    prt%obj = event_particle_const_iterator_get (it%obj)
  end function hepmc_event_particle_iterator_get

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function gen_event_get_nth_particle (evt_obj, n) bind(C)
      import
      type(c_ptr), value :: evt_obj
      integer(c_int), value :: n
    end function gen_event_get_nth_particle
  end interface
  interface
    integer(c_int) function gen_event_get_nth_beam (evt_obj, n) bind(C)
      import
      type(c_ptr), value :: evt_obj
      integer(c_int), value :: n
    end function gen_event_get_nth_beam
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_get_nth_particle
  public :: hepmc_event_get_nth_beam

<HepMC interface: sub interfaces>+≡
  module function hepmc_event_get_nth_particle (evt, n) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: n
  end function hepmc_event_get_nth_particle
  module function hepmc_event_get_nth_beam (evt, n) result (beam_barcode)
    integer :: beam_barcode
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: n
  end function hepmc_event_get_nth_beam

<HepMC interface: procedures>+≡
  module function hepmc_event_get_nth_particle (evt, n) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: n
    integer :: n_tot
    integer(c_int) :: nth
    nth = n
    n_tot = gen_event_get_n_particles (evt%obj)
    if (n > n_tot .or. n < 1) then
      prt%obj = c_null_ptr
      call msg_error ("HepMC interface called for wrong particle ID.")
    else
      prt%obj = gen_event_get_nth_particle (evt%obj, nth)
    end if
  end function hepmc_event_get_nth_particle

```

```

module function hepmc_event_get_nth_beam (evt, n) result (beam_barcode)
  integer :: beam_barcode
  type(hepmc_event_t), intent(in) :: evt
  integer, intent(in) :: n
  integer(c_int) :: bc
  bc = gen_event_get_nth_beam (evt%obj, n)
  beam_barcode = bc
end function hepmc_event_get_nth_beam

```

18.12.10 I/O streams

There is a specific I/O stream type for handling the output of GenEvent objects (i.e., Monte Carlo event samples) to file. Opening the file is done by the constructor, closing by the destructor.

```

<HepMC interface: public>+≡
  public :: hepmc_iostream_t
<HepMC interface: types>+≡
  type :: hepmc_iostream_t
  private
  type(c_ptr) :: obj
end type hepmc_iostream_t

```

Constructor for an output stream associated to a file.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_io_gen_event_out (hepmc3_mode, filename) bind(C)
    import
    integer(c_int), intent(in) :: hepmc3_mode
    character(c_char), dimension(*), intent(in) :: filename
    end function new_io_gen_event_out
  end interface
<HepMC interface: public>+≡
  public :: hepmc_iostream_open_out
<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_iostream_open_out (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    end subroutine hepmc_iostream_open_out
<HepMC interface: procedures>+≡
  module subroutine hepmc_iostream_open_out (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    integer(c_int) :: mode
    mode = hepmc3_mode
    iostream%obj = &
      new_io_gen_event_out (mode, char (filename) // c_null_char)
  end subroutine hepmc_iostream_open_out

```

Constructor for an input stream associated to a file.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_io_gen_event_in (hepmc3_mode, filename) bind(C)
    import
    integer(c_int), intent(in) :: hepmc3_mode
    character(c_char), dimension(*), intent(in) :: filename
    end function new_io_gen_event_in
  end interface

<HepMC interface: public>+≡
  public :: hepmc_iostream_open_in

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_iostream_open_in (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    end subroutine hepmc_iostream_open_in

<HepMC interface: procedures>+≡
  module subroutine hepmc_iostream_open_in (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    integer(c_int) :: mode
    mode = hepmc3_mode
    iostream%obj = &
      new_io_gen_event_in (mode, char (filename) // c_null_char)
  end subroutine hepmc_iostream_open_in

```

Destructor:

```

<HepMC interface: interfaces>+≡
  interface
    subroutine io_gen_event_delete (io_obj) bind(C)
    import
    type(c_ptr), value :: io_obj
    end subroutine io_gen_event_delete
  end interface

<HepMC interface: public>+≡
  public :: hepmc_iostream_close

<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_iostream_close (iostream)
    type(hepmc_iostream_t), intent(inout) :: iostream
    end subroutine hepmc_iostream_close

<HepMC interface: procedures>+≡
  module subroutine hepmc_iostream_close (iostream)
    type(hepmc_iostream_t), intent(inout) :: iostream
    call io_gen_event_delete (iostream%obj)
  end subroutine hepmc_iostream_close

```

Write a single event to the I/O stream.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine io_gen_event_write_event (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end subroutine io_gen_event_write_event
  end interface
  interface
    subroutine io_gen_event_write_event_hepmc2 (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end subroutine io_gen_event_write_event_hepmc2
  end interface
<HepMC interface: public>+≡
  public :: hepmc_iostream_write_event
<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_iostream_write_event (iostream, evt, hepmc3_mode)
    type(hepmc_iostream_t), intent(inout) :: iostream
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in), optional :: hepmc3_mode
  end subroutine hepmc_iostream_write_event
<HepMC interface: procedures>+≡
  module subroutine hepmc_iostream_write_event (iostream, evt, hepmc3_mode)
    type(hepmc_iostream_t), intent(inout) :: iostream
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in), optional :: hepmc3_mode
    integer :: mode
    mode = HEPMC3_MODE_HEPMC3
    if (present (hepmc3_mode)) mode = hepmc3_mode
    call io_gen_event_write_event (iostream%obj, evt%obj)
  end subroutine hepmc_iostream_write_event

```

Read a single event from the I/O stream. Return true if successful.

```

<HepMC interface: interfaces>+≡
  interface
    logical(c_bool) function io_gen_event_read_event (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end function io_gen_event_read_event
  end interface
<HepMC interface: public>+≡
  public :: hepmc_iostream_read_event
<HepMC interface: sub interfaces>+≡
  module subroutine hepmc_iostream_read_event (iostream, evt, ok)
    type(hepmc_iostream_t), intent(inout) :: iostream
    type(hepmc_event_t), intent(inout) :: evt
    logical, intent(out) :: ok
  end subroutine hepmc_iostream_read_event

```

```

<HepMC interface: procedures>+≡
  module subroutine hepmc_iostream_read_event (iostream, evt, ok)
    type(hepmc_iostream_t), intent(inout) :: iostream
    type(hepmc_event_t), intent(inout) :: evt
    logical, intent(out) :: ok
    ok = io_gen_event_read_event (iostream%obj, evt%obj)
  end subroutine hepmc_iostream_read_event

```

18.12.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<hepmc_interface_ut.f90>≡
  <File header>

  module hepmc_interface_ut
    use unit_tests
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE
    use hepmc_interface_util

```

<Standard module head>

<HepMC interface: public test>

contains

<HepMC interface: test driver>

end module hepmc_interface_ut

```

<hepmc_interface_util.f90>≡
  <File header>

```

```

  module hepmc_interface_util

```

<Use kinds>

<Use strings>

```

    use io_units

```

```

    use lorentz

```

```

    use flavors

```

```

    use colors

```

```

    use polarizations

```

```

    use hepmc_interface

```

<Standard module head>

<HepMC interface: test declarations>

contains

<HepMC interface: tests>

```

end module hepmc_interface_util
API: driver for the unit tests below.
<HepMC interface: public test>≡
  public :: hepmc_interface_test
<HepMC interface: test driver>≡
  subroutine hepmc_interface_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <HepMC interface: execute tests>
  end subroutine hepmc_interface_test

```

This test example is an abridged version from the build-from-scratch example in the HepMC distribution. We create two vertices for $p \rightarrow q$ PDF splitting, then a vertex for a $qq \rightarrow W^- g$ hard-interaction process, and finally a vertex for $W^- \rightarrow qq$ decay. The setup is for LHC kinematics.

Extending the original example, we set color flow for the incoming quarks and polarization for the outgoing photon. For the latter, we have to define a particle-data object for the photon, so a flavor object can be correctly initialized.

```

<HepMC interface: execute tests>≡
  if (HEPMC2_AVAILABLE) then
    call test (hepmc_interface_1, "hepmc2_interface_1", &
      "check HepMC2 interface", &
      u, results)
  else if (HEPMC3_AVAILABLE) then
    call test (hepmc_interface_1, "hepmc3_interface_1", &
      "check HepMC3 interface", &
      u, results)
  end if
<HepMC interface: test declarations>≡
  public :: hepmc_interface_1
<HepMC interface: tests>≡
  subroutine hepmc_interface_1 (u)
    use physics_defs, only: VECTOR
    use model_data, only: field_data_t
    integer, intent(in) :: u
    integer :: u_file, iostat
    type(hepmc_event_t) :: evt
    type(hepmc_vertex_t) :: v1, v2, v3, v4
    type(hepmc_particle_t) :: prt1, prt2, prt3, prt4, prt5, prt6, prt7, prt8
    type(hepmc_iostream_t) :: iostream
    type(flavor_t) :: flv
    type(color_t) :: col
    type(polarization_t) :: pol
    type(field_data_t), target :: photon_data
    character(80) :: buffer

    write (u, "(A)")  "* Test output: HepMC interface"
    write (u, "(A)")  "* Purpose: test HepMC interface"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"

```



```

write (u, "(A)")

! Initialize a photon flavor object and some polarization
call photon_data%init (var_str ("PHOTON"), 22)
call photon_data%set (spin_type=VECTOR)
call photon_data%freeze ()
call flv%init (photon_data)
call pol%init_angles &
    (flv, 0.6_default, 1._default, 0.5_default)

! Event initialization
call hepmc_event_init (evt, 20, 1)

write (u, "(A)")  "* p -> q splitting"
write (u, "(A)")

! $p\to q$ splittings
call hepmc_vertex_init (v1)
call hepmc_event_add_vertex (evt, v1)
call hepmc_vertex_init (v2)
call hepmc_event_add_vertex (evt, v2)
call particle_init (prt1, &
    0._default, 0._default, 7000._default, 7000._default, &
    2212, 3)
call hepmc_vertex_add_particle_in (v1, prt1)
call particle_init (prt2, &
    0._default, 0._default, -7000._default, 7000._default, &
    2212, 3)
call hepmc_vertex_add_particle_in (v2, prt2)
call particle_init (prt3, &
    .750_default, -1.569_default, 32.191_default, 32.238_default, &
    1, 3)
call color_init_from_array (col, [501])
call hepmc_particle_set_color (prt3, col)
call hepmc_vertex_add_particle_out (v1, prt3)
call particle_init (prt4, &
    -3.047_default, -19._default, -54.629_default, 57.920_default, &
    -2, 3)
call color_init_from_array (col, [-501])
call hepmc_particle_set_color (prt4, col)
call hepmc_vertex_add_particle_out (v2, prt4)

write (u, "(A)")  "* Hard interaction"
write (u, "(A)")

! Hard interaction
call hepmc_vertex_init (v3)
call hepmc_event_add_vertex (evt, v3)
call hepmc_vertex_add_particle_in (v3, prt3)
call hepmc_vertex_add_particle_in (v3, prt4)
call particle_init (prt6, &
    -3.813_default, 0.113_default, -1.833_default, 4.233_default, &
    22, 1)
call hepmc_particle_set_polarization (prt6, pol)

```

```

call hepmc_vertex_add_particle_out (v3, prt6)
call particle_init (prt5, &
    1.517_default, -20.68_default, -20.605_default, 85.925_default, &
    -24, 3)
call hepmc_vertex_add_particle_out (v3, prt5)
call hepmc_event_set_signal_process_vertex (evt, v3)

! $W^-$ decay
call vertex_init_pos (v4, &
    0.12_default, -0.3_default, 0.05_default, 0.004_default)
call hepmc_event_add_vertex (evt, v4)
call hepmc_vertex_add_particle_in (v4, prt5)
call particle_init (prt7, &
    -2.445_default, 28.816_default, 6.082_default, 29.552_default, &
    1, 1)
call hepmc_vertex_add_particle_out (v4, prt7)
call particle_init (prt8, &
    3.962_default, -49.498_default, -26.687_default, 56.373_default, &
    -2, 1)
call hepmc_vertex_add_particle_out (v4, prt8)

! Event output
call hepmc_event_print (evt)
write (u, "(A)") "Writing to file 'hepmc_test.hepmc'"
write (u, "(A)")

call hepmc_iostream_open_out (iostream , var_str ("hepmc_test.hepmc"), 2)
call hepmc_iostream_write_event (iostream, evt)
call hepmc_iostream_close (iostream)

write (u, "(A)") "Writing completed"

write (u, "(A)")
write (u, "(A)") "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "hepmc_test.hepmc", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:14) == "HepMC::Version") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)") "* Cleanup"
write (u, "(A)")

! Wrapup
! call pol%final ()
call hepmc_event_final (evt)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: hepmc_interface_1"

contains

subroutine vertex_init_pos (v, x, y, z, t)
  type(hepmc_vertex_t), intent(out) :: v
  real(default), intent(in) :: x, y, z, t
  type(vector4_t) :: xx
  xx = vector4_moving (t, vector3_moving ([x, y, z]))
  call hepmc_vertex_init (v, xx)
end subroutine vertex_init_pos

subroutine particle_init (prt, px, py, pz, E, pdg, status)
  type(hepmc_particle_t), intent(out) :: prt
  real(default), intent(in) :: px, py, pz, E
  integer, intent(in) :: pdg, status
  type(vector4_t) :: p
  p = vector4_moving (E, vector3_moving ([px, py, pz]))
  call hepmc_particle_init (prt, p, pdg, status)
end subroutine particle_init

end subroutine hepmc_interface_1

```

18.13 LCIO events

This section provides the interface to the LCIO C++ library for handling Monte-Carlo events.

Each C++ class of LCIO that we use is mirrored by a Fortran type, which contains as its only component the C pointer to the C++ object.

Each C++ method of LCIO that we use has a C wrapper function. This function takes a pointer to the host object as its first argument. Further arguments are either C pointers, or in the case of simple types (integer, real), interoperable C/Fortran objects.

The C wrapper functions have explicit interfaces in the Fortran module. They are called by Fortran wrapper procedures. These are treated as methods of the corresponding Fortran type.

```

(lcio_interface.f90)≡
  <File header>

```

```

module lcio_interface

  use, intrinsic :: iso_c_binding !NODEP!

  <Use kinds>
  <Use strings>
  use lorentz
  use flavors
  use colors
  use helicities

```

```

    use polarizations
    use event_handles, only: event_handle_t

    <Standard module head>

    <LCIO interface: public>

    <LCIO interface: types>

    <LCIO interface: interfaces>

    interface
    <LCIO interface: sub interfaces>
    end interface

    end module lcio_interface

    <lcio_interface_sub.f90>≡
    <File header>

    submodule (lcio_interface) lcio_interface_s

        use constants, only: PI
        use physics_defs, only: ns_per_mm
        use diagnostics

        implicit none

    contains

    <LCIO interface: procedures>

    end submodule lcio_interface_s

```

18.13.1 Interface check

This function can be called in order to verify that we are using the actual LCIO library, and not the dummy version.

```

    <LCIO interface: interfaces>≡
    interface
        logical(c_bool) function lcio_available () bind(C)
        import
        end function lcio_available
    end interface

    <LCIO interface: public>≡
    public :: lcio_is_available

    <LCIO interface: sub interfaces>≡
    module function lcio_is_available () result (flag)
        logical :: flag
    end function lcio_is_available

```

```

<LCIO interface: procedures>≡
  module function lcio_is_available () result (flag)
    logical :: flag
    flag = lcio_available ()
  end function lcio_is_available

```

18.13.2 LCIO Run Header

This is a type for the run header of the LCIO file.

```

<LCIO interface: public>+≡
  public :: lcio_run_header_t

<LCIO interface: types>≡
  type :: lcio_run_header_t
  private
  type(c_ptr) :: obj
  end type lcio_run_header_t

```

The Fortran version has initializer form.

```

<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function new_lcio_run_header (proc_id) bind(C)
      import
      integer(c_int), value :: proc_id
    end function new_lcio_run_header
  end interface

<LCIO interface: interfaces>+≡
  interface
    subroutine run_header_set_simstring &
      (runhdr_obj, simstring) bind(C)
    import
    type(c_ptr), value :: runhdr_obj
    character(c_char), dimension(*), intent(in) :: simstring
  end subroutine run_header_set_simstring
  end interface

<LCIO interface: public>+≡
  public :: lcio_run_header_init

<LCIO interface: sub interfaces>+≡
  module subroutine lcio_run_header_init (runhdr, proc_id, run_id)
    type(lcio_run_header_t), intent(out) :: runhdr
    integer, intent(in), optional :: proc_id, run_id
  end subroutine lcio_run_header_init

<LCIO interface: procedures>+≡
  module subroutine lcio_run_header_init (runhdr, proc_id, run_id)
    type(lcio_run_header_t), intent(out) :: runhdr
    integer, intent(in), optional :: proc_id, run_id
    integer(c_int) :: rid
    rid = 0; if (present (run_id)) rid = run_id
    runhdr%obj = new_lcio_run_header (rid)
    call run_header_set_simstring (runhdr%obj, &

```

```

        "WHIZARD version:" // "<Version>")
    end subroutine lcio_run_header_init

<LCIO interface: interfaces>+≡
    interface
        subroutine write_run_header (lcwrt_obj, runhdr_obj) bind(C)
            import
            type(c_ptr), value :: lcwrt_obj
            type(c_ptr), value :: runhdr_obj
        end subroutine write_run_header
    end interface

<LCIO interface: public>+≡
    public :: lcio_run_header_write

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_run_header_write (wrt, hdr)
        type(lcio_writer_t), intent(inout) :: wrt
        type(lcio_run_header_t), intent(inout) :: hdr
    end subroutine lcio_run_header_write

<LCIO interface: procedures>+≡
    module subroutine lcio_run_header_write (wrt, hdr)
        type(lcio_writer_t), intent(inout) :: wrt
        type(lcio_run_header_t), intent(inout) :: hdr
        call write_run_header (wrt%obj, hdr%obj)
    end subroutine lcio_run_header_write

```

18.13.3 LCIO Event and LC Collection

The main object of LCIO is a LCEventImpl. The object is filled by MCParticle objects, which are set as LCCollection.

```

<LCIO interface: public>+≡
    public :: lccollection_t

<LCIO interface: types>+≡
    type :: lccollection_t
    private
        type(c_ptr) :: obj = c_null_ptr
    end type lccollection_t

```

Initializer.

```

<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function new_lccollection () bind(C)
            import
        end function new_lccollection
    end interface

<LCIO interface: public>+≡
    public :: lcio_event_t

```

```

<LCIO interface: types>+≡
  type, extends (event_handle_t) :: lcio_event_t
  private
    type(c_ptr) :: obj = c_null_ptr
    type(lccollection_t) :: lccoll
  end type lcio_event_t

```

Constructor. Arguments are process ID (integer) and event ID (integer).
The Fortran version has initializer form.

```

<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function new_lcio_event (proc_id, event_id, run_id) bind(C)
    import
      integer(c_int), value :: proc_id, event_id, run_id
    end function new_lcio_event
  end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_event_init

```

```

<LCIO interface: sub interfaces>+≡
  module subroutine lcio_event_init (evt, proc_id, event_id, run_id)
    type(lcio_event_t), intent(out) :: evt
    integer, intent(in), optional :: proc_id, event_id, run_id
  end subroutine lcio_event_init

```

```

<LCIO interface: procedures>+≡
  module subroutine lcio_event_init (evt, proc_id, event_id, run_id)
    type(lcio_event_t), intent(out) :: evt
    integer, intent(in), optional :: proc_id, event_id, run_id
    integer(c_int) :: pid, eid, rid
    pid = 0; if (present (proc_id)) pid = proc_id
    eid = 0; if (present (event_id)) eid = event_id
    rid = 0; if (present (run_id)) rid = run_id
    evt%obj = new_lcio_event (pid, eid, rid)
    evt%lccoll%obj = new_lccollection ()
  end subroutine lcio_event_init

```

Destructor.

```

<LCIO interface: interfaces>+≡
  interface
    subroutine lcio_event_delete (evt_obj) bind(C)
    import
      type(c_ptr), value :: evt_obj
    end subroutine lcio_event_delete
  end interface

```

Show event on screen.

```

<LCIO interface: interfaces>+≡
  interface
    subroutine dump_lcio_event (evt_obj) bind(C)
    import
      type(c_ptr), value :: evt_obj
    end subroutine dump_lcio_event
  end interface

```

```

<LCIO interface: public>+≡
    public :: show_lcio_event

<LCIO interface: sub interfaces>+≡
    module subroutine show_lcio_event (evt)
        type(lcio_event_t), intent(in) :: evt
    end subroutine show_lcio_event

<LCIO interface: procedures>+≡
    module subroutine show_lcio_event (evt)
        type(lcio_event_t), intent(in) :: evt
        if (c_associated (evt%obj)) then
            call dump_lcio_event (evt%obj)
        else
            call msg_error ("LCIO event is not allocated.")
        end if
    end subroutine show_lcio_event

```

Put a single event to file.

```

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_event_to_file (evt_obj, filename) bind(C)
            import
            type(c_ptr), value :: evt_obj
            character(c_char), dimension(*), intent(in) :: filename
        end subroutine lcio_event_to_file
    end interface

<LCIO interface: public>+≡
    public :: write_lcio_event

<LCIO interface: sub interfaces>+≡
    module subroutine write_lcio_event (evt, filename)
        type(lcio_event_t), intent(in) :: evt
        type(string_t), intent(in) :: filename
    end subroutine write_lcio_event

<LCIO interface: procedures>+≡
    module subroutine write_lcio_event (evt, filename)
        type(lcio_event_t), intent(in) :: evt
        type(string_t), intent(in) :: filename
        call lcio_event_to_file (evt%obj, char (filename) // c_null_char)
    end subroutine write_lcio_event

```

Finalize: use the LCIO destructor. Also nullify the pointer explicitly, to be on the safe side.

```

<LCIO interface: public>+≡
    public :: lcio_event_final

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_final (evt, delete)
        type(lcio_event_t), intent(inout) :: evt
        logical, intent(in) :: delete
    end subroutine lcio_event_final

```



```

<LCIO interface: procedures>+≡
  module subroutine lcio_event_final (evt, delete)
    type(lcio_event_t), intent(inout) :: evt
    logical, intent(in) :: delete
    if (c_associated (evt%obj)) then
      if (delete) call lcio_event_delete (evt%obj)
      evt%obj = c_null_ptr
      evt%lccoll%obj = c_null_ptr
    end if
  end subroutine lcio_event_final

```

Nullify: do not call the destructor, just nullify the C pointer. There should be another pointer associated with the object.

```

<LCIO interface: public>+≡
  public :: lcio_event_nullify

<LCIO interface: sub interfaces>+≡
  module subroutine lcio_event_nullify (evt)
    type(lcio_event_t), intent(inout) :: evt
  end subroutine lcio_event_nullify

```

```

<LCIO interface: procedures>+≡
  module subroutine lcio_event_nullify (evt)
    type(lcio_event_t), intent(inout) :: evt
    evt%obj = c_null_ptr
    evt%lccoll%obj = c_null_ptr
  end subroutine lcio_event_nullify

```

Return the actual object as a C pointer. For use in the native C++ interface only.

```

<LCIO interface: public>+≡
  public :: lcio_event_get_c_ptr

<LCIO interface: sub interfaces>+≡
  module function lcio_event_get_c_ptr (evt) result (p)
    type(lcio_event_t), intent(in) :: evt
    type(c_ptr) :: p
  end function lcio_event_get_c_ptr

<LCIO interface: procedures>+≡
  module function lcio_event_get_c_ptr (evt) result (p)
    type(lcio_event_t), intent(in) :: evt
    type(c_ptr) :: p
    p = evt%obj
  end function lcio_event_get_c_ptr

```

```

<LCIO interface: interfaces>+≡
  interface
    subroutine lcio_set_weight (evt_obj, weight) bind(C)
      import
      type(c_ptr), value :: evt_obj
      real(c_double), value :: weight
    end subroutine lcio_set_weight
  end interface

```

```

interface
  subroutine lcio_set_alpha_qcd (evt_obj, alphas) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: alphas
  end subroutine lcio_set_alpha_qcd
end interface
interface
  subroutine lcio_set_scale (evt_obj, scale) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: scale
  end subroutine lcio_set_scale
end interface
interface
  subroutine lcio_set_sqrts (evt_obj, sqrts) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: sqrts
  end subroutine lcio_set_sqrts
end interface
interface
  subroutine lcio_set_xsec (evt_obj, xsec, xsec_err) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: xsec, xsec_err
  end subroutine lcio_set_xsec
end interface
interface
  subroutine lcio_set_beam (evt_obj, pdg, beam) bind(C)
    import
    type(c_ptr), value :: evt_obj
    integer(c_int), value :: pdg, beam
  end subroutine lcio_set_beam
end interface
interface
  subroutine lcio_set_pol (evt_obj, pol, beam) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: pol
    integer(c_int), value :: beam
  end subroutine lcio_set_pol
end interface
interface
  subroutine lcio_set_beam_file (evt_obj, file) bind(C)
    import
    type(c_ptr), value :: evt_obj
    character(len=1, kind=c_char), dimension(*), intent(in) :: file
  end subroutine lcio_set_beam_file
end interface
interface
  subroutine lcio_set_process_name (evt_obj, name) bind(C)
    import
    type(c_ptr), value :: evt_obj

```

```

        character(len=1, kind=c_char), dimension(*), intent(in) :: name
    end subroutine lcio_set_process_name
end interface
interface
    subroutine lcio_set_sqme (evt_obj, sqme) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: sqme
    end subroutine lcio_set_sqme
end interface
interface
    subroutine lcio_set_alt_sqme (evt_obj, sqme, index) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: sqme
        integer(c_int), value :: index
    end subroutine lcio_set_alt_sqme
end interface
interface
    subroutine lcio_set_alt_weight (evt_obj, weight, index) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: weight
        integer(c_int), value :: index
    end subroutine lcio_set_alt_weight
end interface

<LCIO interface: public>+≡
    public :: lcio_event_set_weight

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_weight (evt, weight)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight
    end subroutine lcio_event_set_weight

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_weight (evt, weight)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight
        call lcio_set_weight (evt%obj, real (weight, c_double))
    end subroutine lcio_event_set_weight

<LCIO interface: public>+≡
    public :: lcio_event_set_alpha_qcd

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_alpha_qcd (evt, alphas)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: alphas
    end subroutine lcio_event_set_alpha_qcd

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_alpha_qcd (evt, alphas)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: alphas

```

```

        call lcio_set_alpha_qcd (evt%obj, real (alphas, c_double))
    end subroutine lcio_event_set_alpha_qcd

<LCIO interface: public>+≡
    public :: lcio_event_set_scale

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_scale (evt, scale)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: scale
    end subroutine lcio_event_set_scale

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_scale (evt, scale)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: scale
        call lcio_set_scale (evt%obj, real (scale, c_double))
    end subroutine lcio_event_set_scale

<LCIO interface: public>+≡
    public :: lcio_event_set_sqrts

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_sqrts (evt, sqrts)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqrts
    end subroutine lcio_event_set_sqrts

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_sqrts (evt, sqrts)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqrts
        call lcio_set_sqrts (evt%obj, real (sqrts, c_double))
    end subroutine lcio_event_set_sqrts

<LCIO interface: public>+≡
    public :: lcio_event_set_xsec

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_xsec (evt, xsec, xsec_err)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: xsec, xsec_err
    end subroutine lcio_event_set_xsec

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_xsec (evt, xsec, xsec_err)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: xsec, xsec_err
        call lcio_set_xsec (evt%obj, &
            real (xsec, c_double), real (xsec_err, c_double))
    end subroutine lcio_event_set_xsec

<LCIO interface: public>+≡
    public :: lcio_event_set_beam

```

```

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_beam (evt, pdg, beam)
        type(lcio_event_t), intent(inout) :: evt
        integer, intent(in) :: pdg, beam
    end subroutine lcio_event_set_beam

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_beam (evt, pdg, beam)
        type(lcio_event_t), intent(inout) :: evt
        integer, intent(in) :: pdg, beam
        call lcio_set_beam (evt%obj, &
            int (pdg, c_int), int (beam, c_int))
    end subroutine lcio_event_set_beam

<LCIO interface: public>+≡
    public :: lcio_event_set_polarization

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_polarization (evt, pol, beam)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: pol
        integer, intent(in) :: beam
    end subroutine lcio_event_set_polarization

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_polarization (evt, pol, beam)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: pol
        integer, intent(in) :: beam
        call lcio_set_pol (evt%obj, real (pol, c_double), &
            int (beam, c_int))
    end subroutine lcio_event_set_polarization

<LCIO interface: public>+≡
    public :: lcio_event_set_beam_file

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_beam_file (evt, file)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: file
    end subroutine lcio_event_set_beam_file

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_beam_file (evt, file)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: file
        call lcio_set_beam_file (evt%obj, &
            char (file) // c_null_char)
    end subroutine lcio_event_set_beam_file

<LCIO interface: public>+≡
    public :: lcio_event_set_process_name

```

```

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_process_name (evt, name)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: name
    end subroutine lcio_event_set_process_name

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_process_name (evt, name)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: name
        call lcio_set_process_name (evt%obj, &
            char (name) // c_null_char)
    end subroutine lcio_event_set_process_name

<LCIO interface: public>+≡
    public :: lcio_event_set_alt_sqme

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_alt_sqme (evt, sqme, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
        integer, intent(in) :: index
    end subroutine lcio_event_set_alt_sqme

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_alt_sqme (evt, sqme, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
        integer, intent(in) :: index
        call lcio_set_alt_sqme (evt%obj, real (sqme, c_double), &
            int (index, c_int))
    end subroutine lcio_event_set_alt_sqme

<LCIO interface: public>+≡
    public :: lcio_event_set_sqme

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_sqme (evt, sqme)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
    end subroutine lcio_event_set_sqme

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_sqme (evt, sqme)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
        call lcio_set_sqme (evt%obj, real (sqme, c_double))
    end subroutine lcio_event_set_sqme

<LCIO interface: public>+≡
    public :: lcio_event_set_alt_weight

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_set_alt_weight (evt, weight, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight

```

```

        integer, intent(in) :: index
    end subroutine lcio_event_set_alt_weight

<LCIO interface: procedures>+≡
    module subroutine lcio_event_set_alt_weight (evt, weight, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight
        integer, intent(in) :: index
        call lcio_set_alt_weight (evt%obj, real (weight, c_double), &
            int (index, c_int))
    end subroutine lcio_event_set_alt_weight

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_event_add_collection &
            (evt_obj, lccoll_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj, lccoll_obj
    end subroutine lcio_event_add_collection
end interface

<LCIO interface: public>+≡
    public :: lcio_event_add_coll

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_event_add_coll (evt)
        type(lcio_event_t), intent(inout) :: evt
    end subroutine lcio_event_add_coll

<LCIO interface: procedures>+≡
    module subroutine lcio_event_add_coll (evt)
        type(lcio_event_t), intent(inout) :: evt
        call lcio_event_add_collection (evt%obj, &
            evt%lccoll%obj)
    end subroutine lcio_event_add_coll

```

18.13.4 LCIO Particle

Particle objects have the obvious meaning.

```

<LCIO interface: public>+≡
    public :: lcio_particle_t

<LCIO interface: types>+≡
    type :: lcio_particle_t
    private
        type(c_ptr) :: obj
    end type lcio_particle_t

```

Constructor.

```

<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function new_lcio_particle &
            (px, py, pz, pdg_id, mass, charge, status) bind(C)
    import

```

```

        integer(c_int), value :: pdg_id, status
        real(c_double), value :: px, py, pz, mass, charge
    end function new_lcio_particle
end interface

<LCIO interface: interfaces>+≡
interface
    subroutine add_particle_to_collection &
        (prt_obj, lccoll_obj) bind(C)
    import
        type(c_ptr), value :: prt_obj, lccoll_obj
    end subroutine add_particle_to_collection
end interface

<LCIO interface: public>+≡
public :: lcio_particle_add_to_evt_coll

<LCIO interface: sub interfaces>+≡
module subroutine lcio_particle_add_to_evt_coll &
    (lprt, evt)
    type(lcio_particle_t), intent(in) :: lprt
    type(lcio_event_t), intent(inout) :: evt
end subroutine lcio_particle_add_to_evt_coll

<LCIO interface: procedures>+≡
module subroutine lcio_particle_add_to_evt_coll &
    (lprt, evt)
    type(lcio_particle_t), intent(in) :: lprt
    type(lcio_event_t), intent(inout) :: evt
    call add_particle_to_collection (lprt%obj, evt%lccoll%obj)
end subroutine lcio_particle_add_to_evt_coll

<LCIO interface: public>+≡
public :: lcio_particle_init

<LCIO interface: sub interfaces>+≡
module subroutine lcio_particle_init (prt, p, pdg, charge, status)
    type(lcio_particle_t), intent(out) :: prt
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: charge
    integer, intent(in) :: pdg, status
end subroutine lcio_particle_init

<LCIO interface: procedures>+≡
module subroutine lcio_particle_init (prt, p, pdg, charge, status)
    type(lcio_particle_t), intent(out) :: prt
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: charge
    real(default) :: mass
    real(default) :: px, py, pz
    integer, intent(in) :: pdg, status
    px = vector4_get_component (p, 1)
    py = vector4_get_component (p, 2)
    pz = vector4_get_component (p, 3)
    mass = p**1
    prt%obj = new_lcio_particle (real (px, c_double), real (py, c_double), &
        real (pz, c_double), int (pdg, c_int), &

```



```

        real (mass, c_double), real (charge, c_double), int (status, c_int))
end subroutine lcio_particle_init

```

Set the particle color flow.

<LCIO interface: interfaces>+≡

```

interface
  subroutine lcio_set_color_flow (prt_obj, col1, col2) bind(C)
    import
    type(c_ptr), value :: prt_obj
    integer(c_int), value :: col1, col2
  end subroutine lcio_set_color_flow
end interface

```

Set the particle color. Either from a color_t object or directly from a pair of integers.

<LCIO interface: interfaces>+≡

```

interface lcio_particle_set_color
  module procedure lcio_particle_set_color_col
  module procedure lcio_particle_set_color_int
end interface lcio_particle_set_color

```

<LCIO interface: public>+≡

```

public :: lcio_particle_set_color

```

<LCIO interface: sub interfaces>+≡

```

module subroutine lcio_particle_set_color_col (prt, col)
  type(lcio_particle_t), intent(inout) :: prt
  type(color_t), intent(in) :: col
end subroutine lcio_particle_set_color_col
module subroutine lcio_particle_set_color_int (prt, col)
  type(lcio_particle_t), intent(inout) :: prt
  integer, dimension(2), intent(in) :: col
end subroutine lcio_particle_set_color_int

```

<LCIO interface: procedures>+≡

```

module subroutine lcio_particle_set_color_col (prt, col)
  type(lcio_particle_t), intent(inout) :: prt
  type(color_t), intent(in) :: col
  integer(c_int), dimension(2) :: c
  c(1) = col%get_col ()
  c(2) = col%get_acl ()
  if (c(1) /= 0 .or. c(2) /= 0) then
    call lcio_set_color_flow (prt%obj, c(1), c(2))
  end if
end subroutine lcio_particle_set_color_col

module subroutine lcio_particle_set_color_int (prt, col)
  type(lcio_particle_t), intent(inout) :: prt
  integer, dimension(2), intent(in) :: col
  integer(c_int), dimension(2) :: c
  c = col
  if (c(1) /= 0 .or. c(2) /= 0) then
    call lcio_set_color_flow (prt%obj, c(1), c(2))
  end if
end subroutine lcio_particle_set_color_int

```

Return the particle color as a two-dimensional array (color, anticolor).

```

<LCIO interface: interfaces>+≡
    interface
        integer(c_int) function lcio_particle_flow (prt_obj, col_index) bind(C)
            use iso_c_binding !NODEP!
            type(c_ptr), value :: prt_obj
            integer(c_int), value :: col_index
        end function lcio_particle_flow
    end interface

<LCIO interface: public>+≡
    public :: lcio_particle_get_flow

<LCIO interface: sub interfaces>+≡
    module function lcio_particle_get_flow (prt) result (col)
        integer, dimension(2) :: col
        type(lcio_particle_t), intent(in) :: prt
    end function lcio_particle_get_flow

<LCIO interface: procedures>+≡
    module function lcio_particle_get_flow (prt) result (col)
        integer, dimension(2) :: col
        type(lcio_particle_t), intent(in) :: prt
        col(1) = lcio_particle_flow (prt%obj, 0_c_int)
        col(2) = - lcio_particle_flow (prt%obj, 1_c_int)
    end function lcio_particle_get_flow

```

Return the four-momentum of a LCIO particle.

```

<LCIO interface: interfaces>+≡
    interface
        real(c_double) function lcio_three_momentum (prt_obj, p_index) bind(C)
            use iso_c_binding !NODEP!
            type(c_ptr), value :: prt_obj
            integer(c_int), value :: p_index
        end function lcio_three_momentum
    end interface

<LCIO interface: interfaces>+≡
    interface
        real(c_double) function lcio_energy (prt_obj) bind(C)
            import
            type(c_ptr), intent(in), value :: prt_obj
        end function lcio_energy
    end interface

<LCIO interface: public>+≡
    public :: lcio_particle_get_momentum

<LCIO interface: sub interfaces>+≡
    module function lcio_particle_get_momentum (prt) result (p)
        type(vector4_t) :: p
        type(lcio_particle_t), intent(in) :: prt
    end function lcio_particle_get_momentum

<LCIO interface: procedures>+≡
    module function lcio_particle_get_momentum (prt) result (p)
        type(vector4_t) :: p

```

```

    type(lcio_particle_t), intent(in) :: prt
    real(default) :: E, px, py, pz
    E = lcio_energy (prt%obj)
    px = lcio_three_momentum (prt%obj, 0_c_int)
    py = lcio_three_momentum (prt%obj, 1_c_int)
    pz = lcio_three_momentum (prt%obj, 2_c_int)
    p = vector4_moving ( E, vector3_moving ([ px, py, pz ]))
end function lcio_particle_get_momentum

```

Return the invariant mass squared of the particle object. LCIO stores the signed invariant mass (no squaring).

<LCIO interface: interfaces>+≡

```

interface
    function lcio_mass (prt_obj) result (mass) bind(C)
        import
        real(c_double) :: mass
        type(c_ptr), value :: prt_obj
    end function lcio_mass
end interface

```

<LCIO interface: public>+≡

```

public :: lcio_particle_get_mass_squared

```

<LCIO interface: sub interfaces>+≡

```

module function lcio_particle_get_mass_squared (prt) result (m2)
    real(default) :: m2
    type(lcio_particle_t), intent(in) :: prt
end function lcio_particle_get_mass_squared

```

<LCIO interface: procedures>+≡

```

module function lcio_particle_get_mass_squared (prt) result (m2)
    real(default) :: m2
    type(lcio_particle_t), intent(in) :: prt
    real(default) :: m
    m = lcio_mass (prt%obj)
    m2 = sign (m**2, m)
end function lcio_particle_get_mass_squared

```

Return vertex and production time of a LCIO particle.

<LCIO interface: interfaces>+≡

```

interface
    real(c_double) function lcio_vtx_x (prt) bind(C)
        import
        type(c_ptr), value :: prt
    end function lcio_vtx_x
end interface
interface
    real(c_double) function lcio_vtx_y (prt) bind(C)
        import
        type(c_ptr), value :: prt
    end function lcio_vtx_y
end interface
interface
    real(c_double) function lcio_vtx_z (prt) bind(C)

```

```

        import
        type(c_ptr), value :: prt
    end function lcio_vtx_z
end interface
interface
    real(c_float) function lcio_prt_time (prt) bind(C)
        import
        type(c_ptr), value :: prt
    end function lcio_prt_time
end interface

(Decay) times in LCIO are in nanoseconds, so they need to get converted to
mm for the internal format.
<LCIO interface: public>+≡
    public :: lcio_particle_get_vertex
    public :: lcio_particle_get_time
<LCIO interface: sub interfaces>+≡
    module function lcio_particle_get_vertex (prt) result (vtx)
        type(vector3_t) :: vtx
        type(lcio_particle_t), intent(in) :: prt
    end function lcio_particle_get_vertex
    module function lcio_particle_get_time (prt) result (time)
        real(default) :: time
        type(lcio_particle_t), intent(in) :: prt
    end function lcio_particle_get_time
<LCIO interface: procedures>+≡
    module function lcio_particle_get_vertex (prt) result (vtx)
        type(vector3_t) :: vtx
        type(lcio_particle_t), intent(in) :: prt
        real(default) :: vx, vy, vz
        vx = lcio_vtx_x (prt%obj)
        vy = lcio_vtx_y (prt%obj)
        vz = lcio_vtx_z (prt%obj)
        vtx = vector3_moving ([vx, vy, vz])
    end function lcio_particle_get_vertex

    module function lcio_particle_get_time (prt) result (time)
        real(default) :: time
        type(lcio_particle_t), intent(in) :: prt
        time = lcio_prt_time (prt%obj)
        time = time / ns_per_mm
    end function lcio_particle_get_time

```

18.13.5 Polarization

For polarization there is a three-component float entry foreseen in the LCIO format. Completely generic density matrices can in principle be attached to events as float vectors added to `LCCollection` of the `LCEvent`. This is not yet implemented currently. Here, we restrict ourselves to the same implementation as in HepMC format: we use two entries as the polarization angles, while the first entry gives the degree of polarization (something not specified in the HepMC

format). For massive vector bosons, we arbitrarily choose the convention that the longitudinal (zero) helicity state is mapped to the theta angle $\pi/2$. This works under the condition that helicity is projected onto one of the basis states.

```

(LCIO interface: interfaces)+≡
interface
  subroutine lcio_particle_set_spin (prt_obj, s1, s2, s3) bind(C)
  import
  type(c_ptr), value :: prt_obj
  real(c_double), value :: s1, s2, s3
  end subroutine lcio_particle_set_spin
end interface

(LCIO interface: public)+≡
public :: lcio_polarization_init

(LCIO interface: interfaces)+≡
interface lcio_polarization_init
  module procedure lcio_polarization_init_pol
  module procedure lcio_polarization_init_hel
  module procedure lcio_polarization_init_int
end interface

(LCIO interface: sub interfaces)+≡
module subroutine lcio_polarization_init_pol (prt, pol)
  type(lcio_particle_t), intent(inout) :: prt
  type(polarization_t), intent(in) :: pol
end subroutine lcio_polarization_init_pol
module subroutine lcio_polarization_init_hel (prt, hel)
  type(lcio_particle_t), intent(inout) :: prt
  type(helicity_t), intent(in) :: hel
end subroutine lcio_polarization_init_hel
module subroutine lcio_polarization_init_int (prt, hel)
  type(lcio_particle_t), intent(inout) :: prt
  integer, intent(in) :: hel
end subroutine lcio_polarization_init_int

(LCIO interface: procedures)+≡
module subroutine lcio_polarization_init_pol (prt, pol)
  type(lcio_particle_t), intent(inout) :: prt
  type(polarization_t), intent(in) :: pol
  real(default) :: r, theta, phi
  if (pol%is_polarized ()) then
    call pol%to_angles (r, theta, phi)
    call lcio_particle_set_spin (prt%obj, &
      real(r, c_double), real (theta, c_double), real (phi, c_double))
  end if
end subroutine lcio_polarization_init_pol

module subroutine lcio_polarization_init_hel (prt, hel)
  type(lcio_particle_t), intent(inout) :: prt
  type(helicity_t), intent(in) :: hel
  integer, dimension(2) :: h
  if (hel%is_defined ()) then
    h = hel%to_pair ()
    select case (h(1))
    case (1:)

```

```

        call lcio_particle_set_spin (prt%obj, 1._c_double, &
            0._c_double, 0._c_double)
    case (:-1)
        call lcio_particle_set_spin (prt%obj, 1._c_double, &
            real (pi, c_double), 0._c_double)
    case (0)
        call lcio_particle_set_spin (prt%obj, 1._c_double, &
            real (pi/2, c_double), 0._c_double)
    end select
end if
end subroutine lcio_polarization_init_hel

module subroutine lcio_polarization_init_int (prt, hel)
    type(lcio_particle_t), intent(inout) :: prt
    integer, intent(in) :: hel
    call lcio_particle_set_spin (prt%obj, 0._c_double, &
        0._c_double, real (hel, c_double))
end subroutine lcio_polarization_init_int

```

Recover polarization from LCIO particle (with the abovementioned deficiencies).

<LCIO interface: interfaces>+≡

```

interface
    function lcio_polarization_degree (prt_obj) result (degree) bind(C)
        import
        real(c_double) :: degree
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_degree
end interface
interface
    function lcio_polarization_theta (prt_obj) result (theta) bind(C)
        import
        real(c_double) :: theta
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_theta
end interface
interface
    function lcio_polarization_phi (prt_obj) result (phi) bind(C)
        import
        real(c_double) :: phi
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_phi
end interface

```

<LCIO interface: public>+≡

```

public :: lcio_particle_to_pol

```

<LCIO interface: sub interfaces>+≡

```

module subroutine lcio_particle_to_pol (prt, flv, pol)
    type(lcio_particle_t), intent(in) :: prt
    type(flavor_t), intent(in) :: flv
    type(polarization_t), intent(out) :: pol
end subroutine lcio_particle_to_pol

```

<LCIO interface: procedures>+≡

```

module subroutine lcio_particle_to_pol (prt, flv, pol)

```

```

type(lcio_particle_t), intent(in) :: prt
type(flavor_t), intent(in) :: flv
type(polarization_t), intent(out) :: pol
real(default) :: degree, theta, phi
degree = lcio_polarization_degree (prt%obj)
theta = lcio_polarization_theta (prt%obj)
phi = lcio_polarization_phi (prt%obj)
call pol%init_angles (flv, degree, theta, phi)
end subroutine lcio_particle_to_pol

```

Recover helicity. Here, ϕ and `degree` is ignored and only the sign of $\cos \theta$ is relevant, mapped to positive/negative helicity.

```

<LCIO interface: public>+≡
    public :: lcio_particle_to_hel

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_particle_to_hel (prt, flv, hel)
        type(lcio_particle_t), intent(in) :: prt
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(out) :: hel
    end subroutine lcio_particle_to_hel

<LCIO interface: procedures>+≡
    module subroutine lcio_particle_to_hel (prt, flv, hel)
        type(lcio_particle_t), intent(in) :: prt
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(out) :: hel
        real(default) :: theta
        integer :: hmax
        theta = lcio_polarization_theta (prt%obj)
        hmax = flv%get_spin_type () / 2
        call hel%init (sign (hmax, nint (cos (theta))))
    end subroutine lcio_particle_to_hel

```

Set the vertex of a particle.

```

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_particle_set_vertex (prt_obj, vx, vy, vz) bind(C)
            import
            type(c_ptr), value :: prt_obj
            real(c_double), value :: vx, vy, vz
        end subroutine lcio_particle_set_vertex
    end interface
    interface
        subroutine lcio_particle_set_time (prt_obj, t) bind(C)
            import
            type(c_ptr), value :: prt_obj
            real(c_float), value :: t
        end subroutine lcio_particle_set_time
    end interface

<LCIO interface: public>+≡
    public :: lcio_particle_set_vtx

```

```

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_particle_set_vtx (prt, vtx)
        type(lcio_particle_t), intent(inout) :: prt
        type(vector3_t), intent(in) :: vtx
    end subroutine lcio_particle_set_vtx

<LCIO interface: procedures>+≡
    module subroutine lcio_particle_set_vtx (prt, vtx)
        type(lcio_particle_t), intent(inout) :: prt
        type(vector3_t), intent(in) :: vtx
        call lcio_particle_set_vertex (prt%obj, real(vtx%p(1), c_double), &
            real(vtx%p(2), c_double), real(vtx%p(3), c_double))
    end subroutine lcio_particle_set_vtx

Times in LCIO are in nanoseconds, not in mm, so need to be converted.

<LCIO interface: public>+≡
    public :: lcio_particle_set_t

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_particle_set_t (prt, t)
        type(lcio_particle_t), intent(inout) :: prt
        real(default), intent(in) :: t
    end subroutine lcio_particle_set_t

<LCIO interface: procedures>+≡
    module subroutine lcio_particle_set_t (prt, t)
        type(lcio_particle_t), intent(inout) :: prt
        real(default), intent(in) :: t
        real(default) :: ns_from_t_mm
        ns_from_t_mm = ns_per_mm * t
        call lcio_particle_set_time (prt%obj, real(ns_from_t_mm, c_float))
    end subroutine lcio_particle_set_t

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_particle_add_parent (prt_obj1, prt_obj2) bind(C)
            import
            type(c_ptr), value :: prt_obj1, prt_obj2
        end subroutine lcio_particle_add_parent
    end interface

<LCIO interface: public>+≡
    public :: lcio_particle_set_parent

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_particle_set_parent (daughter, parent)
        type(lcio_particle_t), intent(inout) :: daughter, parent
    end subroutine lcio_particle_set_parent

<LCIO interface: procedures>+≡
    module subroutine lcio_particle_set_parent (daughter, parent)
        type(lcio_particle_t), intent(inout) :: daughter, parent
        call lcio_particle_add_parent (daughter%obj, parent%obj)
    end subroutine lcio_particle_set_parent

```



```

<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_particle_get_generator_status &
    (prt_obj) bind(C)
  import
    type(c_ptr), value :: prt_obj
  end function lcio_particle_get_generator_status
end interface

<LCIO interface: public>+≡
public :: lcio_particle_get_status

<LCIO interface: sub interfaces>+≡
module function lcio_particle_get_status (lptr) result (status)
  integer :: status
  type(lcio_particle_t), intent(in) :: lptr
end function lcio_particle_get_status

<LCIO interface: procedures>+≡
module function lcio_particle_get_status (lptr) result (status)
  integer :: status
  type(lcio_particle_t), intent(in) :: lptr
  status = lcio_particle_get_generator_status (lptr%obj)
end function lcio_particle_get_status

```

Getting the PDG code.

```

<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_particle_get_pdg_code (prt_obj) bind(C)
  import
    type(c_ptr), value :: prt_obj
  end function lcio_particle_get_pdg_code
end interface

<LCIO interface: public>+≡
public :: lcio_particle_get_pdg

<LCIO interface: sub interfaces>+≡
module function lcio_particle_get_pdg (lptr) result (pdg)
  integer :: pdg
  type(lcio_particle_t), intent(in) :: lptr
end function lcio_particle_get_pdg

<LCIO interface: procedures>+≡
module function lcio_particle_get_pdg (lptr) result (pdg)
  integer :: pdg
  type(lcio_particle_t), intent(in) :: lptr
  pdg = lcio_particle_get_pdg_code (lptr%obj)
end function lcio_particle_get_pdg

```

Obtaining the number of parents and daughters of an LCIO particle.

```

<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_n_parents (prt_obj) bind(C)
  import
    type(c_ptr), value :: prt_obj

```

```

        end function lcio_n_parents
    end interface

    <LCIO interface: interfaces>+≡
    interface
        integer(c_int) function lcio_n_daughters (prt_obj) bind(C)
        import
        type(c_ptr), value :: prt_obj
        end function lcio_n_daughters
    end interface

    <LCIO interface: public>+≡
    public :: lcio_particle_get_n_parents

    <LCIO interface: sub interfaces>+≡
    module function lcio_particle_get_n_parents (lptr) result (n_parents)
        integer :: n_parents
        type(lcio_particle_t), intent(in) :: lptr
    end function lcio_particle_get_n_parents

    <LCIO interface: procedures>+≡
    module function lcio_particle_get_n_parents (lptr) result (n_parents)
        integer :: n_parents
        type(lcio_particle_t), intent(in) :: lptr
        n_parents = lcio_n_parents (lptr%obj)
    end function lcio_particle_get_n_parents

    <LCIO interface: public>+≡
    public :: lcio_particle_get_n_children

    <LCIO interface: sub interfaces>+≡
    module function lcio_particle_get_n_children (lptr) result (n_children)
        integer :: n_children
        type(lcio_particle_t), intent(in) :: lptr
    end function lcio_particle_get_n_children

    <LCIO interface: procedures>+≡
    module function lcio_particle_get_n_children (lptr) result (n_children)
        integer :: n_children
        type(lcio_particle_t), intent(in) :: lptr
        n_children = lcio_n_daughters (lptr%obj)
    end function lcio_particle_get_n_children

```

This provides access from the LCIO event `lcio_event_t` to the array entries of the parent and daughter arrays of the LCIO particles.

```

    <LCIO interface: interfaces>+≡
    interface
        integer(c_int) function lcio_event_parent_k &
            (evt_obj, num_part, k_parent) bind (C)
        use iso_c_binding !NODEP!
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: num_part, k_parent
        end function lcio_event_parent_k
    end interface

```

```

<LCIO interface: interfaces>+≡
interface
    integer(c_int) function lcio_event_daughter_k &
        (evt_obj, num_part, k_daughter) bind (C)
    use iso_c_binding !NODEP!
    type(c_ptr), value :: evt_obj
    integer(c_int), value :: num_part, k_daughter
    end function lcio_event_daughter_k
end interface

<LCIO interface: public>+≡
public :: lcio_get_n_parents

<LCIO interface: sub interfaces>+≡
module function lcio_get_n_parents &
    (evt, num_part, k_parent) result (index_parent)
    type(lcio_event_t), intent(in) :: evt
    integer, intent(in) :: num_part, k_parent
    integer :: index_parent
    end function lcio_get_n_parents

<LCIO interface: procedures>+≡
module function lcio_get_n_parents &
    (evt, num_part, k_parent) result (index_parent)
    type(lcio_event_t), intent(in) :: evt
    integer, intent(in) :: num_part, k_parent
    integer :: index_parent
    index_parent = lcio_event_parent_k (evt%obj, int (num_part, c_int), &
        int (k_parent, c_int))
    end function lcio_get_n_parents

<LCIO interface: public>+≡
public :: lcio_get_n_children

<LCIO interface: sub interfaces>+≡
module function lcio_get_n_children &
    (evt, num_part, k_daughter) result (index_daughter)
    type(lcio_event_t), intent(in) :: evt
    integer, intent(in) :: num_part, k_daughter
    integer :: index_daughter
    end function lcio_get_n_children

<LCIO interface: procedures>+≡
module function lcio_get_n_children &
    (evt, num_part, k_daughter) result (index_daughter)
    type(lcio_event_t), intent(in) :: evt
    integer, intent(in) :: num_part, k_daughter
    integer :: index_daughter
    index_daughter = lcio_event_daughter_k (evt%obj, int (num_part, c_int), &
        int (k_daughter, c_int))
    end function lcio_get_n_children

```

18.13.6 LCIO Writer type

There is a specific LCIO Writer type for handling the output of LCEventImpl objects (i.e., Monte Carlo event samples) to file. Opening the file is done by the constructor, closing by the destructor.

```
<LCIO interface: public>+≡
    public :: lcio_writer_t
<LCIO interface: types>+≡
    type :: lcio_writer_t
    private
    type(c_ptr) :: obj
    end type lcio_writer_t
```

Constructor for an output associated to a file.

```
<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function open_lcio_writer_new (filename, complevel) bind(C)
        import
        character(c_char), dimension(*), intent(in) :: filename
        integer(c_int), intent(in) :: complevel
        end function open_lcio_writer_new
    end interface
<LCIO interface: public>+≡
    public :: lcio_writer_open_out
<LCIO interface: sub interfaces>+≡
    module subroutine lcio_writer_open_out (lcio_writer, filename)
        type(lcio_writer_t), intent(out) :: lcio_writer
        type(string_t), intent(in) :: filename
    end subroutine lcio_writer_open_out
<LCIO interface: procedures>+≡
    module subroutine lcio_writer_open_out (lcio_writer, filename)
        type(lcio_writer_t), intent(out) :: lcio_writer
        type(string_t), intent(in) :: filename
        lcio_writer%obj = open_lcio_writer_new (char (filename) // &
            c_null_char, 9_c_int)
    end subroutine lcio_writer_open_out
```

Destructor:

```
<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_writer_delete (io_obj) bind(C)
        import
        type(c_ptr), value :: io_obj
        end subroutine lcio_writer_delete
    end interface
<LCIO interface: public>+≡
    public :: lcio_writer_close
<LCIO interface: sub interfaces>+≡
    module subroutine lcio_writer_close (lciowriter)
        type(lcio_writer_t), intent(inout) :: lciowriter
    end subroutine lcio_writer_close
```

```

<LCIO interface: procedures>+≡
  module subroutine lcio_writer_close (lciowriter)
    type(lcio_writer_t), intent(inout) :: lciowriter
    call lcio_writer_delete (lciowriter%obj)
  end subroutine lcio_writer_close

```

Write a single event to the LCIO writer.

```

<LCIO interface: interfaces>+≡
  interface
    subroutine lcio_write_event (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end subroutine lcio_write_event
  end interface

<LCIO interface: public>+≡
  public :: lcio_event_write

<LCIO interface: sub interfaces>+≡
  module subroutine lcio_event_write (wrt, evt)
    type(lcio_writer_t), intent(inout) :: wrt
    type(lcio_event_t), intent(in) :: evt
  end subroutine lcio_event_write

<LCIO interface: procedures>+≡
  module subroutine lcio_event_write (wrt, evt)
    type(lcio_writer_t), intent(inout) :: wrt
    type(lcio_event_t), intent(in) :: evt
    call lcio_write_event (wrt%obj, evt%obj)
  end subroutine lcio_event_write

```

18.13.7 LCIO Reader type

There is a specific LCIO Reader type for handling the input of LCEventImpl objects (i.e., Monte Carlo event samples) from file. Opening the file is done by the constructor, closing by the destructor.

```

<LCIO interface: public>+≡
  public :: lcio_reader_t

<LCIO interface: types>+≡
  type :: lcio_reader_t
  private
  type(c_ptr) :: obj
end type lcio_reader_t

```

Constructor for an output associated to a file.

```

<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function open_lcio_reader (filename) bind(C)
      import
      character(c_char), dimension(*), intent(in) :: filename
    end function open_lcio_reader
  end interface

```

```

<LCIO interface: public>+≡
    public :: lcio_open_file

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_open_file (lcio_reader, filename)
        type(lcio_reader_t), intent(out) :: lcio_reader
        type(string_t), intent(in) :: filename
    end subroutine lcio_open_file

<LCIO interface: procedures>+≡
    module subroutine lcio_open_file (lcio_reader, filename)
        type(lcio_reader_t), intent(out) :: lcio_reader
        type(string_t), intent(in) :: filename
        lcio_reader%obj = open_lcio_reader (char (filename) // c_null_char)
    end subroutine lcio_open_file

```

Destructor:

```

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_reader_delete (io_obj) bind(C)
            import
            type(c_ptr), value :: io_obj
        end subroutine lcio_reader_delete
    end interface

<LCIO interface: public>+≡
    public :: lcio_reader_close

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_reader_close (lcioreader)
        type(lcio_reader_t), intent(inout) :: lcioreader
    end subroutine lcio_reader_close

<LCIO interface: procedures>+≡
    module subroutine lcio_reader_close (lcioreader)
        type(lcio_reader_t), intent(inout) :: lcioreader
        call lcio_reader_delete (lcioreader%obj)
    end subroutine lcio_reader_close

```

Read a single event from the event file. Return true if successful.

```

<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function read_lcio_event (io_obj) bind(C)
            import
            type(c_ptr), value :: io_obj
        end function read_lcio_event
    end interface

<LCIO interface: public>+≡
    public :: lcio_read_event

<LCIO interface: sub interfaces>+≡
    module subroutine lcio_read_event (lcrdr, evt, ok)
        type(lcio_reader_t), intent(inout) :: lcrdr
        type(lcio_event_t), intent(out) :: evt
        logical, intent(out) :: ok
    end subroutine lcio_read_event

```

```

<LCIO interface: procedures>+≡
  module subroutine lcio_read_event (lcrdr, evt, ok)
    type(lcio_reader_t), intent(inout) :: lcrdr
    type(lcio_event_t), intent(out) :: evt
    logical, intent(out) :: ok
    evt%obj = read_lcio_event (lcrdr%obj)
    ok = c_associated (evt%obj)
  end subroutine lcio_read_event

```

Get the event index.

```

<LCIO interface: interfaces>+≡
  interface
    integer(c_int) function lcio_event_get_event_number (evt_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
  end function lcio_event_get_event_number
end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_event_get_event_index

```

```

<LCIO interface: sub interfaces>+≡
  module function lcio_event_get_event_index (evt) result (i_evt)
    integer :: i_evt
    type(lcio_event_t), intent(in) :: evt
  end function lcio_event_get_event_index

```

```

<LCIO interface: procedures>+≡
  module function lcio_event_get_event_index (evt) result (i_evt)
    integer :: i_evt
    type(lcio_event_t), intent(in) :: evt
    i_evt = lcio_event_get_event_number (evt%obj)
  end function lcio_event_get_event_index

```

Extract the process ID. This is stored (at the moment abusively) in the RUN ID as well as in an additional event parameter.

```

<LCIO interface: interfaces>+≡
  interface
    integer(c_int) function lcio_event_signal_process_id (evt_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
  end function lcio_event_signal_process_id
end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_event_get_process_id

```

```

<LCIO interface: sub interfaces>+≡
  module function lcio_event_get_process_id (evt) result (i_proc)
    integer :: i_proc
    type(lcio_event_t), intent(in) :: evt
  end function lcio_event_get_process_id

```

```

<LCIO interface: procedures>+≡
  module function lcio_event_get_process_id (evt) result (i_proc)
    integer :: i_proc
    type(lcio_event_t), intent(in) :: evt
    i_proc = lcio_event_signal_process_id (evt%obj)
  end function lcio_event_get_process_id

```

Number of particles in an LCIO event.

```

<LCIO interface: interfaces>+≡
  interface
    integer(c_int) function lcio_event_get_n_particles (evt_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
    end function lcio_event_get_n_particles
  end interface

```

```

<LCIO interface:>≡

```

```

<LCIO interface: public>+≡
  public :: lcio_event_get_n_tot

```

```

<LCIO interface: sub interfaces>+≡
  module function lcio_event_get_n_tot (evt) result (n_tot)
    integer :: n_tot
    type(lcio_event_t), intent(in) :: evt
  end function lcio_event_get_n_tot

```

```

<LCIO interface: procedures>+≡
  module function lcio_event_get_n_tot (evt) result (n_tot)
    integer :: n_tot
    type(lcio_event_t), intent(in) :: evt
    n_tot = lcio_event_get_n_particles (evt%obj)
  end function lcio_event_get_n_tot

```

Extracting α_s and the scale.

```

<LCIO interface: interfaces>+≡
  interface
    function lcio_event_get_alpha_qcd (evt_obj) result (as) bind(C)
    import
    real(c_double) :: as
    type(c_ptr), value :: evt_obj
    end function lcio_event_get_alpha_qcd
  end interface
  interface
    function lcio_event_get_scale (evt_obj) result (scale) bind(C)
    import
    real(c_double) :: scale
    type(c_ptr), value :: evt_obj
    end function lcio_event_get_scale
  end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_event_get_alphas

```



```

<LCIO interface: sub interfaces>+≡
    module function lcio_event_get_alphas (evt) result (as)
        type(lcio_event_t), intent(in) :: evt
        real(default) :: as
    end function lcio_event_get_alphas

<LCIO interface: procedures>+≡
    module function lcio_event_get_alphas (evt) result (as)
        type(lcio_event_t), intent(in) :: evt
        real(default) :: as
        as = lcio_event_get_alpha_qcd (evt%obj)
    end function lcio_event_get_alphas

<LCIO interface: public>+≡
    public :: lcio_event_get_scaleval

<LCIO interface: sub interfaces>+≡
    module function lcio_event_get_scaleval (evt) result (scale)
        type(lcio_event_t), intent(in) :: evt
        real(default) :: scale
    end function lcio_event_get_scaleval

<LCIO interface: procedures>+≡
    module function lcio_event_get_scaleval (evt) result (scale)
        type(lcio_event_t), intent(in) :: evt
        real(default) :: scale
        scale = lcio_event_get_scale (evt%obj)
    end function lcio_event_get_scaleval

```

Extracting particles by index from an LCIO event.

```

<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function lcio_event_particle_k (evt_obj, k) bind(C)
        import
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: k
    end function lcio_event_particle_k
    end interface

<LCIO interface: public>+≡
    public :: lcio_event_get_particle

<LCIO interface: sub interfaces>+≡
    module function lcio_event_get_particle (evt, n) result (prt)
        type(lcio_event_t), intent(in) :: evt
        integer, intent(in) :: n
        type(lcio_particle_t) :: prt
    end function lcio_event_get_particle

<LCIO interface: procedures>+≡
    module function lcio_event_get_particle (evt, n) result (prt)
        type(lcio_event_t), intent(in) :: evt
        integer, intent(in) :: n
        type(lcio_particle_t) :: prt
        prt%obj = lcio_event_particle_k (evt%obj, int (n, c_int))
    end function lcio_event_get_particle

```

18.13.8 Unit tests

Test module, followed by the corresponding implementation module.

```
<lcio_interface_ut.f90>≡  
  <File header>  
  
  module lcio_interface_ut  
    use unit_tests  
    use lcio_interface_utl  
  
    <Standard module head>  
  
    <LCIO interface: public test>  
  
    contains  
  
    <LCIO interface: test driver>  
  
  end module lcio_interface_ut  
<lcio_interface_uti.f90>≡  
  <File header>  
  
  module lcio_interface_uti  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use lorentz  
    use flavors  
    use colors  
    use polarizations  
  
    use lcio_interface  
  
    <Standard module head>  
  
    <LCIO interface: test declarations>  
  
    contains  
  
    <LCIO interface: tests>  
  
  end module lcio_interface_uti  
API: driver for the unit tests below.  
<LCIO interface: public test>≡  
  public :: lcio_interface_test  
<LCIO interface: test driver>≡  
  subroutine lcio_interface_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <LCIO interface: execute tests>  
  end subroutine lcio_interface_test
```

```

<LCIO interface: execute tests>≡
  call test (lcio_interface_1, "lcio_interface_1", &
    "check LCIO interface", &
    u, results)

<LCIO interface: test declarations>≡
  public :: lcio_interface_1

<LCIO interface: tests>≡
  subroutine lcio_interface_1 (u)
    use physics_defs, only: VECTOR
    use model_data, only: field_data_t
    integer, intent(in) :: u
    integer :: u_file, iostat
    type(lcio_event_t) :: evt
    type(lcio_particle_t) :: prt1, prt2, prt3, prt4, prt5, prt6, prt7, prt8
    type(flavor_t) :: flv
    type(color_t) :: col
    type(polarization_t) :: pol
    type(field_data_t), target :: photon_data
    character(220) :: buffer

    write (u, "(A)")  "* Test output: LCIO interface"
    write (u, "(A)")  "* Purpose: test LCIO interface"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    ! Initialize a photon flavor object and some polarization
    call photon_data%init (var_str ("PHOTON"), 22)
    call photon_data%set (spin_type=VECTOR)
    call photon_data%freeze ()
    call flv%init (photon_data)
    call pol%init_angles &
      (flv, 0.6_default, 1._default, 0.5_default)

    ! Event initialization
    call lcio_event_init (evt, 20, 1, 42)

    write (u, "(A)")  "* p -> q splitting"
    write (u, "(A)")

    ! $p\to q$ splittings
    call particle_init (prt1, &
      0._default, 0._default, 7000._default, 7000._default, &
      2212, 1._default, 3)
    call particle_init (prt2, &
      0._default, 0._default, -7000._default, 7000._default, &
      2212, 1._default, 3)
    call particle_init (prt3, &
      .750_default, -1.569_default, 32.191_default, 32.238_default, &
      1, -1._default/3._default, 3)
    call color_init_from_array (col, [501])
    call lcio_particle_set_color (prt3, col)

```

```

call lcio_particle_set_parent (prt3, prt1)
call lcio_particle_set_parent (prt3, prt2)
call particle_init (prt4, &
  -3.047_default, -19._default, -54.629_default, 57.920_default, &
  -2, -2._default/3._default, 3)
call color_init_from_array (col, [-501])
call lcio_particle_set_color (prt4, col)
call lcio_particle_set_parent (prt4, prt1)
call lcio_particle_set_parent (prt4, prt2)

write (u, "(A)")  "* Hard interaction"
write (u, "(A)")

! Hard interaction
call particle_init (prt6, &
  -3.813_default, 0.113_default, -1.833_default, 4.233_default, &
  22, 0._default, 1)
call lcio_polarization_init (prt6, pol)
call particle_init (prt5, &
  1.517_default, -20.68_default, -20.605_default, 85.925_default, &
  -24, -1._default, 3)
call lcio_particle_set_parent (prt5, prt3)
call lcio_particle_set_parent (prt5, prt4)
call lcio_particle_set_parent (prt6, prt3)
call lcio_particle_set_parent (prt6, prt4)

! $W^-$ decay
call particle_init (prt7, &
  -2.445_default, 28.816_default, 6.082_default, 29.552_default, &
  1, -1._default/3._default, 1)
call particle_init (prt8, &
  3.962_default, -49.498_default, -26.687_default, 56.373_default, &
  -2, -2._default/3._default, 1)
call lcio_particle_set_t (prt7, 0.12_default)
call lcio_particle_set_t (prt8, 0.12_default)
call lcio_particle_set_vtx &
  (prt7, vector3_moving ([-0.3_default, 0.05_default, 0.004_default]))
call lcio_particle_set_vtx &
  (prt8, vector3_moving ([-0.3_default, 0.05_default, 0.004_default]))
call lcio_particle_set_parent (prt7, prt5)
call lcio_particle_set_parent (prt8, prt5)
call lcio_particle_add_to_evt_coll (prt1, evt)
call lcio_particle_add_to_evt_coll (prt2, evt)
call lcio_particle_add_to_evt_coll (prt3, evt)
call lcio_particle_add_to_evt_coll (prt4, evt)
call lcio_particle_add_to_evt_coll (prt5, evt)
call lcio_particle_add_to_evt_coll (prt6, evt)
call lcio_particle_add_to_evt_coll (prt7, evt)
call lcio_particle_add_to_evt_coll (prt8, evt)
call lcio_event_add_coll (evt)

! Event output
write (u, "(A)")  "Writing in ASCII form to file 'lcio_test.slcio'"
write (u, "(A)")

```

```

call write_lcio_event (evt, var_str ("lcio_test.slcio"))

write (u, "(A)") "Writing completed"

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "lcio_test.slcio", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (trim (buffer) == "") cycle
  if (buffer(1:12) == " - timestamp") buffer = "[...]"
  if (buffer(1:6) == " date:") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

! Wrapup
! call pol%final ()
call lcio_event_final (evt, .true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lcio_interface_1"

contains

subroutine particle_init &
  (prt, px, py, pz, E, pdg, charge, status)
  type(lcio_particle_t), intent(out) :: prt
  real(default), intent(in) :: px, py, pz, E, charge
  integer, intent(in) :: pdg, status
  type(vector4_t) :: p
  p = vector4_moving (E, vector3_moving ([px, py, pz]))
  call lcio_particle_init (prt, p, pdg, charge, status)
end subroutine particle_init

end subroutine lcio_interface_1

```

18.14 HEP Common and Events

This is a separate module that manages data exchange between the common blocks and `event_t` objects. We separate this from the previous module in order to avoid a circular module dependency. It also contains the functions necessary

for communication between `hepmc_event_t` and `event_t` or `lcio_event_t` and `event_t` as well as `particle_set_t` and `particle_t` objects.

`<hep_events.f90>`≡

<File header>

`module hep_events`

<Use kinds>

<Use strings>

`use lorentz`

`use polarizations`

`use model_data`

`use particles`

`use hepmc_interface`

`use lcio_interface`

`use event_base`

<Standard module head>

<HEP events: public>

`interface`

<HEP events: sub interfaces>

`end interface`

`end module hep_events`

`<hep_events_sub.f90>`≡

<File header>

`submodule (hep_events) hep_events_s`

`use system_dependencies, only: HEPMC2_AVAILABLE`

`use system_dependencies, only: HEPMC3_AVAILABLE`

`use diagnostics`

`use numeric_utils`

`use flavors`

`use colors`

`use helicities`

`use subevents, only: PRT_BEAM, PRT_INCOMING, PRT_OUTGOING`

`use subevents, only: PRT_UNDEFINED`

`use subevents, only: PRT_VIRTUAL, PRT_RESONANT, PRT_BEAM_REMNANT`

`use hep_common`

`implicit none`

`contains`

<HEP events: procedures>

`end submodule hep_events_s`

18.14.1 Data Transfer: events

Fill the HEPEUP block, given a WHIZARD event object.

```

<HEP events: public>≡
    public :: hepeup_from_event

<HEP events: sub interfaces>≡
    module subroutine hepeup_from_event &
        (event, keep_beams, keep_remnants, process_index)
        class(generic_event_t), intent(in), target :: event
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        integer, intent(in), optional :: process_index
    end subroutine hepeup_from_event

<HEP events: procedures>≡
    module subroutine hepeup_from_event &
        (event, keep_beams, keep_remnants, process_index)
        class(generic_event_t), intent(in), target :: event
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        integer, intent(in), optional :: process_index
        type(particle_set_t), pointer :: particle_set
        real(default) :: scale, alpha_qcd
        if (event%has_valid_particle_set ()) then
            particle_set => event%get_particle_set_ptr ()
            call hepeup_from_particle_set (particle_set, keep_beams, keep_remnants)
            if (present (process_index)) then
                call hepeup_set_event_parameters (proc_id = process_index)
            end if
            scale = event%get_fac_scale ()
            if (.not. vanishes (scale)) then
                call hepeup_set_event_parameters (scale = scale)
            end if
            alpha_qcd = event%get_alpha_s ()
            if (.not. vanishes (alpha_qcd)) then
                call hepeup_set_event_parameters (alpha_qcd = alpha_qcd)
            end if
            if (event%weight_prc_is_known ()) then
                call hepeup_set_event_parameters (weight = event%get_weight_prc ())
            end if
        else
            call msg_bug ("HEPEUP: event incomplete")
        end if
    end subroutine hepeup_from_event

```

Reverse.

Note: The current implementation sets the particle set of the hard process and is therefore not useful if the event on file is dressed. This should be reconsidered.

Note: setting of scale or alpha is not yet supported by the `event_t` object. Ticket #628.

```

<HEP events: public>+≡
    public :: hepeup_to_event

```

```

<HEP events: sub interfaces>+≡
  module subroutine hepeup_to_event &
    (event, fallback_model, process_index, recover_beams, &
     use_alpha_s, use_scale)
    class(generic_event_t), intent(inout), target :: event
    class(model_data_t), intent(in), target :: fallback_model
    integer, intent(out), optional :: process_index
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alpha_s
    logical, intent(in), optional :: use_scale
  end subroutine hepeup_to_event

```

```

<HEP events: procedures>+≡
  module subroutine hepeup_to_event &
    (event, fallback_model, process_index, recover_beams, &
     use_alpha_s, use_scale)
    class(generic_event_t), intent(inout), target :: event
    class(model_data_t), intent(in), target :: fallback_model
    integer, intent(out), optional :: process_index
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alpha_s
    logical, intent(in), optional :: use_scale
    class(model_data_t), pointer :: model
    real(default) :: weight, scale, alpha_qcd
    type(particle_set_t) :: particle_set
    model => event%get_model_ptr ()
    call hepeup_to_particle_set &
      (particle_set, recover_beams, model, fallback_model)
    call event%set_hard_particle_set (particle_set)
    call particle_set%final ()
    if (present (process_index)) then
      call hepeup_get_event_parameters (proc_id = process_index)
    end if
    call hepeup_get_event_parameters (weight = weight, &
      scale = scale, alpha_qcd = alpha_qcd)
    call event%set_weight_ref (weight)
    if (present (use_alpha_s)) then
      if (use_alpha_s .and. alpha_qcd > 0) &
        call event%set_alpha_qcd_forced (alpha_qcd)
    end if
    if (present (use_scale)) then
      if (use_scale .and. scale > 0) &
        call event%set_scale_forced (scale)
    end if
  end subroutine hepeup_to_event

```

Fill the HEPEVT (event) common block.

The `i_evt` argument overrides the index stored in the `event` object.

```

<HEP events: public>+≡
  public :: hepevt_from_event

<HEP events: sub interfaces>+≡
  module subroutine hepevt_from_event &
    (event, process_index, i_evt, keep_beams, keep_remnants, &
     ensure_order, fill_hepev4)

```



```

class(generic_event_t), intent(in), target :: event
integer, intent(in), optional :: i_evt, process_index
logical, intent(in), optional :: keep_beams
logical, intent(in), optional :: keep_remnants
logical, intent(in), optional :: ensure_order
logical, intent(in), optional :: fill_hepev4
end subroutine hepevt_from_event

<HEP events: procedures>+≡
module subroutine hepevt_from_event &
    (event, process_index, i_evt, keep_beams, keep_remnants, &
     ensure_order, fill_hepev4)
class(generic_event_t), intent(in), target :: event
integer, intent(in), optional :: i_evt, process_index
logical, intent(in), optional :: keep_beams
logical, intent(in), optional :: keep_remnants
logical, intent(in), optional :: ensure_order
logical, intent(in), optional :: fill_hepev4
type(particle_set_t), pointer :: particle_set
real(default) :: alpha_qcd, scale
if (event%has_valid_particle_set ()) then
    particle_set => event%get_particle_set_ptr ()
    call hepevt_from_particle_set (particle_set, keep_beams, &
        keep_remnants, ensure_order, fill_hepev4)
    if (present (process_index)) then
        call hepevt_set_event_parameters (proc_id = process_index)
    end if
    if (event%weight_prc_is_known ()) then
        call hepevt_set_event_parameters (weight = event%get_weight_prc ())
    end if
    if (event%sqme_prc_is_known ()) then
        call hepevt_set_event_parameters &
            (function_value = event%get_sqme_prc ())
    end if
    scale = event%get_fac_scale ()
    if (.not. vanishes (scale)) then
        call hepevt_set_event_parameters (scale = scale)
    end if
    alpha_qcd = event%get_alpha_s ()
    if (.not. vanishes (alpha_qcd)) then
        call hepevt_set_event_parameters (alpha_qcd = alpha_qcd)
    end if
    if (present (i_evt)) then
        call hepevt_set_event_parameters (i_evt = i_evt)
    else if (event%has_index ()) then
        call hepevt_set_event_parameters (i_evt = event%get_index ())
    else
        call hepevt_set_event_parameters (i_evt = 0)
    end if
else
    call msg_bug ("HEPEVT: event incomplete")
end if
end subroutine hepevt_from_event

```

HepMC format

The master output function fills a HepMC GenEvent object that is already initialized, but has no vertices in it.

We first set up the vertex lists and enter the vertices into the HepMC event. Then, we assign first all incoming particles and then all outgoing particles to their associated vertices. Particles which have neither parent nor children entries (this should not happen) are dropped.

Finally, we insert the beam particles. If there are none, use the incoming particles instead. Transform a particle into a `hepmc_particle` object, including color and polarization. The HepMC status is equivalent to the HEPEVT status, in particular: 0 = null entry, 1 = physical particle, 2 = decayed/fragmented SM hadron, tau or muon, 3 = other unphysical particle entry, 4 = incoming particles, 11 = intermediate resonance such as squarks. The use of 11 for intermediate resonances is as done by HERWIG, see <http://herwig.hepforge.org/trac/wiki/FaQs>.

(HEP events: procedures)+≡

```
subroutine particle_to_hepmc (prt, hprt)
  type(particle_t), intent(in) :: prt
  type(hepmc_particle_t), intent(out) :: hprt
  integer :: hepmc_status
  select case (prt%get_status ())
  case (PRT_UNDEFINED)
    hepmc_status = 0
  case (PRT_OUTGOING)
    hepmc_status = 1
  case (PRT_BEAM)
    hepmc_status = 4
  case (PRT_RESONANT)
    hepmc_status = 2
  case (PRT_BEAM_REMNANT)
    if (prt%get_n_children () == 0) then
      hepmc_status = 1
    else
      hepmc_status = 3
    end if
  case default
    hepmc_status = 3
  end select
  call hepmc_particle_init (hprt, &
    prt%get_momentum (), prt%get_pdg (), &
    hepmc_status)
  if (HEPMC2_AVAILABLE) then
    call hepmc_particle_set_color (hprt, prt%get_color ())
    select case (prt%get_polarization_status ())
    case (PRT_DEFINITE_HELICITY)
      call hepmc_particle_set_polarization (hprt, &
        prt%get_helicity ())
    case (PRT_GENERIC_POLARIZATION)
      call hepmc_particle_set_polarization (hprt, &
        prt%get_polarization ())
    end select
  end if
end subroutine particle_to_hepmc
```

For HepMC3, a HepMC particle needs first to be attached to a vertex and an event before non-intrinsic particle properties (color flow and helicity) could be set.

```

<HEP events: public>+=
    public :: hepmc_event_from_particle_set

<HEP events: sub interfaces>+=
    module subroutine hepmc_event_from_particle_set &
        (evt, particle_set, cross_section, error, color)
        type(hepmc_event_t), intent(inout) :: evt
        type(particle_set_t), intent(in) :: particle_set
        real(default), intent(in), optional :: cross_section, error
        logical, intent(in), optional :: color
    end subroutine hepmc_event_from_particle_set

<HEP events: procedures>+=
    module subroutine hepmc_event_from_particle_set &
        (evt, particle_set, cross_section, error, color)
        type(hepmc_event_t), intent(inout) :: evt
        type(particle_set_t), intent(in) :: particle_set
        real(default), intent(in), optional :: cross_section, error
        logical, intent(in), optional :: color
        type(hepmc_vertex_t), dimension(:), allocatable :: v
        type(hepmc_particle_t), dimension(:), allocatable :: hpvt
        type(hepmc_particle_t), dimension(2) :: hbeam
        type(vector4_t), dimension(:), allocatable :: vtx
        logical, dimension(:), allocatable :: is_beam
        integer, dimension(:), allocatable :: v_from, v_to
        integer :: n_vertices, n_tot, i
        logical :: write_color
        write_color = .false.
        if (present (color)) write_color = color
        n_tot = particle_set%get_n_tot ()
        allocate (v_from (n_tot), v_to (n_tot))
        call particle_set%assign_vertices (v_from, v_to, n_vertices)
        allocate (hpvt (n_tot))
        allocate (vtx (n_vertices))
        vtx = vector4_null
        do i = 1, n_tot
            if (v_to(i) /= 0 .or. v_from(i) /= 0) then
                call particle_to_hepmc (particle_set%prt(i), hpvt(i))
                if (v_from(i) /= 0) then
                    vtx(v_from(i)) = particle_set%prt(i)%get_vertex ()
                end if
            end if
        end do
        if (present (cross_section) .and. present(error)) &
            call hepmc_event_set_cross_section (evt, cross_section, error)
        allocate (v (n_vertices))
        do i = 1, n_vertices
            call hepmc_vertex_init (v(i), vtx(i))
            call hepmc_event_add_vertex (evt, v(i))
        end do
        allocate (is_beam (n_tot))

```

```

is_beam = particle_set%prt(1:n_tot)%get_status () == PRT_BEAM
if (.not. any (is_beam)) then
    is_beam = particle_set%prt(1:n_tot)%get_status () == PRT_INCOMING
end if
if (count (is_beam) == 2) then
    hbeam = pack (hprt, is_beam)
    call hepmc_event_set_beam_particles (evt, hbeam(1), hbeam(2))
end if
do i = 1, n_tot
    if (v_to(i) /= 0) then
        call hepmc_vertex_add_particle_in (v(v_to(i)), hprt(i))
    end if
end do
do i = 1, n_tot
    if (v_from(i) /= 0) then
        call hepmc_vertex_add_particle_out (v(v_from(i)), hprt(i))
    end if
end do
FIND_SIGNAL_PROCESS: do i = 1, n_tot
    if (particle_set%prt(i)%get_status () == PRT_INCOMING) then
        call hepmc_event_set_signal_process_vertex (evt, v(v_to(i)))
        exit FIND_SIGNAL_PROCESS
    end if
end do FIND_SIGNAL_PROCESS
if (HEPMC3_AVAILABLE) then
    do i = 1, n_tot
        if (write_color) then
            call hepmc_particle_set_color (hprt(i), &
                particle_set%prt(i)%get_color ())
        end if
        select case (particle_set%prt(i)%get_polarization_status ())
        case (PRT_DEFINITE_HELICITY)
            call hepmc_particle_set_polarization (hprt(i), &
                particle_set%prt(i)%get_helicity ())
        case (PRT_GENERIC_POLARIZATION)
            call hepmc_particle_set_polarization (hprt(i), &
                particle_set%prt(i)%get_polarization ())
        end select
    end do
end if
end subroutine hepmc_event_from_particle_set

```

Initialize a particle from a HepMC particle object. The model is necessary for making a fully qualified flavor component. We have the additional flag `polarized` which tells whether the polarization information should be interpreted or ignored, and the lookup array of barcodes. Note that the lookup array is searched linearly, a possible bottleneck for large particle arrays. If necessary, the barcode array could be replaced by a hash table.

(HEP events: procedures) +=

```

subroutine particle_from_hepmc_particle &
    (prt, hprt, model, fallback_model, polarization, barcode)
type(particle_t), intent(out) :: prt
type(hepmc_particle_t), intent(in) :: hprt

```

```

type(model_data_t), intent(in), target :: model
type(model_data_t), intent(in), target :: fallback_model
type(hepmc_vertex_t) :: vtx
integer, intent(in) :: polarization
integer, dimension(:), intent(in) :: barcode
type(hepmc_polarization_t) :: hpol
type(flavor_t) :: flv
type(color_t) :: col
type(helicity_t) :: hel
type(polarization_t) :: pol
type(vector4_t) :: vertex
integer :: n_parents, n_children
integer, dimension(:), allocatable :: &
    parent_barcode, child_barcode, parent, child
integer :: i
select case (hepmc_particle_get_status (hprt))
case (1); call prt%set_status (PRT_OUTGOING)
case (2); call prt%set_status (PRT_RESONANT)
case (3); call prt%set_status (PRT_VIRTUAL)
end select
if (hepmc_particle_is_beam (hprt)) call prt%set_status (PRT_BEAM)
call flv%init (hepmc_particle_get_pdg (hprt), model, fallback_model)
call col%init (hepmc_particle_get_color (hprt))
call prt%set_flavor (flv)
call prt%set_color (col)
call prt%set_polarization (polarization)
select case (polarization)
case (PRT_DEFINITE_HELICITY)
    hpol = hepmc_particle_get_polarization (hprt)
    call hepmc_polarization_to_hel (hpol, prt%get_flv (), hel)
    call prt%set_helicity (hel)
    call hepmc_polarization_final (hpol)
case (PRT_GENERIC_POLARIZATION)
    hpol = hepmc_particle_get_polarization (hprt)
    call hepmc_polarization_to_pol (hpol, prt%get_flv (), pol)
    call prt%set_pol (pol)
    call hepmc_polarization_final (hpol)
end select
call prt%set_momentum (hepmc_particle_get_momentum (hprt), &
    hepmc_particle_get_mass_squared (hprt))
n_parents = hepmc_particle_get_n_parents (hprt)
n_children = hepmc_particle_get_n_children (hprt)
if (HEPMC2_AVAILABLE) then
    allocate (parent_barcode (n_parents), parent (n_parents))
    allocate (child_barcode (n_children), child (n_children))
    parent_barcode = hepmc_particle_get_parent_barcodes (hprt)
    child_barcode = hepmc_particle_get_child_barcodes (hprt)
    do i = 1, size (barcode)
        where (parent_barcode == barcode(i)) parent = i
        where (child_barcode == barcode(i)) child = i
    end do
    call prt%set_parents (parent)
    call prt%set_children (child)
else if (HEPMC3_AVAILABLE) then

```

```

        allocate (parent_barcode (n_parents), parent (n_parents))
        allocate (child_barcode (n_children), child (n_children))
        parent_barcode = hepmc_particle_get_parent_barcodes (hpvt)
        child_barcode = hepmc_particle_get_child_barcodes (hpvt)
        do i = 1, size (barcode)
            where (parent_barcode == barcode(i)) parent = i
            where (child_barcode == barcode(i)) child = i
        end do
        call prt%set_parents (parent)
        call prt%set_children (child)
    end if
    if (prt%get_status () == PRT_VIRTUAL .and. n_parents == 0) &
        call prt%set_status (PRT_INCOMING)
    if (HEPMC2_AVAILABLE) then
        vtx = hepmc_particle_get_decay_vertex (hpvt)
        if (hepmc_vertex_is_valid (vtx)) then
            vertex = hepmc_vertex_to_vertex (vtx)
            if (vertex /= vector4_null) call prt%set_vertex (vertex)
        end if
    end if
end if
end subroutine particle_from_hepmc_particle

```

If a particle set is initialized from a HepMC event record, we have to specify the treatment of polarization (unpolarized or density matrix) which is common to all particles. Correlated polarization information is not available.

There is some complication in reconstructing incoming particles and beam remnants. First of all, they all will be tagged as virtual. We then define an incoming particle as

```

<HEP events: public>+≡
    public :: hepmc_event_to_particle_set

<HEP events: sub interfaces>+≡
    module subroutine hepmc_event_to_particle_set &
        (particle_set, evt, model, fallback_model, polarization)
        type(particle_set_t), intent(inout), target :: particle_set
        type(hepmc_event_t), intent(in) :: evt
        class(model_data_t), intent(in), target :: model, fallback_model
        integer, intent(in) :: polarization
    end subroutine hepmc_event_to_particle_set

<HEP events: procedures>+≡
    module subroutine hepmc_event_to_particle_set &
        (particle_set, evt, model, fallback_model, polarization)
        type(particle_set_t), intent(inout), target :: particle_set
        type(hepmc_event_t), intent(in) :: evt
        class(model_data_t), intent(in), target :: model, fallback_model
        integer, intent(in) :: polarization
        type(hepmc_event_particle_iterator_t) :: it
        type(hepmc_vertex_t) :: v
        type(hepmc_vertex_particle_in_iterator_t) :: v_it
        type(hepmc_particle_t) :: prt
        integer, dimension(:), allocatable :: barcode, n_parents
        integer :: n_tot, n_beam, i, bc
        n_tot = hepmc_event_get_n_particles(evt)

```

```

allocate (barcode (n_tot))
if (HEPMC2_AVAILABLE) then
  call hePMC_event_particle_iterator_init (it, evt)
  do i = 1, n_tot
    barcode(i) = hePMC_particle_get_barcode &
      (hePMC_event_particle_iterator_get (it))
    call hePMC_event_particle_iterator_advance (it)
  end do
  allocate (particle_set%prt (n_tot))
  call hePMC_event_particle_iterator_reset (it)
  do i = 1, n_tot
    prt = hePMC_event_particle_iterator_get (it)
    call particle_from_hePMC_particle (particle_set%prt(i), &
      prt, model, fallback_model, polarization, barcode)
    call hePMC_event_particle_iterator_advance (it)
  end do
  call hePMC_event_particle_iterator_final (it)
  v = hePMC_event_get_signal_process_vertex (evt)
  if (hePMC_vertex_is_valid (v)) then
    call hePMC_vertex_particle_in_iterator_init (v_it, v)
    do while (hePMC_vertex_particle_in_iterator_is_valid (v_it))
      prt = hePMC_vertex_particle_in_iterator_get (v_it)
      bc = hePMC_particle_get_barcode &
        (hePMC_vertex_particle_in_iterator_get (v_it))
      do i = 1, size(barcode)
        if (bc == barcode(i)) &
          call particle_set%prt(i)%set_status (PRT_INCOMING)
      end do
      call hePMC_vertex_particle_in_iterator_advance (v_it)
    end do
    call hePMC_vertex_particle_in_iterator_final (v_it)
  end if
else if (HEPMC3_AVAILABLE) then
  allocate (particle_set%prt (n_tot))
  do i = 1, n_tot
    barcode(i) = hePMC_particle_get_barcode &
      (hePMC_event_get_nth_particle (evt, i))
  end do
  do i = 1, n_tot
    prt = hePMC_event_get_nth_particle (evt, i)
    call particle_from_hePMC_particle (particle_set%prt(i), &
      prt, model, fallback_model, polarization, barcode)
  end do
end if
do i = 1, n_tot
  if (particle_set%prt(i)%get_status () == PRT_VIRTUAL &
    .and. particle_set%prt(i)%get_n_children () == 0) &
    call particle_set%prt(i)%set_status (PRT_OUTGOING)
end do
if (HEPMC3_AVAILABLE) then
  n_beam = hePMC_event_get_n_beams (evt)
  do i = 1, n_beam
    bc = hePMC_event_get_nth_beam (evt, i)
    if (.not. particle_set%prt(bc)%get_status () == PRT_INCOMING) &

```

```

        call particle_set%prt(bc)%set_status (PRT_BEAM)
    end do
    do i = 1, n_tot
        if (particle_set%prt(i)%get_status () == PRT_VIRTUAL) then
            n_parents = particle_set%prt(i)%get_parents ()
            if (all &
                (particle_set%prt(n_parents)%get_status () == PRT_BEAM)) then
                call particle_set%prt(i)%set_status (PRT_INCOMING)
            end if
        end if
    end do
end if
particle_set%n_tot = n_tot
particle_set%n_beam = &
    count (particle_set%prt%get_status () == PRT_BEAM)
particle_set%n_in = &
    count (particle_set%prt%get_status () == PRT_INCOMING)
particle_set%n_out = &
    count (particle_set%prt%get_status () == PRT_OUTGOING)
particle_set%n_vir = &
    particle_set%n_tot - particle_set%n_in - particle_set%n_out
end subroutine hepmc_event_to_particle_set

```

Fill a WHIZARD event from a HepMC event record. In HepMC the weights are in a weight container. If the size of this container is larger than one, it is ambiguous to assign the event a specific weight. For now we only allow to read in unweighted events.

```

<HEP events: public>+≡
    public :: hepmc_to_event

<HEP events: sub interfaces>+≡
    module subroutine hepmc_to_event &
        (event, hepmc_event, fallback_model, process_index, &
         recover_beams, use_alpha_s, use_scale)
        class(generic_event_t), intent(inout), target :: event
        type(hepmc_event_t), intent(inout) :: hepmc_event
        class(model_data_t), intent(in), target :: fallback_model
        integer, intent(out), optional :: process_index
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: use_alpha_s
        logical, intent(in), optional :: use_scale
    end subroutine hepmc_to_event

<HEP events: procedures>+≡
    module subroutine hepmc_to_event &
        (event, hepmc_event, fallback_model, process_index, &
         recover_beams, use_alpha_s, use_scale)
        class(generic_event_t), intent(inout), target :: event
        type(hepmc_event_t), intent(inout) :: hepmc_event
        class(model_data_t), intent(in), target :: fallback_model
        integer, intent(out), optional :: process_index
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: use_alpha_s
        logical, intent(in), optional :: use_scale
    end subroutine hepmc_to_event

```



```

class(model_data_t), pointer :: model
real(default) :: scale, alpha_qcd
type(particle_set_t) :: particle_set
model => event%get_model_ptr ()
call event%set_index (hepmc_event_get_event_index (hepmc_event))
call hepmc_event_to_particle_set (particle_set, &
    hepmc_event, model, fallback_model, PRT_DEFINITE_HELICITY)
call event%set_hard_particle_set (particle_set)
call particle_set%final ()
call event%set_weight_ref (1._default)
alpha_qcd = hepmc_event_get_alpha_qcd (hepmc_event)
scale = hepmc_event_get_scale (hepmc_event)
if (present (use_alpha_s)) then
    if (use_alpha_s .and. alpha_qcd > 0) &
        call event%set_alpha_qcd_forced (alpha_qcd)
end if
if (present (use_scale)) then
    if (use_scale .and. scale > 0) &
        call event%set_scale_forced (scale)
end if
end subroutine hepmc_to_event

```

LCIO event format

The master output function fills a LCIO event object that is already initialized, but has no particles in it.

In contrast to HepMC in LCIO there are no vertices (except for tracker and other detector specifications). So we assign first all incoming particles and then all outgoing particles to LCIO particle types. Particles which have neither parent nor children entries (this should not happen) are dropped. Finally, we insert the beam particles. If there are none, use the incoming particles instead.

Transform a particle into a `lcio_particle` object, including color and polarization. The LCIO status is equivalent to the HepMC status, in particular: 0 = null entry, 1 = physical particle, 2 = decayed/fragmented SM hadron, tau or muon, 3 = other unphysical particle entry, 4 = incoming particles, 11 = intermediate resonance such as squarks. The use of 11 for intermediate resonances is as done by HERWIG, see <http://herwig.hepforge.org/trac/wiki/FaQs>.

A beam-remnant particle (e.g., ISR photon) that has no children is tagged as outgoing, otherwise unphysical.

```

<HEP events: public>+≡
    public :: particle_to_lcio

<HEP events: sub interfaces>+≡
    module subroutine particle_to_lcio (prt, lprt)
        type(particle_t), intent(in) :: prt
        type(lcio_particle_t), intent(out) :: lprt
    end subroutine particle_to_lcio

<HEP events: procedures>+≡
    module subroutine particle_to_lcio (prt, lprt)
        type(particle_t), intent(in) :: prt
        type(lcio_particle_t), intent(out) :: lprt
    end subroutine particle_to_lcio

```

```

integer :: lcio_status
type(vector4_t) :: vtx
select case (prt%get_status ())
case (PRT_UNDEFINED)
    lcio_status = 0
case (PRT_OUTGOING)
    lcio_status = 1
case (PRT_BEAM_REMNANT)
    if (prt%get_n_children () == 0) then
        lcio_status = 1
    else
        lcio_status = 3
    end if
case (PRT_BEAM)
    lcio_status = 4
case (PRT_RESONANT)
    lcio_status = 2
case default
    lcio_status = 3
end select
call lcio_particle_init (lprt, &
    prt%get_momentum (), &
    prt%get_pdg (), &
    prt%flv%get_charge (), &
    lcio_status)
call lcio_particle_set_color (lprt, prt%get_color ())
vtx = prt%get_vertex ()
call lcio_particle_set_vtx (lprt, space_part (vtx))
call lcio_particle_set_t (lprt, vtx%p(0))
select case (prt%get_polarization_status ())
case (PRT_DEFINITE_HELICITY)
    call lcio_polarization_init (lprt, prt%get_helicity ())
case (PRT_GENERIC_POLARIZATION)
    call lcio_polarization_init (lprt, prt%get_polarization ())
end select
end subroutine particle_to_lcio

```

Initialize a particle from a LCIO particle object. The model is necessary for making a fully qualified flavor component.

<HEP events: public>+≡

public :: particle_from_lcio_particle

<HEP events: sub interfaces>+≡

```

module subroutine particle_from_lcio_particle &
    (prt, lprt, model, fallback_model, daughters, parents, polarization)
type(particle_t), intent(out) :: prt
type(lcio_particle_t), intent(in) :: lprt
type(model_data_t), intent(in), target :: model
type(model_data_t), intent(in), target :: fallback_model
integer, dimension(:), intent(in) :: daughters, parents
integer, intent(in) :: polarization
end subroutine particle_from_lcio_particle

```

<HEP events: procedures>+≡

module subroutine particle_from_lcio_particle &

```

    (prt, lprt, model, fallback_model, daughters, parents, polarization)
    type(particle_t), intent(out) :: prt
    type(lcio_particle_t), intent(in) :: lprt
    type(model_data_t), intent(in), target :: model
    type(model_data_t), intent(in), target :: fallback_model
    integer, dimension(:), intent(in) :: daughters, parents
    integer, intent(in) :: polarization
    type(vector4_t) :: vtx4
    type(flavor_t) :: flv
    type(color_t) :: col
    type(helicity_t) :: hel
    type(polarization_t) :: pol
    select case (lcio_particle_get_status (lprt))
    case (1); call prt%set_status (PRT_OUTGOING)
    case (2); call prt%set_status (PRT_RESONANT)
    case (3)
        select case (size (parents))
        case (0)
            call prt%set_status (PRT_INCOMING)
        case default
            call prt%set_status (PRT_VIRTUAL)
        end select
    case (4); call prt%set_status (PRT_BEAM)
    end select
    call flv%init (lcio_particle_get_pdg (lprt), model, fallback_model)
    call col%init (lcio_particle_get_flow (lprt))
    if (flv%is_beam_remnant ()) call prt%set_status (PRT_BEAM_REMNANT)
    call prt%set_flavor (flv)
    call prt%set_color (col)
    call prt%set_polarization (polarization)
    select case (polarization)
    case (PRT_DEFINITE_HELICITY)
        call lcio_particle_to_hel (lprt, prt%get_flv (), hel)
        call prt%set_helicity (hel)
    case (PRT_GENERIC_POLARIZATION)
        call lcio_particle_to_pol (lprt, prt%get_flv (), pol)
        call prt%set_pol (pol)
    end select
    call prt%set_momentum (lcio_particle_get_momentum (lprt), &
        lcio_particle_get_mass_squared (lprt))
    call prt%set_parents (parents)
    call prt%set_children (daughters)
    vtx4 = vector4_moving (lcio_particle_get_time (lprt), &
        lcio_particle_get_vertex (lprt))
    if (vtx4 /= vector4_null) call prt%set_vertex (vtx4)
end subroutine particle_from_lcio_particle

```

<HEP events: public>+≡

```
public :: lcio_event_from_particle_set
```

<HEP events: sub interfaces>+≡

```

module subroutine lcio_event_from_particle_set (evt, particle_set)
    type(lcio_event_t), intent(inout) :: evt
    type(particle_set_t), intent(in) :: particle_set

```

```

end subroutine lcio_event_from_particle_set

<HEP events: procedures>+=
module subroutine lcio_event_from_particle_set (evt, particle_set)
  type(lcio_event_t), intent(inout) :: evt
  type(particle_set_t), intent(in) :: particle_set
  type(lcio_particle_t), dimension(:), allocatable :: lprt
  type(particle_set_t), target :: pset_filtered
  integer, dimension(:), allocatable :: parent
  integer :: n_tot, i, j, n_beam, n_parents, type, beam_count

  call particle_set%filter_particles ( pset_filtered, &
    real_parents = .true. , keep_beams = .true. , keep_virtuals = .false.)
  n_tot = pset_filtered%n_tot
  n_beam = count (pset_filtered%prt%get_status () == PRT_BEAM)
  if (n_beam == 0) then
    type = PRT_INCOMING
  else
    type = PRT_BEAM
  end if
  beam_count = 0
  allocate (lprt (n_tot))
  do i = 1, n_tot
    call particle_to_lcio (pset_filtered%prt(i), lprt(i))
    n_parents = pset_filtered%prt(i)%get_n_parents ()
    if (n_parents /= 0) then
      allocate (parent (n_parents))
      parent = pset_filtered%prt(i)%get_parents ()
      do j = 1, n_parents
        call lcio_particle_set_parent (lprt(i), lprt(parent(j)))
      end do
      deallocate (parent)
    end if
    if (pset_filtered%prt(i)%get_status () == type) then
      beam_count = beam_count + 1
      call lcio_event_set_beam &
        (evt, pset_filtered%prt(i)%get_pdg (), beam_count)
    end if
    call lcio_particle_add_to_evt_coll (lprt(i), evt)
  end do
  call lcio_event_add_coll (evt)
end subroutine lcio_event_from_particle_set

```

If a particle set is initialized from a LCIO event record, we have to specify the treatment of polarization (unpolarized or density matrix) which is common to all particles. Correlated polarization information is not available.

```

<HEP events: public>+=
public :: lcio_event_to_particle_set

<HEP events: sub interfaces>+=
module subroutine lcio_event_to_particle_set &
  (particle_set, evt, model, fallback_model, polarization)
  type(particle_set_t), intent(inout), target :: particle_set
  type(lcio_event_t), intent(in) :: evt

```

```

        class(model_data_t), intent(in), target :: model, fallback_model
        integer, intent(in) :: polarization
    end subroutine lcio_event_to_particle_set
<HEP events: procedures>+≡
module subroutine lcio_event_to_particle_set &
    (particle_set, evt, model, fallback_model, polarization)
    type(particle_set_t), intent(inout), target :: particle_set
    type(lcio_event_t), intent(in) :: evt
    class(model_data_t), intent(in), target :: model, fallback_model
    integer, intent(in) :: polarization
    type(lcio_particle_t) :: prt
    integer, dimension(:), allocatable :: parents, daughters
    integer :: n_tot, i, j, n_parents, n_children
    n_tot = lcio_event_get_n_tot (evt)
    allocate (particle_set%prt (n_tot))
    do i = 1, n_tot
        prt = lcio_event_get_particle (evt, i-1)
        n_parents = lcio_particle_get_n_parents (prt)
        n_children = lcio_particle_get_n_children (prt)
        allocate (daughters (n_children))
        allocate (parents (n_parents))
        if (n_children > 0) then
            do j = 1, n_children
                daughters(j) = lcio_get_n_children (evt,i,j)
            end do
        end if
        if (n_parents > 0) then
            do j = 1, n_parents
                parents(j) = lcio_get_n_parents (evt,i,j)
            end do
        end if
        call particle_from_lcio_particle (particle_set%prt(i), &
            prt, model, fallback_model, &
            daughters, parents, polarization)
        deallocate (daughters, parents)
    end do
    do i = 1, n_tot
        if (particle_set%prt(i)%get_status () == PRT_VIRTUAL) then
            CHECK_BEAM: do j = 1, particle_set%prt(i)%get_n_parents ()
                if (particle_set%prt(j)%get_status () == PRT_BEAM) &
                    call particle_set%prt(i)%set_status (PRT_INCOMING)
                exit CHECK_BEAM
            end do CHECK_BEAM
        end if
    end do
    particle_set%n_tot = n_tot
    particle_set%n_beam = &
        count (particle_set%prt%get_status () == PRT_BEAM)
    particle_set%n_in = &
        count (particle_set%prt%get_status () == PRT_INCOMING)
    particle_set%n_out = &
        count (particle_set%prt%get_status () == PRT_OUTGOING)
    particle_set%n_vir = &
        particle_set%n_tot - particle_set%n_in - particle_set%n_out

```

```

end subroutine lcio_event_to_particle_set

<HEP events: public>+≡
public :: lcio_to_event

<HEP events: sub interfaces>+≡
module subroutine lcio_to_event &
    (event, lcio_event, fallback_model, process_index, recover_beams, &
     use_alpha_s, use_scale)
    class(generic_event_t), intent(inout), target :: event
    type(lcio_event_t), intent(inout) :: lcio_event
    class(model_data_t), intent(in), target :: fallback_model
    integer, intent(out), optional :: process_index
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alpha_s
    logical, intent(in), optional :: use_scale
end subroutine lcio_to_event

<HEP events: procedures>+≡
module subroutine lcio_to_event &
    (event, lcio_event, fallback_model, process_index, recover_beams, &
     use_alpha_s, use_scale)
    class(generic_event_t), intent(inout), target :: event
    type(lcio_event_t), intent(inout) :: lcio_event
    class(model_data_t), intent(in), target :: fallback_model
    integer, intent(out), optional :: process_index
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alpha_s
    logical, intent(in), optional :: use_scale
    class(model_data_t), pointer :: model
    real(default) :: scale, alpha_qcd
    type(particle_set_t) :: particle_set
    model => event%get_model_ptr ()
    call lcio_event_to_particle_set (particle_set, &
        lcio_event, model, fallback_model, PRT_DEFINITE_HELICITY)
    call event%set_hard_particle_set (particle_set)
    call particle_set%final ()
    call event%set_weight_ref (1._default)
    alpha_qcd = lcio_event_get_alphas (lcio_event)
    scale = lcio_event_get_scaleval (lcio_event)
    if (present (use_alpha_s)) then
        if (use_alpha_s .and. alpha_qcd > 0) &
            call event%set_alpha_qcd_forced (alpha_qcd)
    end if
    if (present (use_scale)) then
        if (use_scale .and. scale > 0) &
            call event%set_scale_forced (scale)
    end if
end subroutine lcio_to_event

```

18.14.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨hep_events_ut.f90⟩≡
  ⟨File header⟩

  module hep_events_ut
    use unit_tests
    use hePMC_interface, only: HEPMC_IS_AVAILABLE
    use system_dependencies, only: HEPMC2_AVAILABLE
    use hep_events_util

    ⟨Standard module head⟩

    ⟨HEP events: public test⟩

    contains

    ⟨HEP events: test driver⟩

  end module hep_events_ut
⟨hep_events_util.f90⟩≡
  ⟨File header⟩

  module hep_events_util

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices, only: FM_SELECT_HELICITY, FM_FACTOR_HELICITY
    use interactions
    use evaluators
    use model_data
    use particles
    use subevents
    use hePMC_interface

    use hep_events

    ⟨Standard module head⟩

    ⟨HEP events: test declarations⟩

    contains

    ⟨HEP events: tests⟩

  end module hep_events_util
API: driver for the unit tests below.
⟨HEP events: public test⟩≡
  public :: hep_events_test
⟨HEP events: test driver⟩≡

```

```

subroutine hep_events_test (u, results)
  integer, intent(in) :: u
  type(test_results_t), intent(inout) :: results
  <HEP events: execute tests>
end subroutine hep_events_test

```

If HepMC is available, check the routines via HepMC.

Set up a chain of production and decay and factorize the result into particles.

The process is $d\bar{d} \rightarrow Z \rightarrow q\bar{q}$.

```

<HEP events: execute tests>≡
  if (hepmc_is_available ()) then
    call test (hep_events_1, "hep_events_1", &
      "check HepMC event routines", &
      u, results)
  end if

<HEP events: test declarations>≡
  public :: hep_events_1

<HEP events: tests>≡
  subroutine hep_events_1 (u)
    use os_interface
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(3) :: flv
    type(color_t), dimension(3) :: col
    type(helicity_t), dimension(3) :: hel
    type(quantum_numbers_t), dimension(3) :: qn
    type(vector4_t), dimension(3) :: p
    type(interaction_t), target :: int1, int2
    type(quantum_numbers_mask_t) :: qn_mask_conn
    type(evaluator_t), target :: eval
    type(interaction_t), pointer :: int
    type(particle_set_t) :: particle_set1, particle_set2
    type(hepmc_event_t) :: hepmc_event
    type(hepmc_iostream_t) :: iostream
    real(default) :: cross_section, error, weight
    logical :: ok

    write (u, "(A)")  "* Test output: HEP events"
    write (u, "(A)")  "* Purpose: test HepMC event routines"
    write (u, "(A)")

    write (u, "(A)")  "* Reading model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* Initializing production process"

    call int1%basic_init (2, 0, 1, set_relations=.true.)
    call flv%init ([1, -1, 23], model)
    call col%init_col_acl ([0, 0, 0], [0, 0, 0])
    call hel(3)%init ( 1, 1)

```



```

call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.25_default, 0._default))
call hel(3)%init ( 1,-1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0._default, 0.25_default))
call hel(3)%init (-1, 1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0._default,-0.25_default))
call hel(3)%init (-1,-1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.25_default, 0._default))
call hel(3)%init ( 0, 0)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.5_default, 0._default))
call int1%freeze ()
p(1) = vector4_moving (45._default, 45._default, 3)
p(2) = vector4_moving (45._default,-45._default, 3)
p(3) = p(1) + p(2)
call int1%set_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Setup decay process"

call int2%basic_init (1, 0, 2, set_relations=.true.)
call flv%init ([23, 1, -1], model)
call col%init_col_acl ([0, 501, 0], [0, 0, 501])
call hel%init ([1, 1, 1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([1, 1, 1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default, 0.1_default))
call hel%init ([-1,-1,-1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default,-0.1_default))
call hel%init ([-1,-1,-1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call hel%init ([0,-1, 1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0, 1,-1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call flv%init ([23, 2, -2], model)
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))

```

```

call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call int2%freeze ()
p(2) = vector4_moving (45._default, 45._default, 2)
p(3) = vector4_moving (45._default,-45._default, 2)
call int2%set_momenta (p)
call int2%set_source_link (1, int1, 3)
call int1%basic_write (u)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Concatenate production and decay"

call eval%init_product (int1, int2, qn_mask_conn, &
    connections_are_resonant=.true.)
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, polarized)"
write (u, "(A)")

int => eval%interaction_t
call particle_set1%init &
    (ok, int, int, FM_FACTOR_HELICITY, &
    [0.2_default, 0.2_default], .false., .true.)
call particle_set1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (in/out only, selected helicity)"
write (u, "(A)")

int => eval%interaction_t
call particle_set2%init &
    (ok, int, int, FM_SELECT_HELICITY, &
    [0.9_default, 0.9_default], .false., .false.)
call particle_set2%write (u)
call particle_set2%final ()

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, selected helicity)"
write (u, "(A)")

int => eval%interaction_t
call particle_set2%init &
    (ok, int, int, FM_SELECT_HELICITY, &
    [0.7_default, 0.7_default], .false., .true.)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer particle_set to HepMC, print, and output to"
write (u, "(A)")  "      hep_events.hepmc.dat"

```

```

write (u, "(A)")

cross_section = 42.0_default
error = 17.0_default
weight = 1.0_default
call hepmc_event_init (hepmc_event, 11, 127)
call hepmc_event_from_particle_set (hepmc_event, particle_set2, &
    cross_section, error, .true.)
call hepmc_event_add_weight (hepmc_event, weight, .true.)
call hepmc_event_print (hepmc_event)
call hepmc_iostream_open_out &
    (iostream, var_str ("hep_events.hepmc.dat"), 2)
call hepmc_iostream_write_event (iostream, hepmc_event)
call hepmc_iostream_close (iostream)

write (u, "(A)")
write (u, "(A)")  "* Recover from HepMC file"
write (u, "(A)")

call particle_set2%final ()
call hepmc_event_final (hepmc_event)
call hepmc_event_init (hepmc_event)
call hepmc_iostream_open_in &
    (iostream, var_str ("hep_events.hepmc.dat"), HEPMC3_MODE_HEPMC3)
call hepmc_iostream_read_event (iostream, hepmc_event, ok=ok)
call hepmc_iostream_close (iostream)
call hepmc_event_to_particle_set (particle_set2, &
    hepmc_event, model, model, PRT_DEFINITE_HELICITY)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set1%final ()
call particle_set2%final ()
call eval%final ()
call int1%final ()
call int2%final ()
call hepmc_event_final (hepmc_event)
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: hep_events_1"

end subroutine hep_events_1

```

18.15 LHEF Input/Output

The LHEF event record is standardized. It is an ASCII format. We try our best at using it for both input and output.

(eio_lhef.f90)≡

```

    <File header>

module eio_lhef

    <Use kinds>
    <Use strings>
    use xml
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO LHEF: public>

    <EIO LHEF: types>

    interface
    <EIO LHEF: sub interfaces>
    end interface

end module eio_lhef

<eio_lhef_sub.f90>≡
    <File header>

submodule (eio_lhef) eio_lhef_s

    use io_units
    use string_utils
    use numeric_utils
    use diagnostics
    use os_interface
    use hep_common
    use hep_events

    implicit none

contains

    <EIO LHEF: procedures>

end submodule eio_lhef_s

```

18.15.1 Type

With sufficient confidence that it will always be three characters, we can store the version string with a default value.

```

<EIO LHEF: public>≡
    public :: eio_lhef_t

```

```

<EIO LHEF: types>≡
  type, extends (eio_t) :: eio_lhef_t
    logical :: writing = .false.
    logical :: reading = .false.
    integer :: unit = 0
    type(event_sample_data_t) :: data
    type(cstream_t) :: cstream
    character(3) :: version = "1.0"
    logical :: keep_beams = .false.
    logical :: keep_remnants = .true.
    logical :: keep_virtuals = .false.
    logical :: recover_beams = .true.
    logical :: unweighted = .true.
    logical :: write_sqme_ref = .false.
    logical :: write_sqme_prc = .false.
    logical :: write_sqme_alt = .false.
    logical :: use_alphas_from_file = .false.
    logical :: use_scale_from_file = .false.
    integer :: n_alt = 0
    integer, dimension(:), allocatable :: proc_num_id
    integer :: i_weight_sqme = 0
    type(xml_tag_t) :: tag_lhef, tag_head, tag_init, tag_event
    type(xml_tag_t), allocatable :: tag_whiz_info
    type(xml_tag_t), allocatable :: tag_gen_n, tag_gen_v
    type(xml_tag_t), allocatable :: tag_generator, tag_xsecinfo
    type(xml_tag_t), allocatable :: tag_sqme_ref, tag_sqme_prc
    type(xml_tag_t), dimension(:), allocatable :: tag_sqme_alt, tag_wgts_alt
    type(xml_tag_t), allocatable :: tag_weight, tag_weightinfo, tag_weights
  contains
    <EIO LHEF: eio_lhef: TBP>
  end type eio_lhef_t

```

18.15.2 Specific Methods

Set parameters that are specifically used with LHEF.

```

<EIO LHEF: eio_lhef: TBP>≡
  procedure :: set_parameters => eio_lhef_set_parameters

<EIO LHEF: sub interfaces>≡
  module subroutine eio_lhef_set_parameters (eio, &
    keep_beams, keep_remnants, recover_beams, &
    use_alphas_from_file, use_scale_from_file, &
    version, extension, write_sqme_ref, write_sqme_prc, write_sqme_alt)
    class(eio_lhef_t), intent(inout) :: eio
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file
    logical, intent(in), optional :: use_scale_from_file
    character(*), intent(in), optional :: version
    type(string_t), intent(in), optional :: extension
    logical, intent(in), optional :: write_sqme_ref
    logical, intent(in), optional :: write_sqme_prc

```

```

        logical, intent(in), optional :: write_sqme_alt
    end subroutine eio_lhef_set_parameters

<EIO LHEF: procedures>≡
module subroutine eio_lhef_set_parameters (eio, &
    keep_beams, keep_remnants, recover_beams, &
    use_alphas_from_file, use_scale_from_file, &
    version, extension, write_sqme_ref, write_sqme_prc, write_sqme_alt)
class(eio_lhef_t), intent(inout) :: eio
logical, intent(in), optional :: keep_beams
logical, intent(in), optional :: keep_remnants
logical, intent(in), optional :: recover_beams
logical, intent(in), optional :: use_alphas_from_file
logical, intent(in), optional :: use_scale_from_file
character(*), intent(in), optional :: version
type(string_t), intent(in), optional :: extension
logical, intent(in), optional :: write_sqme_ref
logical, intent(in), optional :: write_sqme_prc
logical, intent(in), optional :: write_sqme_alt
if (present (keep_beams)) eio%keep_beams = keep_beams
if (present (keep_remnants)) eio%keep_remnants = keep_remnants
if (present (recover_beams)) eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (version)) then
    select case (version)
    case ("1.0", "2.0", "3.0")
        eio%version = version
    case default
        call msg_error ("LHEF version " // version &
            // " is not supported. Inserting 2.0")
        eio%version = "2.0"
    end select
end if
if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "lhe"
end if
if (present (write_sqme_ref)) eio%write_sqme_ref = write_sqme_ref
if (present (write_sqme_prc)) eio%write_sqme_prc = write_sqme_prc
if (present (write_sqme_alt)) eio%write_sqme_alt = write_sqme_alt
end subroutine eio_lhef_set_parameters

```

18.15.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: write => eio_lhef_write

```

<EIO LHEF: sub interfaces>+≡

```

module subroutine eio_lhef_write (object, unit)
  class(eio_lhef_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine eio_lhef_write

```

<EIO LHEF: procedures>+≡

```

module subroutine eio_lhef_write (object, unit)
  class(eio_lhef_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "LHEF event stream:"
  if (object%writing) then
    write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
  else if (object%reading) then
    write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
  else
    write (u, "(3x,A)") "[closed]"
  end if
  write (u, "(3x,A,L1)") "Keep beams      = ", object%keep_beams
  write (u, "(3x,A,L1)") "Keep remnants  = ", object%keep_remnants
  write (u, "(3x,A,L1)") "Recover beams   = ", object%recover_beams
  write (u, "(3x,A,L1)") "Alpha_s from file = ", &
    object%use_alphas_from_file
  write (u, "(3x,A,L1)") "Scale from file  = ", &
    object%use_scale_from_file
  write (u, "(3x,A,A)") "Version          = ", object%version
  write (u, "(3x,A,A,A)") "File extension    = '", &
    char (object%extension), "'"
  if (allocated (object%proc_num_id)) then
    write (u, "(3x,A)") "Numerical process IDs:"
    do i = 1, size (object%proc_num_id)
      write (u, "(5x,I0,': ',I0)") i, object%proc_num_id(i)
    end do
  end if
end subroutine eio_lhef_write

```

Finalizer: close any open file.

<EIO LHEF: eio_lhef: TBP>+≡

```

procedure :: final => eio_lhef_final

```

<EIO LHEF: sub interfaces>+≡

```

module subroutine eio_lhef_final (object)
  class(eio_lhef_t), intent(inout) :: object
end subroutine eio_lhef_final

```

<EIO LHEF: procedures>+≡

```

module subroutine eio_lhef_final (object)
  class(eio_lhef_t), intent(inout) :: object
  if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
  if (object%writing) then
    write (msg_buffer, "(A,A,A)") "Events: closing LHEF file '", &
      char (object%filename), "'"
    call msg_message ()
  end if
end subroutine eio_lhef_final

```

```

        call object%write_footer ()
        close (object%unit)
        object%writing = .false.
    else if (object%reading) then
        write (msg_buffer, "(A,A,A)") "Events: closing LHEF file '", &
            char (object%filename), "'"
        call msg_message ()
        call object%cstream%final ()
        close (object%unit)
        object%reading = .false.
    end if
end subroutine eio_lhef_final

```

Common initialization for input and output.

(EIO LHEF: eio_lhef: TBP)+≡

```

    procedure :: common_init => eio_lhef_common_init

```

(EIO LHEF: sub interfaces)+≡

```

    module subroutine eio_lhef_common_init (eio, sample, data, extension)
        class(eio_lhef_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
    end subroutine eio_lhef_common_init

```

(EIO LHEF: procedures)+≡

```

    module subroutine eio_lhef_common_init (eio, sample, data, extension)
        class(eio_lhef_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        if (.not. present (data)) &
            call msg_bug ("LHEF initialization: missing data")
        eio%data = data
        eio%unweighted = data%unweighted
        if (eio%unweighted) then
            select case (data%norm_mode)
            case (NORM_UNIT)
            case default; call msg_fatal &
                ("LHEF: normalization for unweighted events must be '1'")
            end select
        else
            select case (data%norm_mode)
            case (NORM_SIGMA)
            case default; call msg_fatal &
                ("LHEF: normalization for weighted events must be 'sigma'")
            end select
        end if
        eio%n_alt = data%n_alt
        eio%sample = sample
        if (present (extension)) then
            eio%extension = extension
        end if
        call eio%set_filename ()
        eio%unit = free_unit ()
    end subroutine eio_lhef_common_init

```



```

        call eio%init_tags (data)
        allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
    end subroutine eio_lhef_common_init

```

Initialize the tag objects. Some tags depend on the LHEF version. In particular, the tags that in LHEF 2.0 identify individual weights by name in each event block, in LHEF 3.0 are replaced by info tags in the init block and a single `weights` tag in the event block. The name attributes of those tags are specific for WHIZARD.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: init_tags => eio_lhef_init_tags

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_init_tags (eio, data)
        class(eio_lhef_t), intent(inout) :: eio
        type(event_sample_data_t), intent(in) :: data
    end subroutine eio_lhef_init_tags

<EIO LHEF: procedures>+≡
    module subroutine eio_lhef_init_tags (eio, data)
        class(eio_lhef_t), intent(inout) :: eio
        type(event_sample_data_t), intent(in) :: data
        real(default), parameter :: pb_per_fb = 1.e-3_default
        real(default) :: xsec_width
        integer :: i
        call eio%tag_lhef%init ( &
            var_str ("LesHouchesEvents"), &
            [xml_attribute (var_str ("version"), var_str (eio%version))], &
            .true.)
        call eio%tag_head%init ( &
            var_str ("header"), &
            .true.)
        call eio%tag_init%init ( &
            var_str ("init"), &
            .true.)
        call eio%tag_event%init (var_str ("event"), &
            .true.)
        allocate (eio%tag_whiz_info)
        call eio%tag_whiz_info%init (var_str ("WhizardInfo"), .true.)
        select case (eio%version)
        case ("1.0")
            allocate (eio%tag_gen_n)
            call eio%tag_gen_n%init ( &
                var_str ("generator_name"), &
                .true.)
            allocate (eio%tag_gen_v)
            call eio%tag_gen_v%init ( &
                var_str ("generator_version"), &
                .true.)
        end select
        select case (eio%version)
        case ("2.0", "3.0")
            allocate (eio%tag_generator)
            call eio%tag_generator%init ( &

```

```

        var_str ("generator"), &
        [xml_attribute (var_str ("version"), var_str ("<Version>"))], &
        .true.)
allocate (eio%tag_xsecinfo)
if (data%n_beam == 2) then
    xsec_width = data%total_cross_section * pb_per_fb
else
    xsec_width = data%total_cross_section
end if
call eio%tag_xsecinfo%init ( &
    var_str ("xsecinfo"), &
    [xml_attribute (var_str ("neve"), str (data%n_evt)), &
    xml_attribute (var_str ("totxsec"), &
        str (xsec_width))])
end select
select case (eio%version)
case ("2.0")
    allocate (eio%tag_weight)
    call eio%tag_weight%init (var_str ("weight"), &
        [xml_attribute (var_str ("name"))])
    if (eio%write_sqme_ref) then
        allocate (eio%tag_sqme_ref)
        call eio%tag_sqme_ref%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_ref"))], &
            .true.)
    end if
    if (eio%write_sqme_prc) then
        allocate (eio%tag_sqme_prc)
        call eio%tag_sqme_prc%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_prc"))], &
            .true.)
    end if
    if (eio%n_alt > 0) then
        if (eio%write_sqme_alt) then
            allocate (eio%tag_sqme_alt (1))
            call eio%tag_sqme_alt(1)%init (var_str ("weight"), &
                [xml_attribute (var_str ("name"), var_str ("sqme_alt"))], &
                .true.)
        end if
        allocate (eio%tag_wgts_alt (1))
        call eio%tag_wgts_alt(1)%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("wgts_alt"))], &
            .true.)
    end if
case ("3.0")
    if (eio%write_sqme_ref) then
        allocate (eio%tag_sqme_ref)
        call eio%tag_sqme_ref%init (var_str ("weightinfo"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_ref"))])
    end if
    if (eio%write_sqme_prc) then
        allocate (eio%tag_sqme_prc)
        call eio%tag_sqme_prc%init (var_str ("weightinfo"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_prc"))])
    end if

```

```

end if
if (eio%n_alt > 0) then
  if (eio%write_sqme_alt) then
    allocate (eio%tag_sqme_alt (eio%n_alt))
    do i = 1, eio%n_alt
      call eio%tag_sqme_alt(i)%init (var_str ("weightinfo"), &
        [xml_attribute (var_str ("name"), &
          var_str ("sqme_alt") // str (i))])
    end do
  end if
  allocate (eio%tag_wgts_alt (eio%n_alt))
  do i = 1, eio%n_alt
    call eio%tag_wgts_alt(i)%init (var_str ("weightinfo"), &
      [xml_attribute (var_str ("name"), &
        var_str ("wgts_alt") // str (i))])
  end do
end if
allocate (eio%tag_weightinfo)
call eio%tag_weightinfo%init (var_str ("weightinfo"), &
  [xml_attribute (var_str ("name"))])
allocate (eio%tag_weights)
call eio%tag_weights%init (var_str ("weights"), .true.)
end select
end subroutine eio_lhef_init_tags

```

Initialize event writing.

(EIO LHEF: eio_lhef: TBP)+≡

```

procedure :: init_out => eio_lhef_init_out

```

(EIO LHEF: sub interfaces)+≡

```

module subroutine eio_lhef_init_out (eio, sample, data, success, extension)
  class(eio_lhef_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
end subroutine eio_lhef_init_out

```

(EIO LHEF: procedures)+≡

```

module subroutine eio_lhef_init_out (eio, sample, data, success, extension)
  class(eio_lhef_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
  integer :: u, i
  logical :: is_width
  is_width = data%n_beam == 1
  call eio%set_splitting (data)
  call eio%common_init (sample, data, extension)
  write (msg_buffer, "(A,A,A)") "Events: writing to LHEF file '", &
    char (eio%filename), "'"
  call msg_message ()
  eio%writing = .true.
  u = eio%unit

```

```

open (u, file = char (eio%filename), &
      action = "write", status = "replace")
call eio%write_header (is_width)
call heprup_init &
      (data%pdg_beam, &
       data%energy_beam, &
       n_processes = data%n_proc, &
       unweighted = data%unweighted, &
       negative_weights = data%negative_weights)
do i = 1, data%n_proc
  call heprup_set_process_parameters (i = i, &
    process_id = data%proc_num_id(i), &
    cross_section = data%cross_section(i), &
    error = data%error(i), &
    is_width = is_width)
end do
call eio%tag_init%write (u); write (u, *)
call heprup_write_lhef (u)
select case (eio%version)
case ("2.0"); call eio%write_init_20 (data)
case ("3.0"); call eio%write_init_30 (data)
end select
call eio%tag_init%close (u); write (u, *)
if (present (success)) success = .true.
end subroutine eio_lhef_init_out

```

Initialize event reading. First read the LHEF tag and version, then read the header and skip over its contents, then read the init block. (We require the opening and closing tags of the init block to be placed on separate lines without extra stuff.)

For input, we do not (yet?) support split event files.

(EIO LHEF: eio_lhef: TBP)+≡

```
procedure :: init_in => eio_lhef_init_in
```

(EIO LHEF: sub interfaces)+≡

```

module subroutine eio_lhef_init_in (eio, sample, data, success, extension)
  class(eio_lhef_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(inout), optional :: data
  logical, intent(out), optional :: success
end subroutine eio_lhef_init_in

```

(EIO LHEF: procedures)+≡

```

module subroutine eio_lhef_init_in (eio, sample, data, success, extension)
  class(eio_lhef_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(inout), optional :: data
  logical, intent(out), optional :: success
  logical :: exist, ok, closing
  type(event_sample_data_t) :: data_file
  type(string_t) :: string
  integer :: u

```

```

eio%split = .false.
call eio%common_init (sample, data, extension)
write (msg_buffer, "(A,A,A)") "Events: reading from LHEF file '", &
    char (eio%filename), "'"
call msg_message ()
inquire (file = char (eio%filename), exist = exist)
if (.not. exist) call msg_fatal ("Events: LHEF file not found.")
eio%reading = .true.
u = eio%unit
open (u, file = char (eio%filename), &
    action = "read", status = "old")
call eio%cstream%init (u)
call eio%read_header ()
call eio%tag_init%read (eio%cstream, ok)
if (.not. ok) call err_init
select case (eio%version)
case ("1.0"); call eio%read_init_10 (data_file)
    call eio%tag_init%read_content (eio%cstream, string, closing)
    if (string /= "" .or. .not. closing) call err_init
case ("2.0"); call eio%read_init_20 (data_file)
case ("3.0"); call eio%read_init_30 (data_file)
end select
call eio%merge_data (data, data_file)
if (present (success)) success = .true.

contains

subroutine err_init
    call msg_fatal ("LHEF: syntax error in init tag")
end subroutine err_init

end subroutine eio_lhef_init_in

```

Merge event sample data: we can check the data in the file against our assumptions and set or reset parameters.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: merge_data => eio_merge_data

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_merge_data (eio, data, data_file)
        class(eio_lhef_t), intent(inout) :: eio
        type(event_sample_data_t), intent(inout) :: data
        type(event_sample_data_t), intent(in) :: data_file
    end subroutine eio_merge_data

<EIO LHEF: procedures>+≡
    module subroutine eio_merge_data (eio, data, data_file)
        class(eio_lhef_t), intent(inout) :: eio
        type(event_sample_data_t), intent(inout) :: data
        type(event_sample_data_t), intent(in) :: data_file
        real, parameter :: tolerance = 1000 * epsilon (1._default)
        if (data%unweighted .neqv. data_file%unweighted) call err_weights
        if (data%negative_weights .neqv. data_file%negative_weights) &
            call err_weights
        if (data%norm_mode /= data_file%norm_mode) call err_norm

```

```

if (data%n_beam /= data_file%n_beam) call err_beams
if (any (data%pdg_beam /= data_file%pdg_beam)) call err_beams
if (any (abs ((data%energy_beam - data_file%energy_beam)) &
    > (data%energy_beam + data_file%energy_beam) * tolerance)) &
    call err_beams
if (data%n_proc /= data_file%n_proc) call err_proc
if (any (data%proc_num_id /= data_file%proc_num_id)) call err_proc
where (data%cross_section == 0)
    data%cross_section = data_file%cross_section
    data%error = data_file%error
end where
data%total_cross_section = sum (data%cross_section)
if (data_file%n_evt > 0) then
    if (data%n_evt > 0 .and. data_file%n_evt /= data%n_evt) call err_n_evt
    data%n_evt = data_file%n_evt
end if
contains
subroutine err_weights
    call msg_fatal ("LHEF: mismatch in event weight properties")
end subroutine err_weights
subroutine err_norm
    call msg_fatal ("LHEF: mismatch in event normalization")
end subroutine err_norm
subroutine err_beams
    call msg_fatal ("LHEF: mismatch in beam properties")
end subroutine err_beams
subroutine err_proc
    call msg_fatal ("LHEF: mismatch in process definitions")
end subroutine err_proc
subroutine err_n_evt
    call msg_error ("LHEF: mismatch in specified number of events (ignored)")
end subroutine err_n_evt
end subroutine eio_merge_data

```

Switch from input to output: reopen the file for reading.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: switch_inout => eio_lhef_switch_inout

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_switch_inout (eio, success)
        class(eio_lhef_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_lhef_switch_inout

<EIO LHEF: procedures>+≡
    module subroutine eio_lhef_switch_inout (eio, success)
        class(eio_lhef_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("LHEF: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_lhef_switch_inout

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common

block contents are still intact.)

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: split_out => eio_lhef_split_out

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_split_out (eio)
        class(eio_lhef_t), intent(inout) :: eio
    end subroutine eio_lhef_split_out

<EIO LHEF: procedures>+≡
    module subroutine eio_lhef_split_out (eio)
        class(eio_lhef_t), intent(inout) :: eio
        integer :: u
        if (eio%split) then
            eio%split_index = eio%split_index + 1
            call eio%set_filename ()
            write (msg_buffer, "(A,A,A)") "Events: writing to LHEF file '", &
                char (eio%filename), "'"
            call msg_message ()
            call eio%write_footer ()
            u = eio%unit
            close (u)
            open (u, file = char (eio%filename), &
                action = "write", status = "replace")
            call eio%write_header ()
            call eio%tag_init%write (u); write (u, *)
            call heprup_write_lhef (u)
            select case (eio%version)
            case ("2.0"); call eio%write_init_20 (eio%data)
            case ("3.0"); call eio%write_init_30 (eio%data)
            end select
            call eio%tag_init%close (u); write (u, *)
        end if
    end subroutine eio_lhef_split_out

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: output => eio_lhef_output

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_lhef_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_lhef_output

<EIO LHEF: procedures>+≡
    module subroutine eio_lhef_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_lhef_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event

```

```

integer, intent(in) :: i_prc
logical, intent(in), optional :: reading, passed, pacify
class(event_handle_t), intent(inout), optional :: event_handle
integer :: u
u = given_output_unit (eio%unit); if (u < 0) return
if (present (passed)) then
    if (.not. passed) return
end if
if (eio%writing) then
    call hepeup_from_event (event, &
        process_index = eio%proc_num_id (i_prc), &
        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants)
    write (u, '(A)') "<event>"
    call hepeup_write_lhef (eio%unit)
    select case (eio%version)
        case ("2.0"); call eio%write_event_20 (event)
        case ("3.0"); call eio%write_event_30 (event)
    end select
    write (u, '(A)') "</event>"
else
    call eio%write ()
    call msg_fatal ("LHEF file is not open for writing")
end if
end subroutine eio_lhef_output

```

Input an event. Upon input of `i_prc`, we can just read in the whole HEPEUP common block. These data are known to come first. The `i_prc` value can be deduced from the IDPRUP value by a table lookup.

Reading the common block bypasses the `cstream` which accesses the input unit. This is consistent with the LHEF specification. After the common-block data have been swallowed, we can resume reading from stream.

We don't catch actual I/O errors. However, we return a negative value in `iostat` if we reached the terminating `</LesHouchesEvents>` tag.

<EIO LHEF: eio_lhef: TBP>+≡

```

procedure :: input_i_prc => eio_lhef_input_i_prc

```

<EIO LHEF: sub interfaces>+≡

```

module subroutine eio_lhef_input_i_prc (eio, i_prc, iostat)
    class(eio_lhef_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
end subroutine eio_lhef_input_i_prc

```

<EIO LHEF: procedures>+≡

```

module subroutine eio_lhef_input_i_prc (eio, i_prc, iostat)
    class(eio_lhef_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    integer :: i, proc_num_id
    type(string_t) :: s
    logical :: ok
    iostat = 0
    call eio%tag_lhef%read_content (eio%cstream, s, ok)

```



```

if (ok) then
  if (s == "") then
    iostat = -1
  else
    call err_close
  end if
  return
else
  call eio%cstream%revert_record (s)
end if
call eio%tag_event%read (eio%cstream, ok)
if (.not. ok) then
  call err_evt1
  return
end if
call hepeup_read_lhef (eio%unit)
call hepeup_get_event_parameters (proc_id = proc_num_id)
i_prc = 0
FIND_I_PRC: do i = 1, size (eio%proc_num_id)
  if (eio%proc_num_id(i) == proc_num_id) then
    i_prc = i
    exit FIND_I_PRC
  end if
end do FIND_I_PRC
if (i_prc == 0) call err_index
contains
subroutine err_close
  call msg_error ("LHEF: reading events: syntax error in closing tag")
  iostat = 1
end subroutine
subroutine err_evt1
  call msg_error ("LHEF: reading events: invalid event tag, &
    &aborting read")
  iostat = 2
end subroutine err_evt1
subroutine err_index
  call msg_error ("LHEF: reading events: undefined process ID " &
    // char (str (proc_num_id)) // ", aborting read")
  iostat = 3
end subroutine err_index
end subroutine eio_lhef_input_i_prc

```

Since we have already read the event information from file, this input routine can transfer the common-block contents to the event record. Also, we read any further information in the event record.

Since LHEF does not give this information, we must assume that the MCI group, term, and channel can all be safely set to 1. This works if there is only one MCI group and term. The channel doesn't matter for the matrix element.

The event index is incremented, as if the event was generated. The LHEF format does not support event indices.

```

<EIO LHEF: eio lhef: TBP>+≡
  procedure :: input_event => eio_lhef_input_event

```

```

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_input_event (eio, event, iostat, event_handle)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine eio_lhef_input_event

```

```

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_input_event (eio, event, iostat, event_handle)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    type(string_t) :: s
    logical :: closing
    iostat = 0
    call event%reset_contents ()
    call event%select (1, 1, 1)
    call hepeup_to_event (event, eio%fallback_model, &
      recover_beams = eio%recover_beams, &
      use_alpha_s = eio%use_alphas_from_file, &
      use_scale = eio%use_scale_from_file)
    select case (eio%version)
    case ("1.0")
      call eio%tag_event%read_content (eio%cstream, s, closing = closing)
      if (s /= "" .or. .not. closing) call err_evt2
    case ("2.0"); call eio%read_event_20 (event)
    case ("3.0"); call eio%read_event_30 (event)
    end select
    call event%increment_index ()
  contains
    subroutine err_evt2
      call msg_error ("LHEF: reading events: syntax error in event record, &
        &aborting read")
      iostat = 2
    end subroutine err_evt2

  end subroutine eio_lhef_input_event

```

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: skip => eio_lhef_skip

```

```

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_skip (eio, iostat)
    class(eio_lhef_t), intent(inout) :: eio
    integer, intent(out) :: iostat
  end subroutine eio_lhef_skip

```

```

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_skip (eio, iostat)
    class(eio_lhef_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    if (eio%reading) then
      read (eio%unit, iostat = iostat)
    end if
  end subroutine eio_lhef_skip

```

```

else
  call eio%write ()
  call msg_fatal ("Raw event file is not open for reading")
end if
end subroutine eio_lhef_skip

```

18.15.4 Les Houches Event File: header/footer

These two routines write the header and footer for the Les Houches Event File format (LHEF).

The current version writes no information except for the generator name and version (v.1.0 only).

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_header => eio_lhef_write_header
  procedure :: write_footer => eio_lhef_write_footer

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_write_header (eio, is_width)
    class(eio_lhef_t), intent(in) :: eio
    logical, intent(in), optional :: is_width
  end subroutine eio_lhef_write_header
  module subroutine eio_lhef_write_footer (eio)
    class(eio_lhef_t), intent(in) :: eio
  end subroutine eio_lhef_write_footer

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_write_header (eio, is_width)
    class(eio_lhef_t), intent(in) :: eio
    logical, intent(in), optional :: is_width
    logical :: is_w
    integer :: u
    u = given_output_unit (eio%unit); if (u < 0) return
    is_w = .false.
    if (present (is_width)) is_w = is_width
    call eio%tag_lhef%write (u); write (u, *)
    call eio%tag_head%write (u); write (u, *)
    select case (eio%version)
    case ("1.0")
      write (u, "(2x)", advance = "no")
      call eio%tag_gen_n%write (var_str ("WHIZARD"), u)
      write (u, *)
      write (u, "(2x)", advance = "no")
      call eio%tag_gen_v%write (var_str ("<Version>"), u)
      write (u, *)
    end select
    if (is_w) then
      call eio%tag_whiz_info%write (u); write (u, *)
      write (u, "(A)") &
        "# Special LHE event setup for decays, units in GeV"
      call eio%tag_whiz_info%close (u); write (u, *)
    end if
    call eio%tag_head%close (u); write (u, *)
  end subroutine eio_lhef_write_header

```

```

module subroutine eio_lhef_write_footer (eio)
  class(eio_lhef_t), intent(in) :: eio
  integer :: u
  u = given_output_unit (eio%unit); if (u < 0) return
  call eio%tag_lhef%close (u)
end subroutine eio_lhef_write_footer

```

Reading the header just means finding the tags and ignoring any contents. When done, we should stand just after the header tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_header => eio_lhef_read_header

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_read_header (eio)
    class(eio_lhef_t), intent(inout) :: eio
  end subroutine eio_lhef_read_header

<EIO LHEF: procedures>+≡
module subroutine eio_lhef_read_header (eio)
  class(eio_lhef_t), intent(inout) :: eio
  logical :: success, closing
  type(string_t) :: content
  call eio%tag_lhef%read (eio%cstream, success)
  if (.not. success .or. .not. eio%tag_lhef%has_content) call err_lhef
  if (eio%tag_lhef%get_attribute (1) /= eio%version) call err_version
  call eio%tag_head%read (eio%cstream, success)
  if (.not. success) call err_header
  if (eio%tag_head%has_content) then
    SKIP_HEADER_CONTENT: do
      call eio%tag_head%read_content (eio%cstream, content, closing)
      if (closing) exit SKIP_HEADER_CONTENT
    end do SKIP_HEADER_CONTENT
  end if
contains
  subroutine err_lhef
    call msg_fatal ("LHEF: LesHouchesEvents tag absent or corrupted")
  end subroutine err_lhef
  subroutine err_header
    call msg_fatal ("LHEF: header tag absent or corrupted")
  end subroutine err_header
  subroutine err_version
    call msg_error ("LHEF: version mismatch: expected " &
      // eio%version // ", found " &
      // char (eio%tag_lhef%get_attribute (1)))
  end subroutine err_version
end subroutine eio_lhef_read_header

```

18.15.5 Version-Specific Code: 1.0

In version 1.0, the init tag contains just HEPUP data. While a `cstream` is connected to the input unit, we bypass it temporarily for the purpose of reading the HEPUP contents. This is consistent with the LHEF standard.

This routine does not read the closing tag of the init block.

```

<EIO LHEF: eio lhef: TBP>+≡
  procedure :: read_init_10 => eio_lhef_read_init_10

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_read_init_10 (eio, data)
    class(eio_lhef_t), intent(in) :: eio
    type(event_sample_data_t), intent(out) :: data
  end subroutine eio_lhef_read_init_10

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_read_init_10 (eio, data)
    class(eio_lhef_t), intent(in) :: eio
    type(event_sample_data_t), intent(out) :: data
    integer :: n_proc, i
    logical :: is_width
    call heprup_read_lhef (eio%unit)
    call heprup_get_run_parameters (n_processes = n_proc)
    call data%init (n_proc)
    if (IDBMUP(2) == 0) then
      data%n_beam = 1
      is_width = .true.
    else
      data%n_beam = 2
      is_width = .false.
    end if
    call heprup_get_run_parameters ( &
      unweighted = data%unweighted, &
      negative_weights = data%negative_weights, &
      beam_pdg = data%pdg_beam, &
      beam_energy = data%energy_beam)
    if (data%unweighted) then
      data%norm_mode = NORM_UNIT
    else
      data%norm_mode = NORM_SIGMA
    end if
    do i = 1, n_proc
      call heprup_get_process_parameters (i, &
        process_id = data%proc_num_id(i), &
        cross_section = data%cross_section(i), &
        error = data%error(i), &
        is_width = is_width)
    end do
  end subroutine eio_lhef_read_init_10

```

18.15.6 Version-Specific Code: 2.0

This is the init information for the 2.0 format, after the HEPRUP data. We have the following tags:

- **generator** Generator name and version.
- **xsecinfo** Cross section and weights data. We have the total cross section and number of events (assuming that the event file is intact), but

information on minimum and maximum weights is not available before the file is complete. We just write the mandatory tags. (Note that the default values of the other tags describe a uniform unit weight, but we can determine most values only after the sample is complete.)

- **cutsinfo** This optional tag is too specific to represent the possibilities of WHIZARD, so we skip it.
- **procinfo** This optional tag is useful for giving details of NLO calculations. Skipped.
- **mergetype** Optional, also not applicable.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_init_20 => eio_lhef_write_init_20

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_write_init_20 (eio, data)
    class(eio_lhef_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
  end subroutine eio_lhef_write_init_20

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_write_init_20 (eio, data)
    class(eio_lhef_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
    integer :: u
    u = eio%unit
    call eio%tag_generator%write (u)
    write (u, "(A)", advance="no") "WHIZARD"
    call eio%tag_generator%close (u); write (u, *)
    call eio%tag_xsecinfo%write (u); write (u, *)
  end subroutine eio_lhef_write_init_20

```

When reading the init block, we first call the 1.0 routine that fills HEPUP. Then we consider the possible tags. Only the **generator** and **xsecinfo** tags are of interest. We skip everything else except for the closing tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_init_20 => eio_lhef_read_init_20

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_read_init_20 (eio, data)
    class(eio_lhef_t), intent(inout) :: eio
    type(event_sample_data_t), intent(out) :: data
  end subroutine eio_lhef_read_init_20

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_read_init_20 (eio, data)
    class(eio_lhef_t), intent(inout) :: eio
    type(event_sample_data_t), intent(out) :: data
    real(default), parameter :: pb_per_fb = 1.e-3_default
    type(string_t) :: content
    logical :: found, closing
    call eio_lhef_read_init_10 (eio, data)
    SCAN_INIT_TAGS: do
      call eio%tag_generator%read (eio%cstream, found)

```

```

    if (found) then
        if (.not. eio%tag_generator%has_content) call err_generator
        call eio%tag_generator%read_content (eio%cstream, content, closing)
        call msg_message ("LHEF: Event file has been generated by " &
            // char (content) // " " &
            // char (eio%tag_generator%get_attribute (1)))
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_xsecinfo%read (eio%cstream, found)
    if (found) then
        if (eio%tag_xsecinfo%has_content) call err_xsecinfo
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_init%read_content (eio%cstream, content, closing)
    if (closing) then
        if (content /= "") call err_init
        exit SCAN_INIT_TAGS
    end if
end do SCAN_INIT_TAGS
data%n_evt = &
    read_ival (eio%tag_xsecinfo%get_attribute (1))
if (data%n_beam == 1) then
    data%total_cross_section = &
        read_rval (eio%tag_xsecinfo%get_attribute (2))
else
    data%total_cross_section = &
        read_rval (eio%tag_xsecinfo%get_attribute (2)) / pb_per_fb
end if
contains
subroutine err_generator
    call msg_fatal ("LHEF: invalid generator tag")
end subroutine err_generator
subroutine err_xsecinfo
    call msg_fatal ("LHEF: invalid xsecinfo tag")
end subroutine err_xsecinfo
subroutine err_init
    call msg_fatal ("LHEF: syntax error after init tag")
end subroutine err_init
end subroutine eio_lhef_read_init_20

```

This is additional event-specific information for the 2.0 format, after the HEP-EUP data. We can specify weights, starting from the master weight and adding alternative weights. The alternative weights are collected in a common tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: write_event_20 => eio_lhef_write_event_20

<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_write_event_20 (eio, event)
        class(eio_lhef_t), intent(in) :: eio
        class(generic_event_t), intent(in) :: event
    end subroutine eio_lhef_write_event_20

<EIO LHEF: procedures>+≡
    module subroutine eio_lhef_write_event_20 (eio, event)

```

```

class(eio_lhef_t), intent(in) :: eio
class(generic_event_t), intent(in) :: event
type(string_t) :: s
integer :: i, u
u = eio%unit
if (eio%write_sqme_ref) then
    s = str (event%get_sqme_ref ())
    call eio%tag_sqme_ref%write (s, u); write (u, *)
end if
if (eio%write_sqme_prc) then
    s = str (event%get_sqme_prc ())
    call eio%tag_sqme_prc%write (s, u); write (u, *)
end if
if (eio%n_alt > 0) then
    if (eio%write_sqme_alt) then
        s = str (event%get_sqme_alt(1))
        do i = 2, eio%n_alt
            s = s // " " // str (event%get_sqme_alt(i)); write (u, *)
        end do
        call eio%tag_sqme_alt(1)%write (s, u)
    end if
    s = str (event%get_weight_alt(1))
    do i = 2, eio%n_alt
        s = s // " " // str (event%get_weight_alt(i)); write (u, *)
    end do
    call eio%tag_wgts_alt(1)%write (s, u)
end if
end subroutine eio_lhef_write_event_20

```

Read extra event data. If there is a weight entry labeled `sqme_prc`, we take this as the squared matrix-element value (the new *reference* value `sqme_ref`). Other tags, including tags written by the above writer, are skipped.

(EIO LHEF: eio_lhef: TBP)+≡

```
procedure :: read_event_20 => eio_lhef_read_event_20
```

(EIO LHEF: sub interfaces)+≡

```

module subroutine eio_lhef_read_event_20 (eio, event)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout) :: event
end subroutine eio_lhef_read_event_20

```

(EIO LHEF: procedures)+≡

```

module subroutine eio_lhef_read_event_20 (eio, event)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout) :: event
    type(string_t) :: content
    logical :: found, closing
    SCAN_EVENT_TAGS: do
        call eio%tag_weight%read (eio%cstream, found)
        if (found) then
            if (.not. eio%tag_weight%has_content) call err_weight
            call eio%tag_weight%read_content (eio%cstream, content, closing)
            if (.not. closing) call err_weight
            if (eio%tag_weight%get_attribute (1) == "sqme_prc") then

```



```

        call event%set_sqme_ref (read_rval (content))
    end if
    cycle SCAN_EVENT_TAGS
end if
call eio%tag_event%read_content (eio%cstream, content, closing)
if (closing) then
    if (content /= "") call err_event
    exit SCAN_EVENT_TAGS
end if
end do SCAN_EVENT_TAGS
contains
subroutine err_weight
    call msg_fatal ("LHEF: invalid weight tag in event record")
end subroutine err_weight
subroutine err_event
    call msg_fatal ("LHEF: syntax error after event tag")
end subroutine err_event
end subroutine eio_lhef_read_event_20

```

18.15.7 Version-Specific Code: 3.0

This is the init information for the 3.0 format, after the HEPUP data. We have the following tags:

- **generator** Generator name and version.
- **xsecinfo** Cross section and weights data. We have the total cross section and number of events (assuming that the event file is intact), but information on minimum and maximum weights is not available before the file is complete. We just write the mandatory tags. (Note that the default values of the other tags describe a uniform unit weight, but we can determine most values only after the sample is complete.)
- **cutsinfo** This optional tag is too specific to represent the possibilities of WHIZARD, so we skip it.
- **procinfo** This optional tag is useful for giving details of NLO calculations. Skipped.
- **weightinfo** Determine the meaning of optional weights, whose values are given in the event record.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: write_init_30 => eio_lhef_write_init_30
<EIO LHEF: sub interfaces>+≡
    module subroutine eio_lhef_write_init_30 (eio, data)
        class(eio_lhef_t), intent(in) :: eio
        type(event_sample_data_t), intent(in) :: data
    end subroutine eio_lhef_write_init_30

```

```

<EIO LHEF: procedures>+≡
module subroutine eio_lhef_write_init_30 (eio, data)
  class(eio_lhef_t), intent(in) :: eio
  type(event_sample_data_t), intent(in) :: data
  integer :: u, i
  u = given_output_unit (eio%unit)
  call eio%tag_generator%write (u)
  write (u, "(A)", advance="no") "WHIZARD"
  call eio%tag_generator%close (u); write (u, *)
  call eio%tag_xsecinfo%write (u); write (u, *)
  if (eio%write_sqme_ref) then
    call eio%tag_sqme_ref%write (u); write (u, *)
  end if
  if (eio%write_sqme_prc) then
    call eio%tag_sqme_prc%write (u); write (u, *)
  end if
  if (eio%write_sqme_alt) then
    do i = 1, eio%n_alt
      call eio%tag_sqme_alt(i)%write (u); write (u, *)
    end do
  end if
  do i = 1, eio%n_alt
    call eio%tag_wgts_alt(i)%write (u); write (u, *)
  end do
end subroutine eio_lhef_write_init_30

```

When reading the init block, we first call the 1.0 routine that fills HEPUP. Then we consider the possible tags. Only the `generator` and `xsecinfo` tags are of interest. We skip everything else except for the closing tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
procedure :: read_init_30 => eio_lhef_read_init_30

<EIO LHEF: sub interfaces>+≡
module subroutine eio_lhef_read_init_30 (eio, data)
  class(eio_lhef_t), intent(inout) :: eio
  type(event_sample_data_t), intent(out) :: data
end subroutine eio_lhef_read_init_30

<EIO LHEF: procedures>+≡
module subroutine eio_lhef_read_init_30 (eio, data)
  class(eio_lhef_t), intent(inout) :: eio
  type(event_sample_data_t), intent(out) :: data
  real(default), parameter :: pb_per_fb = 1.e-3_default
  type(string_t) :: content
  logical :: found, closing
  integer :: n_weightinfo
  call eio_lhef_read_init_10 (eio, data)
  n_weightinfo = 0
  eio%i_weight_sqme = 0
  SCAN_INIT_TAGS: do
    call eio%tag_generator%read (eio%cstream, found)
    if (found) then
      if (.not. eio%tag_generator%has_content) call err_generator
      call eio%tag_generator%read_content (eio%cstream, content, closing)
    end if
  end do

```

```

        call msg_message ("LHEF: Event file has been generated by " &
            // char (content) // " " &
            // char (eio%tag_generator%get_attribute (1)))
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_xsecinfo%read (eio%cstream, found)
    if (found) then
        if (eio%tag_xsecinfo%has_content) call err_xsecinfo
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_weightinfo%read (eio%cstream, found)
    if (found) then
        if (eio%tag_weightinfo%has_content) call err_xsecinfo
        n_weightinfo = n_weightinfo + 1
        if (eio%tag_weightinfo%get_attribute (1) == "sqme_prc") then
            eio%i_weight_sqme = n_weightinfo
        end if
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_init%read_content (eio%cstream, content, closing)
    if (closing) then
        if (content /= "") call err_init
        exit SCAN_INIT_TAGS
    end if
end do SCAN_INIT_TAGS
data%n_evt = &
    read_ival (eio%tag_xsecinfo%get_attribute (1))
if (data%n_beam == 1) then
    data%total_cross_section = &
        read_rval (eio%tag_xsecinfo%get_attribute (2))
else
    data%total_cross_section = &
        read_rval (eio%tag_xsecinfo%get_attribute (2)) / pb_per_fb
end if
contains
subroutine err_generator
    call msg_fatal ("LHEF: invalid generator tag")
end subroutine err_generator
subroutine err_xsecinfo
    call msg_fatal ("LHEF: invalid xsecinfo tag")
end subroutine err_xsecinfo
subroutine err_init
    call msg_fatal ("LHEF: syntax error after init tag")
end subroutine err_init
end subroutine eio_lhef_read_init_30

```

This is additional event-specific information for the 3.0 format, after the HEP-EUP data. We can specify weights, starting from the master weight and adding alternative weights. The weight tags are already allocated, so we just have to transfer the weight values to strings, assemble them and write them to file. All weights are collected in a single tag.

Note: If efficiency turns out to be an issue, we may revert to traditional character buffer writing. However, we need to know the maximum length.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_event_30 => eio_lhef_write_event_30

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_write_event_30 (eio, event)
    class(eio_lhef_t), intent(in) :: eio
    class(generic_event_t), intent(in) :: event
    end subroutine eio_lhef_write_event_30

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_write_event_30 (eio, event)
    class(eio_lhef_t), intent(in) :: eio
    class(generic_event_t), intent(in) :: event
    type(string_t) :: s
    integer :: u, i
    u = eio%unit
    s = ""
    if (eio%write_sqme_ref) then
      s = s // str (event%get_sqme_ref ()) // " "
    end if
    if (eio%write_sqme_prc) then
      s = s // str (event%get_sqme_prc ()) // " "
    end if
    if (eio%n_alt > 0) then
      if (eio%write_sqme_alt) then
        s = s // str (event%get_sqme_alt(1)) // " "
        do i = 2, eio%n_alt
          s = s // str (event%get_sqme_alt(i)) // " "
        end do
      end if
      s = s // str (event%get_weight_alt(1)) // " "
      do i = 2, eio%n_alt
        s = s // str (event%get_weight_alt(i)) // " "
      end do
    end if
    if (len_trim (s) > 0) then
      call eio%tag_weights%write (trim (s), u); write (u, *)
    end if
  end subroutine eio_lhef_write_event_30

```

Read extra event data. If there is a `weights` tag and if there was a `weightinfo` entry labeled `sqme_prc`, we extract the corresponding entry from the `weights` string and store this as the event's squared matrix-element value. Other tags, including tags written by the above writer, are skipped.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_event_30 => eio_lhef_read_event_30

<EIO LHEF: sub interfaces>+≡
  module subroutine eio_lhef_read_event_30 (eio, event)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout) :: event
    end subroutine eio_lhef_read_event_30

<EIO LHEF: procedures>+≡
  module subroutine eio_lhef_read_event_30 (eio, event)

```

```

class(eio_lhef_t), intent(inout) :: eio
class(generic_event_t), intent(inout) :: event
type(string_t) :: content, string
logical :: found, closing
integer :: i
SCAN_EVENT_TAGS: do
  call eio%tag_weights%read (eio%cstream, found)
  if (found) then
    if (.not. eio%tag_weights%has_content) call err_weights
    call eio%tag_weights%read_content (eio%cstream, content, closing)
    if (.not. closing) call err_weights
    if (eio%i_weight_sqme > 0) then
      SCAN_WEIGHTS: do i = 1, eio%i_weight_sqme
        call split (content, string, " ")
        content = adjustl (content)
        if (i == eio%i_weight_sqme) then
          call event%set_sqme_ref (read_rval (string))
          exit SCAN_WEIGHTS
        end if
      end do SCAN_WEIGHTS
    end if
    cycle SCAN_EVENT_TAGS
  end if
  call eio%tag_event%read_content (eio%cstream, content, closing)
  if (closing) then
    if (content /= "") call err_event
    exit SCAN_EVENT_TAGS
  end if
end do SCAN_EVENT_TAGS
contains
subroutine err_weights
  call msg_fatal ("LHEF: invalid weights tag in event record")
end subroutine err_weights
subroutine err_event
  call msg_fatal ("LHEF: syntax error after event tag")
end subroutine err_event
end subroutine eio_lhef_read_event_30

```

18.15.8 Unit tests

Test module, followed by the corresponding implementation module.

(eio_lhef_ut.f90)≡

⟨File header⟩

```

module eio_lhef_ut
  use unit_tests
  use eio_lhef_uti

```

⟨Standard module head⟩

⟨EIO LHEF: public test⟩

```

contains

  <EIO LHEF: test driver>

  end module eio_lhef_ut

  <eio_lhef_uti.f90>≡
  <File header>

  module eio_lhef_uti

    <Use kinds>
    <Use strings>
    use io_units
    use model_data
    use event_base
    use eio_data
    use eio_base

    use eio_lhef

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
    use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    <Standard module head>

    <EIO LHEF: test declarations>

contains

  <EIO LHEF: tests>

  end module eio_lhef_uti
API: driver for the unit tests below.
  <EIO LHEF: public test>≡
    public :: eio_lhef_test
  <EIO LHEF: test driver>≡
    subroutine eio_lhef_test (u, results)
      integer, intent(in) :: u
      type(test_results_t), intent(inout) :: results
    <EIO LHEF: execute tests>
    end subroutine eio_lhef_test

```

Version 1.0 Output

We test the implementation of all I/O methods. We start with output according to version 1.0.

```

  <EIO LHEF: execute tests>≡
    call test (eio_lhef_1, "eio_lhef_1", &
      "write version 1.0", &
      u, results)

```

```

<EIO LHEF: test declarations>≡
    public :: eio_lhef_1

<EIO LHEF: tests>≡
    subroutine eio_lhef_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_lhef_1"
        write (u, "(A)")  "* Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%unweighted = .true.
        data%norm_mode = NORM_UNIT
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_lhef_1"

        allocate (eio_lhef_t :: eio)
        select type (eio)
        type is (eio_lhef_t)
            call eio%set_parameters ()
        end select

        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])

        call eio%output (event, i_prc = 1)
        call eio%write (u)
        call eio%final ()

        write (u, "(A)")
        write (u, "(A)")  "* File contents:"
        write (u, "(A)")

```

```

u_file = free_unit ()
open (u_file, file = char (sample // "." // eio%extension), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (buffer(1:21) == " <generator_version>")  buffer = "[...]"
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
  call eio%set_parameters ()
end select

select type (eio)
type is (eio_lhef_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_1"

end subroutine eio_lhef_1

```

Version 2.0 Output

Version 2.0 has added a lot of options to the LHEF format. We implement some of them.

```

<EIO LHEF: execute tests>+≡
  call test (eio_lhef_2, "eio_lhef_2", &
    "write version 2.0", &
    u, results)

<EIO LHEF: test declarations>+≡
  public :: eio_lhef_2

<EIO LHEF: tests>+≡
  subroutine eio_lhef_2 (u)

```



```

integer, intent(in) :: u
class(generic_event_t), pointer :: event
type(event_sample_data_t) :: data
class(eio_t), allocatable :: eio
type(string_t) :: sample
integer :: u_file, iostat
character(80) :: buffer

write (u, "(A)")  "* Test output: eio_lhef_2"
write (u, "(A)")  "* Purpose: generate an event and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%unweighted = .false.
data%norm_mode = NORM_SIGMA
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lhef_2"

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters (version = "2.0", write_sqme_prc = .true.)
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // "." // eio%extension), &

```

```

        action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:10) == "<generator") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_2"

end subroutine eio_lhef_2

```

Version 3.0 Output

Version 3.0 is an update which removes some tags (which we didn't use anyway) and suggests a new treatment of weights.

```

<EIO LHEF: execute tests>+≡
    call test (eio_lhef_3, "eio_lhef_3", &
        "write version 3.0", &
        u, results)

<EIO LHEF: test declarations>+≡
    public :: eio_lhef_3

<EIO LHEF: tests>+≡
    subroutine eio_lhef_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_lhef_3"
        write (u, "(A)")  "* Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%unweighted = .false.
        data%norm_mode = NORM_SIGMA
        data%n_evt = 1

```

```

data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lhef_3"

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters (version = "3.0", write_sqme_prc = .true.)
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lhe"), &
      action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:10) == "<generator") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_3"

end subroutine eio_lhef_3

```

Version 1.0 Input

Check input of a version-1.0 conforming LHEF file.

```
(EIO LHEF: execute tests)+≡
    call test (eio_lhef_4, "eio_lhef_4", &
        "read version 1.0", &
        u, results)

(EIO LHEF: test declarations)+≡
    public :: eio_lhef_4

(EIO LHEF: tests)+≡
    subroutine eio_lhef_4 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat, i_prc

        write (u, "(A)")  "*" Test output: eio_lhef_4"
        write (u, "(A)")  "*" Purpose: read a LHEF 1.0 file"
        write (u, "(A)")

        write (u, "(A)")  "*" Write a LHEF data file"
        write (u, "(A)")

        u_file = free_unit ()
        sample = "eio_lhef_4"
        open (u_file, file = char (sample // ".lhe"), &
            status = "replace", action = "readwrite")

        write (u_file, "(A)")  '<LesHouchesEvents version="1.0">'
        write (u_file, "(A)")  '<header>'
        write (u_file, "(A)")  '  <arbitrary_tag opt="foo">content</arbitrary_tag>'
        write (u_file, "(A)")  '  Text'
        write (u_file, "(A)")  '  <another_tag />'
        write (u_file, "(A)")  '</header>'
        write (u_file, "(A)")  '<init>'
        write (u_file, "(A)")  '  25 25  5.0000000000E+02  5.0000000000E+02 &
            & -1 -1 -1 -1 3 1'
        write (u_file, "(A)")  '  1.0000000000E-01  1.0000000000E-03 &
            & 1.0000000000E+00 42'
        write (u_file, "(A)")  '</init>'
        write (u_file, "(A)")  '<event>'
        write (u_file, "(A)")  '  4 42  3.0574068604E+08  1.0000000000E+03 &
            & -1.0000000000E+00 -1.0000000000E+00'
        write (u_file, "(A)")  '  25 -1 0 0 0 0  0.0000000000E+00  0.0000000000E+00 &
            & 4.8412291828E+02  5.0000000000E+02  1.2500000000E+02 &
            & 0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  '  25 -1 0 0 0 0  0.0000000000E+00  0.0000000000E+00 &
            & -4.8412291828E+02  5.0000000000E+02  1.2500000000E+02 &
            & 0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  '  25 1 1 2 0 0 -1.4960220911E+02 -4.6042825611E+02 &
```

```

& 0.0000000000E+00 5.0000000000E+02 1.2500000000E+02 &
& 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 1 1 2 0 0 1.4960220911E+02 4.6042825611E+02 &
& 0.0000000000E+00 5.0000000000E+02 1.2500000000E+02 &
& 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") '</event>'
write (u_file, "(A)") '</LesHouchesEvents>'
close (u_file)

write (u, "(A)")  " * Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  " * Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, *)

select type (eio)
type is (eio_lhef_t)
    call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  " * Read event"
write (u, "(A)")

```

```

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
    write (u, "(A,I0,A,I0)") "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)") "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_4"

end subroutine eio_lhef_4

```

Version 2.0 Input

Check input of a version-2.0 conforming LHEF file.

```

<EIO LHEF: execute tests>+≡
    call test (eio_lhef_5, "eio_lhef_5", &
        "read version 2.0", &
        u, results)

<EIO LHEF: test declarations>+≡
    public :: eio_lhef_5

<EIO LHEF: tests>+≡
    subroutine eio_lhef_5 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat, i_prc

```

```

write (u, "(A)")  "* Test output: eio_lhef_5"
write (u, "(A)")  "* Purpose: read a LHEF 2.0 file"
write (u, "(A)")

write (u, "(A)")  "* Write a LHEF data file"
write (u, "(A)")

u_file = free_unit ()
sample = "eio_lhef_5"
open (u_file, file = char (sample // ".lhe"), &
      status = "replace", action = "readwrite")

write (u_file, "(A)")  '<LesHouchesEvents version="2.0">'
write (u_file, "(A)")  '<header>'
write (u_file, "(A)")  '</header>'
write (u_file, "(A)")  '<init>'
write (u_file, "(A)")  ' 25 25 5.0000000000E+02 5.0000000000E+02 &
&-1 -1 -1 -1 4 1'
write (u_file, "(A)")  ' 1.0000000000E-01 1.0000000000E-03 &
& 0.0000000000E+00 42'
write (u_file, "(A)")  '<generator version="2.2.3">WHIZARD&
&</generator>'
write (u_file, "(A)")  '<xsecinfo neve="1" totxsec="1.0000000000E-01" />'
write (u_file, "(A)")  '</init>'
write (u_file, "(A)")  '<event>'
write (u_file, "(A)")  ' 4 42 3.0574068604E+08 1.0000000000E+03 &
&-1.0000000000E+00 -1.0000000000E+00'
write (u_file, "(A)")  ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)")  ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 -4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)")  ' 25 1 1 2 0 0 -1.4960220911E+02 &
&-4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)")  ' 25 1 1 2 0 0 1.4960220911E+02 &
& 4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)")  '<weight name="sqme_prc">1.0000000000E+00</weight>'
write (u_file, "(A)")  '</event>'
write (u_file, "(A)")  '</LesHouchesEvents>'
close (u_file)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)

```

```

        call eio%set_parameters (version = "2.0", recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%unweighted = .false.
data%norm_mode = NORM_SIGMA
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, *)

select type (eio)
type is (eio_lhef_t)
    call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")

```



```

write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_5"

end subroutine eio_lhef_5

```

Version 3.0 Input

Check input of a version-3.0 conforming LHEF file.

```

<EIO LHEF: execute tests>+≡
  call test (eio_lhef_6, "eio_lhef_6", &
    "read version 3.0", &
    u, results)

<EIO LHEF: test declarations>+≡
  public :: eio_lhef_6

<EIO LHEF: tests>+≡
  subroutine eio_lhef_6 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat, i_prc

    write (u, "(A)")  "* Test output: eio_lhef_6"
    write (u, "(A)")  "* Purpose: read a LHEF 3.0 file"
    write (u, "(A)")

    write (u, "(A)")  "* Write a LHEF data file"
    write (u, "(A)")

    u_file = free_unit ()
    sample = "eio_lhef_6"
    open (u_file, file = char (sample // ".lhe"), &
      status = "replace", action = "readwrite")

    write (u_file, "(A)")  '<LesHouchesEvents version="3.0">'
    write (u_file, "(A)")  '<header>'
    write (u_file, "(A)")  '</header>'
    write (u_file, "(A)")  '<init>'
    write (u_file, "(A)")  ' 25 25  5.0000000000E+02  5.0000000000E+02 &
      &-1 -1 -1 -1 4 1'
    write (u_file, "(A)")  ' 1.0000000000E-01  1.0000000000E-03 &
      & 0.0000000000E+00 42'

```

```

write (u_file, "(A)") '<generator version="2.2.3">WHIZARD&
&</generator>'
write (u_file, "(A)") '<xsecinfo neve="1" totxsec="1.0000000000E-01" />'
write (u_file, "(A)") '<weightinfo name="sqme_prc" />'
write (u_file, "(A)") '</init>'
write (u_file, "(A)") '<event>'
write (u_file, "(A)") ' 4 42 3.0574068604E+08 1.0000000000E+03 &
&-1.0000000000E+00 -1.0000000000E+00'
write (u_file, "(A)") ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 -4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 1 1 2 0 0 -1.4960220911E+02 &
&-4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 1 1 2 0 0 1.4960220911E+02 &
& 4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") '<weights>1.0000000000E+00</weights>'
write (u_file, "(A)") '</event>'
write (u_file, "(A)") '</LesHouchesEvents>'
close (u_file)

write (u, "(A)") "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
call eio%set_parameters (version = "3.0", recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%unweighted = .false.
data%norm_mode = NORM_SIGMA
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)") "* Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

```

```

write (u, *)

select type (eio)
type is (eio_lhef_t)
  call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
  write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
    " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_6"

end subroutine eio_lhef_6

```

18.16 STDHEP File Formats

Here, we implement the two existing STDHEP file formats, one based on the HEPRUP/HEPEUP common blocks, the other based on the HEPEVT common

block. The second one is actually the standard STDHEP format.

```

<eio_stdhep.f90>≡
  <File header>

  module eio_stdhep

    use kinds, only: i32, i64
  <Use strings>
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

  <Standard module head>

  <EIO stdhep: public>

  <EIO stdhep: types>

    interface
  <EIO stdhep: sub interfaces>
    end interface

  end module eio_stdhep
<eio_stdhep_sub.f90>≡
  <File header>

  submodule (eio_stdhep) eio_stdhep_s

    use io_units
    use string_utils
    use diagnostics
    use hep_common
    use hep_events

    implicit none

  <EIO stdhep: variables>

  contains

  <EIO stdhep: procedures>

  end submodule eio_stdhep_s

```

18.16.1 Type

```

<EIO stdhep: public>≡
  public :: eio_stdhep_t

<EIO stdhep: types>≡
  type, abstract, extends (eio_t) :: eio_stdhep_t
    logical :: writing = .false.

```

```

        logical :: reading = .false.
        integer :: unit = 0
        logical :: keep_beams = .false.
        logical :: keep_remnants = .true.
        logical :: ensure_order = .false.
        logical :: recover_beams = .false.
        logical :: use_alphas_from_file = .false.
        logical :: use_scale_from_file = .false.
        integer, dimension(:), allocatable :: proc_num_id
        integer(i64) :: n_events_expected = 0
    contains
        <EIO stdhep: eio stdhep: TBP>
    end type eio_stdhep_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepevt_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepevt_t
    end type eio_stdhep_hepevt_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepeup_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepeup_t
    end type eio_stdhep_hepeup_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepev4_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepev4_t
    end type eio_stdhep_hepev4_t

```

18.16.2 Specific Methods

Set parameters that are specifically used with STDHEP file formats.

```

<EIO stdhep: eio stdhep: TBP>≡
    procedure :: set_parameters => eio_stdhep_set_parameters

<EIO stdhep: sub interfaces>≡
    module subroutine eio_stdhep_set_parameters (eio, &
        keep_beams, keep_remnants, ensure_order, recover_beams, &
        use_alphas_from_file, use_scale_from_file, extension)
        class(eio_stdhep_t), intent(inout) :: eio
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: ensure_order
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: use_alphas_from_file
        logical, intent(in), optional :: use_scale_from_file
        type(string_t), intent(in), optional :: extension
    end subroutine eio_stdhep_set_parameters

```

```

<EIO stdhep: procedures>≡
module subroutine eio_stdhep_set_parameters (eio, &
    keep_beams, keep_remnants, ensure_order, recover_beams, &
    use_alphas_from_file, use_scale_from_file, extension)
class(eio_stdhep_t), intent(inout) :: eio
logical, intent(in), optional :: keep_beams
logical, intent(in), optional :: keep_remnants
logical, intent(in), optional :: ensure_order
logical, intent(in), optional :: recover_beams
logical, intent(in), optional :: use_alphas_from_file
logical, intent(in), optional :: use_scale_from_file
type(string_t), intent(in), optional :: extension
if (present (keep_beams)) eio%keep_beams = keep_beams
if (present (keep_remnants)) eio%keep_remnants = keep_remnants
if (present (ensure_order)) eio%ensure_order = ensure_order
if (present (recover_beams)) eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (extension)) then
    eio%extension = extension
else
    select type (eio)
    type is (eio_stdhep_hepevt_t)
        eio%extension = "hep"
    type is (eio_stdhep_hepev4_t)
        eio%extension = "ev4.hep"
    type is (eio_stdhep_hepeup_t)
        eio%extension = "up.hep"
    end select
end if
end subroutine eio_stdhep_set_parameters

```

18.16.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO stdhep: eio stdhep: TBP>+≡
procedure :: write => eio_stdhep_write

<EIO stdhep: sub interfaces>+≡
module subroutine eio_stdhep_write (object, unit)
class(eio_stdhep_t), intent(in) :: object
integer, intent(in), optional :: unit
end subroutine eio_stdhep_write

<EIO stdhep: procedures>+≡
module subroutine eio_stdhep_write (object, unit)
class(eio_stdhep_t), intent(in) :: object
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit)

```

```

write (u, "(1x,A)") "STDHEP event stream:"
if (object%writing) then
  write (u, "(3x,A,A)") "Writing to file = ", char (object%filename)
else if (object%reading) then
  write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
else
  write (u, "(3x,A)") "[closed]"
end if
write (u, "(3x,A,L1)") "Keep beams = ", object%keep_beams
write (u, "(3x,A,L1)") "Keep remnants = ", object%keep_remnants
write (u, "(3x,A,L1)") "Recover beams = ", object%recover_beams
write (u, "(3x,A,L1)") "Alpha_s from file = ", &
  object%use_alphas_from_file
write (u, "(3x,A,L1)") "Scale from file = ", &
  object%use_scale_from_file
if (allocated (object%proc_num_id)) then
  write (u, "(3x,A)") "Numerical process IDs:"
  do i = 1, size (object%proc_num_id)
    write (u, "(5x,I0,': ',I0)") i, object%proc_num_id(i)
  end do
end if
end subroutine eio_stdhep_write

```

Finalizer: close any open file.

<EIO stdhep: eio stdhep: TBP>+≡

```

procedure :: final => eio_stdhep_final

```

<EIO stdhep: sub interfaces>+≡

```

module subroutine eio_stdhep_final (object)
  class(eio_stdhep_t), intent(inout) :: object
end subroutine eio_stdhep_final

```

<EIO stdhep: procedures>+≡

```

module subroutine eio_stdhep_final (object)
  class(eio_stdhep_t), intent(inout) :: object
  if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
  if (object%writing) then
    write (msg_buffer, "(A,A,A)") "Events: closing STDHEP file '", &
      char (object%filename), "'"
    call msg_message ()
    call stdhep_write (200)
    call stdhep_end ()
    object%writing = .false.
  else if (object%reading) then
    write (msg_buffer, "(A,A,A)") "Events: closing STDHEP file '", &
      char (object%filename), "'"
    call msg_message ()
    object%reading = .false.
  end if
end subroutine eio_stdhep_final

```

Common initialization for input and output.

<EIO stdhep: eio stdhep: TBP>+≡

```

procedure :: common_init => eio_stdhep_common_init

```

```

<EIO stdhep: sub interfaces>+≡
  module subroutine eio_stdhep_common_init (eio, sample, data, extension)
    class(eio_stdhep_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
  end subroutine eio_stdhep_common_init

<EIO stdhep: procedures>+≡
  module subroutine eio_stdhep_common_init (eio, sample, data, extension)
    class(eio_stdhep_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
    if (.not. present (data)) &
      call msg_bug ("STDHEP initialization: missing data")
    if (present (extension)) then
      eio%extension = extension
    end if
    eio%sample = sample
    call eio%set_filename ()
    eio%unit = free_unit ()
    allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
  end subroutine eio_stdhep_common_init

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common block contents are still intact.)

```

<EIO stdhep: eio stdhep: TBP>+≡
  procedure :: split_out => eio_stdhep_split_out

<EIO stdhep: sub interfaces>+≡
  module subroutine eio_stdhep_split_out (eio)
    class(eio_stdhep_t), intent(inout) :: eio
  end subroutine eio_stdhep_split_out

<EIO stdhep: procedures>+≡
  module subroutine eio_stdhep_split_out (eio)
    class(eio_stdhep_t), intent(inout) :: eio
    if (eio%split) then
      eio%split_index = eio%split_index + 1
      call eio%set_filename ()
      write (msg_buffer, "(A,A,A)") "Events: writing to STDHEP file '", &
        char (eio%filename), "'"
      call msg_message ()
      call stdhep_write (200)
      call stdhep_end ()
      select type (eio)
      type is (eio_stdhep_hepeup_t)
        call stdhep_init_out (char (eio%filename), &
          "WHIZARD <Version>", eio%n_events_expected)
        call stdhep_write (100)
        call stdhep_write (STDHEP_HEPRUP)
      type is (eio_stdhep_hepevt_t)
        call stdhep_init_out (char (eio%filename), &

```



```

        "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    type is (eio_stdhep_hepev4_t)
    call stdhep_init_out (char (eio%filename), &
        "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    end select
end if
end subroutine eio_stdhep_split_out

```

Initialize event writing.

<EIO stdhep: eio stdhep: TBP>+≡

```

    procedure :: init_out => eio_stdhep_init_out

```

<EIO stdhep: sub interfaces>+≡

```

    module subroutine eio_stdhep_init_out &
        (eio, sample, data, success, extension)
    class(eio_stdhep_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    end subroutine eio_stdhep_init_out

```

<EIO stdhep: procedures>+≡

```

    module subroutine eio_stdhep_init_out &
        (eio, sample, data, success, extension)
    class(eio_stdhep_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    logical :: is_width
    integer :: i
    if (.not. present (data)) &
        call msg_bug ("STDHEP initialization: missing data")
    is_width = data%n_beam == 1
    call eio%set_splitting (data)
    call eio%common_init (sample, data, extension)
    eio%n_events_expected = data%n_evt
    write (msg_buffer, "(A,A,A)") "Events: writing to STDHEP file '", &
        char (eio%filename), ""
    call msg_message ()
    eio%writing = .true.
    select type (eio)
    type is (eio_stdhep_hepeup_t)
        call heprup_init &
            (data%pdg_beam, &
            data%energy_beam, &
            n_processes = data%n_proc, &
            unweighted = data%unweighted, &
            negative_weights = data%negative_weights)
        do i = 1, data%n_proc
            call heprup_set_process_parameters (i = i, &
                process_id = data%proc_num_id(i), &

```

```

        cross_section = data%cross_section(i), &
        error = data%error(i), &
        is_width = is_width)
    end do
    call stdhep_init_out (char (eio%filename), &
        "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    call stdhep_write (STDHEP_HEPRUP)
    type is (eio_stdhep_hepevt_t)
    call stdhep_init_out (char (eio%filename), &
        "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    type is (eio_stdhep_hepev4_t)
    call stdhep_init_out (char (eio%filename), &
        "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    end select
    if (present (success)) success = .true.
end subroutine eio_stdhep_init_out

```

Initialize event reading.

<EIO stdhep: eio stdhep: TBP>+≡

```

    procedure :: init_in => eio_stdhep_init_in

```

<EIO stdhep: sub interfaces>+≡

```

    module subroutine eio_stdhep_init_in &
        (eio, sample, data, success, extension)
        class(eio_stdhep_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_stdhep_init_in

```

<EIO stdhep: procedures>+≡

```

    module subroutine eio_stdhep_init_in &
        (eio, sample, data, success, extension)
        class(eio_stdhep_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        integer :: ilbl, lok
        logical :: exist
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: reading from STDHEP file '", &
            char (eio%filename), "'"
        call msg_message ()
        inquire (file = char (eio%filename), exist = exist)
        if (.not. exist) call msg_fatal ("Events: STDHEP file not found.")
        eio%reading = .true.
        call stdhep_init_in (char (eio%filename), eio%n_events_expected)
        call stdhep_read (ilbl, lok)
        if (lok /= 0) then
            call stdhep_end ()
        end if
    end subroutine eio_stdhep_init_in

```

```

        write (msg_buffer, "(A)") "Events: STDHEP file appears to" // &
            " be empty."
        call msg_message ()
    end if
    if (ilbl == 100) then
        write (msg_buffer, "(A)") "Events: reading in STDHEP events"
        call msg_message ()
    end if
    if (present (success)) success = .false.
end subroutine eio_stdhep_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: switch_inout => eio_stdhep_switch_inout

<EIO stdhep: sub interfaces>+≡
    module subroutine eio_stdhep_switch_inout (eio, success)
        class(eio_stdhep_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_stdhep_switch_inout

<EIO stdhep: procedures>+≡
    module subroutine eio_stdhep_switch_inout (eio, success)
        class(eio_stdhep_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("STDHEP: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_stdhep_switch_inout

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: output => eio_stdhep_output

<EIO stdhep: sub interfaces>+≡
    module subroutine eio_stdhep_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_stdhep_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_stdhep_output

<EIO stdhep: procedures>+≡
    module subroutine eio_stdhep_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_stdhep_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        if (present (passed)) then
            if (.not. passed) return
        end if
    end if

```

```

if (eio%writing) then
  select type (eio)
  type is (eio_stdhep_hepeup_t)
    call hepeup_from_event (event, &
      process_index = eio%proc_num_id (i_prc), &
      keep_beams = eio%keep_beams, &
      keep_remnants = eio%keep_remnants)
    call stdhep_write (STDHEP_HEPEUP)
  type is (eio_stdhep_hepevt_t)
    call hepevt_from_event (event, &
      keep_beams = eio%keep_beams, &
      keep_remnants = eio%keep_remnants, &
      ensure_order = eio%ensure_order)
    call stdhep_write (STDHEP_HEPEVT)
  type is (eio_stdhep_hepev4_t)
    call hepevt_from_event (event, &
      process_index = eio%proc_num_id (i_prc), &
      keep_beams = eio%keep_beams, &
      keep_remnants = eio%keep_remnants, &
      ensure_order = eio%ensure_order, &
      fill_hepev4 = .true.)
    call stdhep_write (STDHEP_HEPEV4)
  end select
else
  call eio%write ()
  call msg_fatal ("STDHEP file is not open for writing")
end if
end subroutine eio_stdhep_output

```

Input an event. We do not allow to read in STDHEP files written via the HEPEVT common block as there is no control on the process ID. This implies that the event index cannot be read; it is simply incremented to count the current event sample.

```

<EIO stdhep: eio stdhep: TBP>+≡
  procedure :: input_i_prc => eio_stdhep_input_i_prc
  procedure :: input_event => eio_stdhep_input_event

<EIO stdhep: sub interfaces>+≡
  module subroutine eio_stdhep_input_i_prc (eio, i_prc, iostat)
    class(eio_stdhep_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
  end subroutine eio_stdhep_input_i_prc
  module subroutine eio_stdhep_input_event (eio, event, iostat, event_handle)
    class(eio_stdhep_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine eio_stdhep_input_event

<EIO stdhep: procedures>+≡
  module subroutine eio_stdhep_input_i_prc (eio, i_prc, iostat)
    class(eio_stdhep_t), intent(inout) :: eio
    integer, intent(out) :: i_prc

```

```

integer, intent(out) :: iostat
integer :: i, ilbl, proc_num_id
iostat = 0
select type (eio)
type is (eio_stdhep_hepevt_t)
  if (size (eio%proc_num_id) > 1) then
    call msg_fatal ("Events: only single processes allowed " // &
      "with the STDHEP HEPEVT format.")
  else
    proc_num_id = eio%proc_num_id (1)
    call stdhep_read (ilbl, lok)
  end if
type is (eio_stdhep_hepev4_t)
  call stdhep_read (ilbl, lok)
  proc_num_id = idruplh
type is (eio_stdhep_hepeup_t)
  call stdhep_read (ilbl, lok)
  if (lok /= 0) call msg_error ("Events: STDHEP appears to be " // &
    "empty or corrupted.")
  if (ilbl == 12) then
    call stdhep_read (ilbl, lok)
  end if
  if (ilbl == 11) then
    proc_num_id = IDPRUP
  end if
end select
FIND_I_PRC: do i = 1, size (eio%proc_num_id)
  if (eio%proc_num_id(i) == proc_num_id) then
    i_prc = i
    exit FIND_I_PRC
  end if
end do FIND_I_PRC
if (i_prc == 0) call err_index
contains
subroutine err_index
  call msg_error ("STDHEP: reading events: undefined process ID " &
    // char (str (proc_num_id)) // ", aborting read")
  iostat = 1
end subroutine err_index
end subroutine eio_stdhep_input_i_prc

module subroutine eio_stdhep_input_event (eio, event, iostat, event_handle)
  class(eio_stdhep_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  iostat = 0
  call event%reset_contents ()
  call event%select (1, 1, 1)
  call hepeup_to_event (event, eio%fallback_model, &
    recover_beams = eio%recover_beams, &
    use_alpha_s = eio%use_alphas_from_file, &
    use_scale = eio%use_scale_from_file)
  call event%increment_index ()

```

```

        end subroutine eio_stdhep_input_event

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: skip => eio_stdhep_skip

<EIO stdhep: sub interfaces>+≡
    module subroutine eio_stdhep_skip (eio, iostat)
        class(eio_stdhep_t), intent(inout) :: eio
        integer, intent(out) :: iostat
    end subroutine eio_stdhep_skip

<EIO stdhep: procedures>+≡
    module subroutine eio_stdhep_skip (eio, iostat)
        class(eio_stdhep_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        if (eio%reading) then
            read (eio%unit, iostat = iostat)
        else
            call eio%write ()
            call msg_fatal ("Raw event file is not open for reading")
        end if
    end subroutine eio_stdhep_skip

```

STDHEP specific routines.

```

<EIO stdhep: public>+≡
    public :: stdhep_init_out
    public :: stdhep_init_in
    public :: stdhep_write
    public :: stdhep_end

<EIO stdhep: sub interfaces>+≡
    module subroutine stdhep_init_out (file, title, nevt)
        character(len=*), intent(in) :: file, title
        integer(i64), intent(in) :: nevt
    end subroutine stdhep_init_out
    module subroutine stdhep_init_in (file, nevt)
        character(len=*), intent(in) :: file
        integer(i64), intent(out) :: nevt
    end subroutine stdhep_init_in
    module subroutine stdhep_write (ilbl)
        integer, intent(in) :: ilbl
    end subroutine stdhep_write
    module subroutine stdhep_read (ilbl, lok)
        integer, intent(out) :: ilbl, lok
    end subroutine stdhep_read
    module subroutine stdhep_end ()
    end subroutine stdhep_end

<EIO stdhep: procedures>+≡
    module subroutine stdhep_init_out (file, title, nevt)
        character(len=*), intent(in) :: file, title
        integer(i64), intent(in) :: nevt
        integer(i32) :: nevt32
        nevt32 = min (nevt, int (huge (1_i32), i64))
        call stdxwinit (file, title, nevt32, istr, lok)
    end subroutine stdhep_init_out

```

```

end subroutine stdhep_init_out

module subroutine stdhep_init_in (file, nevt)
  character(len=*), intent(in) :: file
  integer(i64), intent(out) :: nevt
  integer(i32) :: nevt32
  call stdxrinit (file, nevt32, istr, lok)
  if (lok /= 0) call msg_fatal ("STDHEP: error in reading file '" // &
    file // "'.")
  nevt = int (nevt32, i64)
end subroutine stdhep_init_in

module subroutine stdhep_write (ilbl)
  integer, intent(in) :: ilbl
  call stdxwrt (ilbl, istr, lok)
end subroutine stdhep_write

module subroutine stdhep_read (ilbl, lok)
  integer, intent(out) :: ilbl, lok
  call stdxrd (ilbl, istr, lok)
  if (lok /= 0) return
end subroutine stdhep_read

module subroutine stdhep_end ()
  call stdxend (istr)
end subroutine stdhep_end

```

18.16.4 Variables

<EIO stdhep: variables>≡

```

integer, save :: istr, lok
integer, parameter :: &
  STDHEP_HEPEVT = 1, STDHEP_HEPEV4 = 4, &
  STDHEP_HEPEUP = 11, STDHEP_HEPRUP = 12

```

18.16.5 Unit tests

Test module, followed by the corresponding implementation module.

<eio_stdhep_ut.f90>≡

<File header>

```

module eio_stdhep_ut
  use unit_tests
  use eio_stdhep_ut_i

```

<Standard module head>

<EIO stdhep: public test>

contains

<EIO stdhep: test driver>

```

    end module eio_stdhep_ut

    <eio_stdhep_util.f90>≡
    <File header>

    module eio_stdhep_util

    <Use kinds>
    <Use strings>
        use io_units
        use model_data
        use event_base
        use eio_data
        use eio_base
        use xdr_wo_stdhep

        use eio_stdhep

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
        use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    <Standard module head>

    <EIO stdhep: test declarations>

    contains

    <EIO stdhep: tests>

    end module eio_stdhep_util
API: driver for the unit tests below.
    <EIO stdhep: public test>≡
        public :: eio_stdhep_test
    <EIO stdhep: test driver>≡
        subroutine eio_stdhep_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO stdhep: execute tests>
        end subroutine eio_stdhep_test

```

Test I/O methods

We test the implementation of the STDHEP HEPEVT I/O method:

```

    <EIO stdhep: execute tests>≡
        call test (eio_stdhep_1, "eio_stdhep_1", &
            "read and write event contents, format [stdhep]", &
            u, results)
    <EIO stdhep: test declarations>≡
        public :: eio_stdhep_1

```



```

<EIO stdhep: tests>≡
subroutine eio_stdhep_1 (u)
  integer, intent(in) :: u
  class(generic_event_t), pointer :: event
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  type(string_t) :: sample
  integer :: u_file, iostat
  character(215) :: buffer

  write (u, "(A)")  "* Test output: eio_stdhep_1"
  write (u, "(A)")  "* Purpose: generate an event in STDHEP HEPEVT format"
  write (u, "(A)")  "* and write weight to file"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize test process"

  call eio_prepare_test (event)

  call data%init (1)
  data%n_evt = 1
  data%n_beam = 2
  data%pdg_beam = 25
  data%energy_beam = 500
  data%proc_num_id = [42]
  data%cross_section(1) = 100
  data%error(1) = 1
  data%total_cross_section = sum (data%cross_section)

  write (u, "(A)")
  write (u, "(A)")  "* Generate and write an event"
  write (u, "(A)")

  sample = "eio_stdhep_1"

  allocate (eio_stdhep_hepevt_t :: eio)
  select type (eio)
  type is (eio_stdhep_hepevt_t)
    call eio%set_parameters ()
  end select

  call eio%init_out (sample, data)
  call event%generate (1, [0._default, 0._default])
  call event%set_index (61) ! not supported by reader, actually
  call event%evaluate_expressions ()
  call event%pacify_particle_set ()

  call eio%output (event, i_prc = 1)
  call eio%write (u)
  call eio%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Write STDHEP file contents to ASCII file"
  write (u, "(A)")

```

```

call write_stdhep_event &
    (sample // ".hep", var_str ("eio_stdhep_1.hep.out"), 1)

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of STDHEP file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_stdhep_1.hep.out", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat)  buffer
    if (iostat /= 0) exit
    if (trim (buffer) == "") cycle
    if (buffer(1:18) == "    total blocks: ") &
        buffer = "    total blocks: [...]"
    if (buffer(1:25) == "    title: WHIZARD") &
        buffer = "    title: WHIZARD [version]"
    if (buffer(1:17) == "    date:") &
        buffer = "    date: [...]"
    if (buffer(1:17) == "    closing date:") &
        buffer = "    closing date: [...]"
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_stdhep_hepevt_t :: eio)

select type (eio)
type is (eio_stdhep_hepevt_t)
    call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_1"

end subroutine eio_stdhep_1

```

We test the implementation of the STDHEP HEPEUP I/O method:

```

(EIO_stdhep: execute tests)+≡
    call test (eio_stdhep_2, "eio_stdhep_2", &

```

```

        "read and write event contents, format [stdhep]", &
        u, results)

<EIO stdhep: test declarations>+≡
    public :: eio_stdhep_2

<EIO stdhep: tests>+≡
    subroutine eio_stdhep_2 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(model_data_t), pointer :: fallback_model
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(215) :: buffer

        write (u, "(A)")  "* Test output: eio_stdhep_2"
        write (u, "(A)")  "*   Purpose: generate an event in STDHEP HEPEUP format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        allocate (fallback_model)
        call eio_prepare_fallback_model (fallback_model)
        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_stdhep_2"

        allocate (eio_stdhep_hepeup_t :: eio)
        select type (eio)
        type is (eio_stdhep_hepeup_t)
            call eio%set_parameters ()
        end select
        call eio%set_fallback_model (fallback_model)

        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%set_index (62) ! not supported by reader, actually
        call event%evaluate_expressions ()

```

```

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Write STDHEP file contents to ASCII file"
write (u, "(A)")

call write_stdhep_event &
      (sample // ".up.hep", var_str ("eio_stdhep_2.hep.out"), 2)

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of STDHEP file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_stdhep_2.hep.out", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (iostat /= 0) exit
  if (trim (buffer) == "") cycle
  if (buffer(1:18) == "      total blocks: ") &
    buffer = "      total blocks: [...]"
  if (buffer(1:25) == "          title: WHIZARD") &
    buffer = "          title: WHIZARD [version]"
  if (buffer(1:17) == "          date:") &
    buffer = "          date: [...]"
  if (buffer(1:17) == "      closing date:") &
    buffer = "      closing date: [...]"
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_stdhep_hepeup_t :: eio)

select type (eio)
type is (eio_stdhep_hepeup_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_2"

end subroutine eio_stdhep_2

```

Check input from a StdHep file, HEPEVT block.

```

<EIO stdhep: execute tests>+≡
  call test (eio_stdhep_3, "eio_stdhep_3", &
    "read StdHep file, HEPEVT block", &
    u, results)

<EIO stdhep: test declarations>+≡
  public :: eio_stdhep_3

<EIO stdhep: tests>+≡
  subroutine eio_stdhep_3 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: iostat, i_prc

    write (u, "(A)")  "* Test output: eio_stdhep_3"
    write (u, "(A)")  "* Purpose: read a StdHep file, HEPEVT block"
    write (u, "(A)")

    write (u, "(A)")  "* Write a StdHep data file, HEPEVT block"
    write (u, "(A)")

    allocate (fallback_model)
    call eio_prepare_fallback_model (fallback_model)
    call eio_prepare_test (event)

    call data%init (1)
    data%n_evt = 1
    data%n_beam = 2
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    data%cross_section(1) = 100
    data%error(1) = 1
    data%total_cross_section = sum (data%cross_section)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_stdhep_3"

    allocate (eio_stdhep_hepevt_t :: eio)
    select type (eio)
    type is (eio_stdhep_hepevt_t)

```

```

        call eio%set_parameters ()
end select
call eio%set_fallback_model (fallback_model)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (63) ! not supported by reader, actually
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (eio)
deallocate (fallback_model)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_stdhep_hepevt_t :: eio)
select type (eio)
type is (eio_stdhep_hepevt_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

```

```

select type (eio)
type is (eio_stdhep_hepevt_t)
    write (u, "(A,I0,A,I0)") "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)") "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_3"

end subroutine eio_stdhep_3

```

Check input from a StdHep file, HEPEVT block.

```

<EIO stdhep: execute tests>+≡
    call test (eio_stdhep_4, "eio_stdhep_4", &
        "read StdHep file, HEPRUP/HEPEUP block", &
        u, results)

<EIO stdhep: test declarations>+≡
    public :: eio_stdhep_4

<EIO stdhep: tests>+≡
    subroutine eio_stdhep_4 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: iostat, i_prc

        write (u, "(A)")  "* Test output: eio_stdhep_3"
        write (u, "(A)")  "* Purpose: read a StdHep file, HEPRUP/HEPEUP block"
        write (u, "(A)")

        write (u, "(A)")  "* Write a StdHep data file, HEPRUP/HEPEUP block"

```

```

write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event, HEPEUP/HEPRUP"
write (u, "(A)")

sample = "eio_stdhep_4"

allocate (eio_stdhep_hepeup_t :: eio)
select type (eio)
type is (eio_stdhep_hepeup_t)
    call eio%set_parameters ()
end select
call eio%set_fallback_model (fallback_model)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (64)  ! not supported by reader, actually
call event%evaluate_expressions ()
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (eio)
deallocate (fallback_model)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_stdhep_hepeup_t :: eio)
select type (eio)
type is (eio_stdhep_hepeup_t)

```



```

        call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_stdhep_hepeup_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_4"

```

```
end subroutine eio_stdhep_4
```

18.17 HepMC Output

The HepMC event record is standardized. It is an ASCII format. We try our best at using it for both input and output.

```
<eio_hepmc.f90>≡
  <File header>

  module eio_hepmc

    <Use kinds>
    <Use strings>
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base
    use hepmc_interface

    <Standard module head>

    <EIO HepMC: public>

    <EIO HepMC: types>

    interface
    <EIO HepMC: sub interfaces>
    end interface

  end module eio_hepmc

<eio_hepmc_sub.f90>≡
  <File header>

  submodule (eio_hepmc) eio_hepmc_s

    use io_units
    use string_utils
    use diagnostics
    use particles
    use model_data
    use hep_events

    implicit none

  contains

    <EIO HepMC: procedures>

  end submodule eio_hepmc_s
```

18.17.1 Type

A type `hepmc_event` is introduced as container to store HepMC event data, particularly for splitting the reading into read out of the process index and the proper event data.

Note: the `keep_beams` flag is not supported. Beams will always be written. Tools like `Rivet` can use the cross section information of a HepMC file for scaling plots. As there is no header in HepMC and this is written for every event, we make it optional with `output_cross_section`.

```
(EIO HepMC: public)≡
    public :: eio_hepmc_t

(EIO HepMC: types)≡
    type, extends (eio_t) :: eio_hepmc_t
        logical :: writing = .false.
        logical :: reading = .false.
        type(event_sample_data_t) :: data
        ! logical :: keep_beams = .false.
        logical :: recover_beams = .false.
        logical :: use_alphas_from_file = .false.
        logical :: use_scale_from_file = .false.
        logical :: output_cross_section = .false.
        integer :: hepmc3_mode = HEPMC3_MODE_HEPMC3
        logical :: hepmc3_flows = .false.
        type(hepmc_iostream_t) :: iostream
        type(hepmc_event_t) :: hepmc_event
        integer, dimension(:), allocatable :: proc_num_id
    contains
        (EIO HepMC: eio_hepmc: TBP)
    end type eio_hepmc_t
```

18.17.2 Specific Methods

Set parameters that are specifically used with HepMC.

```
(EIO HepMC: eio_hepmc: TBP)≡
    procedure :: set_parameters => eio_hepmc_set_parameters

(EIO HepMC: sub interfaces)≡
    module subroutine eio_hepmc_set_parameters &
        (eio, recover_beams, use_alphas_from_file, &
         use_scale_from_file, extension, output_cross_section, &
         hepmc3_mode, hepmc3_write_flows)
        class(eio_hepmc_t), intent(inout) :: eio
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: use_alphas_from_file
        logical, intent(in), optional :: use_scale_from_file
        logical, intent(in), optional :: output_cross_section
        type(string_t), intent(in), optional :: extension
        integer, intent(in), optional :: hepmc3_mode
        logical, intent(in), optional :: hepmc3_write_flows
    end subroutine eio_hepmc_set_parameters
```

```

(EIO HepMC: procedures)≡
  module subroutine eio_hepmc_set_parameters &
    (eio, recover_beams, use_alphas_from_file, &
     use_scale_from_file, extension, output_cross_section, &
     hepmc3_mode, hepmc3_write_flows)
    class(eio_hepmc_t), intent(inout) :: eio
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file
    logical, intent(in), optional :: use_scale_from_file
    logical, intent(in), optional :: output_cross_section
    type(string_t), intent(in), optional :: extension
    integer, intent(in), optional :: hepmc3_mode
    logical, intent(in), optional :: hepmc3_write_flows
    if (present (recover_beams)) &
      eio%recover_beams = recover_beams
    if (present (use_alphas_from_file)) &
      eio%use_alphas_from_file = use_alphas_from_file
    if (present (use_scale_from_file)) &
      eio%use_scale_from_file = use_scale_from_file
    if (present (extension)) then
      eio%extension = extension
    else
      eio%extension = "hepmc"
    end if
    if (present (output_cross_section)) &
      eio%output_cross_section = output_cross_section
    if (present (hepmc3_mode)) &
      eio%hepmc3_mode = hepmc3_mode
    if (present (hepmc3_write_flows)) &
      eio%hepmc3_flows = hepmc3_write_flows
  end subroutine eio_hepmc_set_parameters

```

18.17.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

(EIO HepMC: eio hepmc: TBP)+≡
  procedure :: write => eio_hepmc_write

(EIO HepMC: sub interfaces)+≡
  module subroutine eio_hepmc_write (object, unit)
    class(eio_hepmc_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine eio_hepmc_write

(EIO HepMC: procedures)+≡
  module subroutine eio_hepmc_write (object, unit)
    class(eio_hepmc_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "HepMC event stream:"
    if (object%writing) then

```

```

        write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
    else if (object%reading) then
        write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
    else
        write (u, "(3x,A)") "[closed]"
    end if
    write (u, "(3x,A,L1)") "Recover beams      = ", object%recover_beams
    write (u, "(3x,A,L1)") "Alpha_s from file = ", &
        object%use_alphas_from_file
    write (u, "(3x,A,L1)") "Scale from file  = ", &
        object%use_scale_from_file
    write (u, "(3x,A,A,A)") "File extension  = '", &
        char (object%extension), "'"
    write (u, "(3x,A,I0)") "HepMC3 mode      = ", object%hepmc3_mode
    write (u, "(3x,A,L1)") "HepMC3 flows     = ", object%hepmc3_flows
    if (allocated (object%proc_num_id)) then
        write (u, "(3x,A)") "Numerical process IDs:"
        do i = 1, size (object%proc_num_id)
            write (u, "(5x,I0,': ',I0)") i, object%proc_num_id(i)
        end do
    end if
end subroutine eio_hepmc_write

```

Finalizer: close any open file.

(EIO HepMC: eio hepmc: TBP)+≡

```

    procedure :: final => eio_hepmc_final

```

(EIO HepMC: sub interfaces)+≡

```

    module subroutine eio_hepmc_final (object)
        class(eio_hepmc_t), intent(inout) :: object
    end subroutine eio_hepmc_final

```

(EIO HepMC: procedures)+≡

```

    module subroutine eio_hepmc_final (object)
        class(eio_hepmc_t), intent(inout) :: object
        if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
        if (object%writing) then
            write (msg_buffer, "(A,A,A)") "Events: closing HepMC file '", &
                char (object%filename), "'"
            call msg_message ()
            call hepmc_iostream_close (object%iostream)
            object%writing = .false.
        else if (object%reading) then
            write (msg_buffer, "(A,A,A)") "Events: closing HepMC file '", &
                char (object%filename), "'"
            call msg_message ()
            call hepmc_iostream_close (object%iostream)
            object%reading = .false.
        end if
    end subroutine eio_hepmc_final

```

Split event file: increment the counter, close the current file, open a new one.
 If the file needs a header, repeat it for the new file.

(EIO HepMC: eio hepmc: TBP)+≡

```

        procedure :: split_out => eio_hepmc_split_out
<EIO HepMC: sub interfaces>+≡
        module subroutine eio_hepmc_split_out (eio)
            class(eio_hepmc_t), intent(inout) :: eio
        end subroutine eio_hepmc_split_out
<EIO HepMC: procedures>+≡
        module subroutine eio_hepmc_split_out (eio)
            class(eio_hepmc_t), intent(inout) :: eio
            if (eio%split) then
                eio%split_index = eio%split_index + 1
                call eio%set_filename ()
                write (msg_buffer, "(A,A,A)") "Events: writing to HepMC file '", &
                    char (eio%filename), "'"
                call msg_message ()
                call hepmc_iostream_close (eio%iostream)
                call hepmc_iostream_open_out (eio%iostream, &
                    eio%filename, eio%hepmc3_mode)
            end if
        end subroutine eio_hepmc_split_out

```

Common initialization for input and output.

```

<EIO HepMC: eio hepmc: TBP>+≡
        procedure :: common_init => eio_hepmc_common_init
<EIO HepMC: sub interfaces>+≡
        module subroutine eio_hepmc_common_init (eio, sample, data, extension)
            class(eio_hepmc_t), intent(inout) :: eio
            type(string_t), intent(in) :: sample
            type(string_t), intent(in), optional :: extension
            type(event_sample_data_t), intent(in), optional :: data
        end subroutine eio_hepmc_common_init
<EIO HepMC: procedures>+≡
        module subroutine eio_hepmc_common_init (eio, sample, data, extension)
            class(eio_hepmc_t), intent(inout) :: eio
            type(string_t), intent(in) :: sample
            type(string_t), intent(in), optional :: extension
            type(event_sample_data_t), intent(in), optional :: data
            if (.not. present (data)) &
                call msg_bug ("HepMC initialization: missing data")
            eio%data = data
            ! We could relax this condition now with weighted hepmc events
            if (data%unweighted) then
                select case (data%norm_mode)
                case (NORM_UNIT)
                case default; call msg_fatal &
                    ("HepMC: normalization for unweighted events must be '1'")
                end select
            end if
            eio%sample = sample
            if (present (extension)) then
                eio%extension = extension
            end if
            call eio%set_filename ()

```

```

        allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
    end subroutine eio_hepmc_common_init

```

Initialize event writing.

```

<EIO HepMC: eio_hepmc: TBP>+≡
    procedure :: init_out => eio_hepmc_init_out

<EIO HepMC: sub interfaces>+≡
    module subroutine eio_hepmc_init_out (eio, sample, data, success, extension)
        class(eio_hepmc_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_hepmc_init_out

<EIO HepMC: procedures>+≡
    module subroutine eio_hepmc_init_out (eio, sample, data, success, extension)
        class(eio_hepmc_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        call eio%set_splitting (data)
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: writing to HepMC file '", &
            char (eio%filename), ""
        call msg_message ()
        eio%writing = .true.
        call hepmc_iostream_open_out (eio%iostream, &
            eio%filename, eio%hepmc3_mode)
        if (present (success)) success = .true.
    end subroutine eio_hepmc_init_out

```

Initialize event reading. For input, we do not (yet) support split event files.

```

<EIO HepMC: eio_hepmc: TBP>+≡
    procedure :: init_in => eio_hepmc_init_in

<EIO HepMC: sub interfaces>+≡
    module subroutine eio_hepmc_init_in (eio, sample, data, success, extension)
        class(eio_hepmc_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_hepmc_init_in

<EIO HepMC: procedures>+≡
    module subroutine eio_hepmc_init_in (eio, sample, data, success, extension)
        class(eio_hepmc_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        logical :: exist

```

```

eio%split = .false.
call eio%common_init (sample, data, extension)
write (msg_buffer, "(A,A,A)") "Events: reading from HepMC file '", &
    char (eio%filename), "'"
call msg_message ()
inquire (file = char (eio%filename), exist = exist)
if (.not. exist) call msg_fatal ("Events: HepMC file not found.")
eio%reading = .true.
call hepmc_iostream_open_in (eio%iostream, &
    eio%filename, eio%hepmc3_mode)
if (present (success)) success = .true.
end subroutine eio_hepmc_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO HepMC: eio_hepmc: TBP>+≡
    procedure :: switch_inout => eio_hepmc_switch_inout

<EIO HepMC: sub interfaces>+≡
    module subroutine eio_hepmc_switch_inout (eio, success)
        class(eio_hepmc_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_hepmc_switch_inout

<EIO HepMC: procedures>+≡
    module subroutine eio_hepmc_switch_inout (eio, success)
        class(eio_hepmc_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("HepMC: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_hepmc_switch_inout

```

Output an event to the allocated HepMC output stream. For the moment, we set `alpha_qed` always to -1. There should be methods for the handling of α in `me_methods` in the same way as for α_s .

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it there (i.e., the enclosed C pointer).

```

<EIO HepMC: eio_hepmc: TBP>+≡
    procedure :: output => eio_hepmc_output

<EIO HepMC: sub interfaces>+≡
    module subroutine eio_hepmc_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_hepmc_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_hepmc_output

<EIO HepMC: procedures>+≡
    module subroutine eio_hepmc_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_hepmc_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc

```



```

logical, intent(in), optional :: reading, passed, pacify
class(event_handle_t), intent(inout), optional :: event_handle
type(particle_set_t), pointer :: pset_ptr
if (present (passed)) then
    if (.not. passed) return
end if
if (eio%writing) then
    pset_ptr => event%get_particle_set_ptr ()
    call hepmc_event_init (eio%hepmc_event, &
        proc_id = eio%proc_num_id(i_prc), &
        event_id = event%get_index ())
    if (eio%output_cross_section .and. eio%data%n_beam == 2) then
        call hepmc_event_from_particle_set (eio%hepmc_event, pset_ptr, &
            eio%data%cross_section(i_prc), eio%data%error(i_prc), &
            color = eio%hepmc3_flows)
    else
        call hepmc_event_from_particle_set (eio%hepmc_event, pset_ptr, &
            color = eio%hepmc3_flows)
    end if
    call hepmc_event_set_scale (eio%hepmc_event, event%get_fac_scale ())
    call hepmc_event_set_alpha_qcd (eio%hepmc_event, event%get_alpha_s ())
    call hepmc_event_set_alpha_qed (eio%hepmc_event, -1._default)
    if (.not. eio%data%unweighted .or. eio%data%negative_weights) then
        select case (eio%data%norm_mode)
        case (NORM_UNIT,NORM_N_EVT)
            call hepmc_event_add_weight &
                (eio%hepmc_event, event%weight_prc, .false.)
        case default
            call hepmc_event_add_weight &
                (eio%hepmc_event, event%weight_prc, .true.)
        end select
    end if
    call hepmc_iostream_write_event (eio%iostream, &
        eio%hepmc_event, eio%hepmc3_mode)
    call maybe_transfer_event_to_handle (eio%hepmc_event, event_handle)
    call hepmc_event_final (eio%hepmc_event)
else
    call eio%write ()
    call msg_fatal ("HepMC file is not open for writing")
end if
end subroutine eio_hepmc_output

```

Input an event.

(EIO HepMC: eio hepmc: TBP)+≡

```

procedure :: input_i_prc => eio_hepmc_input_i_prc
procedure :: input_event => eio_hepmc_input_event

```

(EIO HepMC: sub interfaces)+≡

```

module subroutine eio_hepmc_input_i_prc (eio, i_prc, iostat)
    class(eio_hepmc_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
end subroutine eio_hepmc_input_i_prc
module subroutine eio_hepmc_input_event (eio, event, iostat, event_handle)

```

```

        class(eio_hepmc_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_hepmc_input_event

```

(EIO HepMC: procedures)+≡

```

module subroutine eio_hepmc_input_i_prc (eio, i_prc, iostat)
    class(eio_hepmc_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    logical :: ok
    integer :: i, proc_num_id
    iostat = 0
    call hepmc_event_init (eio%hepmc_event)
    call hepmc_iostream_read_event (eio%iostream, &
        eio%hepmc_event, ok=ok)
    proc_num_id = hepmc_event_get_process_id (eio%hepmc_event)
    if (.not. ok) then
        iostat = -1
        return
    end if
    i_prc = 0
    FIND_I_PRC: do i = 1, size (eio%proc_num_id)
        if (eio%proc_num_id(i) == proc_num_id) then
            i_prc = i
            exit FIND_I_PRC
        end if
    end do FIND_I_PRC
    if (i_prc == 0) call err_index
contains
    subroutine err_index
        call msg_error ("HepMC: reading events: undefined process ID " &
            // char (str (proc_num_id)) // ", aborting read")
        iostat = 1
    end subroutine err_index
end subroutine eio_hepmc_input_i_prc

module subroutine eio_hepmc_input_event (eio, event, iostat, event_handle)
    class(eio_hepmc_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    iostat = 0
    call event%reset_contents ()
    call event%select (1, 1, 1)
    call hepmc_to_event (event, eio%hepmc_event, &
        eio%fallback_model, &
        recover_beams = eio%recover_beams, &
        use_alpha_s = eio%use_alphas_from_file, &
        use_scale = eio%use_scale_from_file)
    call maybe_transfer_event_to_handle (eio%hepmc_event, event_handle)
    call hepmc_event_final (eio%hepmc_event)
end subroutine eio_hepmc_input_event

```

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it to the handle (i.e., the enclosed C pointer). Nullify the original pointer, so the event does not get destroyed.

```

<EIO HepMC: procedures>+≡
  subroutine maybe_transfer_event_to_handle (hepmc_event, event_handle)
    type(hepmc_event_t), intent(inout) :: hepmc_event
    class(event_handle_t), intent(inout), optional :: event_handle
    if (present (event_handle)) then
      select type (event_handle)
      type is (hepmc_event_t)
        call hepmc_event_final (event_handle) ! just in case
        event_handle = hepmc_event
        call hepmc_event_nullify (hepmc_event) ! avoid destructor call
      end select
    end if
  end subroutine maybe_transfer_event_to_handle

```

```

<EIO HepMC: eio hepmc: TBP>+≡
  procedure :: skip => eio_hepmc_skip

```

```

<EIO HepMC: sub interfaces>+≡
  module subroutine eio_hepmc_skip (eio, iostat)
    class(eio_hepmc_t), intent(inout) :: eio
    integer, intent(out) :: iostat
  end subroutine eio_hepmc_skip

```

```

<EIO HepMC: procedures>+≡
  module subroutine eio_hepmc_skip (eio, iostat)
    class(eio_hepmc_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_hepmc_skip

```

18.17.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_hepmc_ut.f90>≡
  <File header>

  module eio_hepmc_ut
    use unit_tests
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE
    use eio_hepmc_util

    <Standard module head>

    <EIO HepMC: public test>

    contains

    <EIO HepMC: test driver>

```

```

    end module eio_hepmc_ut

    <eio_hepmc_util.f90>≡
    <File header>

    module eio_hepmc_util

    <Use kinds>
    <Use strings>
        use system_dependencies, only: HEPMC2_AVAILABLE
        use system_dependencies, only: HEPMC3_AVAILABLE
        use io_units
        use diagnostics
        use model_data
        use event_base
        use eio_data
        use eio_base

        use eio_hepmc

        use eio_base_util, only: eio_prepare_test, eio_cleanup_test
        use eio_base_util, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    <Standard module head>

    <EIO HepMC: test declarations>

    contains

    <EIO HepMC: tests>

    end module eio_hepmc_util
API: driver for the unit tests below.
    <EIO HepMC: public test>≡
        public :: eio_hepmc_test

    <EIO HepMC: test driver>≡
        subroutine eio_hepmc_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO HepMC: execute tests>
        end subroutine eio_hepmc_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

    <EIO HepMC: execute tests>≡
        if (HEPMC2_AVAILABLE) then
            call test (eio_hepmc_1, "eio_hepmc2_1", &
                "write event contents", &
                u, results)
        else if (HEPMC3_AVAILABLE) then

```

```

        call test (eio_hepmc_1, "eio_hepmc3_1", &
            "write event contents", &
            u, results)
    end if
<EIO HepMC: test declarations>≡
    public :: eio_hepmc_1
<EIO HepMC: tests>≡
    subroutine eio_hepmc_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(116) :: buffer

        write (u, "(A)")  "* Test output: eio_hepmc_1"
        write (u, "(A)")  "* Purpose: write a HepMC file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted=.false.)

        call data%init (1)
        data%n_beam = 2
        data%unweighted = .true.
        data%norm_mode = NORM_UNIT
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_hepmc_1"

        allocate (eio_hepmc_t :: eio)
        select type (eio)
        type is (eio_hepmc_t)
            call eio%set_parameters ()
        end select

        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%set_index (55)

        call eio%output (event, i_prc = 1)
        call eio%write (u)

```

```

call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents (blanking out last two digits):"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepmc"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0) exit
  if (trim (buffer) == "") cycle
  if (buffer(1:14) == "HepMC::Version") cycle
  if (HEPMC2_AVAILABLE) then
    if (buffer(1:10) == "P 10001 25") &
      call buffer_blanker (buffer, 32, 55, 78)
    if (buffer(1:10) == "P 10002 25") &
      call buffer_blanker (buffer, 33, 56, 79)
    if (buffer(1:10) == "P 10003 25") &
      call buffer_blanker (buffer, 29, 53, 78, 101)
    if (buffer(1:10) == "P 10004 25") &
      call buffer_blanker (buffer, 28, 51, 76, 99)
  else if (HEPMC3_AVAILABLE) then
    if (buffer(1:8) == "P 1 0 25") &
      call buffer_blanker (buffer, 26, 49, 72)
    if (buffer(1:8) == "P 2 0 25") &
      call buffer_blanker (buffer, 26, 49, 73)
    if (buffer(1:9) == "P 3 -1 25") &
      call buffer_blanker (buffer, 28, 52, 75)
    if (buffer(1:9) == "P 4 -1 25") &
      call buffer_blanker (buffer, 27, 50, 73)
  end if
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_hepmc_t :: eio)

select type (eio)
type is (eio_hepmc_t)
  call eio%set_parameters ()
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_hepmc_1"

contains

subroutine buffer_blanker (buf, pos1, pos2, pos3, pos4)
  character(len=*), intent(inout) :: buf
  integer, intent(in) :: pos1, pos2, pos3
  integer, intent(in), optional :: pos4
  type(string_t) :: line
  line = var_str (trim (buf))
  line = replace (line, pos1, "XX")
  line = replace (line, pos2, "XX")
  line = replace (line, pos3, "XX")
  if (present (pos4)) then
    line = replace (line, pos4, "XX")
  end if
  line = replace (line, "4999999999999", "5000000000000")
  buf = char (line)
end subroutine buffer_blanker

end subroutine eio_hepmc_1

```

Test also the reading of HepMC events.

```

<EIO HepMC: execute tests>+≡
  if (HEPMC2_AVAILABLE) then
    call test (eio_hepmc_2, "eio_hepmc2_2", &
      "read event contents", &
      u, results)
  else if (HEPMC3_AVAILABLE) then
    call test (eio_hepmc_2, "eio_hepmc3_2", &
      "read event contents", &
      u, results)
  end if

<EIO HepMC: test declarations>+≡
  public :: eio_hepmc_2

<EIO HepMC: tests>+≡
  subroutine eio_hepmc_2 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat, i_prc

    write (u, "(A)")  "* Test output: eio_hepmc_2"
    write (u, "(A)")  "* Purpose: read a HepMC event"
    write (u, "(A)")

    write (u, "(A)")  "* Write a HepMC data file"
    write (u, "(A)")

```

```

u_file = free_unit ()
sample = "eio_hepmc_2"
open (u_file, file = char (sample // ".hepmc"), &
      status = "replace", action = "readwrite")

if (HEPMC2_AVAILABLE) then
  write (u_file, "(A)") "HepMC::Version 2.06.09"
  write (u_file, "(A)") "HepMC::IO_GenEvent-START_EVENT_LISTING"
  write (u_file, "(A)") "E 66 -1 -1.0000000000000000e+00 &
    &-1.0000000000000000e+00 &
    &-1.0000000000000000e+00 42 0 1 10001 10002 0 0"
  write (u_file, "(A)") "U GEV MM"
  write (u_file, "(A)") "V -1 0 0 0 0 0 2 2 0"
  write (u_file, "(A)") "P 10001 25 0 0 4.8412291827592713e+02 &
    &5.0000000000000000e+02 &
    &1.2499999999999999e+02 3 0 0 -1 0"
  write (u_file, "(A)") "P 10002 25 0 0 -4.8412291827592713e+02 &
    &5.0000000000000000e+02 &
    &1.2499999999999999e+02 3 0 0 -1 0"
  write (u_file, "(A)") "P 10003 25 -1.4960220911365536e+02 &
    &-4.6042825611414656e+02 &
    &0 5.0000000000000000e+02 1.2500000000000000e+02 1 0 0 0 0"
  write (u_file, "(A)") "P 10004 25 1.4960220911365536e+02 &
    &4.6042825611414656e+02 &
    &0 5.0000000000000000e+02 1.2500000000000000e+02 1 0 0 0 0"
  write (u_file, "(A)") "HepMC::IO_GenEvent-END_EVENT_LISTING"
else if (HEPMC3_AVAILABLE) then
  write (u_file, "(A)") "HepMC::Version 3.01.01"
  write (u_file, "(A)") "HepMC::Ascii3-START_EVENT_LISTING"
  write (u_file, "(A)") "E 55 1 4"
  write (u_file, "(A)") "U GEV MM"
  write (u_file, "(A)") "A 0 alphaQCD -1"
  write (u_file, "(A)") "A 0 event_scale 1000"
  write (u_file, "(A)") "A 0 signal_process_id 42"
  write (u_file, "(A)") "P 1 0 25 0.0000000000000000e+00 &
    &0.0000000000000000e+00 4.8412291827592713e+02 &
    &5.0000000000000000e+02 1.2499999999999999e+02 3"
  write (u_file, "(A)") "P 2 0 25 0.0000000000000000e+00 &
    &0.0000000000000000e+00 -4.8412291827592713e+02 &
    &5.0000000000000000e+02 1.2499999999999999e+02 3"
  write (u_file, "(A)") "V -1 0 [1,2]"
  write (u_file, "(A)") "P 3 -1 25 -1.4960220911365536e+02 &
    &-4.6042825611414656e+02 0.0000000000000000e+00 &
    &5.0000000000000000e+02 1.2500000000000000e+02 1"
  write (u_file, "(A)") "P 4 -1 25 1.4960220911365536e+02 &
    &4.6042825611414656e+02 0.0000000000000000e+00 &
    &5.0000000000000000e+02 1.2500000000000000e+02 1"
  write (u_file, "(A)") "HepMC::Ascii3-END_EVENT_LISTING"
else
  call msg_fatal &
    ("Trying to execute eio_hepmc unit tests without a linked HepMC")
end if
close (u_file)

```



```

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted=.false.)

allocate (eio_hepmc_t :: eio)
select type (eio)
type is (eio_hepmc_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_hepmc_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_hepmc_2"

end subroutine eio_hepmc_2

```

Test also the correct normalization of weighted HepMC events.

```

<EIO HepMC: execute tests>+≡
  if (HEPMC2_AVAILABLE) then
    call test (eio_hepmc_3, "eio_hepmc2_3", &
      "write event contents", &
      u, results)
  else if (HEPMC3_AVAILABLE) then
    call test (eio_hepmc_3, "eio_hepmc3_3", &
      "event contents weighted, '1' normalization", &
      u, results)
  end if

<EIO HepMC: test declarations>+≡
  public :: eio_hepmc_3

<EIO HepMC: tests>+≡
  subroutine eio_hepmc_3 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(126) :: buffer

    write (u, "(A)")  "* Test output: eio_hepmc_3"
    write (u, "(A)")  "* Purpose: test correct HepMC normalization"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted=.false., &
      sample_norm = var_str ("1"))

    call data%init (1)
    data%n_beam = 2
    data%unweighted = .false.
    data%norm_mode = NORM_UNIT
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]

```

```

data%cross_section(1) = 20
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_hepmc_3"

allocate (eio_hepmc_t :: eio)
select type (eio)
type is (eio_hepmc_t)
    call eio%set_parameters ()
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (55)

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents (blanking out last two digits):"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepmc"), &
      action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat)  buffer
    if (iostat /= 0) exit
    if (trim (buffer) == "") cycle
    if (buffer(1:14) == "HepMC::Version") cycle
    if (HEPMC2_AVAILABLE) then
        if (buffer(1:4) == "E 55") then
            buffer = replace (buffer, 113, "XXXXXXXX")
        end if
        if (buffer(1:10) == "P 10001 25") &
            call buffer_blanker (buffer, 32, 55, 78)
        if (buffer(1:10) == "P 10002 25") &
            call buffer_blanker (buffer, 33, 56, 79)
        if (buffer(1:10) == "P 10003 25") &
            call buffer_blanker (buffer, 29, 53, 78, 101)
        if (buffer(1:10) == "P 10004 25") &
            call buffer_blanker (buffer, 28, 51, 76, 99)
    else if (HEPMC3_AVAILABLE) then
        if (buffer(1:4) == "W 3.") then
            buffer = replace (buffer, 11, "XXXXXXXXXXXXXXXXXX")
        end if
        if (buffer(1:8) == "P 1 0 25") &
            call buffer_blanker (buffer, 26, 49, 72, 118)
    end if
end do

```

```

        if (buffer(1:8) == "P 2 0 25") &
            call buffer_blanker (buffer, 26, 49, 73, 119)
        if (buffer(1:9) == "P 3 -1 25") &
            call buffer_blanker (buffer, 28, 52, 75, 121)
        if (buffer(1:9) == "P 4 -1 25") &
            call buffer_blanker (buffer, 27, 50, 73, 119)
        end if
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Reset data"
    write (u, "(A)")

    deallocate (eio)
    allocate (eio_hepmc_t :: eio)

    select type (eio)
    type is (eio_hepmc_t)
        call eio%set_parameters ()
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_hepmc_3"

contains

    subroutine buffer_blanker (buf, pos1, pos2, pos3, pos4)
        character(len=*) , intent(inout) :: buf
        integer, intent(in) :: pos1, pos2, pos3
        integer, intent(in), optional :: pos4
        type(string_t) :: line
        line = var_str (trim (buf))
        line = replace (line, pos1, "XX")
        line = replace (line, pos2, "XX")
        line = replace (line, pos3, "XX")
        if (present (pos4)) then
            line = replace (line, pos4, "XX")
        end if
        line = replace (line, "4999999999999", "5000000000000")
        buf = char (line)
    end subroutine buffer_blanker

end subroutine eio_hepmc_3

```

18.18 LCIO Output

The LCIO event record is standardized for the use with Linear e^+e^- colliders. It is a binary event format. We try our best at using it for both input and output.

```
<eio_lcio.f90>≡  
  <File header>  
  
  module eio_lcio  
  
    <Use kinds>  
    <Use strings>  
    use event_base  
    use event_handles, only: event_handle_t  
    use eio_data  
    use eio_base  
    use lcio_interface  
  
    <Standard module head>  
  
    <EIO LCIO: public>  
  
    <EIO LCIO: types>  
  
    interface  
    <EIO LCIO: sub interfaces>  
    end interface  
  
  end module eio_lcio  
  
<eio_lcio_sub.f90>≡  
  <File header>  
  
  submodule (eio_lcio) eio_lcio_s  
  
    use io_units  
    use string_utils  
    use diagnostics  
    use particles  
    use hep_events  
  
    implicit none  
  
    contains  
  
    <EIO LCIO: procedures>  
  
  end submodule eio_lcio_s
```

18.18.1 Type

A type `lcio_event` is introduced as container to store LCIO event data, particularly for splitting the reading into read out of the process index and the proper

event data.

Note: the `keep_beams` flag is not supported.

```
<EIO LCIO: public>≡
  public :: eio_lcio_t

<EIO LCIO: types>≡
  type, extends (eio_t) :: eio_lcio_t
    logical :: writing = .false.
    logical :: reading = .false.
    type(event_sample_data_t) :: data
    logical :: recover_beams = .false.
    logical :: use_alphas_from_file = .false.
    logical :: use_scale_from_file = .false.
    logical :: proc_as_run_id = .true.
    integer :: n_alt = 0
    integer :: lcio_run_id = 0
    type(lcio_writer_t) :: lcio_writer
    type(lcio_reader_t) :: lcio_reader
    type(lcio_run_header_t) :: lcio_run_hdr
    type(lcio_event_t) :: lcio_event
    integer, dimension(:), allocatable :: proc_num_id
  contains
    <EIO LCIO: eio lcio: TBP>
  end type eio_lcio_t
```

18.18.2 Specific Methods

Set parameters that are specifically used with LCIO.

```
<EIO LCIO: eio lcio: TBP>≡
  procedure :: set_parameters => eio_lcio_set_parameters

<EIO LCIO: sub interfaces>≡
  module subroutine eio_lcio_set_parameters &
    (eio, recover_beams, use_alphas_from_file, use_scale_from_file, &
     extension, proc_as_run_id, lcio_run_id)
    class(eio_lcio_t), intent(inout) :: eio
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file
    logical, intent(in), optional :: use_scale_from_file
    logical, intent(in), optional :: proc_as_run_id
    integer, intent(in), optional :: lcio_run_id
    type(string_t), intent(in), optional :: extension
  end subroutine eio_lcio_set_parameters

<EIO LCIO: procedures>≡
  module subroutine eio_lcio_set_parameters &
    (eio, recover_beams, use_alphas_from_file, use_scale_from_file, &
     extension, proc_as_run_id, lcio_run_id)
    class(eio_lcio_t), intent(inout) :: eio
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file
    logical, intent(in), optional :: use_scale_from_file
    logical, intent(in), optional :: proc_as_run_id
    integer, intent(in), optional :: lcio_run_id
```

```

type(string_t), intent(in), optional :: extension
if (present (recover_beams)) eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (proc_as_run_id)) &
    eio%proc_as_run_id = proc_as_run_id
if (present (lcio_run_id)) &
    eio%lcio_run_id = lcio_run_id
if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "slcio"
end if
end subroutine eio_lcio_set_parameters

```

18.18.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: write => eio_lcio_write

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_write (object, unit)
        class(eio_lcio_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_lcio_write

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_write (object, unit)
        class(eio_lcio_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "LCIO event stream:"
        if (object%writing) then
            write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
        else if (object%reading) then
            write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
        else
            write (u, "(3x,A)") "[closed]"
        end if
        write (u, "(3x,A,L1)") "Recover beams      = ", object%recover_beams
        write (u, "(3x,A,L1)") "Alpha_s from file = ", &
            object%use_alphas_from_file
        write (u, "(3x,A,L1)") "Scale from file  = ", &
            object%use_scale_from_file
        write (u, "(3x,A,L1)") "Process as run ID = ", &
            object%proc_as_run_id
        write (u, "(3x,A,I0)") "LCIO run ID      = ", &
            object%lcio_run_id
    end subroutine eio_lcio_write

```

```

write (u, "(3x,A,A,A)")      "File extension    = '", &
char (object%extension), ""
if (allocated (object%proc_num_id)) then
write (u, "(3x,A)")  "Numerical process IDs:"
do i = 1, size (object%proc_num_id)
write (u, "(5x,I0,': ',I0)")  i, object%proc_num_id(i)
end do
end if
end subroutine eio_lcio_write

```

Finalizer: close any open file.

```

<EIO LCIO: eio_lcio: TBP>+≡
  procedure :: final => eio_lcio_final

<EIO LCIO: sub interfaces>+≡
  module subroutine eio_lcio_final (object)
    class(eio_lcio_t), intent(inout) :: object
    end subroutine eio_lcio_final

<EIO LCIO: procedures>+≡
  module subroutine eio_lcio_final (object)
    class(eio_lcio_t), intent(inout) :: object
    if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
    if (object%writing) then
      write (msg_buffer, "(A,A,A)") "Events: closing LCIO file '", &
char (object%filename), ""
      call msg_message ()
      call lcio_writer_close (object%lcio_writer)
      object%writing = .false.
    else if (object%reading) then
      write (msg_buffer, "(A,A,A)") "Events: closing LCIO file '", &
char (object%filename), ""
      call msg_message ()
      call lcio_reader_close (object%lcio_reader)
      object%reading = .false.
    end if
  end subroutine eio_lcio_final

```

Split event file: increment the counter, close the current file, open a new one.
If the file needs a header, repeat it for the new file.

```

<EIO LCIO: eio_lcio: TBP>+≡
  procedure :: split_out => eio_lcio_split_out

<EIO LCIO: sub interfaces>+≡
  module subroutine eio_lcio_split_out (eio)
    class(eio_lcio_t), intent(inout) :: eio
    end subroutine eio_lcio_split_out

<EIO LCIO: procedures>+≡
  module subroutine eio_lcio_split_out (eio)
    class(eio_lcio_t), intent(inout) :: eio
    if (eio%split) then
      eio%split_index = eio%split_index + 1
      call eio%set_filename ()
      write (msg_buffer, "(A,A,A)") "Events: writing to LCIO file '", &

```



```

        char (eio%filename), "'")
    call msg_message ()
    call lcio_writer_close (eio%lcio_writer)
    call lcio_writer_open_out (eio%lcio_writer, eio%filename)
end if
end subroutine eio_lcio_split_out

```

Common initialization for input and output.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: common_init => eio_lcio_common_init

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_common_init (eio, sample, data, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
    end subroutine eio_lcio_common_init

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_common_init (eio, sample, data, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        if (.not. present (data)) &
            call msg_bug ("LCIO initialization: missing data")
        eio%data = data
        if (data%unweighted) then
            select case (data%norm_mode)
            case (NORM_UNIT)
            case default; call msg_fatal &
                ("LCIO: normalization for unweighted events must be '1'")
            end select
        else
            call msg_fatal ("LCIO: events must be unweighted")
        end if
        eio%n_alt = data%n_alt
        eio%sample = sample
        if (present (extension)) then
            eio%extension = extension
        end if
        call eio%set_filename ()
        allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
    end subroutine eio_lcio_common_init

```

Initialize event writing.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: init_out => eio_lcio_init_out

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_init_out &
        (eio, sample, data, success, extension)
        class(eio_lcio_t), intent(inout) :: eio

```

```

        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_lcio_init_out

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_init_out &
        (eio, sample, data, success, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        call eio%set_splitting (data)
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: writing to LCIO file '", &
            char (eio%filename), ""
        call msg_message ()
        eio%writing = .true.
        call lcio_writer_open_out (eio%lcio_writer, eio%filename)
        call lcio_run_header_init (eio%lcio_run_hdr)
        call lcio_run_header_write (eio%lcio_writer, eio%lcio_run_hdr)
        if (present (success)) success = .true.
    end subroutine eio_lcio_init_out

```

Initialize event reading. For input, we do not (yet) support split event files.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: init_in => eio_lcio_init_in

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_init_in (eio, sample, data, success, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
    end subroutine eio_lcio_init_in

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_init_in (eio, sample, data, success, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        logical :: exist
        eio%split = .false.
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: reading from LCIO file '", &
            char (eio%filename), ""
        call msg_message ()
        inquire (file = char (eio%filename), exist = exist)
        if (.not. exist) call msg_fatal ("Events: LCIO file not found.")
        eio%reading = .true.
    end subroutine eio_lcio_init_in

```

```

    call lcio_open_file (eio%lcio_reader, eio%filename)
    if (present (success)) success = .true.
end subroutine eio_lcio_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: switch_inout => eio_lcio_switch_inout

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_switch_inout (eio, success)
        class(eio_lcio_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_lcio_switch_inout

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_switch_inout (eio, success)
        class(eio_lcio_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("LCIO: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_lcio_switch_inout

```

Output an event to the allocated LCIO writer.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: output => eio_lcio_output

<EIO LCIO: sub interfaces>+≡
    module subroutine eio_lcio_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_lcio_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_lcio_output

<EIO LCIO: procedures>+≡
    module subroutine eio_lcio_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_lcio_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        type(particle_set_t), pointer :: pset_ptr
        real(default) :: sqme_prc, weight
        real(default), dimension(:), allocatable :: pol
        integer :: i
        if (present (passed)) then
            if (.not. passed) return
        end if
        if (eio%writing) then
            pset_ptr => event%get_particle_set_ptr ()
            if (eio%proc_as_run_id) then
                call lcio_event_init (eio%lcio_event, &

```

```

        proc_id = eio%proc_num_id (i_prc), &
        event_id = event%get_index (), &
        run_id = eio%proc_num_id (i_prc))
    else
        call lcio_event_init (eio%lcio_event, &
            proc_id = eio%proc_num_id (i_prc), &
            event_id = event%get_index (), &
            run_id = eio%lcio_run_id)
    end if
    call lcio_event_from_particle_set (eio%lcio_event, pset_ptr)
    call lcio_event_set_weight (eio%lcio_event, event%weight_prc)
    call lcio_event_set_sqrts (eio%lcio_event, event%get_sqrts ())
    call lcio_event_set_sqme (eio%lcio_event, event%get_sqme_prc ())
    call lcio_event_set_scale (eio%lcio_event, event%get_fac_scale ())
    call lcio_event_set_alpha_qcd (eio%lcio_event, event%get_alpha_s ())
    if (eio%data%n_beam == 2) then
        call lcio_event_set_xsec (eio%lcio_event, eio%data%cross_section(i_prc), &
            eio%data%error(i_prc))
    end if
    pol = event%get_polarization ()
    do i = 1, eio%data%n_beam
        call lcio_event_set_polarization (eio%lcio_event, pol(i), i)
    end do
    call lcio_event_set_beam_file (eio%lcio_event, &
        event%get_beam_file ())
    call lcio_event_set_process_name (eio%lcio_event, &
        event%get_process_name ())
    do i = 1, eio%n_alt
        sqme_prc = event%get_sqme_alt(i)
        weight = event%get_weight_alt(i)
        call lcio_event_set_alt_sqme (eio%lcio_event, sqme_prc, i)
        call lcio_event_set_alt_weight (eio%lcio_event, weight, i)
    end do
    call lcio_event_write (eio%lcio_writer, eio%lcio_event)
    call maybe_transfer_event_to_handle (eio%lcio_event, &
        event_handle, .true.)
    call lcio_event_final (eio%lcio_event, .true.)
else
    call eio%write ()
    call msg_fatal ("LCIO file is not open for writing")
end if
end subroutine eio_lcio_output

```

Input an event.

[WK 22-04-21] We do no longer fix the `i_mci` and `i_term` indices to 1, this can now be done by `simulation_recalculate`.

<EIO LCIO: eio lcio: TBP>+≡

```

    procedure :: input_i_prc => eio_lcio_input_i_prc
    procedure :: input_event => eio_lcio_input_event

```

<EIO LCIO: sub interfaces>+≡

```

    module subroutine eio_lcio_input_i_prc (eio, i_prc, iostat)
    class(eio_lcio_t), intent(inout) :: eio
    integer, intent(out) :: i_prc

```

```

        integer, intent(out) :: iostat
    end subroutine eio_lcio_input_i_prc
    module subroutine eio_lcio_input_event (eio, event, iostat, event_handle)
        class(eio_lcio_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_lcio_input_event

    (EIO LCIO: procedures)+≡
    module subroutine eio_lcio_input_i_prc (eio, i_prc, iostat)
        class(eio_lcio_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        logical :: ok
        integer :: i, proc_num_id
        iostat = 0
        call lcio_read_event (eio%lcio_reader, eio%lcio_event, ok)
        if (.not. ok) then
            iostat = -1
            return
        end if
        proc_num_id = lcio_event_get_process_id (eio%lcio_event)
        i_prc = 0
        FIND_I_PRC: do i = 1, size (eio%proc_num_id)
            if (eio%proc_num_id(i) == proc_num_id) then
                i_prc = i
                exit FIND_I_PRC
            end if
        end do FIND_I_PRC
        if (i_prc == 0) call err_index
contains
        subroutine err_index
            call msg_error ("LCIO: reading events: undefined process ID " &
                // char (str (proc_num_id)) // ", aborting read")
            iostat = 1
        end subroutine err_index
    end subroutine eio_lcio_input_i_prc

    module subroutine eio_lcio_input_event (eio, event, iostat, event_handle)
        class(eio_lcio_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        iostat = 0
        call event%reset_contents ()
        call event%select (0, 0, 1)
        call event%set_index (lcio_event_get_event_index (eio%lcio_event))
        call lcio_to_event (event, eio%lcio_event, eio%fallback_model, &
            recover_beams = eio%recover_beams, &
            use_alpha_s = eio%use_alphas_from_file, &
            use_scale = eio%use_scale_from_file)
        call maybe_transfer_event_to_handle (eio%lcio_event, &
            event_handle, .false.)
        call lcio_event_final (eio%lcio_event, .false.)

```

```
end subroutine eio_lcio_input_event
```

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it to the handle (i.e., the enclosed C pointer). Nullify the original pointer, so the event does not get destroyed.

```
<EIO LCIO: procedures>+≡
subroutine maybe_transfer_event_to_handle (lcio_event, event_handle, delete)
  type(lcio_event_t), intent(inout) :: lcio_event
  class(event_handle_t), intent(inout), optional :: event_handle
  logical, intent(in) :: delete
  if (present (event_handle)) then
    select type (event_handle)
    type is (lcio_event_t)
      call lcio_event_final (event_handle, delete) ! just in case
      event_handle = lcio_event
      call lcio_event_nullify (lcio_event) ! avoid destructor call
    end select
  end if
end subroutine maybe_transfer_event_to_handle
```

```
<EIO LCIO: eio lcio: TBP>+≡
procedure :: skip => eio_lcio_skip
```

```
<EIO LCIO: sub interfaces>+≡
module subroutine eio_lcio_skip (eio, iostat)
  class(eio_lcio_t), intent(inout) :: eio
  integer, intent(out) :: iostat
end subroutine eio_lcio_skip
```

```
<EIO LCIO: procedures>+≡
module subroutine eio_lcio_skip (eio, iostat)
  class(eio_lcio_t), intent(inout) :: eio
  integer, intent(out) :: iostat
  iostat = 0
end subroutine eio_lcio_skip
```

18.18.4 Unit tests

Test module, followed by the corresponding implementation module.

```
<eio_lcio_ut.f90>≡
<File header>

module eio_lcio_ut
  use unit_tests
  use eio_lcio_utl

  <Standard module head>

  <EIO LCIO: public test>

contains
```

```

    <EIO LCIO: test driver>

    end module eio_lcio_ut

    <eio_lcio_uti.f90>≡
    <File header>

    module eio_lcio_uti

    <Use kinds>
    <Use strings>
        use io_units
        use model_data
        use particles
        use event_base
        use eio_data
        use eio_base
        use hep_events
        use lcio_interface

        use eio_lcio

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
        use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    <Standard module head>

    <EIO LCIO: test declarations>

    contains

    <EIO LCIO: tests>

    end module eio_lcio_uti
API: driver for the unit tests below.
    <EIO LCIO: public test>≡
        public :: eio_lcio_test
    <EIO LCIO: test driver>≡
        subroutine eio_lcio_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO LCIO: execute tests>
        end subroutine eio_lcio_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

    <EIO LCIO: execute tests>≡
        call test (eio_lcio_1, "eio_lcio_1", &
            "write event contents", &
            u, results)

```

```

<EIO LCIO: test declarations>≡
    public :: eio_lcio_1

<EIO LCIO: tests>≡
    subroutine eio_lcio_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(particle_set_t), pointer :: pset_ptr
        type(string_t) :: sample
        integer :: u_file, iostat
        character(215) :: buffer

        write (u, "(A)")  "* Test output: eio_lcio_1"
        write (u, "(A)")  "* Purpose: write a LCIO file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event)

        call data%init (1)
        data%n_beam = 2
        data%unweighted = .true.
        data%norm_mode = NORM_UNIT
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_lcio_1"

        allocate (eio_lcio_t :: eio)
        select type (eio)
        type is (eio_lcio_t)
            call eio%set_parameters ()
        end select

        call eio%init_out (sample, data)

        call event%generate (1, [0._default, 0._default])
        call event%set_index (77)
        call event%pacify_particle_set ()

        call eio%output (event, i_prc = 1)
        call eio%write (u)
        call eio%final ()
    end subroutine eio_lcio_1

```



```

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_lcio_t :: eio)

select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters ()
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write LCIO file contents to ASCII file"
write (u, "(A)")

select type (eio)
type is (eio_lcio_t)
    call lcio_event_init (eio%lcio_event, &
        proc_id = 42, &
        event_id = event%get_index ())
    pset_ptr => event%get_particle_set_ptr ()
    call lcio_event_from_particle_set &
        (eio%lcio_event, pset_ptr)
    call write_lcio_event (eio%lcio_event, var_str ("test_file.slcio"))
    call lcio_event_final (eio%lcio_event, .true.)
end select

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of LCIO file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "test_file.slcio", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (iostat /= 0) exit
    if (trim (buffer) == "") cycle
    if (buffer(1:12) == " - timestamp") cycle
    if (buffer(1:6) == " date:") cycle
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lcio_1"

```

```
end subroutine eio_lcio_1
```

Test also the reading of LCIO events.

```
<EIO LCIO: execute tests>+≡
  call test (eio_lcio_2, "eio_lcio_2", &
    "read event contents", &
    u, results)

<EIO LCIO: test declarations>+≡
  public :: eio_lcio_2

<EIO LCIO: tests>+≡
  subroutine eio_lcio_2 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: iostat, i_prc

    write (u, "(A)")  "* Test output: eio_lcio_2"
    write (u, "(A)")  "* Purpose: read a LCIO event"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    allocate (fallback_model)
    call eio_prepare_fallback_model (fallback_model)
    call eio_prepare_test (event)

    call data%init (1)
    data%n_beam = 2
    data%unweighted = .true.
    data%norm_mode = NORM_UNIT
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    data%cross_section(1) = 100
    data%error(1) = 1
    data%total_cross_section = sum (data%cross_section)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_lcio_2"

    allocate (eio_lcio_t :: eio)
    select type (eio)
    type is (eio_lcio_t)
      call eio%set_parameters (recover_beams = .false.)
    end select
    call eio%set_fallback_model (fallback_model)
```

```

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (88)
call event%evaluate_expressions ()
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()
deallocate (eio)

call event%reset_contents ()
call event%reset_index ()

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

allocate (eio_lcio_t :: eio)
select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lcio_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

```

```

call event%select (1, 1, 1)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,IO)") "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lcio_2"

end subroutine eio_lcio_2

```

Chapter 19

Phase Space

The abstract representation of a type that parameterizes phase space, with methods for construction and evaluation.

phs_base Abstract phase-space representation.

A simple implementation:

phs_none This implements a non-functional dummy module for the phase space. A process which uses this module cannot be integrated. The purpose of this module is to provide a placeholder for processes which do not require phase-space evaluation. They may still allow for evaluating matrix elements.

phs_single Parameterize the phase space of a single particle, i.e., the solid angle. This is useful only for very restricted problems, but it avoids the complexity of a generic approach in those trivial cases.

The standard implementation is called *wood* phase space. It consists of several auxiliary modules and the actual implementation module.

mappings Generate invariant masses and decay angles from given random numbers (or the inverse operation). Each mapping pertains to a particular node in a phase-space tree. Different mappings account for uniform distributions, resonances, zero-mass behavior, and so on.

phs_trees Phase space parameterizations for scattering processes are defined recursively as if there was an initial particle decaying. This module sets up a representation in terms of abstract trees, where each node gets a unique binary number. Each tree is stored as an array of branches, where integers indicate the connections. This emulates pointers in a transparent way. Real pointers would also be possible, but seem to be less efficient for this particular case.

phs_forests The type defined by this module collects the decay trees corresponding to a given process and the applicable mappings. To set this up, a file is read which is either written by the user or by the **cascades** module functions. The module also contains the routines that evaluate phase space, i.e., generate momenta from random numbers and back.

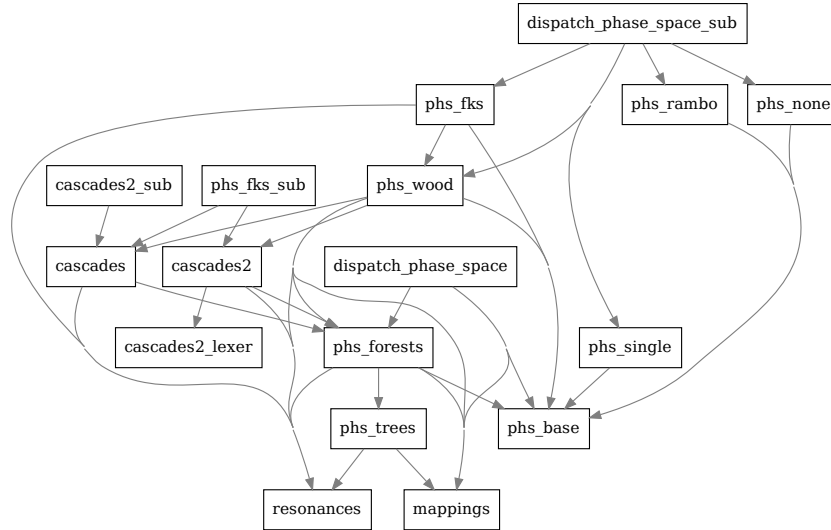


Figure 19.1: Module dependencies in `src/phase_space`.

cascades This module is a pseudo Feynman diagram generator with the particular purpose of finding the phase space parameterizations best suited for a given process. It uses a model file to set up the possible vertices, generates all possible diagrams, identifies resonances and singularities, and simplifies the list by merging equivalent diagrams and dropping irrelevant ones. This process can be controlled at several points by user-defined parameters. Note that it depends on the particular values of particle masses, so it cannot be done before reading the input file.

phs_wood Make the functionality available in form of an implementation of the abstract phase-space type.

phs_fks Phase-space parameterization with modifications for the FKS scheme.

19.1 Abstract phase-space module

In this module we define an abstract base type (and a trivial test implementation) for multi-channel phase-space parameterizations.

```
<phs_base.f90>≡  
  <File header>  
  
  module phs_base  
  
    <Use kinds>  
    <Use strings>  
    use lorentz  
    use model_data  
    use flavors  
    use process_constants  
  
    <Standard module head>  
  
    <PHS base: public>  
  
    <PHS base: types>  
  
    <PHS base: interfaces>  
  
    interface  
    <PHS base: sub interfaces>  
    end interface  
  
    contains  
  
    <PHS base: main procedures>  
  
  end module phs_base  
<phs_base_sub.f90>≡  
  <File header>  
  
  submodule (phs_base) phs_base_s  
  
    use io_units  
    use constants, only: TWOPI, TWOPI4  
    use string_utils, only: split_string  
    use format_defs, only: FMT_19  
    use numeric_utils  
    use diagnostics  
    use md5  
    use physics_defs  
  
    implicit none  
  
  contains  
  
  <PHS base: procedures>
```

```
end submodule phs_base_s
```

19.1.1 Phase-space channels

The kinematics configuration may generate multiple parameterizations of phase space. Some of those have specific properties, such as a resonance in the s channel.

Channel properties

This is the abstract type for the channel properties. We need them as a data transfer container, so everything is public and transparent.

```
⟨PHS base: public⟩≡
  public :: channel_prop_t

⟨PHS base: types⟩≡
  type, abstract :: channel_prop_t
  contains
    procedure (channel_prop_to_string), deferred :: to_string
    generic :: operator (==) => is_equal
    procedure (channel_eq), deferred :: is_equal
  end type channel_prop_t

⟨PHS base: interfaces⟩≡
  abstract interface
    function channel_prop_to_string (object) result (string)
      import
      class(channel_prop_t), intent(in) :: object
      type(string_t) :: string
    end function channel_prop_to_string
  end interface

⟨PHS base: interfaces⟩+≡
  abstract interface
    function channel_eq (prop1, prop2) result (flag)
      import
      class(channel_prop_t), intent(in) :: prop1, prop2
      logical :: flag
    end function channel_eq
  end interface
```

Here is a resonance as a channel property. Mass and width are stored here in physical units.

```
⟨PHS base: public⟩+≡
  public :: resonance_t

⟨PHS base: types⟩+≡
  type, extends (channel_prop_t) :: resonance_t
    real(default) :: mass = 0
    real(default) :: width = 0
  contains
```



```

    procedure :: to_string => resonance_to_string
    procedure :: is_equal => resonance_is_equal
end type resonance_t

```

Print mass and width.

```

<PHS base: sub interfaces>≡
    module function resonance_to_string (object) result (string)
        class(resonance_t), intent(in) :: object
        type(string_t) :: string
    end function resonance_to_string

<PHS base: procedures>≡
    module function resonance_to_string (object) result (string)
        class(resonance_t), intent(in) :: object
        type(string_t) :: string
        character(32) :: buffer
        string = "resonant: m ="
        write (buffer, "(" // FMT_19 // ")") object%mass
        string = string // trim (buffer) // " GeV, w ="
        write (buffer, "(" // FMT_19 // ")") object%width
        string = string // trim (buffer) // " GeV"
    end function resonance_to_string

```

Equality.

```

<PHS base: sub interfaces>+≡
    module function resonance_is_equal (prop1, prop2) result (flag)
        class(resonance_t), intent(in) :: prop1
        class(channel_prop_t), intent(in) :: prop2
        logical :: flag
    end function resonance_is_equal

<PHS base: procedures>+≡
    module function resonance_is_equal (prop1, prop2) result (flag)
        class(resonance_t), intent(in) :: prop1
        class(channel_prop_t), intent(in) :: prop2
        logical :: flag
        select type (prop2)
            type is (resonance_t)
                flag = prop1%mass == prop2%mass .and. prop1%width == prop2%width
            class default
                flag = .false.
        end select
    end function resonance_is_equal

```

This is the limiting case of a resonance, namely an on-shell particle. We just store the mass in physical units.

```

<PHS base: public>+≡
    public :: on_shell_t

<PHS base: types>+≡
    type, extends (channel_prop_t) :: on_shell_t
        real(default) :: mass = 0
    contains

```

```

    procedure :: to_string => on_shell_to_string
    procedure :: is_equal => on_shell_is_equal
end type on_shell_t

```

Print mass and width.

```

<PHS base: sub interfaces>+≡
    module function on_shell_to_string (object) result (string)
        class(on_shell_t), intent(in) :: object
        type(string_t) :: string
    end function on_shell_to_string

<PHS base: procedures>+≡
    module function on_shell_to_string (object) result (string)
        class(on_shell_t), intent(in) :: object
        type(string_t) :: string
        character(32) :: buffer
        string = "on shell: m ="
        write (buffer, "(" // FMT_19 // ")") object%mass
        string = string // trim (buffer) // " GeV"
    end function on_shell_to_string

```

Equality.

```

<PHS base: sub interfaces>+≡
    module function on_shell_is_equal (prop1, prop2) result (flag)
        class(on_shell_t), intent(in) :: prop1
        class(channel_prop_t), intent(in) :: prop2
        logical :: flag
    end function on_shell_is_equal

<PHS base: procedures>+≡
    module function on_shell_is_equal (prop1, prop2) result (flag)
        class(on_shell_t), intent(in) :: prop1
        class(channel_prop_t), intent(in) :: prop2
        logical :: flag
        select type (prop2)
        type is (on_shell_t)
            flag = prop1%mass == prop2%mass
        class default
            flag = .false.
        end select
    end function on_shell_is_equal

```

Channel equivalences

This type describes an equivalence. The current channel is equivalent to channel `c`. The equivalence involves a permutation `perm` of integration dimensions and, within each integration dimension, a mapping `mode`.

```

<PHS base: types>+≡
    type :: phs_equivalence_t
        integer :: c = 0
        integer, dimension(:), allocatable :: perm
        integer, dimension(:), allocatable :: mode

```

```

contains
  <PHS base: phs equivalence: TBP>
end type phs_equivalence_t

```

The mapping modes are

```

<PHS base: types>+≡
  integer, parameter, public :: &
    EQ_IDENTITY = 0, EQ_INVERT = 1, EQ_SYMMETRIC = 2, EQ_INVARIANT = 3

```

In particular, if a channel is equivalent to itself in the EQ_SYMMETRIC mode, the integrand can be assumed to be symmetric w.r.t. a reflection $x \rightarrow 1 - x$ of the corresponding integration variable.

These are the associated tags, for output:

```

<PHS base: types>+≡
  character, dimension(0:3), parameter :: TAG = ["+", "-", ":", "x"]

```

Write an equivalence.

```

<PHS base: phs equivalence: TBP>≡
  procedure :: write => phs_equivalence_write

<PHS base: sub interfaces>+≡
  module subroutine phs_equivalence_write (object, unit)
    class(phs_equivalence_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine phs_equivalence_write

<PHS base: procedures>+≡
  module subroutine phs_equivalence_write (object, unit)
    class(phs_equivalence_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, j
    u = given_output_unit (unit)
    write (u, "(5x,'= ',1x,I0,1x)", advance = "no") object%c
    if (allocated (object%perm)) then
      write (u, "(A)", advance = "no") "("
      do j = 1, size (object%perm)
        if (j > 1) write (u, "(1x)", advance = "no")
        write (u, "(I0,A1)", advance = "no") &
          object%perm(j), TAG(object%mode(j))
      end do
      write (u, "(A)") ")"
    else
      write (u, "(A)")
    end if
  end subroutine phs_equivalence_write

```

Initialize an equivalence. This allocates the perm and mode arrays with equal size.

```

<PHS base: phs equivalence: TBP>+≡
  procedure :: init => phs_equivalence_init

```

```

<PHS base: sub interfaces>+≡
    module subroutine phs_equivalence_init (eq, n_dim)
        class(phs_equivalence_t), intent(out) :: eq
        integer, intent(in) :: n_dim
    end subroutine phs_equivalence_init

```

```

<PHS base: procedures>+≡
    module subroutine phs_equivalence_init (eq, n_dim)
        class(phs_equivalence_t), intent(out) :: eq
        integer, intent(in) :: n_dim
        allocate (eq%perm (n_dim), source = 0)
        allocate (eq%mode (n_dim), source = EQ_IDENTITY)
    end subroutine phs_equivalence_init

```

Channel objects

The channel entry holds (optionally) specific properties.

`sf_channel` is the structure-function channel that corresponds to this phase-space channel. The structure-function channel may be set up with a specific mapping that depends on the phase-space channel properties. (The default setting is to leave the properties empty.)

```

<PHS base: public>+≡
    public :: phs_channel_t

<PHS base: types>+≡
    type :: phs_channel_t
        class(channel_prop_t), allocatable :: prop
        integer :: sf_channel = 1
        type(phs_equivalence_t), dimension(:), allocatable :: eq
    contains
        <PHS base: phs channel: TBP>
    end type phs_channel_t

```

Output.

```

<PHS base: phs channel: TBP>≡
    procedure :: write => phs_channel_write

<PHS base: sub interfaces>+≡
    module subroutine phs_channel_write (object, unit)
        class(phs_channel_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine phs_channel_write

<PHS base: procedures>+≡
    module subroutine phs_channel_write (object, unit)
        class(phs_channel_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, j
        u = given_output_unit (unit)
        write (u, "(1x,I0)", advance="no") object%sf_channel
        if (allocated (object%prop)) then
            write (u, "(1x,A)") char (object%prop%to_string ())
        else
            write (u, *)

```

```

end if
if (allocated (object%eq)) then
  do j = 1, size (object%eq)
    call object%eq(j)%write (u)
  end do
end if
end subroutine phs_channel_write

```

Identify the channel with an s-channel resonance. Gfortran 7/8/9 bug: has to remain in the main module.

```

<PHS base: phs channel: TBP>+≡
  procedure :: set_resonant => channel_set_resonant

<PHS base: main procedures>≡
  subroutine channel_set_resonant (channel, mass, width)
    class(phs_channel_t), intent(inout) :: channel
    real(default), intent(in) :: mass, width
    allocate (resonance_t :: channel%prop)
    select type (prop => channel%prop)
    type is (resonance_t)
      prop%mass = mass
      prop%width = width
    end select
  end subroutine channel_set_resonant

```

Identify the channel with an on-shell particle. Gfortran 7/8/9 bug: has to remain in the main module.

```

<PHS base: phs channel: TBP>+≡
  procedure :: set_on_shell => channel_set_on_shell

<PHS base: main procedures>+≡
  subroutine channel_set_on_shell (channel, mass)
    class(phs_channel_t), intent(inout) :: channel
    real(default), intent(in) :: mass
    allocate (on_shell_t :: channel%prop)
    select type (prop => channel%prop)
    type is (on_shell_t)
      prop%mass = mass
    end select
  end subroutine channel_set_on_shell

```

19.1.2 Property collection

We can set up a list of all distinct channel properties for a given set of channels.

```

<PHS base: public>+≡
  public :: phs_channel_collection_t

<PHS base: types>+≡
  type :: prop_entry_t
    integer :: i = 0
    class(channel_prop_t), allocatable :: prop
    type(prop_entry_t), pointer :: next => null ()

```

```

end type prop_entry_t

type :: phs_channel_collection_t
  integer :: n = 0
  type(prop_entry_t), pointer :: first => null ()
contains
  <PHS base: phs channel collection: TBP>
end type phs_channel_collection_t

```

Finalizer for the list.

```

<PHS base: phs channel collection: TBP>≡
  procedure :: final => phs_channel_collection_final

<PHS base: sub interfaces>+≡
  module subroutine phs_channel_collection_final (object)
    class(phs_channel_collection_t), intent(inout) :: object
    end subroutine phs_channel_collection_final

<PHS base: procedures>+≡
  module subroutine phs_channel_collection_final (object)
    class(phs_channel_collection_t), intent(inout) :: object
    type(prop_entry_t), pointer :: entry
    do while (associated (object%first))
      entry => object%first
      object%first => entry%next
      deallocate (entry)
    end do
  end subroutine phs_channel_collection_final

```

Output.

```

<PHS base: phs channel collection: TBP>+≡
  procedure :: write => phs_channel_collection_write

<PHS base: sub interfaces>+≡
  module subroutine phs_channel_collection_write (object, unit)
    class(phs_channel_collection_t), intent(in) :: object
    integer, intent(in), optional :: unit
    end subroutine phs_channel_collection_write

<PHS base: procedures>+≡
  module subroutine phs_channel_collection_write (object, unit)
    class(phs_channel_collection_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(prop_entry_t), pointer :: entry
    integer :: u
    u = given_output_unit (unit)
    entry => object%first
    do while (associated (entry))
      if (allocated (entry%prop)) then
        write (u, "(1x,I0,1x,A)" entry%i, char (entry%prop%to_string ()))
      else
        write (u, "(1x,I0)" entry%i
      end if
      entry => entry%next
    end do
  end subroutine phs_channel_collection_write

```

```
end subroutine phs_channel_collection_write
```

Push a new property to the stack if it is not yet included. Simultaneously, set the `sf_channel` entry in the phase-space channel object to the index of the matching entry, or the new entry if there was no match.

```
<PHS base: phs channel collection: TBP>+≡
  procedure :: push => phs_channel_collection_push

<PHS base: sub interfaces>+≡
  module subroutine phs_channel_collection_push (coll, channel)
    class(phs_channel_collection_t), intent(inout) :: coll
    type(phs_channel_t), intent(inout) :: channel
  end subroutine phs_channel_collection_push

<PHS base: procedures>+≡
  module subroutine phs_channel_collection_push (coll, channel)
    class(phs_channel_collection_t), intent(inout) :: coll
    type(phs_channel_t), intent(inout) :: channel
    type(prop_entry_t), pointer :: entry, new
    if (associated (coll%first)) then
      entry => coll%first
    do
      if (allocated (entry%prop)) then
        if (allocated (channel%prop)) then
          if (entry%prop == channel%prop) then
            channel%sf_channel = entry%i
            return
          end if
        end if
      else if (.not. allocated (channel%prop)) then
        channel%sf_channel = entry%i
        return
      end if
      if (associated (entry%next)) then
        entry => entry%next
      else
        exit
      end if
    end do
    allocate (new)
    entry%next => new
  else
    allocate (new)
    coll%first => new
  end if
  coll%n = coll%n + 1
  new%i = coll%n
  channel%sf_channel = new%i
  if (allocated (channel%prop)) then
    allocate (new%prop, source = channel%prop)
  end if
end subroutine phs_channel_collection_push
```

Return the number of collected distinct channels.

```

<PHS base: phs channel collection: TBP>+≡
  procedure :: get_n => phs_channel_collection_get_n

<PHS base: sub interfaces>+≡
  module function phs_channel_collection_get_n (coll) result (n)
    class(phs_channel_collection_t), intent(in) :: coll
    integer :: n
  end function phs_channel_collection_get_n

<PHS base: procedures>+≡
  module function phs_channel_collection_get_n (coll) result (n)
    class(phs_channel_collection_t), intent(in) :: coll
    integer :: n
    n = coll%n
  end function phs_channel_collection_get_n

```

Return a specific channel (property object).

```

<PHS base: phs channel collection: TBP>+≡
  procedure :: get_entry => phs_channel_collection_get_entry

<PHS base: sub interfaces>+≡
  module subroutine phs_channel_collection_get_entry (coll, i, prop)
    class(phs_channel_collection_t), intent(in) :: coll
    integer, intent(in) :: i
    class(channel_prop_t), intent(out), allocatable :: prop
  end subroutine phs_channel_collection_get_entry

<PHS base: procedures>+≡
  module subroutine phs_channel_collection_get_entry (coll, i, prop)
    class(phs_channel_collection_t), intent(in) :: coll
    integer, intent(in) :: i
    class(channel_prop_t), intent(out), allocatable :: prop
    type(prop_entry_t), pointer :: entry
    integer :: k
    if (i > 0 .and. i <= coll%n) then
      entry => coll%first
      do k = 2, i
        entry => entry%next
      end do
      if (allocated (entry%prop)) then
        if (allocated (prop)) deallocate (prop)
        allocate (prop, source = entry%prop)
      end if
    else
      call msg_bug ("PHS channel collection: get entry: illegal index")
    end if
  end subroutine phs_channel_collection_get_entry

```

19.1.3 Kinematics configuration

Here, we store the universal information that is specifically relevant for phase-space generation. It is a subset of the process data, supplemented by basic information on phase-space parameterization channels.

A concrete implementation will contain more data, that describe the phase space in detail.

MD5 sums: the phase space setup depends on the process, it depends on the model parameters (the masses, that is), and on the configuration parameters. (It does not depend on the QCD setup.)

```

<PHS base: public>+≡
    public :: phs_config_t

<PHS base: types>+≡
    type, abstract :: phs_config_t
        ! private
        type(string_t) :: id
        integer :: n_in = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        integer :: n_state = 0
        integer :: n_par = 0
        integer :: n_channel = 0
        real(default) :: sqrts = 0
        logical :: sqrts_fixed = .true.
        logical :: lab_is_cm = .true.
        logical :: azimuthal_dependence = .false.
        integer, dimension(:), allocatable :: dim_flat
        logical :: provides_equivalences = .false.
        logical :: provides_chains = .false.
        logical :: vis_channels = .false.
        integer, dimension(:), allocatable :: chain
        class(model_data_t), pointer :: model => null ()
        type(flavor_t), dimension(:, :), allocatable :: flv
        type(phs_channel_t), dimension(:), allocatable :: channel
        character(32) :: md5sum_process = ""
        character(32) :: md5sum_model_par = ""
        character(32) :: md5sum_phs_config = ""
        integer :: nlo_type
    contains
        <PHS base: phs config: TBP>
    end type phs_config_t

```

Finalizer, deferred.

```

<PHS base: phs config: TBP>≡
    procedure (phs_config_final), deferred :: final

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_config_final (object)
            import
            class(phs_config_t), intent(inout) :: object
        end subroutine phs_config_final
    end interface

```

Output. We provide an implementation for the output of the base-type contents and an interface for the actual write method.

```

<PHS base: phs config: TBP>+≡

```

```

        procedure (phs_config_write), deferred :: write
        procedure :: base_write => phs_config_write

<PHS base: sub interfaces>+≡
        module subroutine phs_config_write (object, unit, include_id)
            class(phs_config_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: include_id
        end subroutine phs_config_write

<PHS base: procedures>+≡
        module subroutine phs_config_write (object, unit, include_id)
            class(phs_config_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: include_id
            integer :: u, i, j
            integer :: n_tot_flv
            logical :: use_id
            n_tot_flv = object%n_tot
            u = given_output_unit (unit)
            use_id = .true.; if (present (include_id)) use_id = include_id
            if (use_id) write (u, "(3x,A,A,A)") "ID          = ", char (object%id), ""
            write (u, "(3x,A,I0)") "n_in          = ", object%n_in
            write (u, "(3x,A,I0)") "n_out          = ", object%n_out
            write (u, "(3x,A,I0)") "n_tot          = ", object%n_tot
            write (u, "(3x,A,I0)") "n_state        = ", object%n_state
            write (u, "(3x,A,I0)") "n_par          = ", object%n_par
            write (u, "(3x,A,I0)") "n_channel      = ", object%n_channel
            write (u, "(3x,A," // FMT_19 // ")") "sqrts          = ", object%sqrts
            write (u, "(3x,A,L1)") "s_fixed        = ", object%sqrts_fixed
            write (u, "(3x,A,L1)") "lab_is_cm      = ", object%lab_is_cm
            write (u, "(3x,A,L1)") "azim.dep.      = ", object%azimuthal_dependence
            if (allocated (object%dim_flat)) then
                write (u, "(3x,A,I0)") "flat dim. = ", object%dim_flat
            end if
            write (u, "(1x,A)") "Flavor combinations:"
            do i = 1, object%n_state
                write (u, "(3x,I0,':')", advance="no") i
                ! do j = 1, object%n_tot
                do j = 1, n_tot_flv
                    write (u, "(1x,A)", advance="no") char (object%flv(j,i)%get_name ())
                end do
                write (u, "(A)")
            end do
            if (allocated (object%channel)) then
                write (u, "(1x,A)") "Phase-space / structure-function channels:"
                do i = 1, object%n_channel
                    write (u, "(3x,I0,':')", advance="no") i
                    call object%channel(i)%write (u)
                end do
            end if
            if (object%md5sum_process /= "") then
                write (u, "(3x,A,A,A)") "MD5 sum (process)      = ', &
                    object%md5sum_process, ""
            end if

```

```

if (object%md5sum_model_par /= "") then
  write (u, "(3x,A,A,A)") "MD5 sum (model par) = ', &
    object%md5sum_model_par, "'
end if
if (object%md5sum_phs_config /= "") then
  write (u, "(3x,A,A,A)") "MD5 sum (phs config) = ', &
    object%md5sum_phs_config, "'
end if
end subroutine phs_config_write

```

Similarly, a basic initializer and an interface. The model pointer is taken as an argument; we may verify that this has the expected model name.

The intent is *inout*. We want to be able to set parameters in advance.

(PHS base: phs config: TBP)+≡

```

procedure :: init => phs_config_init

```

(PHS base: sub interfaces)+≡

```

module subroutine phs_config_init (phs_config, data, model)
  class(phs_config_t), intent(inout) :: phs_config
  type(process_constants_t), intent(in) :: data
  class(model_data_t), intent(in), target :: model
end subroutine phs_config_init

```

(PHS base: procedures)+≡

```

module subroutine phs_config_init (phs_config, data, model)
  class(phs_config_t), intent(inout) :: phs_config
  type(process_constants_t), intent(in) :: data
  class(model_data_t), intent(in), target :: model
  integer :: i, j
  phs_config%id = data%id
  phs_config%n_in = data%n_in
  phs_config%n_out = data%n_out
  phs_config%n_tot = data%n_in + data%n_out
  phs_config%n_state = data%n_flv
  if (data%model_name == model%get_name ()) then
    phs_config%model => model
  else
    call msg_bug ("phs_config_init: model name mismatch")
  end if
  allocate (phs_config%flv (phs_config%n_tot, phs_config%n_state))
  do i = 1, phs_config%n_state
    do j = 1, phs_config%n_tot
      call phs_config%flv(j,i)%init (data%flv_state(j,i), &
        phs_config%model)
    end do
  end do
  phs_config%md5sum_process = data%md5sum
end subroutine phs_config_init

```

WK 2018-04-05: This procedure appears to be redundant?

(XXX PHS base: phs config: TBP)≡

```

procedure :: set_component_index => phs_config_set_component_index

```

```

<XXX PHS base: procedures>≡
  subroutine phs_config_set_component_index (phs_config, index)
    class(phs_config_t), intent(inout) :: phs_config
    integer, intent(in) :: index
    type(string_t), dimension(:), allocatable :: id
    type(string_t) :: suffix
    integer :: i, n
    suffix = var_str ('i') // int2string (index)
    call split_string (phs_config%id, var_str ('_'), id)
    phs_config%id = var_str ('')
    n = size (id) - 1
    do i = 1, n
      phs_config%id = phs_config%id // id(i) // var_str ('_')
    end do
    phs_config%id = phs_config%id // suffix
  end subroutine phs_config_set_component_index

```

This procedure should complete the phase-space configuration. We need the `sqrts` value as overall scale, which is known only after the beams have been defined. The procedure should determine the number of channels, their properties (if any), and allocate and fill the channel array accordingly.

```

<PHS base: phs config: TBP>+≡
  procedure (phs_config_configure), deferred :: configure

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_config_configure (phs_config, sqrts, &
      sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
      nlo_type, subdir)
    import
    class(phs_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
  end subroutine phs_config_configure
end interface

```

Manually assign structure-function channel indices to the phase-space channel objects. (Used by a test routine.)

```

<PHS base: phs config: TBP>+≡
  procedure :: set_sf_channel => phs_config_set_sf_channel

<PHS base: sub interfaces>+≡
  module subroutine phs_config_set_sf_channel (phs_config, sf_channel)
    class(phs_config_t), intent(inout) :: phs_config
    integer, dimension(:), intent(in) :: sf_channel
  end subroutine phs_config_set_sf_channel

```

```

<PHS base: procedures>+≡
module subroutine phs_config_set_sf_channel (phs_config, sf_channel)
  class(phs_config_t), intent(inout) :: phs_config
  integer, dimension(:), intent(in) :: sf_channel
  phs_config%channel%sf_channel = sf_channel
end subroutine phs_config_set_sf_channel

```

Collect new channels not yet in the collection from this phase-space configuration object. At the same time, assign structure-function channels.

```

<PHS base: phs config: TBP>+≡
  procedure :: collect_channels => phs_config_collect_channels

<PHS base: sub interfaces>+≡
  module subroutine phs_config_collect_channels (phs_config, coll)
    class(phs_config_t), intent(inout) :: phs_config
    type(phs_channel_collection_t), intent(inout) :: coll
  end subroutine phs_config_collect_channels

```

```

<PHS base: procedures>+≡
module subroutine phs_config_collect_channels (phs_config, coll)
  class(phs_config_t), intent(inout) :: phs_config
  type(phs_channel_collection_t), intent(inout) :: coll
  integer :: c
  do c = 1, phs_config%n_channel
    call coll%push (phs_config%channel(c))
  end do
end subroutine phs_config_collect_channels

```

Compute the MD5 sum. We abuse the `write` method. In type implementations, `write` should only display information that is relevant for the MD5 sum. The data include the process MD5 sum which is taken from the process constants, and the MD5 sum of the model parameters. This may change, so it is computed here.

```

<PHS base: phs config: TBP>+≡
  procedure :: compute_md5sum => phs_config_compute_md5sum

<PHS base: sub interfaces>+≡
  module subroutine phs_config_compute_md5sum (phs_config, include_id)
    class(phs_config_t), intent(inout) :: phs_config
    logical, intent(in), optional :: include_id
  end subroutine phs_config_compute_md5sum

<PHS base: procedures>+≡
module subroutine phs_config_compute_md5sum (phs_config, include_id)
  class(phs_config_t), intent(inout) :: phs_config
  logical, intent(in), optional :: include_id
  integer :: u
  phs_config%md5sum_model_par = phs_config%model%get_parameters_md5sum ()
  phs_config%md5sum_phs_config = ""
  u = free_unit ()
  open (u, status = "scratch", action = "readwrite")
  call phs_config%write (u, include_id)
  rewind (u)
  phs_config%md5sum_phs_config = md5sum (u)

```

```

        close (u)
    end subroutine phs_config_compute_md5sum

```

Print an informative message after phase-space configuration.

```

<PHS base: phs config: TBP>+≡
    procedure (phs_startup_message), deferred :: startup_message
    procedure :: base_startup_message => phs_startup_message

<PHS base: sub interfaces>+≡
    module subroutine phs_startup_message (phs_config, unit)
        class(phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
    end subroutine phs_startup_message

<PHS base: procedures>+≡
    module subroutine phs_startup_message (phs_config, unit)
        class(phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        write (msg_buffer, "(A,3(1x,I0,1x,A))") &
            "Phase space:", &
            phs_config%n_channel, "channels", &
            phs_config%n_par, "dimensions"
        call msg_message (unit = unit)
    end subroutine phs_startup_message

```

This procedure should be implemented such that the phase-space configuration object allocates a phase-space instance of matching type.

```

<PHS base: phs config: TBP>+≡
    procedure (phs_config_allocate_instance), nopass, deferred :: &
        allocate_instance

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_config_allocate_instance (phs)
            import
            class(phs_t), intent(inout), pointer :: phs
        end subroutine phs_config_allocate_instance
    end interface

```

19.1.4 Extract data

Return the number of MC input parameters.

```

<PHS base: phs config: TBP>+≡
    procedure :: get_n_par => phs_config_get_n_par

<PHS base: sub interfaces>+≡
    module function phs_config_get_n_par (phs_config) result (n)
        class(phs_config_t), intent(in) :: phs_config
        integer :: n
    end function phs_config_get_n_par

```

```

<PHS base: procedures>+≡
module function phs_config_get_n_par (phs_config) result (n)
  class(phs_config_t), intent(in) :: phs_config
  integer :: n
  n = phs_config%n_par
end function phs_config_get_n_par

```

Return dimensions (parameter indices) for which the phase-space dimension is flat, so integration and event generation can be simplified.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_flat_dimensions => phs_config_get_flat_dimensions

<PHS base: sub interfaces>+≡
  module function phs_config_get_flat_dimensions &
    (phs_config) result (dim_flat)
    class(phs_config_t), intent(in) :: phs_config
    integer, dimension(:), allocatable :: dim_flat
  end function phs_config_get_flat_dimensions

```

```

<PHS base: procedures>+≡
module function phs_config_get_flat_dimensions &
  (phs_config) result (dim_flat)
  class(phs_config_t), intent(in) :: phs_config
  integer, dimension(:), allocatable :: dim_flat
  if (allocated (phs_config%dim_flat)) then
    allocate (dim_flat (size (phs_config%dim_flat)))
    dim_flat = phs_config%dim_flat
  else
    allocate (dim_flat (0))
  end if
end function phs_config_get_flat_dimensions

```

Return the number of phase-space channels.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_n_channel => phs_config_get_n_channel

<PHS base: sub interfaces>+≡
  module function phs_config_get_n_channel (phs_config) result (n)
    class(phs_config_t), intent(in) :: phs_config
    integer :: n
  end function phs_config_get_n_channel

<PHS base: procedures>+≡
module function phs_config_get_n_channel (phs_config) result (n)
  class(phs_config_t), intent(in) :: phs_config
  integer :: n
  n = phs_config%n_channel
end function phs_config_get_n_channel

```

Return the structure-function channel that corresponds to the phase-space channel c. If the channel array is not allocated (which happens if there is no structure function), return zero.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_sf_channel => phs_config_get_sf_channel

```

```

(PHS base: sub interfaces)+≡
  module function phs_config_get_sf_channel (phs_config, c) result (c_sf)
    class(phs_config_t), intent(in) :: phs_config
    integer, intent(in) :: c
    integer :: c_sf
  end function phs_config_get_sf_channel

```

```

(PHS base: procedures)+≡
  module function phs_config_get_sf_channel (phs_config, c) result (c_sf)
    class(phs_config_t), intent(in) :: phs_config
    integer, intent(in) :: c
    integer :: c_sf
    if (allocated (phs_config%channel)) then
      c_sf = phs_config%channel(c)%sf_channel
    else
      c_sf = 0
    end if
  end function phs_config_get_sf_channel

```

Return the mass(es) of the incoming particle(s). We take the first flavor combination in the array, assuming that masses must be degenerate among flavors.

```

(PHS base: phs config: TBP)+≡
  procedure :: get_masses_in => phs_config_get_masses_in

(PHS base: sub interfaces)+≡
  module subroutine phs_config_get_masses_in (phs_config, m)
    class(phs_config_t), intent(in) :: phs_config
    real(default), dimension(:), intent(out) :: m
  end subroutine phs_config_get_masses_in

(PHS base: procedures)+≡
  module subroutine phs_config_get_masses_in (phs_config, m)
    class(phs_config_t), intent(in) :: phs_config
    real(default), dimension(:), intent(out) :: m
    integer :: i
    do i = 1, phs_config%n_in
      m(i) = phs_config%flv(i,1)%get_mass ()
    end do
  end subroutine phs_config_get_masses_in

```

Return the MD5 sum of the configuration.

```

(PHS base: phs config: TBP)+≡
  procedure :: get_md5sum => phs_config_get_md5sum

(PHS base: sub interfaces)+≡
  module function phs_config_get_md5sum (phs_config) result (md5sum)
    class(phs_config_t), intent(in) :: phs_config
    character(32) :: md5sum
  end function phs_config_get_md5sum

(PHS base: procedures)+≡
  module function phs_config_get_md5sum (phs_config) result (md5sum)
    class(phs_config_t), intent(in) :: phs_config
    character(32) :: md5sum
    md5sum = phs_config%md5sum_phs_config
  end function phs_config_get_md5sum

```



```
end function phs_config_get_md5sum
```

19.1.5 Phase-space point instance

The `phs_t` object holds the workspace for phase-space generation. In the base object, we have the MC input parameters `r` and the Jacobian factor `f`, for each channel, and the incoming and outgoing momenta.

Note: The `active_channel` array is not used yet, all elements are initialized with `.true..` It should be touched by the integrator if it decides to drop irrelevant channels.

```
<PHS base: public>+≡
  public :: phs_t

<PHS base: types>+≡
  type, abstract :: phs_t
    class(phs_config_t), pointer :: config => null ()
    logical :: r_defined = .false.
    integer :: selected_channel = 0
    logical, dimension(:), allocatable :: active_channel
    real(default), dimension(:, :), allocatable :: r
    real(default), dimension(:), allocatable :: f
    real(default), dimension(:), allocatable :: m_in
    real(default), dimension(:), allocatable :: m_out
    real(default) :: flux = 0
    real(default) :: volume = 0
    type(lorentz_transformation_t) :: lt_cm_to_lab
    logical :: p_defined = .false.
    real(default) :: qrts_hat = 0
    type(vector4_t), dimension(:), allocatable :: p
    logical :: q_defined = .false.
    type(vector4_t), dimension(:), allocatable :: q
  contains
    <PHS base: phs: TBP>
  end type phs_t
```

Output. Since phase space may get complicated, we include a `verbose` option for the abstract `write` procedure.

```
<PHS base: phs: TBP>≡
  procedure (phs_write), deferred :: write

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_write (object, unit, verbose)
      import
      class(phs_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: verbose
    end subroutine phs_write
  end interface
```

This procedure can be called to print the contents of the base type.

```

<PHS base: phs: TBP>+≡
    procedure :: base_write => phs_base_write

<PHS base: sub interfaces>+≡
    module subroutine phs_base_write (object, unit)
        class(phs_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine phs_base_write

<PHS base: procedures>+≡
    module subroutine phs_base_write (object, unit)
        class(phs_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, c, i
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "Partonic phase space: parameters"
        if (object%r_defined) then
            write (u, *)
        else
            write (u, "(1x,A)") "[undefined]"
        end if
        write (u, "(3x,A,999(1x," // FMT_19 // ")") "m_in   =", object%m_in
        write (u, "(3x,A,999(1x," // FMT_19 // ")") "m_out   =", object%m_out
        write (u, "(3x,A," // FMT_19 // ")") "Flux    =", object%flux
        write (u, "(3x,A," // FMT_19 // ")") "Volume  =", object%volume
        if (allocated (object%f)) then
            do c = 1, size (object%r, 2)
                write (u, "(1x,A,I0,A)", advance="no") "Channel #", c, ":"
                if (c == object%selected_channel) then
                    write (u, "(1x,A)") "[selected]"
                else
                    write (u, *)
                end if
                write (u, "(3x,A)", advance="no") "r ="
                do i = 1, size (object%r, 1)
                    write (u, "(1x,F9.7)", advance="no") object%r(i,c)
                end do
                write (u, *)
                write (u, "(3x,A,1x,ES13.7)") "f =", object%f(c)
            end do
        end if
        write (u, "(1x,A)") "Partonic phase space: momenta"
        if (object%p_defined) then
            write (u, "(3x,A," // FMT_19 // ")") "sqrts  =", object%sqrts_hat
        end if
        write (u, "(1x,A)", advance="no") "Incoming:"
        if (object%p_defined) then
            write (u, *)
        else
            write (u, "(1x,A)") "[undefined]"
        end if
        if (allocated (object%p)) then
            do i = 1, size (object%p)
                call vector4_write (object%p(i), u)
            end do
        end if
    end subroutine phs_base_write

```

```

        end do
    end if
    write (u, "(1x,A)", advance="no") "Outgoing:"
    if (object%q_defined) then
        write (u, *)
    else
        write (u, "(1x,A)") "[undefined]"
    end if
    if (allocated (object%q)) then
        do i = 1, size (object%q)
            call vector4_write (object%q(i), u)
        end do
    end if
    if (object%p_defined .and. .not. object%config%lab_is_cm) then
        write (u, "(1x,A)") "Transformation c.m -> lab frame"
        call lorentz_transformation_write (object%lt_cm_to_lab, u)
    end if
end subroutine phs_base_write

```

Finalizer. The base type does not need it, but extensions may.

```

<PHS base: phs: TBP>+≡
    procedure (phs_final), deferred :: final

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_final (object)
            import
            class(phs_t), intent(inout) :: object
        end subroutine phs_final
    end interface

```

Initializer. Everything should be contained in the `process_data` configuration object, so we can require a universal interface.

```

<PHS base: phs: TBP>+≡
    procedure (phs_init), deferred :: init

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_init (phs, phs_config)
            import
            class(phs_t), intent(out) :: phs
            class(phs_config_t), intent(in), target :: phs_config
        end subroutine phs_init
    end interface

```

The base version will just allocate the arrays. It should be called at the beginning of the implementation of `phs_init`.

```

<PHS base: phs: TBP>+≡
    procedure :: base_init => phs_base_init

<PHS base: sub interfaces>+≡
    module subroutine phs_base_init (phs, phs_config)
        class(phs_t), intent(out) :: phs

```

```

        class(phs_config_t), intent(in), target :: phs_config
    end subroutine phs_base_init

<PHS base: procedures>+≡
module subroutine phs_base_init (phs, phs_config)
    class(phs_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    phs%config => phs_config
    allocate (phs%active_channel (phs%config%n_channel))
    phs%active_channel = .true.
    allocate (phs%r (phs%config%n_par, phs%config%n_channel)); phs%r = 0
    allocate (phs%f (phs%config%n_channel)); phs%f = 0
    allocate (phs%p (phs%config%n_in))
    allocate (phs%m_in (phs%config%n_in), &
        source = phs_config%flv(:phs_config%n_in, 1)%get_mass ())
    allocate (phs%q (phs%config%n_out))
    allocate (phs%m_out (phs%config%n_out), &
        source = phs_config%flv(phs_config%n_in+1:, 1)%get_mass ())
    call phs%compute_flux ()
end subroutine phs_base_init

```

Manually select a channel.

```

<PHS base: phs: TBP>+≡
    procedure :: select_channel => phs_base_select_channel

<PHS base: sub interfaces>+≡
    module subroutine phs_base_select_channel (phs, channel)
        class(phs_t), intent(inout) :: phs
        integer, intent(in), optional :: channel
    end subroutine phs_base_select_channel

<PHS base: procedures>+≡
module subroutine phs_base_select_channel (phs, channel)
    class(phs_t), intent(inout) :: phs
    integer, intent(in), optional :: channel
    if (present (channel)) then
        phs%selected_channel = channel
    else
        phs%selected_channel = 0
    end if
end subroutine phs_base_select_channel

```

Set incoming momenta. Assume that array shapes match. If requested, compute the Lorentz transformation from the c.m. to the lab frame and apply that transformation to the incoming momenta.

In the c.m. frame, the sum of three-momenta is zero. In a scattering process, the z axis is the direction of the first beam, the second beam is along the negative z axis. The transformation from the c.m. to the lab frame is a rotation from the z axis to the boost axis followed by a boost, such that the c.m. momenta are transformed into the lab-frame momenta. In a decay process, we just boost along the flight direction, without rotation.

```

<PHS base: phs: TBP>+≡
    procedure :: set_incoming_momenta => phs_set_incoming_momenta

```

```

<PHS base: sub interfaces>+≡
    module subroutine phs_set_incoming_momenta (phs, p)
        class(phs_t), intent(inout) :: phs
        type(vector4_t), dimension(:), intent(in) :: p
    end subroutine phs_set_incoming_momenta

<PHS base: procedures>+≡
    module subroutine phs_set_incoming_momenta (phs, p)
        class(phs_t), intent(inout) :: phs
        type(vector4_t), dimension(:), intent(in) :: p
        type(vector4_t) :: p0, p1
        type(lorentz_transformation_t) :: lt0
        integer :: i
        phs%p = p
        if (phs%config%lab_is_cm) then
            phs%sqrts_hat = phs%config%sqrts
            phs%p = p
            phs%lt_cm_to_lab = identity
        else
            p0 = sum (p)
            if (phs%config%sqrts_fixed) then
                phs%sqrts_hat = phs%config%sqrts
            else
                phs%sqrts_hat = p0 ** 1
            end if
            lt0 = boost (p0, phs%sqrts_hat)
            select case (phs%config%n_in)
            case (1)
                phs%lt_cm_to_lab = lt0
            case (2)
                p1 = inverse (lt0) * p(1)
                phs%lt_cm_to_lab = lt0 * rotation_to_2nd (3, space_part (p1))
            end select
            phs%p = inverse (phs%lt_cm_to_lab) * p
        end if
        phs%p_defined = .true.
    end subroutine phs_set_incoming_momenta

```

Set outgoing momenta. Assume that array shapes match. The incoming momenta must be known, so we can apply the Lorentz transformation from c.m. to lab (inverse) to the momenta.

```

<PHS base: phs: TBP>+≡
    procedure :: set_outgoing_momenta => phs_set_outgoing_momenta

<PHS base: sub interfaces>+≡
    module subroutine phs_set_outgoing_momenta (phs, q)
        class(phs_t), intent(inout) :: phs
        type(vector4_t), dimension(:), intent(in) :: q
    end subroutine phs_set_outgoing_momenta

<PHS base: procedures>+≡
    module subroutine phs_set_outgoing_momenta (phs, q)
        class(phs_t), intent(inout) :: phs
        type(vector4_t), dimension(:), intent(in) :: q
        integer :: i

```

```

    if (phs%p_defined) then
      if (phs%config%lab_is_cm) then
        phs%q = q
      else
        phs%q = inverse (phs%lt_cm_to_lab) * q
      end if
      phs%q_defined = .true.
    end if
  end subroutine phs_set_outgoing_momenta

```

Return outgoing momenta. Apply the c.m. to lab transformation if necessary.

<PHS base: phs: TBP>+≡

```

  procedure :: get_outgoing_momenta => phs_get_outgoing_momenta

```

<PHS base: sub interfaces>+≡

```

  module subroutine phs_get_outgoing_momenta (phs, q)
    class(phs_t), intent(in) :: phs
    type(vector4_t), dimension(:), intent(out) :: q
  end subroutine phs_get_outgoing_momenta

```

<PHS base: procedures>+≡

```

  module subroutine phs_get_outgoing_momenta (phs, q)
    class(phs_t), intent(in) :: phs
    type(vector4_t), dimension(:), intent(out) :: q
    if (phs%p_defined .and. phs%q_defined) then
      if (phs%config%lab_is_cm) then
        q = phs%q
      else
        q = phs%lt_cm_to_lab * phs%q
      end if
    else
      q = vector4_null
    end if
  end subroutine phs_get_outgoing_momenta

```

<PHS base: phs: TBP>+≡

```

  procedure :: lab_is_cm => phs_lab_is_cm

```

<PHS base: sub interfaces>+≡

```

  module function phs_lab_is_cm (phs) result (lab_is_cm)
    logical :: lab_is_cm
    class(phs_t), intent(in) :: phs
  end function phs_lab_is_cm

```

<PHS base: procedures>+≡

```

  module function phs_lab_is_cm (phs) result (lab_is_cm)
    logical :: lab_is_cm
    class(phs_t), intent(in) :: phs
    lab_is_cm = phs%config%lab_is_cm
  end function phs_lab_is_cm

```

<PHS base: phs: TBP>+≡

```

  procedure :: get_n_tot => phs_get_n_tot

```

```

<PHS base: sub interfaces>+≡
    elemental module function phs_get_n_tot (phs) result (n_tot)
        integer :: n_tot
        class(phs_t), intent(in) :: phs
    end function phs_get_n_tot

<PHS base: procedures>+≡
    elemental module function phs_get_n_tot (phs) result (n_tot)
        integer :: n_tot
        class(phs_t), intent(in) :: phs
        n_tot = phs%config%n_tot
    end function phs_get_n_tot

<PHS base: phs: TBP>+≡
    procedure :: set_lorentz_transformation => phs_set_lorentz_transformation

<PHS base: sub interfaces>+≡
    module subroutine phs_set_lorentz_transformation (phs, lt)
        class(phs_t), intent(inout) :: phs
        type(lorentz_transformation_t), intent(in) :: lt
    end subroutine phs_set_lorentz_transformation

<PHS base: procedures>+≡
    module subroutine phs_set_lorentz_transformation (phs, lt)
        class(phs_t), intent(inout) :: phs
        type(lorentz_transformation_t), intent(in) :: lt
        phs%lt_cm_to_lab = lt
    end subroutine phs_set_lorentz_transformation

<PHS base: phs: TBP>+≡
    procedure :: get_lorentz_transformation => phs_get_lorentz_transformation

<PHS base: sub interfaces>+≡
    module function phs_get_lorentz_transformation (phs) result (lt)
        type(lorentz_transformation_t) :: lt
        class(phs_t), intent(in) :: phs
    end function phs_get_lorentz_transformation

<PHS base: procedures>+≡
    module function phs_get_lorentz_transformation (phs) result (lt)
        type(lorentz_transformation_t) :: lt
        class(phs_t), intent(in) :: phs
        lt = phs%lt_cm_to_lab
    end function phs_get_lorentz_transformation

```

Return the input parameter array for a channel.

```

<PHS base: phs: TBP>+≡
    procedure :: get_mcpair => phs_get_mcpair

<PHS base: sub interfaces>+≡
    module subroutine phs_get_mcpair (phs, c, r)
        class(phs_t), intent(in) :: phs
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
    end subroutine phs_get_mcpair

```

```

<PHS base: procedures>+≡
  module subroutine phs_get_mcpair (phs, c, r)
    class(phs_t), intent(in) :: phs
    integer, intent(in) :: c
    real(default), dimension(:), intent(out) :: r
    if (phs%r_defined) then
      r = phs%r(:,c)
    else
      r = 0
    end if
  end subroutine phs_get_mcpair

```

Return the Jacobian factor for a channel.

```

<PHS base: phs: TBP>+≡
  procedure :: get_f => phs_get_f

<PHS base: sub interfaces>+≡
  module function phs_get_f (phs, c) result (f)
    class(phs_t), intent(in) :: phs
    integer, intent(in) :: c
    real(default) :: f
  end function phs_get_f

```

```

<PHS base: procedures>+≡
  module function phs_get_f (phs, c) result (f)
    class(phs_t), intent(in) :: phs
    integer, intent(in) :: c
    real(default) :: f
    if (phs%r_defined) then
      f = phs%f(c)
    else
      f = 0
    end if
  end function phs_get_f

```

Return the overall factor, which is the product of the flux factor for the incoming partons and the phase-space volume for the outgoing partons.

```

<PHS base: phs: TBP>+≡
  procedure :: get_overall_factor => phs_get_overall_factor

<PHS base: sub interfaces>+≡
  module function phs_get_overall_factor (phs) result (f)
    class(phs_t), intent(in) :: phs
    real(default) :: f
  end function phs_get_overall_factor

<PHS base: procedures>+≡
  module function phs_get_overall_factor (phs) result (f)
    class(phs_t), intent(in) :: phs
    real(default) :: f
    f = phs%flux * phs%volume
  end function phs_get_overall_factor

```


Compute flux factor. We do this during initialization (when the incoming momenta \mathbf{p} are undefined), unless `sqrts` is variable. We do this again once for each phase-space point, but then we skip the calculation if `sqrts` is fixed.

There are three different flux factors.

1. For a decaying massive particle, the factor is

$$f = (2\pi)^4/(2M) \quad (19.1)$$

2. For a $2 \rightarrow n$ scattering process with $n > 1$, the factor is

$$f = (2\pi)^4/(2\sqrt{\lambda}) \quad (19.2)$$

where for massless incoming particles, $\sqrt{\lambda} = s$.

3. For a $2 \rightarrow 1$ on-shell production process, the factor includes an extra $1/(2\pi)^3$ factor and a $1/m^2$ factor from the phase-space delta function $\delta(x_1x_2 - m^2/s)$, which originate from the one-particle phase space that we integrate out.

$$f = 2\pi/(2sm^2) \quad (19.3)$$

The delta function is handled by the structure-function parameterization.

```

<PHS base: phs: TBP>+=
  procedure :: compute_flux => phs_compute_flux
  procedure :: compute_base_flux => phs_compute_flux

<PHS base: sub interfaces>+=
  module subroutine phs_compute_flux (phs)
    class(phs_t), intent(inout) :: phs
  end subroutine phs_compute_flux

<PHS base: procedures>+=
  module subroutine phs_compute_flux (phs)
    class(phs_t), intent(inout) :: phs
    real(default) :: s_hat, lda
    select case (phs%config%n_in)
    case (1)
      if (.not. phs%p_defined) then
        phs%flux = twopi4 / (2 * phs%m_in(1))
      end if
    case (2)
      if (phs%p_defined) then
        if (phs%config%sqrts_fixed) then
          return
        else
          s_hat = sum (phs%p) ** 2
        end if
      else
        if (phs%config%sqrts_fixed) then
          s_hat = phs%config%sqrts ** 2
        else
          return
        end if
      end if
    select case (phs%config%n_out)

```

```

case (2:)
  lda = lambda (s_hat, phs%m_in(1) ** 2, phs%m_in(2) ** 2)
  if (lda > 0) then
    phs%flux = conv * twopi4 / (2 * sqrt (lda))
  else
    phs%flux = 0
  end if
case (1)
  phs%flux = conv * twopi &
    / (2 * phs%config%sqrts ** 2 * phs%m_out(1) ** 2)
case default
  phs%flux = 0
end select
end select
end subroutine phs_compute_flux

```

Evaluate the phase-space point for a particular channel and compute momenta, Jacobian, and phase-space volume. This is, of course, deferred to the implementation.

```

<PHS base: phs: TBP>+≡
  procedure (phs_evaluate_selected_channel), deferred :: &
    evaluate_selected_channel

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_evaluate_selected_channel (phs, c_in, r_in)
      import
      class(phs_t), intent(inout) :: phs
      integer, intent(in) :: c_in
      real(default), dimension(:), intent(in) :: r_in
    end subroutine phs_evaluate_selected_channel
  end interface

```

Compute the inverse mappings to completely fill the **r** and **f** arrays, for the non-selected channels.

```

<PHS base: phs: TBP>+≡
  procedure (phs_evaluate_other_channels), deferred :: &
    evaluate_other_channels

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_evaluate_other_channels (phs, c_in)
      import
      class(phs_t), intent(inout) :: phs
      integer, intent(in) :: c_in
    end subroutine phs_evaluate_other_channels
  end interface

```

Inverse evaluation. If all momenta are known, we compute the inverse mappings to fill the **r** and **f** arrays.

```

<PHS base: phs: TBP>+≡
  procedure (phs_inverse), deferred :: inverse

```

```

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_inverse (phs)
      import
      class(phs_t), intent(inout) :: phs
    end subroutine phs_inverse
  end interface

<PHS base: phs: TBP>+≡
  procedure :: get_sqrts => phs_get_sqrts

<PHS base: sub interfaces>+≡
  module function phs_get_sqrts (phs) result (sqrts)
    real(default) :: sqrts
    class(phs_t), intent(in) :: phs
  end function phs_get_sqrts

<PHS base: procedures>+≡
  module function phs_get_sqrts (phs) result (sqrts)
    real(default) :: sqrts
    class(phs_t), intent(in) :: phs
    sqrts = phs%config%sqrts
  end function phs_get_sqrts

```

Uniform angular distribution

These procedures implement the uniform angular distribution, generated from two parameters x_1 and x_2 :

$$\cos \theta = 1 - 2x_1, \quad \phi = 2\pi x_2 \quad (19.4)$$

We generate a rotation (Lorentz transformation) which rotates the positive z axis into this point on the unit sphere. This rotation is applied to the \mathbf{p} momenta, which are assumed to be back-to-back, on-shell, and with the correct mass.

We do not compute a Jacobian (constant). The uniform distribution is assumed to be normalized.

```

<PHS base: public>+≡
  public :: compute_kinematics_solid_angle

<PHS base: sub interfaces>+≡
  module subroutine compute_kinematics_solid_angle (p, q, x)
    type(vector4_t), dimension(2), intent(in) :: p
    type(vector4_t), dimension(2), intent(out) :: q
    real(default), dimension(2), intent(in) :: x
  end subroutine compute_kinematics_solid_angle

<PHS base: procedures>+≡
  module subroutine compute_kinematics_solid_angle (p, q, x)
    type(vector4_t), dimension(2), intent(in) :: p
    type(vector4_t), dimension(2), intent(out) :: q
    real(default), dimension(2), intent(in) :: x
    real(default) :: ct, st, phi
    type(lorentz_transformation_t) :: rot
    integer :: i

```

```

ct = 1 - 2*x(1)
st = sqrt (1 - ct**2)
phi = twopi * x(2)
rot = rotation (phi, 3) * rotation (ct, st, 2)
do i = 1, 2
    q(i) = rot * p(i)
end do
end subroutine compute_kinematics_solid_angle

```

This is the inverse transformation. We assume that the outgoing momenta are rotated versions of the incoming momenta, back-to-back. Thus, we determine the angles from $q(1)$ alone. p is unused.

```

<PHS base: public>+≡
    public :: inverse_kinematics_solid_angle

<PHS base: sub interfaces>+≡
    module subroutine inverse_kinematics_solid_angle (p, q, x)
        type(vector4_t), dimension(:), intent(in) :: p
        type(vector4_t), dimension(2), intent(in) :: q
        real(default), dimension(2), intent(out) :: x
    end subroutine inverse_kinematics_solid_angle

<PHS base: procedures>+≡
    module subroutine inverse_kinematics_solid_angle (p, q, x)
        type(vector4_t), dimension(:), intent(in) :: p
        type(vector4_t), dimension(2), intent(in) :: q
        real(default), dimension(2), intent(out) :: x
        real(default) :: ct, phi
        ct = polar_angle_ct (q(1))
        phi = azimuthal_angle (q(1))
        x(1) = (1 - ct) / 2
        x(2) = phi / twopi
    end subroutine inverse_kinematics_solid_angle

```

19.1.6 Auxiliary stuff

The `pacify` subroutine, which is provided by the Lorentz module, has the purpose of setting numbers to zero which are (by comparing with a `tolerance` parameter) considered equivalent with zero. This is useful for numerical checks.

```

<PHS base: public>+≡
    public :: pacify

<PHS base: interfaces>+≡
    interface pacify
        module procedure pacify_phs
    end interface pacify

<PHS base: sub interfaces>+≡
    module subroutine pacify_phs (phs)
        class(phs_t), intent(inout) :: phs
    end subroutine pacify_phs

```

```

<PHS base: procedures>+≡
  module subroutine pacify_phs (phs)
    class(phs_t), intent(inout) :: phs
    if (phs%p_defined) then
      call pacify (phs%p, 30 * epsilon (1._default) * phs%config%sqrts)
      call pacify (phs%lt_cm_to_lab, 30 * epsilon (1._default))
    end if
    if (phs%q_defined) then
      call pacify (phs%q, 30 * epsilon (1._default) * phs%config%sqrts)
    end if
  end subroutine pacify_phs

```

19.1.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_base_ut.f90>≡
  <File header>

  module phs_base_ut
    use unit_tests
    use phs_base_uti

    <Standard module head>

    <PHS base: public test>

    <PHS base: public test auxiliary>

    contains

    <PHS base: test driver>

  end module phs_base_ut

<phs_base_uti.f90>≡
  <File header>

  module phs_base_uti

    <Use kinds>
    <Use strings>
    use diagnostics
    use io_units
    use format_defs, only: FMT_19
    use physics_defs, only: BORN
    use lorentz
    use flavors
    use model_data
    use process_constants

    use phs_base

    <Standard module head>

```

```

    <PHS base: public test auxiliary>

    <PHS base: test declarations>

    <PHS base: test types>

contains

    <PHS base: tests>

    <PHS base: test auxiliary>

end module phs_base_util
API: driver for the unit tests below.
<PHS base: public test>≡
    public :: phs_base_test
<PHS base: test driver>≡
    subroutine phs_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS base: execute tests>
    end subroutine phs_base_test

```

Test process data

We provide a procedure that initializes a test case for the process constants. This set of process data contains just the minimal contents that we need for the phase space. The rest is left uninitialized.

```

<PHS base: public test auxiliary>≡
    public :: init_test_process_data
<PHS base: test auxiliary>≡
    subroutine init_test_process_data (id, data)
        type(process_constants_t), intent(out) :: data
        type(string_t), intent(in), optional :: id
        if (present (id)) then
            data%id = id
        else
            data%id = "testproc"
        end if
        data%model_name = "Test"
        data%n_in = 2
        data%n_out = 2
        data%n_flv = 1
        allocate (data%flv_state (data%n_in + data%n_out, data%n_flv))
        data%flv_state = 25
    end subroutine init_test_process_data

```

This is the variant for a decay process.

```

<PHS base: public test auxiliary>+≡
    public :: init_test_decay_data

```

```

<PHS base: test auxiliary>+≡
subroutine init_test_decay_data (id, data)
  type(process_constants_t), intent(out) :: data
  type(string_t), intent(in), optional :: id
  if (present (id)) then
    data%id = id
  else
    data%id = "testproc"
  end if
  data%model_name = "Test"
  data%n_in = 1
  data%n_out = 2
  data%n_flv = 1
  allocate (data%flv_state (data%n_in + data%n_out, data%n_flv))
  data%flv_state(:,1) = [25, 6, -6]
end subroutine init_test_decay_data

```

Test kinematics configuration

This is a trivial implementation of the `phs_config_t` configuration object.

```

<PHS base: public test auxiliary>+≡
  public :: phs_test_config_t

<PHS base: test types>≡
type, extends (phs_config_t) :: phs_test_config_t
  logical :: create_equivalences = .false.
contains
  procedure :: final => phs_test_config_final
  procedure :: write => phs_test_config_write
  procedure :: configure => phs_test_config_configure
  procedure :: startup_message => phs_test_config_startup_message
  procedure, nopass :: allocate_instance => phs_test_config_allocate_instance
end type phs_test_config_t

```

The finalizer is empty.

```

<PHS base: test auxiliary>+≡
subroutine phs_test_config_final (object)
  class(phs_test_config_t), intent(inout) :: object
end subroutine phs_test_config_final

```

The `lab_is_cm` parameter is not tested here; we defer this to the `phs_single` implementation.

```

<PHS base: test auxiliary>+≡
subroutine phs_test_config_write (object, unit, include_id)
  class(phs_test_config_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: include_id
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Partonic phase-space configuration:"
  call object%base_write (unit)
end subroutine phs_test_config_write

```

```

subroutine phs_test_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
class(phs_test_config_t), intent(inout) :: phs_config
real(default), intent(in) :: sqrts
logical, intent(in), optional :: sqrts_fixed
logical, intent(in), optional :: lab_is_cm
logical, intent(in), optional :: azimuthal_dependence
logical, intent(in), optional :: rebuild
logical, intent(in), optional :: ignore_mismatch
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: subdir
phs_config%n_channel = 2
phs_config%n_par = 2
phs_config%sqrts = sqrts
if (.not. present (nlo_type)) &
    phs_config%nlo_type = BORN
if (present (sqrts_fixed)) then
    phs_config%sqrts_fixed = sqrts_fixed
end if
if (present (lab_is_cm)) then
    phs_config%lab_is_cm = lab_is_cm
end if
if (present (azimuthal_dependence)) then
    phs_config%azimuthal_dependence = azimuthal_dependence
end if
if (allocated (phs_config%channel)) deallocate (phs_config%channel)
allocate (phs_config%channel (phs_config%n_channel))
if (phs_config%create_equivalences) then
    call setup_test_equivalences (phs_config)
    call setup_test_channel_props (phs_config)
end if
call phs_config%compute_md5sum ()
end subroutine phs_test_config_configure

```

If requested, we make up an arbitrary set of equivalences.

(PHS base: test auxiliary)+≡

```

subroutine setup_test_equivalences (phs_config)
class(phs_test_config_t), intent(inout) :: phs_config
integer :: i
associate (channel => phs_config%channel(1))
    allocate (channel%eq (2))
    do i = 1, size (channel%eq)
        call channel%eq(i)%init (phs_config%n_par)
    end do
    associate (eq => channel%eq(1))
        eq%c = 1; eq%perm = [1, 2]; eq%mode = [EQ_IDENTITY, EQ_SYMMETRIC]
    end associate
    associate (eq => channel%eq(2))
        eq%c = 2; eq%perm = [2, 1]; eq%mode = [EQ_INVARIANT, EQ_IDENTITY]
    end associate
end associate
end subroutine setup_test_equivalences

```


Ditto, for channel properties.

```

(PHS base: test auxiliary)+≡
  subroutine setup_test_channel_props (phs_config)
    class(phs_test_config_t), intent(inout) :: phs_config
    associate (channel => phs_config%channel(2))
      call channel%set_resonant (140._default, 3.1415_default)
    end associate
  end subroutine setup_test_channel_props

```

Startup message

```

(PHS base: test auxiliary)+≡
  subroutine phs_test_config_startup_message (phs_config, unit)
    class(phs_test_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
    call phs_config%base_startup_message (unit)
    write (msg_buffer, "(A)") "Phase space: Test"
    call msg_message (unit = unit)
  end subroutine phs_test_config_startup_message

```

The instance type that matches `phs_test_config_t` is `phs_test_t`.

```

(PHS base: test auxiliary)+≡
  subroutine phs_test_config_allocate_instance (phs)
    class(phs_t), intent(inout), pointer :: phs
    allocate (phs_test_t :: phs)
  end subroutine phs_test_config_allocate_instance

```

Test kinematics implementation

This implementation of kinematics generates a simple two-particle configuration from the incoming momenta. The incoming momenta must be in the c.m. system, all masses equal.

There are two channels: one generates $\cos\theta$ and ϕ uniformly, in the other channel we map the r_1 parameter which belongs to $\cos\theta$.

We should store the mass parameter that we need.

```

(PHS base: public test auxiliary)+≡
  public :: phs_test_t

(PHS base: test types)+≡
  type, extends (phs_t) :: phs_test_t
    real(default) :: m = 0
    real(default), dimension(:), allocatable :: x
  contains
    (PHS base: phs test: TBP)
  end type phs_test_t

```

Output. The specific data are displayed only if `verbose` is set.

```

(PHS base: phs test: TBP)≡
  procedure :: write => phs_test_write

```

```

<PHS base: test auxiliary>+≡
  subroutine phs_test_write (object, unit, verbose)
    class(phs_test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    logical :: verb
    u = given_output_unit (unit)
    verb = .false.; if (present (verbose)) verb = verbose
    if (verb) then
      write (u, "(1x,A)") "Partonic phase space: data"
      write (u, "(3x,A," // FMT_19 // ")") "m = ", object%m
    end if
    call object%base_write (u)
  end subroutine phs_test_write

```

The finalizer is empty.

```

<PHS base: phs test: TBP>+≡
  procedure :: final => phs_test_final

<PHS base: test auxiliary>+≡
  subroutine phs_test_final (object)
    class(phs_test_t), intent(inout) :: object
  end subroutine phs_test_final

```

Initialization: set the mass value.

```

<PHS base: phs test: TBP>+≡
  procedure :: init => phs_test_init

<PHS base: test auxiliary>+≡
  subroutine phs_test_init (phs, phs_config)
    class(phs_test_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
    phs%m = phs%config%flv(1,1)%get_mass ()
    allocate (phs%x (phs_config%n_par), source = 0._default)
  end subroutine phs_test_init

```

Evaluation. In channel 1, we uniformly generate $\cos\theta$ and ϕ , with Jacobian normalized to one. In channel 2, we prepend a mapping $r_1 \rightarrow r_1^{(1/3)}$ with Jacobian $f = 3r_1^2$.

The component **x** is allocated in the first subroutine, used and deallocated in the second one.

```

<PHS base: phs test: TBP>+≡
  procedure :: evaluate_selected_channel => phs_test_evaluate_selected_channel
  procedure :: evaluate_other_channels => phs_test_evaluate_other_channels

<PHS base: test auxiliary>+≡
  subroutine phs_test_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_test_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    if (phs%p_defined) then

```

```

        call phs%select_channel (c_in)
        phs%r(:,c_in) = r_in
        select case (c_in)
        case (1)
            phs%x = r_in
        case (2)
            phs%x(1) = r_in(1) ** (1 / 3._default)
            phs%x(2) = r_in(2)
        end select
        call compute_kinematics_solid_angle (phs%p, phs%q, phs%x)
        phs%volume = 1
        phs%q_defined = .true.
    end if
end subroutine phs_test_evaluate_selected_channel

subroutine phs_test_evaluate_other_channels (phs, c_in)
    class(phs_test_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    integer :: c, n_channel
    if (phs%p_defined) then
        n_channel = phs%config%n_channel
        do c = 1, n_channel
            if (c /= c_in) then
                call inverse_kinematics_solid_angle (phs%p, phs%q, phs%x)
                select case (c)
                case (1)
                    phs%r(:,c) = phs%x
                case (2)
                    phs%r(1,c) = phs%x(1) ** 3
                    phs%r(2,c) = phs%x(2)
                end select
            end if
        end do
        phs%f(1) = 1
        if (phs%r(1,2) /= 0) then
            phs%f(2) = 1 / (3 * phs%r(1,2) ** (2/3._default))
        else
            phs%f(2) = 0
        end if
        phs%r_defined = .true.
    end if
end subroutine phs_test_evaluate_other_channels

```

Inverse evaluation.

```

<PHS base: phs test: TBP>+≡
    procedure :: inverse => phs_test_inverse

<PHS base: test auxiliary>+≡
    subroutine phs_test_inverse (phs)
        class(phs_test_t), intent(inout) :: phs
        integer :: c, n_channel
        real(default), dimension(:), allocatable :: x
        if (phs%p_defined .and. phs%q_defined) then
            call phs%select_channel ()

```

```

n_channel = phs%config%n_channel
allocate (x (phs%config%n_par))
do c = 1, n_channel
  call inverse_kinematics_solid_angle (phs%p, phs%q, x)
  select case (c)
  case (1)
    phs%r(:,c) = x
  case (2)
    phs%r(1,c) = x(1) ** 3
    phs%r(2,c) = x(2)
  end select
end do
phs%f(1) = 1
if (phs%r(1,2) /= 0) then
  phs%f(2) = 1 / (3 * phs%r(1,2) ** (2/3._default))
else
  phs%f(2) = 0
end if
phs%volume = 1
phs%r_defined = .true.
end if
end subroutine phs_test_inverse

```

Phase-space configuration data

Construct and display a test phase-space configuration object.

```

<PHS base: execute tests>≡
  call test (phs_base_1, "phs_base_1", &
    "phase-space configuration", &
    u, results)

<PHS base: test declarations>≡
  public :: phs_base_1

<PHS base: tests>≡
  subroutine phs_base_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable :: phs_data

    write (u, "(A)")  "* Test output: phs_base_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test phase-space configuration data"
    write (u, "(A)")

    call model%init_test ()

    write (u, "(A)")  "* Initialize a process and a matching &
      &phase-space configuration"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_base_1"), process_data)

```

```

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_1"

end subroutine phs_base_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS base: execute tests>+≡
call test (phs_base_2, "phs_base_2", &
  "phase-space evaluation", &
  u, results)

<PHS base: test declarations>+≡
public :: phs_base_2

<PHS base: tests>+≡
subroutine phs_base_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(process_constants_t) :: process_data
  real(default) :: sqrts, E
  class(phs_config_t), allocatable, target :: phs_data
  class(phs_t), pointer :: phs => null ()
  type(vector4_t), dimension(2) :: p, q

  write (u, "(A)")  "* Test output: phs_base_2"
  write (u, "(A)")  "* Purpose: test simple two-channel phase space"
  write (u, "(A)")

  call model%init_test ()
  call flv%init (25, model)

  write (u, "(A)")  "* Initialize a process and a matching &
    &phase-space configuration"
  write (u, "(A)")

  call init_test_process_data (var_str ("phs_base_2"), process_data)

  allocate (phs_test_config_t :: phs_data)
  call phs_data%init (process_data, model)

  sqrts = 1000._default
  call phs_data%configure (sqrts)

```

```

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
select type (phs)
type is (phs_test_t)
    call phs%init (phs_data)
end select

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrt(s) / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E,-sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point in channel 1 &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point in channel 2 &
    &for x = 0.125, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (2, [0.125_default, 0.125_default])
call phs%evaluate_other_channels (2)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrt(s) = 1000._default

```

```

select type (phs_data)
type is (phs_test_config_t)
    call phs_data%configure (sqrts)
end select

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_2"

end subroutine phs_base_2

```

Phase-space equivalences

Construct a test phase-space configuration which contains channel equivalences.

```

<PHS base: execute tests>+≡
    call test (phs_base_3, "phs_base_3", &
        "channel equivalences", &
        u, results)

<PHS base: test declarations>+≡
    public :: phs_base_3

<PHS base: tests>+≡
    subroutine phs_base_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data

        write (u, "(A)")  "* Test output: phs_base_3"
        write (u, "(A)")  "* Purpose: construct phase-space configuration data &
            &with equivalences"
        write (u, "(A)")

        call model%init_test ()

        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_base_3"), process_data)

```

```

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_test_config_t)
    phs_data%create_equivalences = .true.
end select

call phs_data%configure (1000._default)
call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_3"

end subroutine phs_base_3

```

MD5 sum checks

Construct a test phase-space configuration, compute and compare MD5 sums.

```

<PHS base: execute tests>+≡
    call test (phs_base_4, "phs_base_4", &
        "MD5 sum", &
        u, results)

<PHS base: test declarations>+≡
    public :: phs_base_4

<PHS base: tests>+≡
    subroutine phs_base_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data

        write (u, "(A)")  "* Test output: phs_base_4"
        write (u, "(A)")  "* Purpose: compute and compare MD5 sums"
        write (u, "(A)")

        call model%init_test ()

        write (u, "(A)")  "* Model parameters"
        write (u, "(A)")

        call model%write (unit = u, &
            show_parameters = .true., &
            show_particles = .false., show_vertices = .false.)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

```



```

call init_test_process_data (var_str ("phs_base_4"), process_data)
process_data%md5sum = "test_process_data_m6sum_12345678"

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%compute_md5sum ()
call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Modify model parameter"
write (u, "(A)")

call model%set_par (var_str ("ms"), 100._default)
call model%write (show_parameters = .true., &
    show_particles = .false., show_vertices = .false.)

write (u, "(A)")
write (u, "(A)")  "* PHS configuration"
write (u, "(A)")

call phs_data%compute_md5sum ()
call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_4"

end subroutine phs_base_4

```

Phase-space channel collection

Set up an array of various phase-space channels and collect them in a list.

```

<PHS base: execute tests>+≡
    call test (phs_base_5, "phs_base_5", &
        "channel collection", &
        u, results)

<PHS base: test declarations>+≡
    public :: phs_base_5

<PHS base: tests>+≡
    subroutine phs_base_5 (u)
        integer, intent(in) :: u
        type(phs_channel_t), dimension(:), allocatable :: channel
        type(phs_channel_collection_t) :: coll
        integer :: i, n

        write (u, "(A)")  "* Test output: phs_base_5"
        write (u, "(A)")  "* Purpose: collect channel properties"
        write (u, "(A)")

```

```

write (u, "(A)")  "* Set up an array of channels"
write (u, "(A)")

n = 6

allocate (channel (n))
call channel(2)%set_resonant (75._default, 3._default)
call channel(4)%set_resonant (130._default, 1._default)
call channel(5)%set_resonant (75._default, 3._default)
call channel(6)%set_on_shell (33._default)

do i = 1, n
    write (u, "(1x,I0)", advance="no") i
    call channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Collect distinct properties"
write (u, "(A)")

do i = 1, n
    call coll%push (channel(i))
end do

write (u, "(1x,A,I0)")  "n = ", coll%get_n ()
write (u, "(A)")

call coll%write (u)

write (u, "(A)")
write (u, "(A)")  "* Channel array with collection index assigned"
write (u, "(A)")

do i = 1, n
    write (u, "(1x,I0)", advance="no") i
    call channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call coll%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_5"

end subroutine phs_base_5

```

19.2 Dummy phase space

This module implements a dummy phase space module for cases where the program structure demands the existence of a phase-space module, but no phase space integration is performed.

```
<phs_none.f90>≡  
  <File header>  
  
  module phs_none  
  
    <Use kinds>  
    <Use strings>  
    use phs_base, only: phs_config_t, phs_t  
  
    <Standard module head>  
  
    <PHS none: public>  
  
    <PHS none: types>  
  
    interface  
    <PHS none: sub interfaces>  
    end interface  
  
    contains  
  
    <PHS none: main procedures>  
  
  end module phs_none  
  
<phs_none_sub.f90>≡  
  <File header>  
  
  submodule (phs_none) phs_none_s  
  
    use io_units, only: given_output_unit  
    use diagnostics, only: msg_message, msg_fatal  
  
    implicit none  
  
    contains  
  
    <PHS none: procedures>  
  
  end submodule phs_none_s
```

19.2.1 Configuration

Nothing to configure, but we provide the type and methods.

```
<PHS none: public>≡  
  public :: phs_none_config_t
```

```

<PHS none: types>≡
  type, extends (phs_config_t) :: phs_none_config_t
  contains
  <PHS none: phs none config: TBP>
  end type phs_none_config_t

```

The finalizer is empty.

```

<PHS none: phs none config: TBP>≡
  procedure :: final => phs_none_config_final

<PHS none: sub interfaces>≡
  module subroutine phs_none_config_final (object)
    class(phs_none_config_t), intent(inout) :: object
  end subroutine phs_none_config_final

<PHS none: procedures>≡
  module subroutine phs_none_config_final (object)
    class(phs_none_config_t), intent(inout) :: object
  end subroutine phs_none_config_final

```

Output. No contents, just an informative line.

```

<PHS none: phs none config: TBP>+≡
  procedure :: write => phs_none_config_write

<PHS none: sub interfaces>+≡
  module subroutine phs_none_config_write (object, unit, include_id)
    class(phs_none_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
  end subroutine phs_none_config_write

<PHS none: procedures>+≡
  module subroutine phs_none_config_write (object, unit, include_id)
    class(phs_none_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") &
      "Partonic phase-space configuration: non-functional dummy"
  end subroutine phs_none_config_write

```

Configuration: we have to implement this method, but it obviously does nothing.

```

<PHS none: phs none config: TBP>+≡
  procedure :: configure => phs_none_config_configure

<PHS none: sub interfaces>+≡
  module subroutine phs_none_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
    class(phs_none_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence

```

```

        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        integer, intent(in), optional :: nlo_type
        type(string_t), intent(in), optional :: subdir
    end subroutine phs_none_config_configure
<PHS none: procedures>+≡
    module subroutine phs_none_config_configure (phs_config, sqrts, &
        sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
        ignore_mismatch, nlo_type, subdir)
        class(phs_none_config_t), intent(inout) :: phs_config
        real(default), intent(in) :: sqrts
        logical, intent(in), optional :: sqrts_fixed
        logical, intent(in), optional :: lab_is_cm
        logical, intent(in), optional :: azimuthal_dependence
        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        integer, intent(in), optional :: nlo_type
        type(string_t), intent(in), optional :: subdir
    end subroutine phs_none_config_configure

Startup message, after configuration is complete.
<PHS none: phs none config: TBP>+≡
    procedure :: startup_message => phs_none_config_startup_message
<PHS none: sub interfaces>+≡
    module subroutine phs_none_config_startup_message (phs_config, unit)
        class(phs_none_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
    end subroutine phs_none_config_startup_message
<PHS none: procedures>+≡
    module subroutine phs_none_config_startup_message (phs_config, unit)
        class(phs_none_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        call msg_message ("Phase space: none")
    end subroutine phs_none_config_startup_message

```

Allocate an instance: the actual phase-space object. Gfortran 7/8/9 bug: has to remain in the main module.

```

<PHS none: phs none config: TBP>+≡
    procedure, nopass :: allocate_instance => phs_none_config_allocate_instance
<PHS none: main procedures>≡
    subroutine phs_none_config_allocate_instance (phs)
        class(phs_t), intent(inout), pointer :: phs
        allocate (phs_none_t :: phs)
    end subroutine phs_none_config_allocate_instance

```

19.2.2 Kinematics implementation

This is considered as empty, but we have to implement the minimal set of methods.

```

<PHS none: public>+≡

```

```

    public :: phs_none_t
  <PHS none: types>+≡
    type, extends (phs_t) :: phs_none_t
    contains
    <PHS none: phs none: TBP>
  end type phs_none_t

```

Output.

```

  <PHS none: phs none: TBP>≡
    procedure :: write => phs_none_write

  <PHS none: sub interfaces>+≡
    module subroutine phs_none_write (object, unit, verbose)
      class(phs_none_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: verbose
    end subroutine phs_none_write

  <PHS none: procedures>+≡
    module subroutine phs_none_write (object, unit, verbose)
      class(phs_none_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: verbose
      integer :: u
      u = given_output_unit (unit)
      write (u, "(A)") "Partonic phase space: none"
    end subroutine phs_none_write

```

The finalizer is empty.

```

  <PHS none: phs none: TBP>+≡
    procedure :: final => phs_none_final

  <PHS none: sub interfaces>+≡
    module subroutine phs_none_final (object)
      class(phs_none_t), intent(inout) :: object
    end subroutine phs_none_final

  <PHS none: procedures>+≡
    module subroutine phs_none_final (object)
      class(phs_none_t), intent(inout) :: object
    end subroutine phs_none_final

```

Initialization, trivial.

```

  <PHS none: phs none: TBP>+≡
    procedure :: init => phs_none_init

  <PHS none: sub interfaces>+≡
    module subroutine phs_none_init (phs, phs_config)
      class(phs_none_t), intent(out) :: phs
      class(phs_config_t), intent(in), target :: phs_config
    end subroutine phs_none_init

```

```

<PHS none: procedures>+≡
  module subroutine phs_none_init (phs, phs_config)
    class(phs_none_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
  end subroutine phs_none_init

```

Evaluation. This must not be called at all.

```

<PHS none: phs none: TBP>+≡
  procedure :: evaluate_selected_channel => phs_none_evaluate_selected_channel
  procedure :: evaluate_other_channels => phs_none_evaluate_other_channels

```

```

<PHS none: sub interfaces>+≡
  module subroutine phs_none_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
  end subroutine phs_none_evaluate_selected_channel
  module subroutine phs_none_evaluate_other_channels (phs, c_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
  end subroutine phs_none_evaluate_other_channels

```

```

<PHS none: procedures>+≡
  module subroutine phs_none_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    call msg_fatal &
      ("Phase space: attempt to evaluate with the 'phs_none' method")
  end subroutine phs_none_evaluate_selected_channel

  module subroutine phs_none_evaluate_other_channels (phs, c_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
  end subroutine phs_none_evaluate_other_channels

```

Inverse evaluation, likewise.

```

<PHS none: phs none: TBP>+≡
  procedure :: inverse => phs_none_inverse

```

```

<PHS none: sub interfaces>+≡
  module subroutine phs_none_inverse (phs)
    class(phs_none_t), intent(inout) :: phs
  end subroutine phs_none_inverse

```

```

<PHS none: procedures>+≡
  module subroutine phs_none_inverse (phs)
    class(phs_none_t), intent(inout) :: phs
    call msg_fatal ("Phase space: attempt to evaluate inverse " // &
      "with the 'phs_none' method")
  end subroutine phs_none_inverse

```

19.2.3 Unit tests

Test module, followed by the corresponding implementation module.

```
<phs_none_ut.f90>≡  
  <File header>  
  
  module phs_none_ut  
    use unit_tests  
    use phs_none_ut_i  
  
    <Standard module head>  
  
    <PHS none: public test>  
  
    contains  
  
    <PHS none: test driver>  
  
  end module phs_none_ut  
  
<phs_none_ut_i.f90>≡  
  <File header>  
  
  module phs_none_ut_i  
  
    <Use kinds>  
    <Use strings>  
    use flavors  
    use lorentz  
    use model_data  
    use process_constants  
    use phs_base  
  
    use phs_none  
  
    use phs_base_ut, only: init_test_process_data, init_test_decay_data  
  
    <Standard module head>  
  
    <PHS none: test declarations>  
  
    contains  
  
    <PHS none: tests>  
  
  end module phs_none_ut_i  
API: driver for the unit tests below.  
<PHS none: public test>≡  
  public :: phs_none_test  
<PHS none: test driver>≡  
  subroutine phs_none_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <PHS none: execute tests>
```



```
end subroutine phs_none_test
```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal_dependence flag.

```
(PHS none: execute tests)≡
  call test (phs_none_1, "phs_none_1", &
    "phase-space configuration dummy", &
    u, results)

(PHS none: test declarations)≡
  public :: phs_none_1

(PHS none: tests)≡
  subroutine phs_none_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable :: phs_data
    real(default) :: sqrts

    write (u, "(A)")  "* Test output: phs_none_1"
    write (u, "(A)")  "* Purpose: display &
      &phase-space configuration data"
    write (u, "(A)")

    allocate (phs_none_config_t :: phs_data)
    call phs_data%init (process_data, model)

    sqrts = 1000._default
    call phs_data%configure (sqrts, azimuthal_dependence=.false.)

    call phs_data%write (u)

    call phs_data%final ()
    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: phs_none_1"

  end subroutine phs_none_1
```

19.3 Single-particle phase space

This module implements the phase space for a single particle, i.e., the solid angle, in a straightforward parameterization with a single channel. The phase-space implementation may be used either for $1 \rightarrow 2$ decays or for $2 \rightarrow 2$ scattering processes, so the number of incoming particles is the only free parameter in the configuration. In the latter case, we should restrict its use to non-resonant s-channel processes, because there is no mapping of the scattering angle.

(We might extend this later to account for generic $2 \rightarrow 2$ situations, e.g., account for a Coulomb singularity or detect an s-channel resonance structure that requires matching structure-function mappings.)

This is derived from the `phs_test` implementation in the `phs_base` module above, even more simplified, but intended for actual use.

```
<phs_single.f90>≡  
  <File header>  
  
  module phs_single  
  
    <Use kinds>  
    <Use strings>  
    use lorentz  
    use phs_base  
  
    <Standard module head>  
  
    <PHS single: public>  
  
    <PHS single: types>  
  
    interface  
    <PHS single: sub interfaces>  
    end interface  
  
    contains  
  
    <PHS single: main procedures>  
  
  end module phs_single  
<phs_single_sub.f90>≡  
  <File header>  
  
  submodule (phs_single) phs_single_s  
  
    use io_units  
    use constants  
    use numeric_utils  
    use diagnostics  
    use physics_defs  
  
    implicit none  
  
    contains
```

```

    <PHS single: procedures>

end submodule phs_single_s

```

19.3.1 Configuration

```

<PHS single: public>≡
    public :: phs_single_config_t

<PHS single: types>≡
    type, extends (phs_config_t) :: phs_single_config_t
    contains
    <PHS single: phs single config: TBP>
end type phs_single_config_t

```

The finalizer is empty.

```

<PHS single: phs single config: TBP>≡
    procedure :: final => phs_single_config_final

<PHS single: sub interfaces>≡
    module subroutine phs_single_config_final (object)
        class(phs_single_config_t), intent(inout) :: object
    end subroutine phs_single_config_final

<PHS single: procedures>≡
    module subroutine phs_single_config_final (object)
        class(phs_single_config_t), intent(inout) :: object
    end subroutine phs_single_config_final

```

Output.

```

<PHS single: phs single config: TBP>+≡
    procedure :: write => phs_single_config_write

<PHS single: sub interfaces>+≡
    module subroutine phs_single_config_write (object, unit, include_id)
        class(phs_single_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
    end subroutine phs_single_config_write

<PHS single: procedures>+≡
    module subroutine phs_single_config_write (object, unit, include_id)
        class(phs_single_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Partonic phase-space configuration (single-particle):"
        call object%base_write (unit)
    end subroutine phs_single_config_write

```

Configuration: there is only one channel and two parameters. The second parameter is the azimuthal angle, which may be a flat dimension.

(PHS single: phs single config: TBP)+≡

```
procedure :: configure => phs_single_config_configure
```

(PHS single: sub interfaces)+≡

```
module subroutine phs_single_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
class(phs_single_config_t), intent(inout) :: phs_config
real(default), intent(in) :: sqrts
logical, intent(in), optional :: sqrts_fixed
logical, intent(in), optional :: lab_is_cm
logical, intent(in), optional :: azimuthal_dependence
logical, intent(in), optional :: rebuild
logical, intent(in), optional :: ignore_mismatch
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: subdir
end subroutine phs_single_config_configure
```

(PHS single: procedures)+≡

```
module subroutine phs_single_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
class(phs_single_config_t), intent(inout) :: phs_config
real(default), intent(in) :: sqrts
logical, intent(in), optional :: sqrts_fixed
logical, intent(in), optional :: lab_is_cm
logical, intent(in), optional :: azimuthal_dependence
logical, intent(in), optional :: rebuild
logical, intent(in), optional :: ignore_mismatch
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: subdir
if (.not. present (nlo_type)) &
    phs_config%nlo_type = BORN
if (phs_config%n_out == 2) then
    phs_config%n_channel = 1
    phs_config%n_par = 2
    phs_config%sqrts = sqrts
    if (present (sqrts_fixed)) phs_config%sqrts_fixed = sqrts_fixed
    if (present (lab_is_cm)) phs_config%lab_is_cm = lab_is_cm
    if (present (azimuthal_dependence)) then
        phs_config%azimuthal_dependence = azimuthal_dependence
        if (.not. azimuthal_dependence) then
            allocate (phs_config%dim_flat (1))
            phs_config%dim_flat(1) = 2
        end if
    end if
    if (allocated (phs_config%channel)) deallocate (phs_config%channel)
    allocate (phs_config%channel (1))
    call phs_config%compute_md5sum ()
else
    call msg_fatal ("Single-particle phase space requires n_out = 2")
end if
end subroutine phs_single_config_configure
```

Startup message, after configuration is complete.

```

<PHS single: phs single config: TBP>+≡
  procedure :: startup_message => phs_single_config_startup_message

<PHS single: sub interfaces>+≡
  module subroutine phs_single_config_startup_message (phs_config, unit)
    class(phs_single_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
  end subroutine phs_single_config_startup_message

<PHS single: procedures>+≡
  module subroutine phs_single_config_startup_message (phs_config, unit)
    class(phs_single_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
    call phs_config%base_startup_message (unit)
    write (msg_buffer, "(A,2(1x,I0,1x,A))") &
      "Phase space: single-particle"
    call msg_message (unit = unit)
  end subroutine phs_single_config_startup_message

```

Allocate an instance: the actual phase-space object. Gfortran 7/8/9 bug, has to remain in the main module.

```

<PHS single: phs single config: TBP>+≡
  procedure, nopass :: allocate_instance => phs_single_config_allocate_instance

<PHS single: main procedures>≡
  subroutine phs_single_config_allocate_instance (phs)
    class(phs_t), intent(inout), pointer :: phs
    allocate (phs_single_t :: phs)
  end subroutine phs_single_config_allocate_instance

```

19.3.2 Kinematics implementation

We generate $\cos\theta$ and ϕ uniformly, covering the solid angle.

Note: The incoming momenta must be in the c.m. system.

```

<PHS single: public>+≡
  public :: phs_single_t

<PHS single: types>+≡
  type, extends (phs_t) :: phs_single_t
  contains
    <PHS single: phs single: TBP>
  end type phs_single_t

```

Output. The `verbose` setting is irrelevant, we just display the contents of the base object.

```

<PHS single: phs single: TBP>≡
  procedure :: write => phs_single_write

```

```

<PHS single: sub interfaces>+≡
  module subroutine phs_single_write (object, unit, verbose)
    class(phs_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine phs_single_write
<PHS single: procedures>+≡
  module subroutine phs_single_write (object, unit, verbose)
    class(phs_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    call object%base_write (u)
  end subroutine phs_single_write

```

The finalizer is empty.

```

<PHS single: phs single: TBP>+≡
  procedure :: final => phs_single_final
<PHS single: sub interfaces>+≡
  module subroutine phs_single_final (object)
    class(phs_single_t), intent(inout) :: object
  end subroutine phs_single_final
<PHS single: procedures>+≡
  module subroutine phs_single_final (object)
    class(phs_single_t), intent(inout) :: object
  end subroutine phs_single_final

```

Initialization. We allocate arrays (`base_init`) and adjust the phase-space volume. The massless two-particle phase space volume is

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.55294034614 \times 10^{-5} \quad (19.5)$$

For a decay with nonvanishing masses (m_3, m_4), there is a correction factor

$$\Phi_2(m)/\Phi_2(0) = \frac{1}{\hat{s}} \lambda^{1/2}(\hat{s}, m_3^2, m_4^2). \quad (19.6)$$

For a scattering process with nonvanishing masses, the correction factor is

$$\Phi_2(m)/\Phi_2(0) = \frac{1}{\hat{s}^2} \lambda^{1/2}(\hat{s}, m_1^2, m_2^2) \lambda^{1/2}(\hat{s}, m_3^2, m_4^2). \quad (19.7)$$

If the energy is fixed, this is constant. Otherwise, we have to account for varying \hat{s} .

```

<PHS single: phs single: TBP>+≡
  procedure :: init => phs_single_init
<PHS single: sub interfaces>+≡
  module subroutine phs_single_init (phs, phs_config)
    class(phs_single_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
  end subroutine phs_single_init

```

```

<PHS single: procedures>+≡
module subroutine phs_single_init (phs, phs_config)
  class(phs_single_t), intent(out) :: phs
  class(phs_config_t), intent(in), target :: phs_config
  call phs%base_init (phs_config)
  phs%volume = 1 / (4 * twopi5)
  call phs%compute_factor ()
end subroutine phs_single_init

```

Compute the correction factor for nonzero masses. We do this during initialization (when the incoming momenta p are undefined), unless `sqrts` is variable. We do this again once for each phase-space point, but then we skip the calculation if `sqrts` is fixed.

```

<PHS single: phs single: TBP>+≡
  procedure :: compute_factor => phs_single_compute_factor

<PHS single: sub interfaces>+≡
  module subroutine phs_single_compute_factor (phs)
    class(phs_single_t), intent(inout) :: phs
  end subroutine phs_single_compute_factor

<PHS single: procedures>+≡
module subroutine phs_single_compute_factor (phs)
  class(phs_single_t), intent(inout) :: phs
  real(default) :: s_hat
  select case (phs%config%n_in)
  case (1)
    if (.not. phs%p_defined) then
      if (sum (phs%m_out) < phs%m_in(1)) then
        s_hat = phs%m_in(1) ** 2
        phs%f(1) = 1 / s_hat &
          * sqrt (lambda (s_hat, phs%m_out(1)**2, phs%m_out(2)**2))
      else
        print *, "m_in = ", phs%m_in
        print *, "m_out = ", phs%m_out
        call msg_fatal ("Decay is kinematically forbidden")
      end if
    end if
  case (2)
    if (phs%config%sqrts_fixed) then
      if (phs%p_defined) return
      s_hat = phs%config%sqrts ** 2
    else
      if (.not. phs%p_defined) return
      s_hat = sum (phs%p) ** 2
    end if
    if (sum (phs%m_in)**2 < s_hat .and. sum (phs%m_out)**2 < s_hat) then
      phs%f(1) = 1 / s_hat * &
        ( lambda (s_hat, phs%m_in (1)**2, phs%m_in (2)**2) &
          * lambda (s_hat, phs%m_out(1)**2, phs%m_out(2)**2) ) &
        ** 0.25_default
    else
      phs%f(1) = 0
    end if
  end if
end if

```

```

        end select
    end subroutine phs_single_compute_factor

```

Evaluation. We uniformly generate $\cos\theta$ and ϕ , with Jacobian normalized to one.

There is only a single channel, so the second subroutine does nothing.

Note: the current implementation works for elastic scattering only.

```

<PHS single: phs single: TBP>+≡
    procedure :: evaluate_selected_channel => phs_single_evaluate_selected_channel
    procedure :: evaluate_other_channels => phs_single_evaluate_other_channels

<PHS single: sub interfaces>+≡
    module subroutine phs_single_evaluate_selected_channel (phs, c_in, r_in)
        class(phs_single_t), intent(inout) :: phs
        integer, intent(in) :: c_in
        real(default), intent(in), dimension(:) :: r_in
    end subroutine phs_single_evaluate_selected_channel
    module subroutine phs_single_evaluate_other_channels (phs, c_in)
        class(phs_single_t), intent(inout) :: phs
        integer, intent(in) :: c_in
    end subroutine phs_single_evaluate_other_channels

<PHS single: procedures>+≡
    module subroutine phs_single_evaluate_selected_channel (phs, c_in, r_in)
        class(phs_single_t), intent(inout) :: phs
        integer, intent(in) :: c_in
        real(default), intent(in), dimension(:) :: r_in
        if (phs%p_defined) then
            call phs%select_channel (c_in)
            phs%r(:,c_in) = r_in
            select case (phs%config%n_in)
            case (2)
                if (all (phs%m_in == phs%m_out)) then
                    call compute_kinematics_solid_angle (phs%p, phs%q, r_in)
                else
                    call msg_bug ("PHS single: inelastic scattering not implemented")
                end if
            case (1)
                call compute_kinematics_solid_angle (phs%decay_p (), phs%q, r_in)
            end select
            call phs%compute_factor ()
            phs%q_defined = .true.
            phs%r_defined = .true.
        end if
    end subroutine phs_single_evaluate_selected_channel

    module subroutine phs_single_evaluate_other_channels (phs, c_in)
        class(phs_single_t), intent(inout) :: phs
        integer, intent(in) :: c_in
    end subroutine phs_single_evaluate_other_channels

```

Auxiliary: split a decaying particle at rest into the decay products, aligned along the z axis.

```

<PHS single: phs single: TBP>+≡

```



```

    procedure :: decay_p => phs_single_decay_p
<PHS single: sub interfaces>+≡
    module function phs_single_decay_p (phs) result (p)
        class(phs_single_t), intent(in) :: phs
        type(vector4_t), dimension(2) :: p
    end function phs_single_decay_p
<PHS single: procedures>+≡
    module function phs_single_decay_p (phs) result (p)
        class(phs_single_t), intent(in) :: phs
        type(vector4_t), dimension(2) :: p
        real(default) :: k
        real(default), dimension(2) :: E
        k = sqrt (lambda (phs%m_in(1) ** 2, phs%m_out(1) ** 2, phs%m_out(2) ** 2)) &
            / (2 * phs%m_in(1))
        E = sqrt (phs%m_out ** 2 + k ** 2)
        p(1) = vector4_moving (E(1), k, 3)
        p(2) = vector4_moving (E(2), -k, 3)
    end function phs_single_decay_p

```

Inverse evaluation.

```

<PHS single: phs single: TBP>+≡
    procedure :: inverse => phs_single_inverse
<PHS single: sub interfaces>+≡
    module subroutine phs_single_inverse (phs)
        class(phs_single_t), intent(inout) :: phs
    end subroutine phs_single_inverse
<PHS single: procedures>+≡
    module subroutine phs_single_inverse (phs)
        class(phs_single_t), intent(inout) :: phs
        real(default), dimension(:), allocatable :: x
        if (phs%p_defined .and. phs%q_defined) then
            call phs%select_channel ()
            allocate (x (phs%config%n_par))
            call inverse_kinematics_solid_angle (phs%p, phs%q, x)
            phs%r(:,1) = x
            call phs%compute_factor ()
            phs%r_defined = .true.
        end if
    end subroutine phs_single_inverse

```

19.3.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_single_ut.f90>≡
<File header>

    module phs_single_ut
        use unit_tests
        use phs_single_util

```

```

    <Standard module head>

    <PHS single: public test>

    contains

    <PHS single: test driver>

    end module phs_single_ut

    <phs_single_uti.f90>≡
    <File header>

    module phs_single_uti

    <Use kinds>
    <Use strings>
    use flavors
    use lorentz
    use model_data
    use process_constants
    use phs_base

    use phs_single

    use phs_base_ut, only: init_test_process_data, init_test_decay_data

    <Standard module head>

    <PHS single: test declarations>

    contains

    <PHS single: tests>

    end module phs_single_uti
API: driver for the unit tests below.
    <PHS single: public test>≡
    public :: phs_single_test
    <PHS single: test driver>≡
    subroutine phs_single_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <PHS single: execute tests>
    end subroutine phs_single_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal_dependence flag.

```

    <PHS single: execute tests>≡
    call test (phs_single_1, "phs_single_1", &

```

```

        "phase-space configuration", &
        u, results)
<PHS single: test declarations>≡
    public :: phs_single_1
<PHS single: tests>≡
    subroutine phs_single_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data
        real(default) :: sqrts

        write (u, "(A)")  "* Test output: phs_single_1"
        write (u, "(A)")  "*   Purpose: initialize and display &
            &phase-space configuration data"
        write (u, "(A)")

        call model%init_test ()

        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_single_1"), process_data)

        allocate (phs_single_config_t :: phs_data)
        call phs_data%init (process_data, model)

        sqrts = 1000._default
        call phs_data%configure (sqrts, azimuthal_dependence=.false.)

        call phs_data%write (u)

        call phs_data%final ()
        call model%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: phs_single_1"

    end subroutine phs_single_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS single: execute tests>+≡
    call test (phs_single_2, "phs_single_2", &
        "phase-space evaluation", &
        u, results)
<PHS single: test declarations>+≡
    public :: phs_single_2

```

```

<PHS single: tests>+≡
subroutine phs_single_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(process_constants_t) :: process_data
  real(default) :: sqrts, E
  class(phs_config_t), allocatable, target :: phs_data
  class(phs_t), pointer :: phs => null ()
  type(vector4_t), dimension(2) :: p, q

  write (u, "(A)")  "* Test output: phs_single_2"
  write (u, "(A)")  "* Purpose: test simple two-channel phase space"
  write (u, "(A)")

  call model%init_test ()
  call flv%init (25, model)

  write (u, "(A)")  "* Initialize a process and a matching &
    &phase-space configuration"
  write (u, "(A)")

  call init_test_process_data (var_str ("phs_single_2"), process_data)

  allocate (phs_single_config_t :: phs_data)
  call phs_data%init (process_data, model)

  sqrts = 1000._default
  call phs_data%configure (sqrts)

  call phs_data%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize the phase-space instance"
  write (u, "(A)")

  call phs_data%allocate_instance (phs)
  call phs%init (phs_data)

  call phs%write (u, verbose=.true.)

  write (u, "(A)")
  write (u, "(A)")  "* Set incoming momenta"
  write (u, "(A)")

  E = sqrts / 2
  p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
  p(2) = vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

  call phs%set_incoming_momenta (p)
  call phs%compute_flux ()
  call phs%write (u)

  write (u, "(A)")

```

```

write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrt_s = 1000._default
call phs_data%configure (sqrt_s)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_2"

end subroutine phs_single_2

```

Phase space for non-c.m. system

Compute kinematics for given parameters, also invert the calculation. Since this will involve cancellations, we call `pacify` to eliminate numerical noise.

```

<PHS single: execute tests>+≡
    call test (phs_single_3, "phs_single_3", &
        "phase-space evaluation in lab frame", &
        u, results)

<PHS single: test declarations>+≡
    public :: phs_single_3

<PHS single: tests>+≡
    subroutine phs_single_3 (u)
        integer, intent(in) :: u

```

```

type(model_data_t), target :: model
type(flavor_t) :: flv
type(process_constants_t) :: process_data
real(default) :: sqrts, E
class(phs_config_t), allocatable, target :: phs_data
class(phs_t), pointer :: phs => null ()
type(vector4_t), dimension(2) :: p, q
type(lorentz_transformation_t) :: lt

write (u, "(A)")  "* Test output: phs_single_3"
write (u, "(A)")  "* Purpose: test simple two-channel phase space"
write (u, "(A)")  "*           without c.m. kinematics assumption"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)

write (u, "(A)")  "* Initialize a process and a matching &
                  &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_single_3"), process_data)

allocate (phs_single_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts, lab_is_cm=.false., sqrts_fixed=.false.)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta in lab system"
write (u, "(A)")

lt = boost (0.1_default, 1) * boost (0.3_default, 3)

E = sqrts / 2
p(1) = lt * vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = lt * vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call vector4_write (p(1), u)
call vector4_write (p(2), u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call pacify (phs)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract outgoing momenta in lab system"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call vector4_write (q(1), u)
call vector4_write (q(2), u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call pacify (phs)
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_3"

end subroutine phs_single_3

```

Decay Phase space evaluation

Compute kinematics for given parameters, also invert the calculation. This time, implement a decay process.

```
(PHS single: execute tests)+≡
    call test (phs_single_4, "phs_single_4", &
               "decay phase-space evaluation", &
               u, results)

(PHS single: test declarations)+≡
    public :: phs_single_4

(PHS single: tests)+≡
    subroutine phs_single_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(1) :: p
        type(vector4_t), dimension(2) :: q

        write (u, "(A)")  "* Test output: phs_single_4"
        write (u, "(A)")  "* Purpose: test simple two-channel phase space"
        write (u, "(A)")

        call model%init_test ()

        call model%set_par (var_str ("ff"), 0.4_default)
        call model%set_par (var_str ("mf"), &
                           model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))
        call flv%init (25, model)

        write (u, "(A)")  "* Initialize a decay and a matching &
                           &phase-space configuration"
        write (u, "(A)")

        call init_test_decay_data (var_str ("phs_single_4"), process_data)

        allocate (phs_single_config_t :: phs_data)
        call phs_data%init(process_data, model)

        call phs_data%configure (flv%get_mass ())

        call phs_data%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize the phase-space instance"
        write (u, "(A)")

        call phs_data%allocate_instance (phs)
        call phs%init (phs_data)

        call phs%write (u, verbose=.true.)
```



```

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

p(1) = vector4_at_rest (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs_data%configure (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_4"

end subroutine phs_single_4

```

19.4 Flat RAMBO phase space

This module implements the flat **RAMBO** phase space for massless and massive particles using the minimal d.o.f $3n - 4$ in a straightforward parameterization with a single channel. We generate n mass systems M_i with $M_0 = \sqrt{s}$ and $M_n = 0$. We let each mass system decay $1 \rightarrow 2$ in a four-momentum conserving way. The four-momenta of the two particles are generated back-to-back where we map the d.o.f. to energy, azimuthal and polar angle. The particle momenta are then boosted to CMS by an appropriate boost using the kinematics of the parent mass system.

```
<phs_rambo.f90>≡
  <File header>

  module phs_rambo

    <Use kinds>
    <Use strings>
    use lorentz
    use phs_base

    <Standard module head>

    <PHS rambo: types>

    <PHS rambo: public>

    interface
    <PHS rambo: sub interfaces>
    end interface

    contains

    <PHS rambo: main procedures>

  end module phs_rambo

<phs_rambo_sub.f90>≡
  <File header>

  submodule (phs_rambo) phs_rambo_s

    use io_units
    use constants
    use numeric_utils
    use format_defs, only: FMT_19
    use permutations, only: factorial
    use diagnostics
    use physics_defs

    implicit none

    <PHS rambo: parameters>
```

```
contains

<PHS rambo: procedures>

end submodule phs_rambo_s
```

19.4.1 Configuration

```
<PHS rambo: public>≡
  public :: phs_rambo_config_t

<PHS rambo: types>≡
  type, extends (phs_config_t) :: phs_rambo_config_t
  contains
  <PHS rambo: phs rambo config: TBP>
  end type phs_rambo_config_t
```

The finalizer is empty.

```
<PHS rambo: phs rambo config: TBP>≡
  procedure :: final => phs_rambo_config_final

<PHS rambo: sub interfaces>≡
  module subroutine phs_rambo_config_final (object)
    class(phs_rambo_config_t), intent(inout) :: object
  end subroutine phs_rambo_config_final

<PHS rambo: procedures>≡
  module subroutine phs_rambo_config_final (object)
    class(phs_rambo_config_t), intent(inout) :: object
  end subroutine phs_rambo_config_final
```

Output.

```
<PHS rambo: phs rambo config: TBP>+≡
  procedure :: write => phs_rambo_config_write

<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_config_write (object, unit, include_id)
    class(phs_rambo_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
  end subroutine phs_rambo_config_write

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_config_write (object, unit, include_id)
    class(phs_rambo_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Partonic, flat phase-space configuration (RAMBO):"
    call object%base_write (unit)
  end subroutine phs_rambo_config_write
```

Configuration: there is only one channel and $3n - 4$ parameters.

(PHS rambo: phs rambo config: TBP)+≡

```
procedure :: configure => phs_rambo_config_configure
```

(PHS rambo: sub interfaces)+≡

```
module subroutine phs_rambo_config_configure (phs_config, sqrts, &
      sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
      ignore_mismatch, nlo_type, subdir)
  class(phs_rambo_config_t), intent(inout) :: phs_config
  real(default), intent(in) :: sqrts
  logical, intent(in), optional :: sqrts_fixed
  logical, intent(in), optional :: lab_is_cm
  logical, intent(in), optional :: azimuthal_dependence
  logical, intent(in), optional :: rebuild
  logical, intent(in), optional :: ignore_mismatch
  integer, intent(in), optional :: nlo_type
  type(string_t), intent(in), optional :: subdir
end subroutine phs_rambo_config_configure
```

(PHS rambo: procedures)+≡

```
module subroutine phs_rambo_config_configure (phs_config, sqrts, &
      sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
      ignore_mismatch, nlo_type, subdir)
  class(phs_rambo_config_t), intent(inout) :: phs_config
  real(default), intent(in) :: sqrts
  logical, intent(in), optional :: sqrts_fixed
  logical, intent(in), optional :: lab_is_cm
  logical, intent(in), optional :: azimuthal_dependence
  logical, intent(in), optional :: rebuild
  logical, intent(in), optional :: ignore_mismatch
  integer, intent(in), optional :: nlo_type
  type(string_t), intent(in), optional :: subdir
  if (.not. present (nlo_type)) &
    phs_config%nlo_type = BORN
  if (phs_config%n_out < 2) then
    call msg_fatal ("RAMBO phase space requires n_out >= 2")
  end if
  phs_config%n_channel = 1
  phs_config%n_par = 3 * phs_config%n_out - 4
  phs_config%sqrts = sqrts
  if (present (sqrts_fixed)) phs_config%sqrts_fixed = sqrts_fixed
  if (present (lab_is_cm)) phs_config%lab_is_cm = lab_is_cm
  if (allocated (phs_config%channel)) deallocate (phs_config%channel)
  allocate (phs_config%channel (1))
  call phs_config%compute_md5sum ()
end subroutine phs_rambo_config_configure
```

Startup message, after configuration is complete.

(PHS rambo: phs rambo config: TBP)+≡

```
procedure :: startup_message => phs_rambo_config_startup_message
```

(PHS rambo: sub interfaces)+≡

```
module subroutine phs_rambo_config_startup_message (phs_config, unit)
  class(phs_rambo_config_t), intent(in) :: phs_config
  integer, intent(in), optional :: unit
```

```

        end subroutine phs_rambo_config_startup_message
<PHS rambo: procedures>+≡
module subroutine phs_rambo_config_startup_message (phs_config, unit)
  class(phs_rambo_config_t), intent(in) :: phs_config
  integer, intent(in), optional :: unit
  call phs_config%base_startup_message (unit)
  write (msg_buffer, "(A,2(1x,I0,1x,A))") &
    "Phase space: flat (RAMBO)"
  call msg_message (unit = unit)
end subroutine phs_rambo_config_startup_message

```

Allocate an instance: the actual phase-space object. Gfortran 7/8/9 bug, has to remain in the main module.

```

<PHS rambo: phs rambo config: TBP>+≡
  procedure, nopass :: allocate_instance => phs_rambo_config_allocate_instance
<PHS rambo: main procedures>≡
  subroutine phs_rambo_config_allocate_instance (phs)
    class(phs_t), intent(inout), pointer :: phs
    allocate (phs_rambo_t :: phs)
  end subroutine phs_rambo_config_allocate_instance

```

19.4.2 Kinematics implementation

We generate $n - 2$ mass systems M_i with $M_0 = \sqrt{s}$ and $M_n = 0...$

Note: The incoming momenta must be in the c.m. system.

```

<PHS rambo: public>+≡
  public :: phs_rambo_t
<PHS rambo: types>+≡
  type, extends (phs_t) :: phs_rambo_t
    real(default), dimension(:), allocatable :: k
    real(default), dimension(:), allocatable :: m
  contains
    <PHS rambo: phs rambo: TBP>
  end type phs_rambo_t

```

Output.

```

<PHS rambo: phs rambo: TBP>≡
  procedure :: write => phs_rambo_write
<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_write (object, unit, verbose)
    class(phs_rambo_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine phs_rambo_write
<PHS rambo: procedures>+≡
  module subroutine phs_rambo_write (object, unit, verbose)
    class(phs_rambo_t), intent(in) :: object
    integer, intent(in), optional :: unit

```

```

logical, intent(in), optional :: verbose
integer :: u
u = given_output_unit (unit)
call object%base_write (u)
write (u, "(1X,A)") "Intermediate masses (massless):"
write (u, "(3X,999(" // FMT_19 // "))") object%k
write (u, "(1X,A)") "Intermediate masses (massive):"
write (u, "(3X,999(" // FMT_19 // "))") object%m
end subroutine phs_rambo_write

```

The finalizer is empty.

```

<PHS rambo: phs rambo: TBP>+≡
  procedure :: final => phs_rambo_final

<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_final (object)
    class(phs_rambo_t), intent(inout) :: object
  end subroutine phs_rambo_final

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_final (object)
    class(phs_rambo_t), intent(inout) :: object
  end subroutine phs_rambo_final

```

Initialization. We allocate arrays (base_init) and adjust the phase-space volume. The energy dependent factor of s^{n-2} is applied later.

```

<PHS rambo: phs rambo: TBP>+≡
  procedure :: init => phs_rambo_init

<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_init (phs, phs_config)
    class(phs_rambo_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
  end subroutine phs_rambo_init

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_init (phs, phs_config)
    class(phs_rambo_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
    associate (n => phs%config%n_out)
      select case (n)
      case (1)
        if (sum (phs%m_out) > phs%m_in (1)) then
          print *, "m_in = ", phs%m_in
          print *, "m_out = ", phs%m_out
          call msg_fatal &
            ("[phs_rambo_init] Decay is kinematically forbidden.")
        end if
      end select
      allocate (phs%k(n), source = 0._default)
      allocate (phs%m(n), source = 0._default)
      phs%volume = 1. / (twopi)**(3 * n) &
        * (pi / 2.)**(n - 1) / (factorial(n - 1) * factorial(n - 2))
    end associate
  end subroutine

```

```
end subroutine phs_rambo_init
```

Evaluation. There is only one channel for RAMBO, so the second subroutine does nothing.

Note: the current implementation works for elastic scattering only.

(PHS rambo: phs rambo: TBP)+≡

```
procedure :: evaluate_selected_channel => phs_rambo_evaluate_selected_channel
procedure :: evaluate_other_channels => phs_rambo_evaluate_other_channels
```

(PHS rambo: sub interfaces)+≡

```
module subroutine phs_rambo_evaluate_selected_channel (phs, c_in, r_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
  real(default), intent(in), dimension(:) :: r_in
end subroutine phs_rambo_evaluate_selected_channel
module subroutine phs_rambo_evaluate_other_channels (phs, c_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
end subroutine phs_rambo_evaluate_other_channels
```

(PHS rambo: procedures)+≡

```
module subroutine phs_rambo_evaluate_selected_channel (phs, c_in, r_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
  real(default), intent(in), dimension(:) :: r_in
  type(vector4_t), dimension(2) :: p_rest, p_boosted
  type(vector4_t) :: q
  real(default), dimension(2) :: r_angle
  integer :: i
  if (.not. phs%p_defined) return
  call phs%select_channel (c_in)
  phs%r(:,c_in) = r_in
  associate (n => phs%config%n_out, m => phs%m)
    call phs%generate_intermediates (r_in(:n - 2))
    q = sum (phs%p)
    do i = 2, n
      r_angle(1) = r_in(n - 5 + 2 * i)
      r_angle(2) = r_in(n - 4 + 2 * i)
      call phs%decay_intermediate (i, r_angle, p_rest)
      p_boosted = boost(q, m(i - 1)) * p_rest
      q = p_boosted(1)
      phs%q(i - 1) = p_boosted(2)
    end do
    phs%q(n) = q
  end associate
  phs%q_defined = .true.
  phs%r_defined = .true.
end subroutine phs_rambo_evaluate_selected_channel

module subroutine phs_rambo_evaluate_other_channels (phs, c_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
end subroutine phs_rambo_evaluate_other_channels
```

Decay intermediate mass system M_{i-1} into a on-shell particle with mass m_{i-1} and subsequent intermediate mass system with fixed M_i .

```

<PHS rambo: phs rambo: TBP>+≡
  procedure, private :: decay_intermediate => phs_rambo_decay_intermediate

<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_decay_intermediate (phs, i, r_angle, p)
    class(phs_rambo_t), intent(in) :: phs
    integer, intent(in) :: i
    real(default), dimension(2), intent(in) :: r_angle
    type(vector4_t), dimension(2), intent(out) :: p
  end subroutine phs_rambo_decay_intermediate

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_decay_intermediate (phs, i, r_angle, p)
    class(phs_rambo_t), intent(in) :: phs
    integer, intent(in) :: i
    real(default), dimension(2), intent(in) :: r_angle
    type(vector4_t), dimension(2), intent(out) :: p
    real(default) :: k_abs, cos_theta, phi
    type(vector3_t) :: k
    real(default), dimension(2) :: E
    cos_theta = 2. * r_angle(1) - 1.
    phi = twopi * r_angle(2)
    if (phi > pi) phi = phi - twopi
    k_abs = sqrt (lambda (phs%m(i - 1)**2, phs%m(i)**2, phs%m_out(i - 1)**2)) &
      / (2. * phs%m(i - 1))
    k = k_abs * [cos(phi) * sqrt(1. - cos_theta**2), &
      sin(phi) * sqrt(1. - cos_theta**2), cos_theta]
    E(1) = sqrt (phs%m(i)**2 + k_abs**2)
    E(2) = sqrt (phs%m_out(i - 1)**2 + k_abs**2)
    p(1) = vector4_moving (E(1), -k)
    p(2) = vector4_moving (E(2), k)
  end subroutine phs_rambo_decay_intermediate

```

Generate intermediate masses.

```

<PHS rambo: parameters>≡
  integer, parameter :: BISECT_MAX_ITERATIONS = 1000
  real(default), parameter :: BISECT_MIN_PRECISION = tiny_10

<PHS rambo: phs rambo: TBP>+≡
  procedure, private :: generate_intermediates => &
    phs_rambo_generate_intermediates
  procedure, private :: invert_intermediates => phs_rambo_invert_intermediates

<PHS rambo: sub interfaces>+≡
  module subroutine phs_rambo_generate_intermediates (phs, r)
    class(phs_rambo_t), intent(inout) :: phs
    real(default), dimension(:), intent(in) :: r
  end subroutine phs_rambo_generate_intermediates
  module subroutine phs_rambo_invert_intermediates (phs)
    class(phs_rambo_t), intent(inout) :: phs
  end subroutine phs_rambo_invert_intermediates

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_generate_intermediates (phs, r)

```



```

class(phs_rambo_t), intent(inout) :: phs
real(default), dimension(:), intent(in) :: r
integer :: i, j
associate (n => phs%config%n_out, k => phs%k, m => phs%m)
  m(1) = invariant_mass (sum (phs%p))
  m(n) = phs%m_out (n)
  call calculate_k (r)
  do i = 2, n - 1
    m(i) = k(i) + sum (phs%m_out (i:n))
  end do
  ! Massless volume times reweighting for massive volume
  phs%f(1) = k(1)**(2 * n - 4) &
    * 8. * rho(m(n - 1), phs%m_out(n), phs%m_out(n - 1))
  do i = 2, n - 1
    phs%f(1) = phs%f(1) * &
      rho(m(i - 1), m(i), phs%m_out(i - 1)) / &
      rho(k(i - 1), k(i), 0._default) * &
      M(i) / K(i)
  end do
end associate
contains
subroutine calculate_k (r)
  real(default), dimension(:), intent(in) :: r
  real(default), dimension(:), allocatable :: u
  integer :: i
  associate (n => phs%config%n_out, k => phs%k, m => phs%m)
    k = 0
    k(1) = m(1) - sum(phs%m_out(1:n))
    allocate (u(2:n - 1), source=0._default)
    call solve_for_u (r, u)
    do i = 2, n - 1
      k(i) = sqrt (u(i) * k(i - 1)**2)
    end do
  end associate
end subroutine calculate_k

subroutine solve_for_u (r, u)
  real(default), dimension(phs%config%n_out - 2), intent(in) :: r
  real(default), dimension(2:phs%config%n_out - 1), intent(out) :: u
  integer :: i, j
  real(default) :: f, f_mid, xl, xr, xmid
  associate (n => phs%config%n_out)
    do i = 2, n - 1
      xl = 0
      xr = 1
      if (r(i - 1) == 1 .or. r(i - 1) == 0) then
        u(i) = r(i - 1)
      else
        do j = 1, BISECT_MAX_ITERATIONS
          xmid = (xl + xr) / 2.
          f = f_rambo (xl, n - i) - r(i - 1)
          f_mid = f_rambo (xmid, n - i) - r(i - 1)
          if (f * f_mid > 0) then
            xl = xmid
          end if
        end do
      end if
    end do
  end associate
end subroutine solve_for_u

```

```

        else
            xr = xmid
        end if
        if (abs(xl - xr) < BISECT_MIN_PRECISION) exit
    end do
    u(i) = xmid
end if
end do
end associate
end subroutine solve_for_u

real(default) function f_rambo(u, n)
    real(default), intent(in) :: u
    integer, intent(in) :: n
    f_rambo = (n + 1) * u**n - n * u**(n + 1)
end function f_rambo

real(default) function rho (M1, M2, m)
    real(default), intent(in) :: M1, M2, m
    real(default) :: MP, MM
    rho = sqrt ((M1**2 - (M2 + m)**2) * (M1**2 - (M2 - m)**2))
    ! MP = (M1 - (M2 + m)) * (M1 + (M2 + m))
    ! MM = (M1 - (M2 - m)) * (M1 + (M2 - m))
    ! rho = sqrt (MP) * sqrt (MM)
    rho = rho / (8._default * M1**2)
end function rho

end subroutine phs_rambo_generate_intermediates

module subroutine phs_rambo_invert_intermediates (phs)
    class(phs_rambo_t), intent(inout) :: phs
    real(default) :: u
    integer :: i
    associate (n => phs%config%n_out, k => phs%k, m => phs%m)
        k = m
        do i = 1, n - 1
            k(i) = k(i) - sum (phs%m_out(i:n))
        end do
        do i = 2, n - 1
            u = (k(i) / k(i - 1))**2
            phs%r(i - 1, 1) = (n + 1 - i) * u**(n - i) &
                - (n - i) * u**(n + 1 - i)
        end do
    end associate
end subroutine phs_rambo_invert_intermediates

```

Inverse evaluation.

```

<PHS rambo: phs rambo: TBP>+≡
    procedure :: inverse => phs_rambo_inverse

<PHS rambo: sub interfaces>+≡
    module subroutine phs_rambo_inverse (phs)
        class(phs_rambo_t), intent(inout) :: phs
    end subroutine phs_rambo_inverse

```

```

<PHS rambo: procedures>+≡
  module subroutine phs_rambo_inverse (phs)
    class(phs_rambo_t), intent(inout) :: phs
    type(vector4_t), dimension(:), allocatable :: q
    type(vector4_t) :: p
    type(lorentz_transformation_t) :: L
    real(default) :: phi, cos_theta
    integer :: i
    if (.not. (phs%p_defined .and. phs%q_defined)) return
    call phs%select_channel ()
    associate (n => phs%config%n_out, m => phs%m)
      allocate(q(n))
      m(1) = invariant_mass (sum (phs%p))
      q(1) = vector4_at_rest (m(1))
      q(n) = phs%q(n)
      do i = 2, n - 1
        q(i) = q(i) + sum (phs%q(i:n))
        m(i) = invariant_mass (q(i))
      end do
      call phs%invert_intermediates ()
      do i = 2, n
        L = inverse (boost (q(i - 1), m(i - 1)))
        p = L * phs%q(i - 1)
        phi = azimuthal_angle (p); cos_theta = polar_angle_ct (p)
        phs%r(n - 5 + 2 * i, 1) = (cos_theta + 1.) / 2.
        phs%r(n - 4 + 2 * i, 1) = phi / twopi
      end do
    end associate
    phs%r_defined = .true.
  end subroutine phs_rambo_inverse

```

19.4.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_rambo_ut.f90>≡
  <File header>

  module phs_rambo_ut
    use unit_tests
    use phs_rambo_uti

    <Standard module head>

    <PHS rambo: public test>

    contains

    <PHS rambo: test driver>

  end module phs_rambo_ut

<phs_rambo_uti.f90>≡
  <File header>

```

```

module phs_rambo_utl

  <Use kinds>
  <Use strings>
  use flavors
  use lorentz
  use model_data
  use process_constants
  use phs_base

  use phs_rambo

  use phs_base_ut, only: init_test_process_data, init_test_decay_data

  <Standard module head>

  <PHS rambo: test declarations>

  contains

  <PHS rambo: tests>

end module phs_rambo_utl
API: driver for the unit tests below.
<PHS rambo: public test>≡
  public :: phs_rambo_test
<PHS rambo: test driver>≡
  subroutine phs_rambo_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <PHS rambo: execute tests>
  end subroutine phs_rambo_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal_dependence flag.

```

<PHS rambo: execute tests>≡
  call test (phs_rambo_1, "phs_rambo_1", &
    "phase-space configuration", &
    u, results)
<PHS rambo: test declarations>≡
  public :: phs_rambo_1
<PHS rambo: tests>≡
  subroutine phs_rambo_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable :: phs_data

```

```

real(default) :: sqrts

write (u, "(A)")  "* Test output: phs_rambo_1"
write (u, "(A)")  "* Purpose: initialize and display &
                    &phase-space configuration data"
write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_rambo_1"), process_data)

allocate (phs_rambo_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_1"

end subroutine phs_rambo_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS rambo: execute tests>+≡
    call test (phs_rambo_2, "phs_rambo_2", &
                "phase-space evaluation", &
                u, results)

<PHS rambo: test declarations>+≡
    public :: phs_rambo_2

<PHS rambo: tests>+≡
    subroutine phs_rambo_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        real(default) :: sqrts, E
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(2) :: p, q

        write (u, "(A)")  "* Test output: phs_rambo_2"
    end subroutine

```

```

write (u, "(A)")  "* Purpose: test simple two-channel phase space"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_rambo_2"), process_data)

allocate (phs_rambo_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrts / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
                    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

```

```

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_2"

end subroutine phs_rambo_2

```

Phase space for non-c.m. system

Compute kinematics for given parameters, also invert the calculation. Since this will involve cancellations, we call `pacify` to eliminate numerical noise.

```

<PHS rambo: execute tests>+≡
  call test (phs_rambo_3, "phs_rambo_3", &
    "phase-space evaluation in lab frame", &
    u, results)

<PHS rambo: test declarations>+≡
  public :: phs_rambo_3

<PHS rambo: tests>+≡
  subroutine phs_rambo_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(process_constants_t) :: process_data
    real(default) :: sqrts, E
    class(phs_config_t), allocatable, target :: phs_data
    class(phs_t), pointer :: phs => null ()
    type(vector4_t), dimension(2) :: p, q
    type(lorentz_transformation_t) :: lt

    write (u, "(A)")  "* Test output: phs_rambo_3"
    write (u, "(A)")  "* Purpose: phase-space evaluation in lab frame"
    write (u, "(A)")

```

```

call model%init_test ()
call flv%init (25, model)

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_rambo_3"), process_data)

allocate (phs_rambo_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts, lab_is_cm=.false., sqrts_fixed=.false.)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta in lab system"
write (u, "(A)")

lt = boost (0.1_default, 1) * boost (0.3_default, 3)

E = sqrts / 2
p(1) = lt * vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = lt * vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call vector4_write (p(1), u)
call vector4_write (p(2), u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
                    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call pacify (phs)
call phs%write (u)

write (u, "(A)")

```



```

write (u, "(A)")  "* Extract outgoing momenta in lab system"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call vector4_write (q(1), u)
call vector4_write (q(2), u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call pacify (phs)
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_3"

end subroutine phs_rambo_3

```

Decay Phase space evaluation

Compute kinematics for given parameters, also invert the calculation. This time, implement a decay process.

```

<PHS rambo: execute tests>+≡
  call test (phs_rambo_4, "phs_rambo_4", &
    "decay phase-space evaluation", &
    u, results)

<PHS rambo: test declarations>+≡
  public :: phs_rambo_4

<PHS rambo: tests>+≡
  subroutine phs_rambo_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model

```

```

type(flavor_t) :: flv
type(process_constants_t) :: process_data
class(phs_config_t), allocatable, target :: phs_data
class(phs_t), pointer :: phs => null ()
type(vector4_t), dimension(1) :: p
type(vector4_t), dimension(2) :: q

write (u, "(A)")  "* Test output: phs_rambo_4"
write (u, "(A)")  "* Purpose: test simple two-channel phase space"
write (u, "(A)")

call model%init_test ()

call model%set_par (var_str ("ff"), 0.4_default)
call model%set_par (var_str ("mf"), &
    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))
call flv%init (25, model)

write (u, "(A)")  "* Initialize a decay and a matching &
    &phase-space configuration"
write (u, "(A)")

call init_test_decay_data (var_str ("phs_rambo_4"), process_data)

allocate (phs_rambo_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%configure (flv%get_mass ())

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

p(1) = vector4_at_rest (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

```

```

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs_data%configure (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_4"

end subroutine phs_rambo_4

```

19.5 Resonance Handler

For various purposes (e.g., shower histories), we should extract the set of resonances and resonant channels from a phase-space tree set. A few methods do kinematics calculations specifically for those resonance data.

```
<resonances.f90>≡  
  <File header>  
  
  module resonances  
  
    <Use kinds>  
    <Use strings>  
    use lorentz  
    use model_data, only: model_data_t  
    use flavors, only: flavor_t  
  
    <Standard module head>  
  
    <Resonances: public>  
  
    <Resonances: parameters>  
  
    <Resonances: types>  
  
    interface  
    <Resonances: sub interfaces>  
    end interface  
  
  end module resonances  
  
<resonances_sub.f90>≡  
  <File header>  
  
  submodule (resonances) resonances_s  
  
    <Use debug>  
    use string_utils, only: str  
    use format_utils, only: write_indent  
    use constants, only: one  
    use io_units  
    use diagnostics  
  
    implicit none  
  
  contains  
  
    <Resonances: procedures>  
  
  end submodule resonances_s
```

19.5.1 Decay products (contributors)

This stores the indices of the particles that contribute to a resonance, i.e., the decay products.

```

<Resonances: public>≡
    public :: resonance_contributors_t

<Resonances: types>≡
    type :: resonance_contributors_t
        integer, dimension(:), allocatable :: c
    contains
        <Resonances: resonance contributors: TBP>
    end type resonance_contributors_t

```

Equality (comparison)

```

<Resonances: resonance contributors: TBP>≡
    procedure, private :: resonance_contributors_equal
    generic :: operator(==) => resonance_contributors_equal

<Resonances: sub interfaces>≡
    elemental module function resonance_contributors_equal &
        (c1, c2) result (equal)
        logical :: equal
        class(resonance_contributors_t), intent(in) :: c1, c2
    end function resonance_contributors_equal

<Resonances: procedures>≡
    elemental module function resonance_contributors_equal &
        (c1, c2) result (equal)
        logical :: equal
        class(resonance_contributors_t), intent(in) :: c1, c2
        equal = allocated (c1%c) .and. allocated (c2%c)
        if (equal) equal = size (c1%c) == size (c2%c)
        if (equal) equal = all (c1%c == c2%c)
    end function resonance_contributors_equal

```

Assignment

```

<Resonances: resonance contributors: TBP>+≡
    procedure, private :: resonance_contributors_assign
    generic :: assignment(=) => resonance_contributors_assign

<Resonances: sub interfaces>+≡
    pure module subroutine resonance_contributors_assign &
        (contributors_out, contributors_in)
        class(resonance_contributors_t), intent(inout) :: contributors_out
        class(resonance_contributors_t), intent(in) :: contributors_in
    end subroutine resonance_contributors_assign

<Resonances: procedures>+≡
    pure module subroutine resonance_contributors_assign &
        (contributors_out, contributors_in)
        class(resonance_contributors_t), intent(inout) :: contributors_out
        class(resonance_contributors_t), intent(in) :: contributors_in
        if (allocated (contributors_out%c)) deallocate (contributors_out%c)
        if (allocated (contributors_in%c)) then

```

```

        allocate (contributors_out%c (size (contributors_in%c)))
        contributors_out%c = contributors_in%c
    end if
end subroutine resonance_contributors_assign

```

19.5.2 Resonance info object

This data structure augments the set of resonance contributors by a flavor object, such that we can perform calculations that take into account the particle properties, including mass and width.

Avoiding nameclash with similar but different `resonance_t` of `phs_base`:

```

<Resonances: public>+≡
    public :: resonance_info_t

<Resonances: types>+≡
    type :: resonance_info_t
        type(flavor_t) :: flavor
        type(resonance_contributors_t) :: contributors
    contains
        <Resonances: resonance info: TBP>
    end type resonance_info_t

<Resonances: resonance info: TBP>≡
    procedure :: copy => resonance_info_copy

<Resonances: sub interfaces>+≡
    module subroutine resonance_info_copy (resonance_in, resonance_out)
        class(resonance_info_t), intent(in) :: resonance_in
        type(resonance_info_t), intent(out) :: resonance_out
    end subroutine resonance_info_copy

<Resonances: procedures>+≡
    module subroutine resonance_info_copy (resonance_in, resonance_out)
        class(resonance_info_t), intent(in) :: resonance_in
        type(resonance_info_t), intent(out) :: resonance_out
        resonance_out%flavor = resonance_in%flavor
        if (allocated (resonance_in%contributors%c)) then
            associate (c => resonance_in%contributors%c)
                allocate (resonance_out%contributors%c (size (c)))
                resonance_out%contributors%c = c
            end associate
        end if
    end subroutine resonance_info_copy

<Resonances: resonance info: TBP>+≡
    procedure :: write => resonance_info_write

<Resonances: sub interfaces>+≡
    module subroutine resonance_info_write (resonance, unit, verbose)
        class(resonance_info_t), intent(in) :: resonance
        integer, optional, intent(in) :: unit
        logical, optional, intent(in) :: verbose
    end subroutine resonance_info_write

```

<Resonances: procedures>+≡

```

module subroutine resonance_info_write (resonance, unit, verbose)
  class(resonance_info_t), intent(in) :: resonance
  integer, optional, intent(in) :: unit
  logical, optional, intent(in) :: verbose
  integer :: u, i
  logical :: verb
  u = given_output_unit (unit); if (u < 0) return
  verb = .true.; if (present (verbose)) verb = verbose
  if (verb) then
    write (u, '(A)', advance='no') "Resonance contributors: "
  else
    write (u, '(1x)', advance="no")
  end if
  if (allocated (resonance%contributors%c)) then
    do i = 1, size(resonance%contributors%c)
      write (u, '(I0,1X)', advance='no') resonance%contributors%c(i)
    end do
  else if (verb) then
    write (u, "(A)", advance="no") "[not allocated]"
  end if
  if (resonance%flavor%is_defined ()) call resonance%flavor%write (u)
  write (u, '(A)')
end subroutine resonance_info_write

```

Create a resonance-info object. The particle info may be available in term of a flavor object or as a PDG code; in the latter case we have to require a model data object that provides mass and width information.

<Resonances: resonance info: TBP>+≡

```

procedure, private :: resonance_info_init_pdg
procedure, private :: resonance_info_init_flv
generic :: init => resonance_info_init_pdg, resonance_info_init_flv

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_info_init_pdg &
  (resonance, mom_id, pdg, model, n_out)
  class(resonance_info_t), intent(out) :: resonance
  integer, intent(in) :: mom_id
  integer, intent(in) :: pdg, n_out
  class(model_data_t), intent(in), target :: model
end subroutine resonance_info_init_pdg
module subroutine resonance_info_init_flv (resonance, mom_id, flv, n_out)
  class(resonance_info_t), intent(out) :: resonance
  integer, intent(in) :: mom_id
  type(flavor_t), intent(in) :: flv
  integer, intent(in) :: n_out
end subroutine resonance_info_init_flv

```

<Resonances: procedures>+≡

```

module subroutine resonance_info_init_pdg &
  (resonance, mom_id, pdg, model, n_out)
  class(resonance_info_t), intent(out) :: resonance
  integer, intent(in) :: mom_id
  integer, intent(in) :: pdg, n_out

```

```

class(model_data_t), intent(in), target :: model
type(flavor_t) :: flv
if (debug_on) call msg_debug (D_PHASESPACE, "resonance_info_init_pdg")
call flv%init (pdg, model)
call resonance%init (mom_id, flv, n_out)
end subroutine resonance_info_init_pdg

module subroutine resonance_info_init_flv (resonance, mom_id, flv, n_out)
class(resonance_info_t), intent(out) :: resonance
integer, intent(in) :: mom_id
type(flavor_t), intent(in) :: flv
integer, intent(in) :: n_out
integer :: i
logical, dimension(n_out) :: contrib
integer, dimension(n_out) :: tmp
if (debug_on) call msg_debug (D_PHASESPACE, "resonance_info_init_flv")
resonance%flavor = flv
do i = 1, n_out
    tmp(i) = i
end do
contrib = btest (mom_id, tmp - 1)
allocate (resonance%contributors%c (count (contrib)))
resonance%contributors%c = pack (tmp, contrib)
end subroutine resonance_info_init_flv

```

<Resonances: resonance info: TBP>+≡

```

procedure, private :: resonance_info_equal
generic :: operator(==) => resonance_info_equal

```

<Resonances: sub interfaces>+≡

```

elemental module function resonance_info_equal (r1, r2) result (equal)
logical :: equal
class(resonance_info_t), intent(in) :: r1, r2
end function resonance_info_equal

```

<Resonances: procedures>+≡

```

elemental module function resonance_info_equal (r1, r2) result (equal)
logical :: equal
class(resonance_info_t), intent(in) :: r1, r2
equal = r1%flavor == r2%flavor .and. r1%contributors == r2%contributors
end function resonance_info_equal

```

With each resonance region we associate a Breit-Wigner function

$$P = \frac{M_{res}^4}{(s - M_{res}^2)^2 + \Gamma_{res}^2 M_{res}^2},$$

where s denotes the invariant mass of the outgoing momenta originating from this resonance. Note that the M_{res}^4 in the nominator makes the mapping a dimensionless quantity.

<Resonances: resonance info: TBP>+≡

```

procedure :: mapping => resonance_info_mapping

```



```

<Resonances: sub interfaces>+≡
  module function resonance_info_mapping (resonance, s) result (bw)
    real(default) :: bw
    class(resonance_info_t), intent(in) :: resonance
    real(default), intent(in) :: s
  end function resonance_info_mapping

```

```

<Resonances: procedures>+≡
  module function resonance_info_mapping (resonance, s) result (bw)
    real(default) :: bw
    class(resonance_info_t), intent(in) :: resonance
    real(default), intent(in) :: s
    real(default) :: m, gamma
    if (resonance%flavor%is_defined ()) then
      m = resonance%flavor%get_mass ()
      gamma = resonance%flavor%get_width ()
      bw = m**4 / ((s - m**2)**2 + gamma**2 * m**2)
    else
      bw = one
    end if
  end function resonance_info_mapping

```

Used for building a resonance tree below.

```

<Resonances: resonance info: TBP>+≡
  procedure, private :: get_n_contributors => resonance_info_get_n_contributors
  procedure, private :: contains => resonance_info_contains

```

```

<Resonances: sub interfaces>+≡
  elemental module function resonance_info_get_n_contributors &
    (resonance) result (n)
    class(resonance_info_t), intent(in) :: resonance
    integer :: n
  end function resonance_info_get_n_contributors
  elemental module function resonance_info_contains &
    (resonance, c) result (flag)
    class(resonance_info_t), intent(in) :: resonance
    integer, intent(in) :: c
    logical :: flag
  end function resonance_info_contains

```

```

<Resonances: procedures>+≡
  elemental module function resonance_info_get_n_contributors &
    (resonance) result (n)
    class(resonance_info_t), intent(in) :: resonance
    integer :: n
    if (allocated (resonance%contributors%c)) then
      n = size (resonance%contributors%c)
    else
      n = 0
    end if
  end function resonance_info_get_n_contributors

  elemental module function resonance_info_contains &
    (resonance, c) result (flag)
    class(resonance_info_t), intent(in) :: resonance

```

```

integer, intent(in) :: c
logical :: flag
if (allocated (resonance%contributors%c)) then
    flag = any (resonance%contributors%c == c)
else
    flag = .false.
end if
end function resonance_info_contains

```

19.5.3 Resonance history object

This data structure stores a set of resonances, i.e., the resonances that appear in a particular Feynman graph or, in the context of phase space, phase space diagram.

```

<Resonances: public>+≡
    public :: resonance_history_t

<Resonances: types>+≡
    type :: resonance_history_t
        type(resonance_info_t), dimension(:), allocatable :: resonances
        integer :: n_resonances = 0
    contains
        <Resonances: resonance history: TBP>
    end type resonance_history_t

```

Clear the resonance history. Assuming that there are no pointer-allocated parts, a straightforward `intent(out)` will do.

```

<Resonances: resonance history: TBP>≡
    procedure :: clear => resonance_history_clear

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_clear (res_hist)
        class(resonance_history_t), intent(out) :: res_hist
    end subroutine resonance_history_clear

<Resonances: procedures>+≡
    module subroutine resonance_history_clear (res_hist)
        class(resonance_history_t), intent(out) :: res_hist
    end subroutine resonance_history_clear

<Resonances: resonance history: TBP>+≡
    procedure :: copy => resonance_history_copy

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_copy (res_hist_in, res_hist_out)
        class(resonance_history_t), intent(in) :: res_hist_in
        type(resonance_history_t), intent(out) :: res_hist_out
    end subroutine resonance_history_copy

<Resonances: procedures>+≡
    module subroutine resonance_history_copy (res_hist_in, res_hist_out)
        class(resonance_history_t), intent(in) :: res_hist_in
        type(resonance_history_t), intent(out) :: res_hist_out

```

```

integer :: i
res_hist_out%n_resonances = res_hist_in%n_resonances
allocate (res_hist_out%resonances (size (res_hist_in%resonances)))
do i = 1, size (res_hist_in%resonances)
    call res_hist_in%resonances(i)%copy (res_hist_out%resonances(i))
end do
end subroutine resonance_history_copy

```

<Resonances: resonance history: TBP>+≡

```

procedure :: write => resonance_history_write

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_history_write (res_hist, unit, verbose, indent)
    class(resonance_history_t), intent(in) :: res_hist
    integer, optional, intent(in) :: unit
    logical, optional, intent(in) :: verbose
    integer, optional, intent(in) :: indent
end subroutine resonance_history_write

```

<Resonances: procedures>+≡

```

module subroutine resonance_history_write (res_hist, unit, verbose, indent)
    class(resonance_history_t), intent(in) :: res_hist
    integer, optional, intent(in) :: unit
    logical, optional, intent(in) :: verbose
    integer, optional, intent(in) :: indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write(u, '(A,I0,A)') "Resonance history with ", &
        res_hist%n_resonances, " resonances:"
    do i = 1, res_hist%n_resonances
        call write_indent (u, indent)
        write (u, "(2x)", advance="no")
        call res_hist%resonances(i)%write (u, verbose)
    end do
end subroutine resonance_history_write

```

Assignment. Indirectly calls type-bound assignment for the contributors.

Strictly speaking, this is redundant. But NAGfor 6.208 intrinsic assignment crashes under certain conditions.

<Resonances: resonance history: TBP>+≡

```

procedure, private :: resonance_history_assign
generic :: assignment(=) => resonance_history_assign

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_history_assign (res_hist_out, res_hist_in)
    class(resonance_history_t), intent(out) :: res_hist_out
    class(resonance_history_t), intent(in) :: res_hist_in
end subroutine resonance_history_assign

```

<Resonances: procedures>+≡

```

module subroutine resonance_history_assign (res_hist_out, res_hist_in)
    class(resonance_history_t), intent(out) :: res_hist_out
    class(resonance_history_t), intent(in) :: res_hist_in
    if (allocated (res_hist_in%resonances)) then

```

```

        res_hist_out%resonances = res_hist_in%resonances
        res_hist_out%n_resonances = res_hist_in%n_resonances
    end if
end subroutine resonance_history_assign

```

Equality. If this turns out to slow down the program, we should change the implementation or use hash codes.

```

<Resonances: resonance history: TBP>+≡
    procedure, private :: resonance_history_equal
    generic :: operator(==) => resonance_history_equal

<Resonances: sub interfaces>+≡
    elemental module function resonance_history_equal (rh1, rh2) result (equal)
        logical :: equal
        class(resonance_history_t), intent(in) :: rh1, rh2
    end function resonance_history_equal

<Resonances: procedures>+≡
    elemental module function resonance_history_equal (rh1, rh2) result (equal)
        logical :: equal
        class(resonance_history_t), intent(in) :: rh1, rh2
        integer :: i
        equal = .false.
        if (rh1%n_resonances == rh2%n_resonances) then
            do i = 1, rh1%n_resonances
                if (.not. rh1%resonances(i) == rh2%resonances(i)) then
                    return
                end if
            end do
            equal = .true.
        end if
    end function resonance_history_equal

```

Check if a resonance history is a strict superset of another one. This is true if the first one is nonempty and the second one is empty. Otherwise, we check if each entry of the second argument appears in the first one.

```

<Resonances: resonance history: TBP>+≡
    procedure, private :: resonance_history_contains
    generic :: operator(.contains.) => resonance_history_contains

<Resonances: sub interfaces>+≡
    elemental module function resonance_history_contains &
        (rh1, rh2) result (flag)
        logical :: flag
        class(resonance_history_t), intent(in) :: rh1, rh2
    end function resonance_history_contains

<Resonances: procedures>+≡
    elemental module function resonance_history_contains &
        (rh1, rh2) result (flag)
        logical :: flag
        class(resonance_history_t), intent(in) :: rh1, rh2
        integer :: i
        if (rh1%n_resonances > rh2%n_resonances) then
            flag = .true.

```

```

        do i = 1, rh2%n_resonances
            flag = flag .and. any (rh1%resonances == rh2%resonances(i))
        end do
    else
        flag = .false.
    end if
end function resonance_history_contains

```

Number of entries for dynamically extending the resonance-info array.

```

<Resonances: parameters>≡
    integer, parameter :: n_max_resonances = 10

<Resonances: resonance history: TBP>+≡
    procedure :: add_resonance => resonance_history_add_resonance

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_add_resonance (res_hist, resonance)
        class(resonance_history_t), intent(inout) :: res_hist
        type(resonance_info_t), intent(in) :: resonance
    end subroutine resonance_history_add_resonance

<Resonances: procedures>+≡
    module subroutine resonance_history_add_resonance (res_hist, resonance)
        class(resonance_history_t), intent(inout) :: res_hist
        type(resonance_info_t), intent(in) :: resonance
        type(resonance_info_t), dimension(:), allocatable :: tmp
        integer :: n, i
        if (debug_on) call msg_debug &
            (D_PHASESPACE, "resonance_history_add_resonance")
        if (.not. allocated (res_hist%resonances)) then
            n = 0
            allocate (res_hist%resonances (1))
        else
            n = res_hist%n_resonances
            allocate (tmp (n))
            do i = 1, n
                call res_hist%resonances(i)%copy (tmp(i))
            end do
            deallocate (res_hist%resonances)
            allocate (res_hist%resonances (n+1))
            do i = 1, n
                call tmp(i)%copy (res_hist%resonances(i))
            end do
            deallocate (tmp)
        end if
        call resonance%copy (res_hist%resonances(n+1))
        res_hist%n_resonances = n + 1
        if (debug_on) call msg_debug &
            (D_PHASESPACE, "res_hist%n_resonances", res_hist%n_resonances)
    end subroutine resonance_history_add_resonance

<Resonances: resonance history: TBP>+≡
    procedure :: remove_resonance => resonance_history_remove_resonance

```

```

⟨Resonances: sub interfaces⟩+≡
  module subroutine resonance_history_remove_resonance (res_hist, i_res)
    class(resonance_history_t), intent(inout) :: res_hist
    integer, intent(in) :: i_res
  end subroutine resonance_history_remove_resonance

```

```

⟨Resonances: procedures⟩+≡
  module subroutine resonance_history_remove_resonance (res_hist, i_res)
    class(resonance_history_t), intent(inout) :: res_hist
    integer, intent(in) :: i_res
    type(resonance_info_t), dimension(:), allocatable :: tmp_1, tmp_2
    integer :: i, j, n
    n = res_hist%n_resonances
    res_hist%n_resonances = n - 1
    if (res_hist%n_resonances == 0) then
      deallocate (res_hist%resonances)
    else
      if (i_res > 1) allocate (tmp_1(1:i_res-1))
      if (i_res < n) allocate (tmp_2(i_res+1:n))
      if (allocated (tmp_1)) then
        do i = 1, i_res - 1
          call res_hist%resonances(i)%copy (tmp_1(i))
        end do
      end if
      if (allocated (tmp_2)) then
        do i = i_res + 1, n
          call res_hist%resonances(i)%copy (tmp_2(i))
        end do
      end if
      deallocate (res_hist%resonances)
      allocate (res_hist%resonances (res_hist%n_resonances))
      j = 1
      if (allocated (tmp_1)) then
        do i = 1, i_res - 1
          call tmp_1(i)%copy (res_hist%resonances(j))
          j = j + 1
        end do
        deallocate (tmp_1)
      end if
      if (allocated (tmp_2)) then
        do i = i_res + 1, n
          call tmp_2(i)%copy (res_hist%resonances(j))
          j = j + 1
        end do
        deallocate (tmp_2)
      end if
    end if
  end subroutine resonance_history_remove_resonance

```

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: add_offset => resonance_history_add_offset

```

```

⟨Resonances: sub interfaces⟩+≡
  module subroutine resonance_history_add_offset (res_hist, n)
    class(resonance_history_t), intent(inout) :: res_hist

```

```

        integer, intent(in) :: n
    end subroutine resonance_history_add_offset

<Resonances: procedures>+≡
module subroutine resonance_history_add_offset (res_hist, n)
    class(resonance_history_t), intent(inout) :: res_hist
    integer, intent(in) :: n
    integer :: i_res
    do i_res = 1, res_hist%n_resonances
        associate (contributors => res_hist%resonances(i_res)%contributors%c)
            contributors = contributors + n
        end associate
    end do
end subroutine resonance_history_add_offset

<Resonances: resonance history: TBP>+≡
    procedure :: contains_leg => resonance_history_contains_leg

<Resonances: sub interfaces>+≡
    module function resonance_history_contains_leg &
        (res_hist, i_leg) result (val)
        logical :: val
        class(resonance_history_t), intent(in) :: res_hist
        integer, intent(in) :: i_leg
    end function resonance_history_contains_leg

<Resonances: procedures>+≡
    module function resonance_history_contains_leg &
        (res_hist, i_leg) result (val)
        logical :: val
        class(resonance_history_t), intent(in) :: res_hist
        integer, intent(in) :: i_leg
        integer :: i_res
        val = .false.
        do i_res = 1, res_hist%n_resonances
            if (any (res_hist%resonances(i_res)%contributors%c == i_leg)) then
                val = .true.
                exit
            end if
        end do
    end function resonance_history_contains_leg

<Resonances: resonance history: TBP>+≡
    procedure :: mapping => resonance_history_mapping

<Resonances: sub interfaces>+≡
    module function resonance_history_mapping &
        (res_hist, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_history_t), intent(in) :: res_hist
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: i_gluon
    end function resonance_history_mapping

```

```

⟨Resonances: procedures⟩+≡
  module function resonance_history_mapping &
    (res_hist, p, i_gluon) result (p_map)
    real(default) :: p_map
    class(resonance_history_t), intent(in) :: res_hist
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in), optional :: i_gluon
    integer :: i_res
    real(default) :: s
    p_map = one
    do i_res = 1, res_hist%n_resonances
      associate (res => res_hist%resonances(i_res))
        s = compute_resonance_mass (p, res%contributors%c, i_gluon)**2
        p_map = p_map * res%mapping (s)
      end associate
    end do
  end function resonance_history_mapping

```

This predicate is true if all resonances in the history have exactly n contributors. For instance, if $n = 2$, all resonances have a two-particle decay.

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: only_has_n_contributors => &
    resonance_history_only_has_n_contributors

⟨Resonances: sub interfaces⟩+≡
  module function resonance_history_only_has_n_contributors &
    (res_hist, n) result (value)
    logical :: value
    class(resonance_history_t), intent(in) :: res_hist
    integer, intent(in) :: n
  end function resonance_history_only_has_n_contributors

⟨Resonances: procedures⟩+≡
  module function resonance_history_only_has_n_contributors &
    (res_hist, n) result (value)
    logical :: value
    class(resonance_history_t), intent(in) :: res_hist
    integer, intent(in) :: n
    integer :: i_res
    value = .true.
    do i_res = 1, res_hist%n_resonances
      associate (res => res_hist%resonances(i_res))
        value = value .and. size (res%contributors%c) == n
      end associate
    end do
  end function resonance_history_only_has_n_contributors

```

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: has_flavor => resonance_history_has_flavor

⟨Resonances: sub interfaces⟩+≡
  module function resonance_history_has_flavor &
    (res_hist, flv) result (has_flv)
    logical :: has_flv

```



```

        class(resonance_history_t), intent(in) :: res_hist
        type(flavor_t), intent(in) :: flv
    end function resonance_history_has_flavor

<Resonances: procedures>+≡
module function resonance_history_has_flavor &
    (res_hist, flv) result (has_flv)
    logical :: has_flv
    class(resonance_history_t), intent(in) :: res_hist
    type(flavor_t), intent(in) :: flv
    integer :: i
    has_flv = .false.
    do i = 1, res_hist%n_resonances
        has_flv = has_flv .or. res_hist%resonances(i)%flavor == flv
    end do
end function resonance_history_has_flavor

```

19.5.4 Kinematics

Evaluate the distance from a resonance. The distance is given by $|p^2 - m^2|/(m\Gamma)$. For $\Gamma \ll m$, this is the relative distance from the resonance peak in units of the half-width.

```

<Resonances: resonance info: TBP>+≡
    procedure :: evaluate_distance => resonance_info_evaluate_distance

<Resonances: sub interfaces>+≡
    module subroutine resonance_info_evaluate_distance (res_info, p, dist)
        class(resonance_info_t), intent(in) :: res_info
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(out) :: dist
    end subroutine resonance_info_evaluate_distance

<Resonances: procedures>+≡
    module subroutine resonance_info_evaluate_distance (res_info, p, dist)
        class(resonance_info_t), intent(in) :: res_info
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(out) :: dist
        real(default) :: m, w
        type(vector4_t) :: q
        m = res_info%flavor%get_mass ()
        w = res_info%flavor%get_width ()
        q = sum (p(res_info%contributors%c))
        dist = abs (q**2 - m**2) / (m * w)
    end subroutine resonance_info_evaluate_distance

```

Evaluate the array of distances from a resonance history. We assume that the array has been allocated with correct size, namely the number of resonances in this history.

```

<Resonances: resonance history: TBP>+≡
    procedure :: evaluate_distances => resonance_history_evaluate_distances

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_history_evaluate_distances (res_hist, p, dist)
  class(resonance_history_t), intent(in) :: res_hist
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), dimension(:), intent(out) :: dist
end subroutine resonance_history_evaluate_distances

```

<Resonances: procedures>+≡

```

module subroutine resonance_history_evaluate_distances (res_hist, p, dist)
  class(resonance_history_t), intent(in) :: res_hist
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), dimension(:), intent(out) :: dist
  integer :: i
  do i = 1, res_hist%n_resonances
    call res_hist%resonances(i)%evaluate_distance (p, dist(i))
  end do
end subroutine resonance_history_evaluate_distances

```

Use the distance to determine a Gaussian turnoff factor for a resonance. The factor is given by a Gaussian function e^{-d^2/σ^2} , where σ is the gw parameter multiplied by the resonance width, and d is the distance (see above). So, for $d = \sigma$, the factor is 0.37, and for $d = 2\sigma$ we get 0.018.

If the gw factor is less or equal to zero, return 1.

<Resonances: resonance info: TBP>+≡

```

procedure :: evaluate_gaussian => resonance_info_evaluate_gaussian

```

<Resonances: sub interfaces>+≡

```

module function resonance_info_evaluate_gaussian &
  (res_info, p, gw) result (factor)
  class(resonance_info_t), intent(in) :: res_info
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: gw
  real(default) :: factor
end function resonance_info_evaluate_gaussian

```

<Resonances: procedures>+≡

```

module function resonance_info_evaluate_gaussian &
  (res_info, p, gw) result (factor)
  class(resonance_info_t), intent(in) :: res_info
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: gw
  real(default) :: factor
  real(default) :: dist, w
  if (gw > 0) then
    w = res_info%flavor%get_width ()
    call res_info%evaluate_distance (p, dist)
    factor = exp (- (dist / (gw * w)) **2)
  else
    factor = 1
  end if
end function resonance_info_evaluate_gaussian

```

The Gaussian factor of the history is the product of all factors.

<Resonances: resonance history: TBP>+≡

```

procedure :: evaluate_gaussian => resonance_history_evaluate_gaussian

```

<Resonances: sub interfaces>+≡

```

module function resonance_history_evaluate_gaussian &
  (res_hist, p, gw) result (factor)
  class(resonance_history_t), intent(in) :: res_hist
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: gw
  real(default) :: factor
end function resonance_history_evaluate_gaussian

```

<Resonances: procedures>+≡

```

module function resonance_history_evaluate_gaussian &
  (res_hist, p, gw) result (factor)
  class(resonance_history_t), intent(in) :: res_hist
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: gw
  real(default), dimension(:), allocatable :: dist
  real(default) :: factor
  integer :: i
  factor = 1
  do i = 1, res_hist%n_resonances
    factor = factor * res_hist%resonances(i)%evaluate_gaussian (p, gw)
  end do
end function resonance_history_evaluate_gaussian

```

Use the distances to determine whether the resonance history can qualify as on-shell. The criterion is whether the distance is greater than the number of width values as given by `on_shell_limit`.

<Resonances: resonance info: TBP>+≡

```

procedure :: is_on_shell => resonance_info_is_on_shell

```

<Resonances: sub interfaces>+≡

```

module function resonance_info_is_on_shell (res_info, p, on_shell_limit) &
  result (flag)
  class(resonance_info_t), intent(in) :: res_info
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: on_shell_limit
  logical :: flag
end function resonance_info_is_on_shell

```

<Resonances: procedures>+≡

```

module function resonance_info_is_on_shell (res_info, p, on_shell_limit) &
  result (flag)
  class(resonance_info_t), intent(in) :: res_info
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: on_shell_limit
  logical :: flag
  real(default) :: dist
  call res_info%evaluate_distance (p, dist)
  flag = dist < on_shell_limit
end function resonance_info_is_on_shell

```

<Resonances: resonance history: TBP>+≡

```

procedure :: is_on_shell => resonance_history_is_on_shell

```

```

<Resonances: sub interfaces>+≡
  module function resonance_history_is_on_shell &
    (res_hist, p, on_shell_limit) result (flag)
    class(resonance_history_t), intent(in) :: res_hist
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: on_shell_limit
    logical :: flag
  end function resonance_history_is_on_shell

<Resonances: procedures>+≡
  module function resonance_history_is_on_shell &
    (res_hist, p, on_shell_limit) result (flag)
    class(resonance_history_t), intent(in) :: res_hist
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: on_shell_limit
    logical :: flag
    integer :: i
    flag = .true.
    do i = 1, res_hist%n_resonances
      flag = flag .and. res_hist%resonances(i)%is_on_shell (p, on_shell_limit)
    end do
  end function resonance_history_is_on_shell

```

19.5.5 OMega restriction strings

One application of the resonance module is creating restriction strings that can be fed into process definitions with the OMega generator. Since OMega counts the incoming particles first, we have to supply `n_in` as an offset.

```

<Resonances: resonance info: TBP>+≡
  procedure :: as_omega_string => resonance_info_as_omega_string

<Resonances: resonance history: TBP>+≡
  procedure :: as_omega_string => resonance_history_as_omega_string

<Resonances: sub interfaces>+≡
  module function resonance_info_as_omega_string &
    (res_info, n_in) result (string)
    class(resonance_info_t), intent(in) :: res_info
    integer, intent(in) :: n_in
    type(string_t) :: string
  end function resonance_info_as_omega_string
  module function resonance_history_as_omega_string &
    (res_hist, n_in) result (string)
    class(resonance_history_t), intent(in) :: res_hist
    integer, intent(in) :: n_in
    type(string_t) :: string
  end function resonance_history_as_omega_string

<Resonances: procedures>+≡
  module function resonance_info_as_omega_string &
    (res_info, n_in) result (string)
    class(resonance_info_t), intent(in) :: res_info
    integer, intent(in) :: n_in
    type(string_t) :: string

```

```

integer :: i
string = ""
if (allocated (res_info%contributors%c)) then
  do i = 1, size (res_info%contributors%c)
    if (i > 1) string = string // "+"
    string = string // str (res_info%contributors%c(i) + n_in)
  end do
  string = string // "~" // res_info%flavor%get_name ()
end if
end function resonance_info_as_omega_string

module function resonance_history_as_omega_string &
  (res_hist, n_in) result (string)
class(resonance_history_t), intent(in) :: res_hist
integer, intent(in) :: n_in
type(string_t) :: string
integer :: i
string = ""
do i = 1, res_hist%n_resonances
  if (i > 1) string = string // " && "
  string = string // res_hist%resonances(i)%as_omega_string (n_in)
end do
end function resonance_history_as_omega_string

```

19.5.6 Resonance history as tree

If we want to organize the resonances and their decay products, it can be useful to have them explicitly as a tree structure. We implement this in the traditional event-record form with the resonances sorted by decreasing number of contributors, and their decay products added as an extra array.

```

<Resonances: public>+≡
  public :: resonance_tree_t

<Resonances: types>+≡
  type :: resonance_branch_t
    integer :: i = 0
    type(flavor_t) :: flv
    integer, dimension(:), allocatable :: r_child
    integer, dimension(:), allocatable :: o_child
  end type resonance_branch_t

  type :: resonance_tree_t
    private
    integer :: n = 0
    type(resonance_branch_t), dimension(:), allocatable :: branch
  contains
    <Resonances: resonance tree: TBP>
  end type resonance_tree_t

<Resonances: resonance tree: TBP>≡
  procedure :: write => resonance_tree_write

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_tree_write (tree, unit, indent)
  class(resonance_tree_t), intent(in) :: tree
  integer, intent(in), optional :: unit, indent
end subroutine resonance_tree_write

```

<Resonances: procedures>+≡

```

module subroutine resonance_tree_write (tree, unit, indent)
  class(resonance_tree_t), intent(in) :: tree
  integer, intent(in), optional :: unit, indent
  integer :: u, b, c
  u = given_output_unit (unit)
  call write_indent (u, indent)
  write (u, "(A)", advance="no") "Resonance tree:"
  if (tree%n > 0) then
    write (u, *)
    do b = 1, tree%n
      call write_indent (u, indent)
      write (u, "(2x,'r',I0,'.',1x)", advance="no") b
      associate (branch => tree%branch(b))
        call branch%flv%write (u)
        write (u, "(1x,'>')", advance="no")
        if (allocated (branch%r_child)) then
          do c = 1, size (branch%r_child)
            write (u, "(1x,'r',I0)", advance="no") branch%r_child(c)
          end do
        end if
        if (allocated (branch%o_child)) then
          do c = 1, size (branch%o_child)
            write (u, "(1x,I0)", advance="no") branch%o_child(c)
          end do
        end if
        write (u, *)
      end associate
    end do
  else
    write (u, "(1x,A)") "[empty]"
  end if
end subroutine resonance_tree_write

```

Contents.

<Resonances: resonance tree: TBP>+≡

```

procedure :: get_n_resonances => resonance_tree_get_n_resonances
procedure :: get_flv => resonance_tree_get_flv

```

<Resonances: sub interfaces>+≡

```

module function resonance_tree_get_n_resonances (tree) result (n)
  class(resonance_tree_t), intent(in) :: tree
  integer :: n
end function resonance_tree_get_n_resonances
module function resonance_tree_get_flv (tree, i) result (flv)
  class(resonance_tree_t), intent(in) :: tree
  integer, intent(in) :: i
  type(flavor_t) :: flv
end function resonance_tree_get_flv

```

```

<Resonances: procedures>+≡
  module function resonance_tree_get_n_resonances (tree) result (n)
    class(resonance_tree_t), intent(in) :: tree
    integer :: n
    n = tree%n
  end function resonance_tree_get_n_resonances

  module function resonance_tree_get_flv (tree, i) result (flv)
    class(resonance_tree_t), intent(in) :: tree
    integer, intent(in) :: i
    type(flavor_t) :: flv
    flv = tree%branch(i)%flv
  end function resonance_tree_get_flv

```

Return the shifted indices of the resonance children for branch i. For a child which is itself a resonance, add `offset_r` to the index value. For the others, add `offset_o`. Combine both in a single array.

```

<Resonances: resonance tree: TBP>+≡
  procedure :: get_children => resonance_tree_get_children

<Resonances: sub interfaces>+≡
  module function resonance_tree_get_children (tree, i, offset_r, offset_o) &
    result (child)
    class(resonance_tree_t), intent(in) :: tree
    integer, intent(in) :: i, offset_r, offset_o
    integer, dimension(:), allocatable :: child
  end function resonance_tree_get_children

<Resonances: procedures>+≡
  module function resonance_tree_get_children (tree, i, offset_r, offset_o) &
    result (child)
    class(resonance_tree_t), intent(in) :: tree
    integer, intent(in) :: i, offset_r, offset_o
    integer, dimension(:), allocatable :: child
    integer :: nr, no
    associate (branch => tree%branch(i))
      nr = size (branch%r_child)
      no = size (branch%o_child)
      allocate (child (nr + no))
      child(1:nr) = branch%r_child + offset_r
      child(nr+1:nr+no) = branch%o_child + offset_o
    end associate
  end function resonance_tree_get_children

```

Transform a resonance history into a resonance tree. Algorithm:

1. Determine a mapping of the resonance array, such that in the new array the resonances are ordered by decreasing number of contributors.
2. Copy the flavor entries to the mapped array.
3. Scan all resonances and, for each one, find a resonance that is its parent. Since the resonances are ordered, later matches overwrite earlier ones. The last match is the correct one. Then scan again and, for each resonance,

collect the resonances that have it as parent. This is the set of child resonances.

4. Analogously, scan all outgoing particles that appear in any of the contributors list. Determine their immediate parent as above, and set the child outgoing parents for the resonances, as above.

```

<Resonances: resonance history: TBP>+≡
  procedure :: to_tree => resonance_history_to_tree

<Resonances: sub interfaces>+≡
  module subroutine resonance_history_to_tree (res_hist, tree)
    class(resonance_history_t), intent(in) :: res_hist
    type(resonance_tree_t), intent(out) :: tree
  end subroutine resonance_history_to_tree

<Resonances: procedures>+≡
  module subroutine resonance_history_to_tree (res_hist, tree)
    class(resonance_history_t), intent(in) :: res_hist
    type(resonance_tree_t), intent(out) :: tree
    integer :: nr
    integer, dimension(:), allocatable :: r_branch, r_source

    nr = res_hist%n_resonances
    tree%n = nr
    allocate (tree%branch (tree%n), r_branch (tree%n), r_source (tree%n))
    if (tree%n > 0) then
      call find_branch_ordering ()
      call set_flavors ()
      call set_child_resonances ()
      call set_child_outgoing ()
    end if

contains

    subroutine find_branch_ordering ()
      integer, dimension(:), allocatable :: nc_array
      integer :: r, ir, nc
      allocate (nc_array (tree%n))
      nc_array(:) = res_hist%resonances%get_n_contributors ()
      ir = 0
      do nc = maxval (nc_array), minval (nc_array), -1
        do r = 1, nr
          if (nc_array(r) == nc) then
            ir = ir + 1
            r_branch(r) = ir
            r_source(ir) = r
          end if
        end do
      end do
    end subroutine find_branch_ordering

    subroutine set_flavors ()
      integer :: r
      do r = 1, nr
        tree%branch(r_branch(r))%flv = res_hist%resonances(r)%flavor
      end do
    end subroutine set_flavors

```



```

        end do
    end subroutine set_flavors

    subroutine set_child_resonances ()
        integer, dimension(:), allocatable :: r_child, r_parent
        integer :: r, ir, pr
        allocate (r_parent (nr), source = 0)
        SCAN_RES: do r = 1, nr
            associate (this_res => res_hist%resonances(r))
                SCAN_PARENT: do ir = 1, nr
                    pr = r_source(ir)
                    if (pr == r) cycle SCAN_PARENT
                    if (all (res_hist%resonances(pr)%contains &
                        (this_res%contributors%c))) then
                        r_parent (r) = pr
                    end if
                end do SCAN_PARENT
            end associate
        end do SCAN_RES
        allocate (r_child (nr), source = [(r, r = 1, nr)])
        do r = 1, nr
            ir = r_branch(r)
            tree%branch(ir)%r_child = r_branch (pack (r_child, r_parent == r))
        end do
    end subroutine set_child_resonances

    subroutine set_child_outgoing ()
        integer, dimension(:), allocatable :: o_child, o_parent
        integer :: o_max, r, o, ir
        o_max = 0
        do r = 1, nr
            associate (this_res => res_hist%resonances(r))
                o_max = max (o_max, maxval (this_res%contributors%c))
            end associate
        end do
        allocate (o_parent (o_max), source=0)
        SCAN_OUT: do o = 1, o_max
            SCAN_PARENT: do ir = 1, nr
                r = r_source(ir)
                associate (this_res => res_hist%resonances(r))
                    if (this_res%contains (o)) o_parent(o) = r
                end associate
            end do SCAN_PARENT
        end do SCAN_OUT
        allocate (o_child (o_max), source = [(o, o = 1, o_max)])
        do r = 1, nr
            ir = r_branch(r)
            tree%branch(ir)%o_child = pack (o_child, o_parent == r)
        end do
    end subroutine set_child_outgoing

    subroutine resonance_history_to_tree

```

19.5.7 Resonance history set

This is an array of resonance histories. The elements are supposed to be unique. That is, entering a new element is successful only if the element does not already exist.

The current implementation uses a straightforward linear search for comparison. If this should become an issue, we may change the implementation to a hash table. To keep this freedom, the set should be an opaque object. In fact, we expect to use it as a transient data structure. Once the set is complete, we transform it into a contiguous array.

```

<Resonances: public>+≡
    public :: resonance_history_set_t

<Resonances: types>+≡
    type :: index_array_t
        integer, dimension(:), allocatable :: i
    end type index_array_t

    type :: resonance_history_set_t
        private
        logical :: complete = .false.
        integer :: n_filter = 0
        type(resonance_history_t), dimension(:), allocatable :: history
        type(index_array_t), dimension(:), allocatable :: contains_this
        type(resonance_tree_t), dimension(:), allocatable :: tree
        integer :: last = 0
    contains
        <Resonances: resonance history set: TBP>
    end type resonance_history_set_t

```

Display.

The tree-format version of the histories is displayed only upon request.

```

<Resonances: resonance history set: TBP>≡
    procedure :: write => resonance_history_set_write

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_set_write &
        (res_set, unit, indent, show_trees)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        logical, intent(in), optional :: show_trees
    end subroutine resonance_history_set_write

<Resonances: procedures>+≡
    module subroutine resonance_history_set_write &
        (res_set, unit, indent, show_trees)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        logical, intent(in), optional :: show_trees
        logical :: s_trees
        integer :: u, i, j, ind
        u = given_output_unit (unit)

```

```

s_trees = .false.; if (present (show_trees)) s_trees = show_trees
ind = 0; if (present (indent)) ind = indent
call write_indent (u, indent)
write (u, "(A)", advance="no") "Resonance history set:"
if (res_set%complete) then
  write (u, *)
else
  write (u, "(1x,A)" "[incomplete]"
end if
do i = 1, res_set%last
  write (u, "(1x,I0,1x)", advance="no") i
  call res_set%history(i)%write (u, verbose=.false., indent=indent)
  if (allocated (res_set%contains_this)) then
    call write_indent (u, indent)
    write (u, "(3x,A)", advance="no") "contained in ("
    do j = 1, size (res_set%contains_this(i)%i)
      if (j>1) write (u, "(", advance="no")
      write (u, "(I0)", advance="no") res_set%contains_this(i)%i(j)
    end do
    write (u, "(A)" ")")
  end if
  if (s_trees .and. allocated (res_set%tree)) then
    call res_set%tree(i)%write (u, ind + 1)
  end if
end do
end subroutine resonance_history_set_write

```

Initialization. The default initial size is 16 elements, to be doubled in size repeatedly as needed.

```

<Resonances: parameters>+≡
  integer, parameter :: resonance_history_set_initial_size = 16

<Resonances: resonance history set: TBP>+≡
  procedure :: init => resonance_history_set_init

<Resonances: sub interfaces>+≡
  module subroutine resonance_history_set_init &
    (res_set, n_filter, initial_size)
    class(resonance_history_set_t), intent(out) :: res_set
    integer, intent(in), optional :: n_filter
    integer, intent(in), optional :: initial_size
  end subroutine resonance_history_set_init

<Resonances: procedures>+≡
  module subroutine resonance_history_set_init &
    (res_set, n_filter, initial_size)
    class(resonance_history_set_t), intent(out) :: res_set
    integer, intent(in), optional :: n_filter
    integer, intent(in), optional :: initial_size
    if (present (n_filter)) res_set%n_filter = n_filter
    if (present (initial_size)) then
      allocate (res_set%history (initial_size))
    else
      allocate (res_set%history (resonance_history_set_initial_size))
    end if
  end if

```

```
end subroutine resonance_history_set_init
```

Enter an entry: append to the array if it does not yet exist, expand as needed.
If a `n_filter` value has been provided, enter the resonance only if it fulfils the requirement.

An empty resonance history is entered only if the `trivial` flag is set.

(Resonances: resonance history set: TBP)+≡

```
procedure :: enter => resonance_history_set_enter
```

(Resonances: sub interfaces)+≡

```
module subroutine resonance_history_set_enter &
  (res_set, res_history, trivial)
  class(resonance_history_set_t), intent(inout) :: res_set
  type(resonance_history_t), intent(in) :: res_history
  logical, intent(in), optional :: trivial
end subroutine resonance_history_set_enter
```

(Resonances: procedures)+≡

```
module subroutine resonance_history_set_enter &
  (res_set, res_history, trivial)
  class(resonance_history_set_t), intent(inout) :: res_set
  type(resonance_history_t), intent(in) :: res_history
  logical, intent(in), optional :: trivial
  integer :: i, new
  if (res_history%n_resonances == 0) then
    if (present (trivial)) then
      if (.not. trivial) return
    else
      return
    end if
  end if
  if (res_set%n_filter > 0) then
    if (.not. res_history%only_has_n_contributors (res_set%n_filter)) return
  end if
  do i = 1, res_set%last
    if (res_set%history(i) == res_history) return
  end do
  new = res_set%last + 1
  if (new > size (res_set%history)) call res_set%expand ()
  res_set%history(new) = res_history
  res_set%last = new
end subroutine resonance_history_set_enter
```

Freeze the resonance history set: determine the array that determines in which other resonance histories a particular history is contained.

This can only be done once, and once this is done, no further histories can be entered.

(Resonances: resonance history set: TBP)+≡

```
procedure :: freeze => resonance_history_set_freeze
```

(Resonances: sub interfaces)+≡

```
module subroutine resonance_history_set_freeze (res_set)
  class(resonance_history_set_t), intent(inout) :: res_set
end subroutine resonance_history_set_freeze
```

<Resonances: procedures>+≡

```

module subroutine resonance_history_set_freeze (res_set)
  class(resonance_history_set_t), intent(inout) :: res_set
  integer :: i, n, c
  logical, dimension(:), allocatable :: contains_this
  integer, dimension(:), allocatable :: index_array
  n = res_set%last
  allocate (contains_this (n))
  allocate (index_array (n), source = [(i, i=1, n)])
  allocate (res_set%contains_this (n))
  do i = 1, n
    contains_this = resonance_history_contains &
      (res_set%history(1:n), res_set%history(i))
    c = count (contains_this)
    allocate (res_set%contains_this(i)%i (c))
    res_set%contains_this(i)%i = pack (index_array, contains_this)
  end do
  allocate (res_set%tree (n))
  do i = 1, n
    call res_set%history(i)%to_tree (res_set%tree(i))
  end do
  res_set%complete = .true.
end subroutine resonance_history_set_freeze

```

Determine the histories (in form of their indices in the array) that can be considered on-shell, given a set of momenta and a maximum distance. The distance from the resonance is measured in multiples of the resonance width.

Note that the momentum array must only contain the outgoing particles.

If a particular history is on-shell, but there is another history which contains this and also is on-shell, only the latter is retained.

<Resonances: resonance history set: TBP>+≡

```

procedure :: determine_on_shell_histories &
  => resonance_history_set_determine_on_shell_histories

```

<Resonances: sub interfaces>+≡

```

module subroutine resonance_history_set_determine_on_shell_histories &
  (res_set, p, on_shell_limit, index_array)
  class(resonance_history_set_t), intent(in) :: res_set
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: on_shell_limit
  integer, dimension(:), allocatable, intent(out) :: index_array
end subroutine resonance_history_set_determine_on_shell_histories

```

<Resonances: procedures>+≡

```

module subroutine resonance_history_set_determine_on_shell_histories &
  (res_set, p, on_shell_limit, index_array)
  class(resonance_history_set_t), intent(in) :: res_set
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), intent(in) :: on_shell_limit
  integer, dimension(:), allocatable, intent(out) :: index_array
  integer :: n, i
  integer, dimension(:), allocatable :: i_array
  if (res_set%complete) then
    n = res_set%last

```

```

allocate (i_array (n), source=0)
do i = 1, n
    if (res_set%history(i)%is_on_shell (p, on_shell_limit)) i_array(i) = i
end do
do i = 1, n
    if (any (i_array(res_set%contains_this(i)%i) /= 0)) then
        i_array(i) = 0
    end if
end do
allocate (index_array (count (i_array /= 0)))
index_array(:) = pack (i_array, i_array /= 0)
end if
end subroutine resonance_history_set_determine_on_shell_histories

```

For the selected history, compute the Gaussian turnoff factor. The turnoff parameter is `gw`.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: evaluate_gaussian => resonance_history_set_evaluate_gaussian

<Resonances: sub interfaces>+≡
    module function resonance_history_set_evaluate_gaussian &
        (res_set, p, gw, i) result (factor)
        class(resonance_history_set_t), intent(in) :: res_set
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: gw
        integer, intent(in) :: i
        real(default) :: factor
    end function resonance_history_set_evaluate_gaussian

<Resonances: procedures>+≡
    module function resonance_history_set_evaluate_gaussian &
        (res_set, p, gw, i) result (factor)
        class(resonance_history_set_t), intent(in) :: res_set
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: gw
        integer, intent(in) :: i
        real(default) :: factor
        factor = res_set%history(i)%evaluate_gaussian (p, gw)
    end function resonance_history_set_evaluate_gaussian

```

Return the number of histories. This is zero if there are none, or if `freeze` has not been called yet.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: get_n_history => resonance_history_set_get_n_history

<Resonances: sub interfaces>+≡
    module function resonance_history_set_get_n_history (res_set) result (n)
        class(resonance_history_set_t), intent(in) :: res_set
        integer :: n
    end function resonance_history_set_get_n_history

<Resonances: procedures>+≡
    module function resonance_history_set_get_n_history (res_set) result (n)
        class(resonance_history_set_t), intent(in) :: res_set
        integer :: n

```

```

    if (res_set%complete) then
        n = res_set%last
    else
        n = 0
    end if
end function resonance_history_set_get_n_history

```

Return a single history.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: get_history => resonance_history_set_get_history

<Resonances: sub interfaces>+≡
    module function resonance_history_set_get_history &
        (res_set, i) result (res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_history_t) :: res_history
    end function resonance_history_set_get_history

<Resonances: procedures>+≡
    module function resonance_history_set_get_history &
        (res_set, i) result (res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_history_t) :: res_history
        if (res_set%complete .and. i <= res_set%last) then
            res_history = res_set%history(i)
        end if
    end function resonance_history_set_get_history

```

Conversion to a plain array, sized correctly.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: to_array => resonance_history_set_to_array

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_set_to_array (res_set, res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
            res_history
    end subroutine resonance_history_set_to_array

<Resonances: procedures>+≡
    module subroutine resonance_history_set_to_array (res_set, res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
            res_history
        if (res_set%complete) then
            allocate (res_history (res_set%last))
            res_history(:) = res_set%history(1:res_set%last)
        end if
    end subroutine resonance_history_set_to_array

```

Return a selected history in tree form.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: get_tree => resonance_history_set_get_tree

```

```

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_set_get_tree (res_set, i, res_tree)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_tree_t), intent(out) :: res_tree
    end subroutine resonance_history_set_get_tree

<Resonances: procedures>+≡
    module subroutine resonance_history_set_get_tree (res_set, i, res_tree)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_tree_t), intent(out) :: res_tree
        if (res_set%complete) then
            res_tree = res_set%tree(i)
        end if
    end subroutine resonance_history_set_get_tree

```

Expand: double the size of the array. We do not need this in the API.

```

<Resonances: resonance history set: TBP>+≡
    procedure, private :: expand => resonance_history_set_expand

<Resonances: sub interfaces>+≡
    module subroutine resonance_history_set_expand (res_set)
        class(resonance_history_set_t), intent(inout) :: res_set
    end subroutine resonance_history_set_expand

<Resonances: procedures>+≡
    module subroutine resonance_history_set_expand (res_set)
        class(resonance_history_set_t), intent(inout) :: res_set
        type(resonance_history_t), dimension(:), allocatable :: history_new
        integer :: s
        s = size (res_set%history)
        allocate (history_new (2 * s))
        history_new(1:s) = res_set%history(1:s)
        call move_alloc (history_new, res_set%history)
    end subroutine resonance_history_set_expand

```

19.5.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<resonances_ut.f90>≡
    <File header>

    module resonances_ut
        use unit_tests
        use resonances_uti

    <Standard module head>

    <Resonances: public test>

    contains

```



```

    <Resonances: test driver>

    end module resonances_ut

    <resonances_util.f90>≡
    <File header>

    module resonances_util

    <Use kinds>
    <Use strings>
        use format_defs, only: FMF_12
        use lorentz, only: vector4_t, vector4_at_rest
        use model_data, only: model_data_t
        use flavors, only: flavor_t

        use resonances, only: resonance_history_t

        use resonances

    <Standard module head>

    <Resonances: test declarations>

    contains

    <Resonances: tests>

    end module resonances_util
API: driver for the unit tests below.
    <Resonances: public test>≡
        public :: resonances_test
    <Resonances: test driver>≡
        subroutine resonances_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <Resonances: execute tests>
        end subroutine resonances_test

```

Basic operations on a resonance history object.

```

    <Resonances: execute tests>≡
        call test (resonances_1, "resonances_1", &
            "check resonance history setup", &
            u, results)
    <Resonances: test declarations>≡
        public :: resonances_1
    <Resonances: tests>≡
        subroutine resonances_1 (u)
            integer, intent(in) :: u
            type(resonance_info_t) :: res_info
            type(resonance_history_t) :: res_history
            type(model_data_t), target :: model

```

```

write (u, "(A)")  "* Test output: resonances_1"
write (u, "(A)")  "* Purpose: test resonance history setup"
write (u, "(A)")

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Empty resonance history"
write (u, "(A)")

call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add resonance"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add another resonance"
write (u, "(A)")

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Remove resonance"
write (u, "(A)")

call res_history%remove_resonance (1)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_1"

end subroutine resonances_1

```

Basic operations on a resonance history object.

(Resonances: execute tests)+≡

```

call test (resonances_2, "resonances_2", &
  "check 0'Mega restriction strings", &

```

```

        u, results)

<Resonances: test declarations>+≡
    public :: resonances_2

<Resonances: tests>+≡
    subroutine resonances_2 (u)
        integer, intent(in) :: u
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(model_data_t), target :: model
        type(string_t) :: restrictions

        write (u, "(A)")  "* Test output: resonances_2"
        write (u, "(A)")  "* Purpose: test OMega restrictions strings &
            &for resonance history"
        write (u, "(A)")

        write (u, "(A)")  "* Read model file"

        call model%init_sm_test ()

        write (u, "(A)")
        write (u, "(A)")  "* Empty resonance history"
        write (u, "(A)")

        restrictions = res_history%as_omega_string (2)
        write (u, "(A,A,A)")  "restrictions = '", char (restrictions), "'"

        write (u, "(A)")
        write (u, "(A)")  "* Add resonance"
        write (u, "(A)")

        call res_info%init (3, -24, model, 5)
        call res_history%add_resonance (res_info)
        restrictions = res_history%as_omega_string (2)
        write (u, "(A,A,A)")  "restrictions = '", char (restrictions), "'"

        write (u, "(A)")
        write (u, "(A)")  "* Add another resonance"
        write (u, "(A)")

        call res_info%init (7, 23, model, 5)
        call res_history%add_resonance (res_info)
        restrictions = res_history%as_omega_string (2)
        write (u, "(A,A,A)")  "restrictions = '", char (restrictions), "'"

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call model%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: resonances_2"

```

```
end subroutine resonances_2
```

Basic operations on a resonance history set.

```
<Resonances: execute tests>+≡
```

```
call test (resonances_3, "resonances_3", &
  "check resonance history set", &
  u, results)
```

```
<Resonances: test declarations>+≡
```

```
public :: resonances_3
```

```
<Resonances: tests>+≡
```

```
subroutine resonances_3 (u)
  integer, intent(in) :: u
  type(resonance_info_t) :: res_info
  type(resonance_history_t) :: res_history
  type(resonance_history_t), dimension(:), allocatable :: res_histories
  type(resonance_history_set_t) :: res_set
  type(model_data_t), target :: model
  integer :: i

  write (u, "(A)")  "* Test output: resonances_3"
  write (u, "(A)")  "* Purpose: test resonance history set"
  write (u, "(A)")

  write (u, "(A)")  "* Read model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* Initialize resonance history set"
  write (u, "(A)")

  call res_set%init (initial_size = 2)

  write (u, "(A)")  "* Add resonance histories, one at a time"
  write (u, "(A)")

  call res_history%write (u)
  call res_set%enter (res_history)
  call res_history%clear ()

  write (u, *)

  call res_info%init (3, -24, model, 5)
  call res_history%add_resonance (res_info)
  call res_history%write (u)
  call res_set%enter (res_history)
  call res_history%clear ()

  write (u, *)

  call res_info%init (3, -24, model, 5)
  call res_history%add_resonance (res_info)
  call res_info%init (7, 23, model, 5)
```

```

call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 25, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "* Result"
write (u, "(A)")

call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Queries"
write (u, "(A)")

write (u, "(A,1x,I0)")  "n_history =", res_set%get_n_history ()

write (u, "(A)")
write (u, "(A)")  "History #2:"

res_history = res_set%get_history (2)
call res_history%write (u, indent=1)
call res_history%clear ()

write (u, "(A)")
write (u, "(A)")  "* Result in array form"

```

```

call res_set%to_array (res_histories)
do i = 1, size (res_histories)
    write (u, *)
    call res_histories(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Re-initialize resonance history set with filter n=2"
write (u, "(A)")

call res_set%init (n_filter = 2)

write (u, "(A)")  "* Add resonance histories, one at a time"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "* Result"
write (u, "(A)")

```

```

call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_3"

end subroutine resonances_3

```

Probe momenta for resonance histories

```

<Resonances: execute tests>+≡
call test (resonances_4, "resonances_4", &
    "resonance history: distance evaluation", &
    u, results)

<Resonances: test declarations>+≡
public :: resonances_4

<Resonances: tests>+≡
subroutine resonances_4 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(model_data_t), target :: model
    type(flavor_t) :: fw, fz
    real(default) :: mw, mz, ww, wz
    type(vector4_t), dimension(3) :: p
    real(default), dimension(2) :: dist
    real(default) :: gw, factor
    integer :: i

    write (u, "(A)")  "* Test output: resonances_4"
    write (u, "(A)")  "* Purpose: test resonance history evaluation"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* W and Z parameters"
    write (u, "(A)")

    call fw%init (24, model)
    call fz%init (23, model)
    mw = fw%get_mass ()
    ww = fw%get_width ()
    mz = fz%get_mass ()
    wz = fz%get_width ()

    write (u, "(A,1x," // FMF_12 // ")")  "mW =", mw
    write (u, "(A,1x," // FMF_12 // ")")  "wW =", ww

```

```

write (u, "(A,1x," // FMF_12 // ")") "mZ =", mz
write (u, "(A,1x," // FMF_12 // ")") "wZ =", wz

write (u, "(A)")
write (u, "(A)") "* Gaussian width parameter"
write (u, "(A)")

gw = 2
write (u, "(A,1x," // FMF_12 // ")") "gw =", gw

write (u, "(A)")
write (u, "(A)") "* Setup resonance histories"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)

call res_history%write (u)

write (u, "(A)")
write (u, "(A)") "* Setup zero momenta"
write (u, "(A)")

do i = 1, 3
    call p(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)") "* Evaluate distances from resonances"
write (u, "(A)")

call res_history%evaluate_distances (p, dist)
write (u, "(A,1x," // FMF_12 // ")") "distance (W) =", dist(1)
write (u, "(A,1x," // FMF_12 // ")") "m/w (W) =", mw / ww
write (u, "(A,1x," // FMF_12 // ")") "distance (Z) =", dist(2)
write (u, "(A,1x," // FMF_12 // ")") "m/w (Z) =", mz / wz

write (u, "(A)")
write (u, "(A)") "* Evaluate Gaussian turnoff factor"
write (u, "(A)")

factor = res_history%evaluate_gaussian (p, gw)
write (u, "(A,1x," // FMF_12 // ")") "gaussian fac =", factor

write (u, "(A)")
write (u, "(A)") "* Set momenta on W peak"
write (u, "(A)")

p(1) = vector4_at_rest (mw/2)
p(2) = vector4_at_rest (mw/2)
do i = 1, 3

```



```

        call p(i)%write (u)
    end do

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate distances from resonances"
    write (u, "(A)")

    call res_history%evaluate_distances (p, dist)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (W) =", dist(1)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (Z) =", dist(2)
    write (u, "(A,1x," // FMF_12 // ")")    "expected      =", &
        abs (mz**2 - mw**2) / (mz*wz)

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate Gaussian turnoff factor"
    write (u, "(A)")

    factor = res_history%evaluate_gaussian (p, gw)
    write (u, "(A,1x," // FMF_12 // ")")    "gaussian fac =", factor
    write (u, "(A,1x," // FMF_12 // ")")    "expected      =", &
        exp (- (abs (mz**2 - mw**2) / (mz*wz))**2 / (gw * wz)**2)

    write (u, "(A)")
    write (u, "(A)")    "* Set momenta on both peaks"
    write (u, "(A)")

    p(3) = vector4_at_rest (mz - mw)
    do i = 1, 3
        call p(i)%write (u)
    end do

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate distances from resonances"
    write (u, "(A)")

    call res_history%evaluate_distances (p, dist)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (W) =", dist(1)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (Z) =", dist(2)

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate Gaussian turnoff factor"
    write (u, "(A)")

    factor = res_history%evaluate_gaussian (p, gw)
    write (u, "(A,1x," // FMF_12 // ")")    "gaussian fac =", factor

    write (u, "(A)")
    write (u, "(A)")    "* Cleanup"

    call model%final ()

    write (u, "(A)")
    write (u, "(A)")    "* Test output end: resonances_4"

```

```
end subroutine resonances_4
```

Probe on-shell test for resonance histories

```
<Resonances: execute tests>+≡
```

```
call test (resonances_5, "resonances_5", &
  "resonance history: on-shell test", &
  u, results)
```

```
<Resonances: test declarations>+≡
```

```
public :: resonances_5
```

```
<Resonances: tests>+≡
```

```
subroutine resonances_5 (u)
  integer, intent(in) :: u
  type(resonance_info_t) :: res_info
  type(resonance_history_t) :: res_history
  type(resonance_history_set_t) :: res_set
  type(model_data_t), target :: model
  type(flavor_t) :: fw, fz
  real(default) :: mw, mz, ww, wz
  real(default) :: on_shell_limit
  integer, dimension(:), allocatable :: on_shell
  type(vector4_t), dimension(4) :: p

  write (u, "(A)")  "* Test output: resonances_5"
  write (u, "(A)")  "* Purpose: resonance history on-shell test"
  write (u, "(A)")

  write (u, "(A)")  "* Read model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* W and Z parameters"
  write (u, "(A)")

  call fw%init (24, model)
  call fz%init (23, model)
  mw = fw%get_mass ()
  ww = fw%get_width ()
  mz = fz%get_mass ()
  wz = fz%get_width ()

  write (u, "(A,1x," // FMF_12 // ")")  "mW =", mw
  write (u, "(A,1x," // FMF_12 // ")")  "wW =", ww
  write (u, "(A,1x," // FMF_12 // ")")  "mZ =", mz
  write (u, "(A,1x," // FMF_12 // ")")  "wZ =", wz

  write (u, "(A)")
  write (u, "(A)")  "* On-shell parameter: distance as multiple of width"
  write (u, "(A)")

  on_shell_limit = 3
  write (u, "(A,1x," // FMF_12 // ")")  "on-shell limit =", on_shell_limit
```

```

write (u, "(A)")
write (u, "(A)")  "* Setup resonance history set"
write (u, "(A)")

call res_set%init ()

call res_info%init (3, -24, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Setup zero momenta"
write (u, "(A)")

call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- resonance (2 widths off)"
write (u, "(A)")

p(1) = vector4_at_rest (82.5_default)
call write_momenta (p)

```

```

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- resonance (4 widths off)"
write (u, "(A)")

p(1) = vector4_at_rest (84.5_default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near Z resonance"
write (u, "(A)")

p(1) = vector4_at_rest (45._default)
p(3) = vector4_at_rest (45._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- and W+ resonances"
write (u, "(A)")

p(1) = vector4_at_rest (40._default)
p(2) = vector4_at_rest (40._default)
p(3) = vector4_at_rest (40._default)
p(4) = vector4_at_rest (40._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- and Z resonances, &
&shadowing single resonances"
write (u, "(A)")

p(1) = vector4_at_rest (40._default)
p(2) = vector4_at_rest (40._default)
p(3) = vector4_at_rest (10._default)
p(4) = vector4_at_rest ( 0._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_5"

contains

subroutine write_momenta (p)
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: i
  do i = 1, size (p)
    call p(i)%write (u)
  end do
end subroutine write_momenta

subroutine write_on_shell_histories (on_shell)
  integer, dimension(:), intent(in) :: on_shell
  integer :: i
  write (u, *)
  write (u, "(A)", advance="no")  "on-shell = ("
  do i = 1, size (on_shell)
    if (i > 1) write (u, "(', ')", advance="no")
    write (u, "(I0)", advance="no")  on_shell(i)
  end do
  write (u, "(')')")
end subroutine write_on_shell_histories

end subroutine resonances_5

```

Organize the resonance history as a tree structure.

```

<Resonances: execute tests>+≡
  call test (resonances_6, "resonances_6", &
    "check resonance history setup", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_6

<Resonances: tests>+≡
  subroutine resonances_6 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_tree_t) :: res_tree
    type(model_data_t), target :: model

    write (u, "(A)")  "* Test output: resonances_6"
    write (u, "(A)")  "* Purpose: retrieve resonance histories as trees"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Empty resonance history"
write (u, "(A)")

call res_history%write (u)

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Single resonance"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Nested resonances"
write (u, "(A)")

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Disjunct resonances"
write (u, "(A)")

call res_history%clear ()

call res_info%init (5, 24, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (7, 6, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (80, -24, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (112, -6, model, 7)
call res_history%add_resonance (res_info)

call res_history%write (u)

```

```

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_6"

end subroutine resonances_6

```

Basic operations on a resonance history set.

```

<Resonances: execute tests>+≡
call test (resonances_7, "resonances_7", &
    "display tree format of history set elements", &
    u, results)

<Resonances: test declarations>+≡
public :: resonances_7

<Resonances: tests>+≡
subroutine resonances_7 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_tree_t) :: res_tree
    type(resonance_history_set_t) :: res_set
    type(model_data_t), target :: model
    type(flavor_t) :: flv

    write (u, "(A)")  "* Test output: resonances_7"
    write (u, "(A)")  "* Purpose: test tree format"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* Initialize, fill and freeze resonance history set"
    write (u, "(A)")

    call res_set%init (initial_size = 2)

    call res_info%init (3, -24, model, 5)
    call res_history%add_resonance (res_info)
    call res_history%clear ()

    call res_info%init (3, -24, model, 5)
    call res_history%add_resonance (res_info)
    call res_info%init (7, 23, model, 5)
    call res_history%add_resonance (res_info)

```

```

call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 25, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

call res_set%write (u, show_trees = .true.)

write (u, "(A)")
write (u, "(A)")  "* Extract tree #1"
write (u, "(A)")

call res_set%get_tree (1, res_tree)
call res_tree%write (u)

write (u, *)
write (u, "(1x,A,1x,I0)")  "n_resonances =", res_tree%get_n_resonances ()

write (u, *)
write (u, "(1x,A,1x)", advance="no")  "flv(r1) ="
flv = res_tree%get_flv (1)
call flv%write (u)
write (u, *)
write (u, "(1x,A,1x)", advance="no")  "flv(r2) ="
flv = res_tree%get_flv (2)
call flv%write (u)
write (u, *)

write (u, *)
write (u, "(1x,A)")  "[offset = 2, 4]"
write (u, "(1x,A,9(1x,I0))")  "children(r1) =", &
    res_tree%get_children(1, 2, 4)
write (u, "(1x,A,9(1x,I0))")  "children(r2) =", &
    res_tree%get_children(2, 2, 4)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```



```
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_7"

end subroutine resonances_7
```

19.6 Mappings

Mappings are objects that encode the transformation of the interval $(0,1)$ to a physical variable m^2 or $\cos\theta$ (and back), as it is used in the phase space parameterization. The mapping objects contain fixed parameters, the associated methods implement the mapping and inverse mapping operations, including the computation of the Jacobian (phase space factor).

```
<mappings.f90>≡
  <File header>

  module mappings

    <Use kinds>
    use kinds, only: TC
    <Use strings>
    use model_data
    use flavors

    <Standard module head>

    <Mappings: public>

    <Mappings: parameters>

    <Mappings: types>

    <Mappings: interfaces>

    interface
    <Mappings: sub interfaces>
    end interface

  end module mappings

<mappings_sub.f90>≡
  <File header>

  submodule (mappings) mappings_s

    use io_units
    use constants, only: pi
    use format_defs, only: FMT_19
    use diagnostics
    use md5

    implicit none

  contains

    <Mappings: procedures>

  end submodule mappings_s
```

19.6.1 Default parameters

This type holds the default parameters, needed for setting the scale in cases where no mass parameter is available. The contents are public.

```
<Mappings: public>≡
    public :: mapping_defaults_t

<Mappings: types>≡
    type :: mapping_defaults_t
        real(default) :: energy_scale = 10
        real(default) :: invariant_mass_scale = 10
        real(default) :: momentum_transfer_scale = 10
        logical :: step_mapping = .true.
        logical :: step_mapping_exp = .true.
        logical :: enable_s_mapping = .false.
    contains
        <Mappings: mapping defaults: TBP>
    end type mapping_defaults_t
```

Output.

```
<Mappings: mapping defaults: TBP>≡
    procedure :: write => mapping_defaults_write

<Mappings: sub interfaces>≡
    module subroutine mapping_defaults_write (object, unit)
        class(mapping_defaults_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine mapping_defaults_write

<Mappings: procedures>≡
    module subroutine mapping_defaults_write (object, unit)
        class(mapping_defaults_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A," // FMT_19 // ")") "energy scale = ", &
            object%energy_scale
        write (u, "(3x,A," // FMT_19 // ")") "mass scale = ", &
            object%invariant_mass_scale
        write (u, "(3x,A," // FMT_19 // ")") "q scale = ", &
            object%momentum_transfer_scale
        write (u, "(3x,A,L1)") "step mapping = ", &
            object%step_mapping
        write (u, "(3x,A,L1)") "step exp. mode = ", &
            object%step_mapping_exp
        write (u, "(3x,A,L1)") "allow s mapping = ", &
            object%enable_s_mapping
    end subroutine mapping_defaults_write

<Mappings: public>+≡
    public :: mapping_defaults_md5sum

<Mappings: sub interfaces>+≡
    module function mapping_defaults_md5sum &
        (mapping_defaults) result (md5sum_map)
```

```

        character(32) :: md5sum_map
        type(mapping_defaults_t), intent(in) :: mapping_defaults
    end function mapping_defaults_md5sum
<Mappings: procedures>+≡
    module function mapping_defaults_md5sum &
        (mapping_defaults) result (md5sum_map)
        character(32) :: md5sum_map
        type(mapping_defaults_t), intent(in) :: mapping_defaults
        integer :: u
        u = free_unit ()
        open (u, status = "scratch")
        write (u, *) mapping_defaults%energy_scale
        write (u, *) mapping_defaults%invariant_mass_scale
        write (u, *) mapping_defaults%momentum_transfer_scale
        write (u, *) mapping_defaults%step_mapping
        write (u, *) mapping_defaults%step_mapping_exp
        write (u, *) mapping_defaults%enable_s_mapping
        rewind (u)
        md5sum_map = md5sum (u)
        close (u)
    end function mapping_defaults_md5sum

```

19.6.2 The Mapping type

Each mapping has a type (e.g., s-channel, infrared), a binary code (redundant, but useful for debugging), and a reference particle. The flavor code of this particle is stored for bookkeeping reasons, what matters are the mass and width of this particle. Furthermore, depending on the type, various mapping parameters can be set and used.

The parameters **a1** to **a3** (for m^2 mappings) and **b1** to **b3** (for $\cos\theta$ mappings) are values that are stored once to speed up the calculation, if **variable_limits** is false. The exact meaning of these parameters depends on the mapping type. The limits are fixed if there is a fixed c.m. energy.

```

<Mappings: public>+≡
    public :: mapping_t
<Mappings: types>+≡
    type :: mapping_t
    private
        integer :: type = NO_MAPPING
        integer(TC) :: bincode
        type(flavor_t) :: flv
        real(default) :: mass = 0
        real(default) :: width = 0
        logical :: a_unknown = .true.
        real(default) :: a1 = 0
        real(default) :: a2 = 0
        real(default) :: a3 = 0
        logical :: b_unknown = .true.
        real(default) :: b1 = 0
        real(default) :: b2 = 0
        real(default) :: b3 = 0

```

```

        logical :: variable_limits = .true.
contains
    <Mappings: mapping: TBP>
end type mapping_t

```

The valid mapping types. The extra type STEP_MAPPING is used only internally.

```

<Mappings: parameters>≡
    <Mapping modes>

```

19.6.3 Screen output

Do not write empty mappings.

```

<Mappings: mapping: TBP>≡
    procedure :: write => mapping_write

<Mappings: sub interfaces>+≡
    module subroutine mapping_write (map, unit, verbose)
        class(mapping_t), intent(in) :: map
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine mapping_write

<Mappings: procedures>+≡
    module subroutine mapping_write (map, unit, verbose)
        class(mapping_t), intent(in) :: map
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        character(len=9) :: str
        u = given_output_unit (unit); if (u < 0) return
        select case (map%type)
        case(S_CHANNEL); str = "s_channel"
        case(COLLINEAR); str = "collinear"
        case(INFRARED); str = "infrared "
        case(RADIATION); str = "radiation"
        case(T_CHANNEL); str = "t_channel"
        case(U_CHANNEL); str = "u_channel"
        case(STEP_MAPPING_E); str = "step_exp"
        case(STEP_MAPPING_H); str = "step_hyp"
        case(ON_SHELL); str = "on_shell"
        case default; str = "???????"
        end select
        if (map%type /= NO_MAPPING) then
            write (u, '(1x,A,I4,A)') &
                "Branch #", map%bincode, ": " // &
                "Mapping (" // str // ") for particle " // &
                "' ' // char (map%flv%get_name ()) // ' '
            if (present (verbose)) then
                if (verbose) then
                    select case (map%type)
                    case (S_CHANNEL, RADIATION, STEP_MAPPING_E, STEP_MAPPING_H)
                        write (u, "(1x,A,3(" // FMT_19 // "))") &
                            " m/w = ", map%mass, map%width
                    case default

```

```

        write (u, "(1x,A,3(" // FMT_19 // "))") &
            " m      = ", map%mass
    end select
    select case (map%type)
    case (S_CHANNEL, T_CHANNEL, U_CHANNEL, &
        STEP_MAPPING_E, STEP_MAPPING_H, &
        COLLINEAR, INFRARED, RADIATION)
        write (u, "(1x,A,3(" // FMT_19 // "))") &
            " a1/2/3 = ", map%a1, map%a2, map%a3
    end select
    select case (map%type)
    case (T_CHANNEL, U_CHANNEL, COLLINEAR)
        write (u, "(1x,A,3(" // FMT_19 // "))") &
            " b1/2/3 = ", map%b1, map%b2, map%b3
    end select
    end if
end if
end if
end subroutine mapping_write

```

19.6.4 Define a mapping

The initialization routine sets the mapping type and the particle (binary code and flavor code) for which the mapping applies (e.g., a Z resonance in branch #3).

(Mappings: mapping: TBP)+≡

```

    procedure :: init => mapping_init

```

(Mappings: sub interfaces)+≡

```

    module subroutine mapping_init (mapping, bincode, type, f, model)
        class(mapping_t), intent(inout) :: mapping
        integer(TC), intent(in) :: bincode
        type(string_t), intent(in) :: type
        integer, intent(in), optional :: f
        class(model_data_t), intent(in), optional, target :: model
    end subroutine mapping_init

```

(Mappings: procedures)+≡

```

    module subroutine mapping_init (mapping, bincode, type, f, model)
        class(mapping_t), intent(inout) :: mapping
        integer(TC), intent(in) :: bincode
        type(string_t), intent(in) :: type
        integer, intent(in), optional :: f
        class(model_data_t), intent(in), optional, target :: model
        mapping%bincode = bincode
        select case (char (type))
        case ("s_channel"); mapping%type = S_CHANNEL
        case ("collinear"); mapping%type = COLLINEAR
        case ("infrared"); mapping%type = INFRARED
        case ("radiation"); mapping%type = RADIATION
        case ("t_channel"); mapping%type = T_CHANNEL
        case ("u_channel"); mapping%type = U_CHANNEL
        case ("step_exp"); mapping%type = STEP_MAPPING_E

```

```

case ("step_hyp"); mapping%type = STEP_MAPPING_H
case ("on_shell"); mapping%type = ON_SHELL
case default
    call msg_bug ("Mappings: encountered undefined mapping key '" &
        // char (type) // "'")
end select
if (present (f) .and. present (model)) call mapping%flv%init (f, model)
end subroutine mapping_init

```

This sets the actual mass and width, using a parameter set. Since the auxiliary parameters will only be determined when the mapping is first called, they are marked as unknown.

```

<Mappings: mapping: TBP>+≡
    procedure :: set_parameters => mapping_set_parameters

<Mappings: sub interfaces>+≡
    module subroutine mapping_set_parameters &
        (map, mapping_defaults, variable_limits)
        class(mapping_t), intent(inout) :: map
        type(mapping_defaults_t), intent(in) :: mapping_defaults
        logical, intent(in) :: variable_limits
    end subroutine mapping_set_parameters

<Mappings: procedures>+≡
    module subroutine mapping_set_parameters &
        (map, mapping_defaults, variable_limits)
        class(mapping_t), intent(inout) :: map
        type(mapping_defaults_t), intent(in) :: mapping_defaults
        logical, intent(in) :: variable_limits
        if (map%type /= NO_MAPPING) then
            map%mass = map%flv%get_mass ()
            map%width = map%flv%get_width ()
            map%variable_limits = variable_limits
            map%a_unknown = .true.
            map%b_unknown = .true.
            select case (map%type)
            case (S_CHANNEL)
                if (map%mass <= 0) then
                    call map%write ()
                    call msg_fatal &
                        & (" S-channel resonance must have positive mass")
                else if (map%width <= 0) then
                    call map%write ()
                    call msg_fatal &
                        & (" S-channel resonance must have positive width")
                end if
            case (RADIATION)
                map%width = max (map%width, mapping_defaults%energy_scale)
            case (INFRARED, COLLINEAR)
                map%mass = max (map%mass, mapping_defaults%invariant_mass_scale)
            case (T_CHANNEL, U_CHANNEL)
                map%mass = max (map%mass, mapping_defaults%momentum_transfer_scale)
            end select
        end if
    end if

```

```
end subroutine mapping_set_parameters
```

For a step mapping the mass and width are set directly, instead of being determined from the flavor parameter (which is meaningless here). They correspond to the effective upper bound of phase space due to a resonance, as opposed to the absolute upper bound.

```
<Mappings: mapping: TBP>+≡
  procedure :: set_step_mapping_parameters => &
    mapping_set_step_mapping_parameters

<Mappings: sub interfaces>+≡
  module subroutine mapping_set_step_mapping_parameters (map, &
    mass, width, variable_limits)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: mass, width
    logical, intent(in) :: variable_limits
  end subroutine mapping_set_step_mapping_parameters

<Mappings: procedures>+≡
  module subroutine mapping_set_step_mapping_parameters (map, &
    mass, width, variable_limits)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: mass, width
    logical, intent(in) :: variable_limits
    select case (map%type)
    case (STEP_MAPPING_E, STEP_MAPPING_H)
      map%variable_limits = variable_limits
      map%a_unknown = .true.
      map%b_unknown = .true.
      map%mass = mass
      map%width = width
    end select
  end subroutine mapping_set_step_mapping_parameters
```

19.6.5 Retrieve contents

Return true if there is any / an s-channel mapping.

```
<Mappings: mapping: TBP>+≡
  procedure :: is_set => mapping_is_set
  procedure :: is_s_channel => mapping_is_s_channel
  procedure :: is_on_shell => mapping_is_on_shell

<Mappings: sub interfaces>+≡
  module function mapping_is_set (mapping) result (flag)
    class(mapping_t), intent(in) :: mapping
    logical :: flag
  end function mapping_is_set
  module function mapping_is_s_channel (mapping) result (flag)
    class(mapping_t), intent(in) :: mapping
    logical :: flag
  end function mapping_is_s_channel
  module function mapping_is_on_shell (mapping) result (flag)
    class(mapping_t), intent(in) :: mapping
```



```

        logical :: flag
    end function mapping_is_on_shell

<Mappings: procedures>+≡
    module function mapping_is_set (mapping) result (flag)
        class(mapping_t), intent(in) :: mapping
        logical :: flag
        flag = mapping%type /= NO_MAPPING
    end function mapping_is_set

    module function mapping_is_s_channel (mapping) result (flag)
        class(mapping_t), intent(in) :: mapping
        logical :: flag
        flag = mapping%type == S_CHANNEL
    end function mapping_is_s_channel

    module function mapping_is_on_shell (mapping) result (flag)
        class(mapping_t), intent(in) :: mapping
        logical :: flag
        flag = mapping%type == ON_SHELL
    end function mapping_is_on_shell

```

Return the binary code for the mapped particle.

```

<Mappings: mapping: TBP>+≡
    procedure :: get_bincode => mapping_get_bincode

<Mappings: sub interfaces>+≡
    module function mapping_get_bincode (mapping) result (bincode)
        class(mapping_t), intent(in) :: mapping
        integer(TC) :: bincode
    end function mapping_get_bincode

<Mappings: procedures>+≡
    module function mapping_get_bincode (mapping) result (bincode)
        class(mapping_t), intent(in) :: mapping
        integer(TC) :: bincode
        bincode = mapping%bincode
    end function mapping_get_bincode

```

Return the flavor object for the mapped particle.

```

<Mappings: mapping: TBP>+≡
    procedure :: get_flv => mapping_get_flv

<Mappings: sub interfaces>+≡
    module function mapping_get_flv (mapping) result (flv)
        class(mapping_t), intent(in) :: mapping
        type(flavor_t) :: flv
    end function mapping_get_flv

<Mappings: procedures>+≡
    module function mapping_get_flv (mapping) result (flv)
        class(mapping_t), intent(in) :: mapping
        type(flavor_t) :: flv
        flv = mapping%flv
    end function mapping_get_flv

```

Return stored mass and width, respectively.

```

<Mappings: mapping: TBP>+≡
  procedure :: get_mass => mapping_get_mass
  procedure :: get_width => mapping_get_width

<Mappings: sub interfaces>+≡
  module function mapping_get_mass (mapping) result (mass)
    class(mapping_t), intent(in) :: mapping
    real(default) :: mass
  end function mapping_get_mass
  module function mapping_get_width (mapping) result (width)
    class(mapping_t), intent(in) :: mapping
    real(default) :: width
  end function mapping_get_width

<Mappings: procedures>+≡
  module function mapping_get_mass (mapping) result (mass)
    class(mapping_t), intent(in) :: mapping
    real(default) :: mass
    mass = mapping%mass
  end function mapping_get_mass

  module function mapping_get_width (mapping) result (width)
    class(mapping_t), intent(in) :: mapping
    real(default) :: width
    width = mapping%width
  end function mapping_get_width

```

19.6.6 Compare mappings

Equality for single mappings and arrays

```

<Mappings: public>+≡
  public :: operator(==)

<Mappings: interfaces>≡
  interface operator(==)
    module procedure mapping_equal
  end interface

<Mappings: sub interfaces>+≡
  module function mapping_equal (m1, m2) result (equal)
    type(mapping_t), intent(in) :: m1, m2
    logical :: equal
  end function mapping_equal

<Mappings: procedures>+≡
  module function mapping_equal (m1, m2) result (equal)
    type(mapping_t), intent(in) :: m1, m2
    logical :: equal
    if (m1%type == m2%type) then
      select case (m1%type)
        case (NO_MAPPING)
          equal = .true.
        case (S_CHANNEL, RADIATION, STEP_MAPPING_E, STEP_MAPPING_H)
          equal = (m1%mass == m2%mass) .and. (m1%width == m2%width)
      end select
    else
      equal = .false.
    end if
  end function mapping_equal

```

```

      case default
        equal = (m1%mass == m2%mass)
      end select
    else
      equal = .false.
    end if
  end function mapping_equal

```

19.6.7 Mappings of the invariant mass

Inserting an x value between 0 and 1, we want to compute the corresponding invariant mass $m^2(x)$ and the jacobian, aka phase space factor $f(x)$. We also need the reverse operation.

In general, the phase space factor f is defined by

$$\frac{1}{s} \int_{m_{\min}^2}^{m_{\max}^2} dm^2 g(m^2) = \int_0^1 dx \frac{1}{s} \frac{dm^2}{dx} g(m^2(x)) = \int_0^1 dx f(x) g(x), \quad (19.8)$$

where thus

$$f(x) = \frac{1}{s} \frac{dm^2}{dx}. \quad (19.9)$$

With this mapping, a function of the form

$$g(m^2) = c \frac{dx(m^2)}{dm^2} \quad (19.10)$$

is mapped to a constant:

$$\frac{1}{s} \int_{m_{\min}^2}^{m_{\max}^2} dm^2 g(m^2) = \int_0^1 dx f(x) g(m^2(x)) = \int_0^1 dx \frac{c}{s}. \quad (19.11)$$

Here is the mapping routine. Input are the available energy squared s , the limits for m^2 , and the x value. Output are the m^2 value and the phase space factor f .

```

<Mappings: mapping: TBP>+≡
  procedure :: compute_msq_from_x => mapping_compute_msq_from_x

<Mappings: sub interfaces>+≡
  module subroutine mapping_compute_msq_from_x &
    (map, s, msq_min, msq_max, msq, f, x)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s, msq_min, msq_max
    real(default), intent(out) :: msq, f
    real(default), intent(in) :: x
  end subroutine mapping_compute_msq_from_x

<Mappings: procedures>+≡
  module subroutine mapping_compute_msq_from_x &
    (map, s, msq_min, msq_max, msq, f, x)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s, msq_min, msq_max
    real(default), intent(out) :: msq, f

```

```

real(default), intent(in) :: x
real(default) :: z, msq0, msq1, tmp
integer :: type
type = map%type
if (s == 0) &
    call msg_fatal (" Applying msq mapping for zero energy")
<Modify mapping type if necessary>
select case(type)
case (NO_MAPPING)
    <Constants for trivial msq mapping>
    <Apply trivial msq mapping>
case (S_CHANNEL)
    <Constants for s-channel resonance mapping>
    <Apply s-channel resonance mapping>
case (COLLINEAR, INFRARED, RADIATION)
    <Constants for s-channel pole mapping>
    <Apply s-channel pole mapping>
case (T_CHANNEL, U_CHANNEL)
    <Constants for t-channel pole mapping>
    <Apply t-channel pole mapping>
case (STEP_MAPPING_E)
    <Constants for exponential step mapping>
    <Apply exponential step mapping>
case (STEP_MAPPING_H)
    <Constants for hyperbolic step mapping>
    <Apply hyperbolic step mapping>
case default
    call msg_fatal ( " Attempt to apply undefined msq mapping")
end select
end subroutine mapping_compute_msq_from_x

```

The inverse mapping

```

<Mappings: mapping: TBP>+≡
    procedure :: compute_x_from_msq => mapping_compute_x_from_msq

<Mappings: sub interfaces>+≡
    module subroutine mapping_compute_x_from_msq &
        (map, s, msq_min, msq_max, msq, f, x)
        class(mapping_t), intent(inout) :: map
        real(default), intent(in) :: s, msq_min, msq_max
        real(default), intent(in) :: msq
        real(default), intent(out) :: f, x
    end subroutine mapping_compute_x_from_msq

<Mappings: procedures>+≡
    module subroutine mapping_compute_x_from_msq &
        (map, s, msq_min, msq_max, msq, f, x)
        class(mapping_t), intent(inout) :: map
        real(default), intent(in) :: s, msq_min, msq_max
        real(default), intent(in) :: msq
        real(default), intent(out) :: f, x
        real(default) :: msq0, msq1, tmp, z
        integer :: type
        type = map%type
        if (s == 0) &

```

```

        call msg_fatal (" Applying inverse msq mapping for zero energy")
    <Modify mapping type if necessary>
    select case (type)
    case (NO_MAPPING)
        <Constants for trivial msq mapping>
        <Apply inverse trivial msq mapping>
    case (S_CHANNEL)
        <Constants for s-channel resonance mapping>
        <Apply inverse s-channel resonance mapping>
    case (COLLINEAR, INFRARED, RADIATION)
        <Constants for s-channel pole mapping>
        <Apply inverse s-channel pole mapping>
    case (T_CHANNEL, U_CHANNEL)
        <Constants for t-channel pole mapping>
        <Apply inverse t-channel pole mapping>
    case (STEP_MAPPING_E)
        <Constants for exponential step mapping>
        <Apply inverse exponential step mapping>
    case (STEP_MAPPING_H)
        <Constants for hyperbolic step mapping>
        <Apply inverse hyperbolic step mapping>
    case default
        call msg_fatal ( " Attempt to apply undefined msq mapping")
    end select
end subroutine mapping_compute_x_from_msq

```

Trivial mapping

We simply map the boundaries of the interval (m_{\min}, m_{\max}) to $(0, 1)$:

$$m^2 = (1 - x)m_{\min}^2 + xm_{\max}^2; \quad (19.12)$$

the inverse is

$$x = \frac{m^2 - m_{\min}^2}{m_{\max}^2 - m_{\min}^2}. \quad (19.13)$$

Hence

$$f(x) = \frac{m_{\max}^2 - m_{\min}^2}{s}, \quad (19.14)$$

and we have, as required,

$$f(x) \frac{dx}{dm^2} = \frac{1}{s}. \quad (19.15)$$

We store the constant parameters the first time the mapping is called – or, if limits vary, recompute them each time.

```

<Constants for trivial msq mapping>≡
    if (map%variable_limits .or. map%a_unknown) then
        map%a1 = 0
        map%a2 = msq_max - msq_min
        map%a3 = map%a2 / s
        map%a_unknown = .false.
    end if

```

```

⟨Apply trivial msq mapping⟩≡
  msq = (1-x) * msq_min + x * msq_max
  f = map%a3
⟨Apply inverse trivial msq mapping⟩≡
  if (map%a2 /= 0) then
    x = (msq - msq_min) / map%a2
  else
    x = 0
  end if
  f = map%a3

```

Resonance or step mapping does not make much sense if the resonance mass is outside the kinematical bounds. If this is the case, revert to `NO_MAPPING`. This is possible even if the kinematical bounds vary from event to event.

```

⟨Modify mapping type if necessary⟩≡
  select case (type)
  case (S_CHANNEL, STEP_MAPPING_E, STEP_MAPPING_H)
    msq0 = map%mass**2
    if (msq0 < msq_min .or. msq0 > msq_max) type = NO_MAPPING
  end select

```

Breit-Wigner mapping

A Breit-Wigner resonance with mass M and width Γ is flattened by the following mapping:

This mapping does not make much sense if the resonance mass is too low. If this is the case, revert to `NO_MAPPING`. There is a tricky point with this if the mass is too high: `msq_max` is not a constant if structure functions are around. However, switching the type depending on the overall energy does not change the integral, it is just another branching point.

$$m^2 = M(M + t\Gamma), \quad (19.16)$$

where

$$t = \tan \left[(1-x) \arctan \frac{m_{\min}^2 - M^2}{M\Gamma} + x \arctan \frac{m_{\max}^2 - M^2}{M\Gamma} \right]. \quad (19.17)$$

The inverse:

$$x = \frac{\arctan \frac{m^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma}}{\arctan \frac{m_{\max}^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma}} \quad (19.18)$$

The phase-space factor of this transformation is

$$f(x) = \frac{M\Gamma}{s} \left(\arctan \frac{m_{\max}^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma} \right) (1 + t^2). \quad (19.19)$$

This maps any function proportional to

$$g(m^2) = \frac{M\Gamma}{(m^2 - M^2)^2 + M^2\Gamma^2} \quad (19.20)$$

to a constant times $1/s$.

```

⟨Constants for s-channel resonance mapping⟩≡

```

```

if (map%variable_limits .or. map%a_unknown) then
  msq0 = map%mass ** 2
  map%a1 = atan ((msq_min - msq0) / (map%mass * map%width))
  map%a2 = atan ((msq_max - msq0) / (map%mass * map%width))
  map%a3 = (map%a2 - map%a1) * (map%mass * map%width) / s
  map%a_unknown = .false.
end if

⟨Apply s-channel resonance mapping⟩≡
  z = (1-x) * map%a1 + x * map%a2
  if (-pi/2 < z .and. z < pi/2) then
    tmp = tan (z)
    msq = map%mass * (map%mass + map%width * tmp)
    f = map%a3 * (1 + tmp**2)
  else
    msq = 0
    f = 0
  end if

⟨Apply inverse s-channel resonance mapping⟩≡
  tmp = (msq - msq0) / (map%mass * map%width)
  x = (atan (tmp) - map%a1) / (map%a2 - map%a1)
  f = map%a3 * (1 + tmp**2)

```

Mapping for massless splittings

This mapping accounts for approximately scale-invariant behavior where $\ln M^2$ is evenly distributed.

$$m^2 = m_{\min}^2 + M^2 (\exp(xL) - 1) \quad (19.21)$$

where

$$L = \ln \left(\frac{m_{\max}^2 - m_{\min}^2}{M^2} + 1 \right). \quad (19.22)$$

The inverse:

$$x = \frac{1}{L} \ln \left(\frac{m^2 - m_{\min}^2}{M^2} + 1 \right) \quad (19.23)$$

The constant M is a characteristic scale. Above this scale ($m^2 - m_{\min}^2 \gg M^2$), this mapping behaves like $x \propto \ln m^2$, while below the scale it reverts to a linear mapping.

The phase-space factor is

$$f(x) = \frac{M^2}{s} \exp(xL) L. \quad (19.24)$$

A function proportional to

$$g(m^2) = \frac{1}{(m^2 - m_{\min}^2) + M^2} \quad (19.25)$$

is mapped to a constant, i.e., a simple pole near m_{\min} with a regulator mass M .

This type of mapping is useful for massless collinear and infrared singularities, where the scale is stored as the mass parameter. In the radiation case

(IR radiation off massive particle), the heavy particle width is the characteristic scale.

```

⟨Constants for s-channel pole mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    if (type == RADIATION) then
      msq0 = map%width**2
    else
      msq0 = map%mass**2
    end if
    map%a1 = msq0
    map%a2 = log ((msq_max - msq_min) / msq0 + 1)
    map%a3 = map%a2 / s
    map%a_unknown = .false.
  end if

⟨Apply s-channel pole mapping⟩≡
  msq1 = map%a1 * exp (x * map%a2)
  msq = msq1 - map%a1 + msq_min
  f = map%a3 * msq1

⟨Apply inverse s-channel pole mapping⟩≡
  msq1 = msq - msq_min + map%a1
  x = log (msq1 / map%a1) / map%a2
  f = map%a3 * msq1

```

Mapping for t-channel poles

This is also approximately scale-invariant, and we use the same type of mapping as before. However, we map $1/x$ singularities at both ends of the interval; again, the mapping becomes linear when the distance is less than M^2 :

$$m^2 = \begin{cases} m_{\min}^2 + M^2 (\exp(xL) - 1) & \text{for } 0 < x < \frac{1}{2} \\ m_{\max}^2 - M^2 (\exp((1-x)L) - 1) & \text{for } \frac{1}{2} \leq x < 1 \end{cases} \quad (19.26)$$

where

$$L = 2 \ln \left(\frac{m_{\max}^2 - m_{\min}^2}{2M^2} + 1 \right). \quad (19.27)$$

The inverse:

$$x = \begin{cases} \frac{1}{L} \ln \left(\frac{m^2 - m_{\min}^2}{M^2} + 1 \right) & \text{for } m^2 < (m_{\max}^2 - m_{\min}^2)/2 \\ 1 - \frac{1}{L} \ln \left(\frac{m_{\max}^2 - m^2}{M^2} + 1 \right) & \text{for } m^2 \geq (m_{\max}^2 - m_{\min}^2)/2 \end{cases} \quad (19.28)$$

The phase-space factor is

$$f(x) = \begin{cases} \frac{M^2}{s} \exp(xL) L. & \text{for } 0 < x < \frac{1}{2} \\ \frac{M^2}{s} \exp((1-x)L) L. & \text{for } \frac{1}{2} \leq x < 1 \end{cases} \quad (19.29)$$

A (continuous) function proportional to

$$g(m^2) = \begin{cases} 1/(m^2 - m_{\min}^2) + M^2 & \text{for } m^2 < (m_{\max}^2 - m_{\min}^2)/2 \\ 1/((m_{\max}^2 - m^2) + M^2) & \text{for } m^2 \geq (m_{\max}^2 - m_{\min}^2)/2 \end{cases} \quad (19.30)$$

is mapped to a constant by this mapping, i.e., poles near both ends of the interval.

```

⟨Constants for t-channel pole mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    msq0 = map%mass**2
    map%a1 = msq0
    map%a2 = 2 * log ((msq_max - msq_min)/(2*msq0) + 1)
    map%a3 = map%a2 / s
    map%a_unknown = .false.
  end if

⟨Apply t-channel pole mapping⟩≡
  if (x < .5_default) then
    msq1 = map%a1 * exp (x * map%a2)
    msq = msq1 - map%a1 + msq_min
  else
    msq1 = map%a1 * exp ((1-x) * map%a2)
    msq = -(msq1 - map%a1) + msq_max
  end if
  f = map%a3 * msq1

⟨Apply inverse t-channel pole mapping⟩≡
  if (msq < (msq_max + msq_min)/2) then
    msq1 = msq - msq_min + map%a1
    x = log (msq1/map%a1) / map%a2
  else
    msq1 = msq_max - msq + map%a1
    x = 1 - log (msq1/map%a1) / map%a2
  end if
  f = map%a3 * msq1

```

19.6.8 Step mapping

Step mapping is useful when the allowed range for a squared-mass variable is large, but only a fraction at the lower end is populated because the particle in question is an (off-shell) decay product of a narrow resonance. I.e., if the resonance was forced to be on-shell, the upper end of the range would be the resonance mass, minus the effective (real or resonance) mass of the particle(s) in the sibling branch of the decay.

The edge of this phase space section has a width which is determined by the width of the parent, plus the width of the sibling branch. (The widths might be added in quadrature, but this precision is probably not important.)

Fermi function

A possible mapping is derived from the Fermi function which has precisely this behavior. The Fermi function is given by

$$f(x) = \frac{1}{1 + \exp \frac{x-\mu}{\gamma}} \quad (19.31)$$

where x is taken as the invariant mass squared, μ is the invariant mass squared of the edge, and γ is the effective width which is given by the widths of the

parent and the sibling branch. (Widths might be added in quadrature, but we do not require this level of precision.)

$$x = \frac{m^2 - m_{\min}^2}{\Delta m^2} \quad (19.32)$$

$$\mu = \frac{m_{\max, \text{eff}}^2 - m_{\min}^2}{\Delta m^2} \quad (19.33)$$

$$\gamma = \frac{2m_{\max, \text{eff}}\Gamma}{\Delta m^2} \quad (19.34)$$

with

$$\Delta m^2 = m_{\max}^2 - m_{\min}^2 \quad (19.35)$$

m^2 is thus given by

$$m^2(x) = xm_{\max}^2 + (1-x)m_{\min}^2 \quad (19.36)$$

For the mapping, we compute the integral $g(x)$ of the Fermi function, normalized such that $g(0) = 0$ and $g(1) = 1$. We introduce the abbreviations

$$\alpha = 1 - \gamma \ln \frac{1 + \beta e^{1/\gamma}}{1 + \beta} \quad (19.37)$$

$$\beta = e^{-\mu/\gamma} \quad (19.38)$$

and obtain

$$g(x) = \frac{1}{\alpha} \left(x - \gamma \ln \frac{1 + \beta e^{x/\gamma}}{1 + \beta} \right) \quad (19.39)$$

The actual mapping is the inverse function $h(y) = g^{-1}(y)$,

$$h(y) = -\gamma \ln \left(e^{-\alpha y/\gamma} (1 + \beta) - \beta \right) \quad (19.40)$$

The Jacobian is

$$\frac{dh}{dy} = \alpha \left(1 - e^{\alpha y/\gamma} \frac{\beta}{1 + \beta} \right)^{-1} \quad (19.41)$$

which is equal to $1/(dg/dx)$, namely

$$\frac{dg}{dx} = \frac{1}{\alpha} \frac{1}{1 + \beta e^{x/\gamma}} \quad (19.42)$$

The final result is

$$\int_{m_{\min}^2}^{m_{\max}^2} dm^2 F(m^2) = \Delta m^2 \int_0^1 dx F(m^2(x)) \quad (19.43)$$

$$= \Delta m^2 \int_0^1 dy F(m^2(h(y))) \frac{dh}{dy} \quad (19.44)$$

Here is the implementation. We fill **a1**, **a2**, **a3** with α, β, γ , respectively.

```

⟨Constants for exponential step mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    map%a3 = max (2 * map%mass * map%width / (msq_max - msq_min), 0.01_default)
    map%a2 = exp (- (map%mass**2 - msq_min) / (msq_max - msq_min) &
                  / map%a3)
    map%a1 = 1 - map%a3 * log ((1 + map%a2 * exp (1 / map%a3)) / (1 + map%a2))
  end if

```

```

⟨Apply exponential step mapping⟩≡
  tmp = exp (- x * map%a1 / map%a3) * (1 + map%a2)
  z = - map%a3 * log (tmp - map%a2)
  msq = z * msq_max + (1 - z) * msq_min
  f = map%a1 / (1 - map%a2 / tmp) * (msq_max - msq_min) / s

⟨Apply inverse exponential step mapping⟩≡
  z = (msq - msq_min) / (msq_max - msq_min)
  tmp = 1 + map%a2 * exp (z / map%a3)
  x = (z - map%a3 * log (tmp / (1 + map%a2))) &
    / map%a1
  f = map%a1 * tmp * (msq_max - msq_min) / s

```

Hyperbolic mapping

The Fermi function has the drawback that it decreases exponentially. It might be preferable to take a function with a power-law decrease, such that the high-mass region is not completely depopulated.

Here, we start with the actual mapping which we take as

$$h(y) = \frac{b}{a-y} - \frac{b}{a} + \mu y \quad (19.45)$$

with the abbreviation

$$a = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4b}{1-\mu}} \right) \quad (19.46)$$

This is a hyperbola in the xy plane. The derivative is

$$\frac{dh}{dy} = \frac{b}{(a-y)^2} + \mu \quad (19.47)$$

The constants correspond to

$$\mu = \frac{m_{\text{max,eff}}^2 - m_{\text{min}}^2}{\Delta m^2} \quad (19.48)$$

$$b = \frac{1}{\mu} \left(\frac{2m_{\text{max,eff}}\Gamma}{\Delta m^2} \right)^2 \quad (19.49)$$

The inverse function is the solution of a quadratic equation,

$$g(x) = \frac{1}{2} \left[\left(a + \frac{x}{\mu} + \frac{b}{a\mu} \right) - \sqrt{\left(a - \frac{x}{\mu} \right)^2 + 2\frac{b}{a\mu} \left(a + \frac{x}{\mu} \right) + \left(\frac{b}{a\mu} \right)^2} \right] \quad (19.50)$$

The constants $a_{1,2,3}$ are identified with a, b, μ .

```

⟨Constants for hyperbolic step mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    map%a3 = (map%mass**2 - msq_min) / (msq_max - msq_min)
    map%a2 = max ((2 * map%mass * map%width / (msq_max - msq_min))**2 &
      / map%a3, 1e-6_default)
    map%a1 = (1 + sqrt (1 + 4 * map%a2 / (1 - map%a3))) / 2
  end if

```

```

⟨Apply hyperbolic step mapping⟩≡
  z = map%a2 / (map%a1 - x) - map%a2 / map%a1 + map%a3 * x
  msq = z * msq_max + (1 - z) * msq_min
  f = (map%a2 / (map%a1 - x)**2 + map%a3) * (msq_max - msq_min) / s

⟨Apply inverse hyperbolic step mapping⟩≡
  z = (msq - msq_min) / (msq_max - msq_min)
  tmp = map%a2 / (map%a1 * map%a3)
  x = ((map%a1 + z / map%a3 + tmp) &
        - sqrt((map%a1 - z / map%a3)**2 + 2 * tmp * (map%a1 + z / map%a3) &
              + tmp**2)) / 2
  f = (map%a2 / (map%a1 - x)**2 + map%a3) * (msq_max - msq_min) / s

```

19.6.9 Mappings of the polar angle

The other type of singularity, a simple pole just outside the integration region, can occur in the integration over $\cos\theta$. This applies to exchange of massless (or light) particles.

Double poles (Coulomb scattering) are also possible, but only in certain cases. These are also handled by the single-pole mapping.

The mapping is analogous to the previous m^2 pole mapping, but with a different normalization and notation of variables:

$$\frac{1}{2} \int_{-1}^1 d\cos\theta g(\theta) = \int_0^1 dx \frac{d\cos\theta}{dx} g(\theta(x)) = \int_0^1 dx f(x) g(x), \quad (19.51)$$

where thus

$$f(x) = \frac{1}{2} \frac{d\cos\theta}{dx}. \quad (19.52)$$

With this mapping, a function of the form

$$g(\theta) = c \frac{dx(\cos\theta)}{d\cos\theta} \quad (19.53)$$

is mapped to a constant:

$$\int_{-1}^1 d\cos\theta g(\theta) = \int_0^1 dx f(x) g(\theta(x)) = \int_0^1 dx c. \quad (19.54)$$

```

⟨Mappings: mapping: TBP⟩+≡
  procedure :: compute_ct_from_x => mapping_compute_ct_from_x

⟨Mappings: sub interfaces⟩+≡
  module subroutine mapping_compute_ct_from_x (map, s, ct, st, f, x)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s
    real(default), intent(out) :: ct, st, f
    real(default), intent(in) :: x
  end subroutine mapping_compute_ct_from_x

⟨Mappings: procedures⟩+≡
  module subroutine mapping_compute_ct_from_x (map, s, ct, st, f, x)
    class(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s
    real(default), intent(out) :: ct, st, f

```

```

real(default), intent(in) :: x
real(default) :: tmp, ct1
select case (map%type)
case (NO_MAPPING, S_CHANNEL, INFRARED, RADIATION, &
      STEP_MAPPING_E, STEP_MAPPING_H)
  <Apply trivial ct mapping>
case (T_CHANNEL, U_CHANNEL, COLLINEAR)
  <Constants for ct pole mapping>
  <Apply ct pole mapping>
case default
  call msg_fatal (" Attempt to apply undefined ct mapping")
end select
end subroutine mapping_compute_ct_from_x

```

<Mappings: mapping: TBP>+≡

```

procedure :: compute_x_from_ct => mapping_compute_x_from_ct

```

<Mappings: sub interfaces>+≡

```

module subroutine mapping_compute_x_from_ct (map, s, ct, f, x)
  class(mapping_t), intent(inout) :: map
  real(default), intent(in) :: s
  real(default), intent(in) :: ct
  real(default), intent(out) :: f, x
end subroutine mapping_compute_x_from_ct

```

<Mappings: procedures>+≡

```

module subroutine mapping_compute_x_from_ct (map, s, ct, f, x)
  class(mapping_t), intent(inout) :: map
  real(default), intent(in) :: s
  real(default), intent(in) :: ct
  real(default), intent(out) :: f, x
  real(default) :: ct1
  select case (map%type)
  case (NO_MAPPING, S_CHANNEL, INFRARED, RADIATION, &
        STEP_MAPPING_E, STEP_MAPPING_H)
    <Apply inverse trivial ct mapping>
  case (T_CHANNEL, U_CHANNEL, COLLINEAR)
    <Constants for ct pole mapping>
    <Apply inverse ct pole mapping>
  case default
    call msg_fatal (" Attempt to apply undefined inverse ct mapping")
  end select
end subroutine mapping_compute_x_from_ct

```

Trivial mapping

This is just the mapping of the interval $(-1, 1)$ to $(0, 1)$:

$$\cos \theta = -1 + 2x \quad (19.55)$$

and

$$f(x) = 1 \quad (19.56)$$

with the inverse

$$x = \frac{1 + \cos \theta}{2} \quad (19.57)$$

```

⟨Apply trivial ct mapping⟩≡
    tmp = 2 * (1-x)
    ct = 1 - tmp
    st = sqrt (tmp * (2-tmp))
    f = 1

⟨Apply inverse trivial ct mapping⟩≡
    x = (ct + 1) / 2
    f = 1

```

Pole mapping

As above for m^2 , we simultaneously map poles at both ends of the $\cos \theta$ interval. The formulae are completely analogous:

$$\cos \theta = \begin{cases} \frac{M^2}{s} [\exp(xL) - 1] - 1 & \text{for } x < \frac{1}{2} \\ -\frac{M^2}{s} [\exp((1-x)L) - 1] + 1 & \text{for } x \geq \frac{1}{2} \end{cases} \quad (19.58)$$

where

$$L = 2 \ln \frac{M^2 + s}{M^2}. \quad (19.59)$$

Inverse:

$$x = \begin{cases} \frac{1}{2L} \ln \frac{1 + \cos \theta + M^2/s}{M^2/s} & \text{for } \cos \theta < 0 \\ 1 - \frac{1}{2L} \ln \frac{1 - \cos \theta + M^2/s}{M^2/s} & \text{for } \cos \theta \geq 0 \end{cases} \quad (19.60)$$

The phase-space factor:

$$f(x) = \begin{cases} \frac{M^2}{s} \exp(xL) L & \text{for } x < \frac{1}{2} \\ \frac{M^2}{s} \exp((1-x)L) L & \text{for } x \geq \frac{1}{2} \end{cases} \quad (19.61)$$

```

⟨Constants for ct pole mapping⟩≡
    if (map%variable_limits .or. map%b_unknown) then
        map%b1 = map%mass**2 / s
        map%b2 = log ((map%b1 + 1) / map%b1)
        map%b3 = 0
        map%b_unknown = .false.
    end if

⟨Apply ct pole mapping⟩≡
    if (x < .5_default) then
        ct1 = map%b1 * exp (2 * x * map%b2)
        ct = ct1 - map%b1 - 1
    else
        ct1 = map%b1 * exp (2 * (1-x) * map%b2)
        ct = -(ct1 - map%b1) + 1
    end if
    if (ct >= -1 .and. ct <= 1) then
        st = sqrt (1 - ct**2)
        f = ct1 * map%b2
    else
        ct = 1; st = 0; f = 0
    end if

```

```

<Apply inverse ct pole mapping>≡
  if (ct < 0) then
    ct1 = ct + map%b1 + 1
    x = log (ct1 / map%b1) / (2 * map%b2)
  else
    ct1 = -ct + map%b1 + 1
    x = 1 - log (ct1 / map%b1) / (2 * map%b2)
  end if
  f = ct1 * map%b2

```

19.7 Phase-space trees

The phase space evaluation is organized in terms of trees, where each branch corresponds to three integrations: m^2 , $\cos\theta$, and ϕ . The complete tree thus makes up a specific parameterization of the multidimensional phase-space integral. For the multi-channel integration, the phase-space tree is a single channel.

The trees imply mappings of formal Feynman tree graphs into arrays of integer numbers: Each branch, corresponding to a particular line in the graph, is assigned an integer code c (with kind value $\text{TC} = \text{tree code}$).

In this integer, each bit determines whether a particular external momentum flows through the line. The external branches therefore have codes 1, 2, 4, 8, ... An internal branch has those bits ORed corresponding to the momenta flowing through it. For example, a branch with momentum $p_1 + p_4$ has code $2^0 + 2^3 = 1 + 8 = 9$.

There is a two-fold ambiguity: Momentum conservation implies that the branch with code

$$c_0 = \sum_{i=1}^{n(\text{ext})} 2^{i-1} \quad (19.62)$$

i.e. the branch with momentum $p_1 + p_2 + \dots p_n$ has momentum zero, which is equivalent to tree code 0 by definition. Correspondingly,

$$c \quad \text{and} \quad c_0 - c = c \text{ XOR } c_0 \quad (19.63)$$

are equivalent. E.g., if there are five externals with codes $c = 1, 2, 4, 8, 16$, then $c = 9$ and $\bar{c} = 31 - 9 = 22$ are equivalent.

This ambiguity may be used to assign a direction to the line: If all momenta are understood as outgoing, $c = 9$ in the example above means $p_1 + p_4$, but $c = 22$ means $p_2 + p_3 + p_5 = -(p_1 + p_4)$.

Here we make use of the ambiguity in a slightly different way. First, the initial particles are singled out as those externals with the highest bits, the IN-bits. (Here: 8 and 16 for a $2 \rightarrow 3$ scattering process, 16 only for a $1 \rightarrow 4$ decay.) Then we invert those codes where all IN-bits are set. For a decay process this maps each tree of an equivalence class onto a unique representative (that one with the smallest integer codes). For a scattering process we proceed further:

The ambiguity remains in all branches where only one IN-bit is set, including the initial particles. If there are only externals with this property, we have an s -channel graph which we leave as it is. In all other cases, an internal with only one IN-bit is a t -channel line, which for phase space integration should be associated with one of the initial momenta as a reference axis. We take that one whose bit is set in the current tree code. (E.g., for branch $c = 9$ we use the initial particle $c = 8$ as reference axis, whereas for the same branch we would take $c = 16$ if it had been assigned $\bar{c} = 31 - 9 = 22$ as tree code.) Thus, different ways of coding the same t -channel graph imply different phase space parameterizations.

s -channel graphs have a unique parameterization. The same sets of parameterizations are used for t -channel graphs, except for the reference frames of their angular parts. We map each t -channel graph onto an s -channel graph as follows:

Working in ascending order, for each t -channel line (whose code has exactly one IN-bit set) the attached initial line is flipped upstream, while the outgoing

line is flipped downstream. (This works only if t -channel graphs are always parameterized beginning at their outer vertices, which we require as a restriction.) After all possible flips have been applied, we have an s -channel graph. We only have to remember the initial particle a vertex was originally attached to.

```

<phs_trees.f90>≡
  <File header>

  module phs_trees

    <Use kinds>
      use kinds, only: TC
    <Use strings>
      use lorentz
      use permutations, only: permutation_t, permutation_size
      use permutations, only: permutation_init, permutation_find
      use permutations, only: tc_decay_level, tc_permute
      use model_data
      use flavors
      use resonances, only: resonance_history_t, resonance_info_t
      use mappings

    <Standard module head>

    <PHS trees: public>

    <PHS trees: types>

    interface
    <PHS trees: sub interfaces>
    end interface

  end module phs_trees

<phs_trees_sub.f90>≡
  <File header>

  submodule (phs_trees) phs_trees_s

    use io_units
    use constants, only: twopi, twopi2, twopi5
    use format_defs, only: FMT_19
    use numeric_utils, only: vanishes
    use diagnostics

    implicit none

  contains

    <PHS trees: procedures>

  end submodule phs_trees_s

```

19.7.1 Particles

We define a particle type which contains only four-momentum and invariant mass squared, and a flag that tells whether the momentum is filled or not.

(PHS trees: public)≡

```
public :: phs_prt_t
```

(PHS trees: types)≡

```
type :: phs_prt_t
private
logical :: defined = .false.
type(vector4_t) :: p
real(default) :: p2
contains
(PHS trees: prt: TBP)
end type phs_prt_t
```

Set contents:

(PHS trees: prt: TBP)≡

```
procedure :: set_defined => phs_prt_set_defined
procedure :: set_undefined => phs_prt_set_undefined
procedure :: set_momentum => phs_prt_set_momentum
procedure :: set_msq => phs_prt_set_msq
```

(PHS trees: sub interfaces)≡

```
elemental module subroutine phs_prt_set_defined (prt)
class(phs_prt_t), intent(inout) :: prt
end subroutine phs_prt_set_defined
elemental module subroutine phs_prt_set_undefined (prt)
class(phs_prt_t), intent(inout) :: prt
end subroutine phs_prt_set_undefined
elemental module subroutine phs_prt_set_momentum (prt, p)
class(phs_prt_t), intent(inout) :: prt
type(vector4_t), intent(in) :: p
end subroutine phs_prt_set_momentum
elemental module subroutine phs_prt_set_msq (prt, p2)
class(phs_prt_t), intent(inout) :: prt
real(default), intent(in) :: p2
end subroutine phs_prt_set_msq
```

(PHS trees: procedures)≡

```
elemental module subroutine phs_prt_set_defined (prt)
class(phs_prt_t), intent(inout) :: prt
prt%defined = .true.
end subroutine phs_prt_set_defined

elemental module subroutine phs_prt_set_undefined (prt)
class(phs_prt_t), intent(inout) :: prt
prt%defined = .false.
end subroutine phs_prt_set_undefined

elemental module subroutine phs_prt_set_momentum (prt, p)
class(phs_prt_t), intent(inout) :: prt
type(vector4_t), intent(in) :: p
prt%p = p
```

```

end subroutine phs_prt_set_momentum

elemental module subroutine phs_prt_set_msq (prt, p2)
  class(phs_prt_t), intent(inout) :: prt
  real(default), intent(in) :: p2
  prt%p2 = p2
end subroutine phs_prt_set_msq

```

Access methods:

```

(PHS trees: prt: TBP)+≡
  procedure :: is_defined => phs_prt_is_defined
  procedure :: get_momentum => phs_prt_get_momentum
  procedure :: get_msq => phs_prt_get_msq

(PHS trees: sub interfaces)+≡
  elemental module function phs_prt_is_defined (prt) result (defined)
    logical :: defined
    class(phs_prt_t), intent(in) :: prt
  end function phs_prt_is_defined
  elemental module function phs_prt_get_momentum (prt) result (p)
    type(vector4_t) :: p
    class(phs_prt_t), intent(in) :: prt
  end function phs_prt_get_momentum
  elemental module function phs_prt_get_msq (prt) result (p2)
    real(default) :: p2
    class(phs_prt_t), intent(in) :: prt
  end function phs_prt_get_msq

(PHS trees: procedures)+≡
  elemental module function phs_prt_is_defined (prt) result (defined)
    logical :: defined
    class(phs_prt_t), intent(in) :: prt
    defined = prt%defined
  end function phs_prt_is_defined

  elemental module function phs_prt_get_momentum (prt) result (p)
    type(vector4_t) :: p
    class(phs_prt_t), intent(in) :: prt
    p = prt%p
  end function phs_prt_get_momentum

  elemental module function phs_prt_get_msq (prt) result (p2)
    real(default) :: p2
    class(phs_prt_t), intent(in) :: prt
    p2 = prt%p2
  end function phs_prt_get_msq

```

Addition of momenta (invariant mass square is computed).

```

(PHS trees: prt: TBP)+≡
  procedure :: combine => phs_prt_combine

(PHS trees: sub interfaces)+≡
  elemental module subroutine phs_prt_combine (prt, prt1, prt2)
    class(phs_prt_t), intent(inout) :: prt

```

```

        type(phs_prt_t), intent(in) :: prt1, prt2
    end subroutine phs_prt_combine

<PHS trees: procedures>+≡
    elemental module subroutine phs_prt_combine (prt, prt1, prt2)
        class(phs_prt_t), intent(inout) :: prt
        type(phs_prt_t), intent(in) :: prt1, prt2
        prt%defined = .true.
        prt%p = prt1%p + prt2%p
        prt%p2 = prt%p ** 2
        call phs_prt_check (prt)
    end subroutine phs_prt_combine

```

Output

```

<PHS trees: prt: TBP>+≡
    procedure :: write => phs_prt_write

<PHS trees: sub interfaces>+≡
    module subroutine phs_prt_write (prt, unit)
        class(phs_prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
    end subroutine phs_prt_write

<PHS trees: procedures>+≡
    module subroutine phs_prt_write (prt, unit)
        class(phs_prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (prt%defined) then
            call vector4_write (prt%p, u)
            write (u, "(1x,A,1x," // FMT_19 // ")") "T = ", prt%p2
        else
            write (u, "(3x,A)") "[undefined]"
        end if
    end subroutine phs_prt_write

<PHS trees: prt: TBP>+≡
    procedure :: check => phs_prt_check

<PHS trees: sub interfaces>+≡
    elemental module subroutine phs_prt_check (prt)
        class(phs_prt_t), intent(inout) :: prt
    end subroutine phs_prt_check

<PHS trees: procedures>+≡
    elemental module subroutine phs_prt_check (prt)
        class(phs_prt_t), intent(inout) :: prt
        if (prt%p2 < 0._default) then
            prt%p2 = 0._default
        end if
    end subroutine phs_prt_check

```

19.7.2 The phase-space tree type

Definition

In the concrete implementation, each branch c may have two *daughters* c_1 and c_2 such that $c_1 + c_2 = c$, a *sibling* c_s and a *mother* c_m such that $c + c_s = c_m$, and a *friend* which is kept during flips, such that it can indicate a fixed reference frame. Absent entries are set $c = 0$.

First, declare the branch type. There is some need to have this public. Give initializations for all components, so no `init` routine is necessary. The branch has some information about the associated coordinates and about connections.

```

(PHS trees: types)+≡
  type :: phs_branch_t
  private
    logical :: set = .false.
    logical :: inverted_decay = .false.
    logical :: inverted_axis = .false.
    integer(TC) :: mother = 0
    integer(TC) :: sibling = 0
    integer(TC) :: friend = 0
    integer(TC) :: origin = 0
    integer(TC), dimension(2) :: daughter = 0
    integer :: firstborn = 0
    logical :: has_children = .false.
    logical :: has_friend = .false.
    logical :: is_real = .false.
  end type phs_branch_t

```

The tree type: No initialization, this is done by `phs_tree_init`. In addition to the branch array which

The branches are collected in an array which holds all possible branches, of which only a few are set. After flips have been applied, the branch $c_M = \sum_{i=1}^{n(\text{fin})} 2^{i-1}$ must be there, indicating the mother of all decay products. In addition, we should check for consistency at the beginning.

`n_branches` is the number of those actually set. `n externals` defines the number of significant bit, and `mask` is a code where all bits are set. Analogous: `n_in` and `mask_in` for the incoming particles.

The mapping array contains the mappings associated to the branches (corresponding indices). The array `mass_sum` contains the sum of the real masses of the external final-state particles associated to the branch. During phase-space evaluation, this determines the boundaries.

```

(PHS trees: public)+≡
  public :: phs_tree_t

(PHS trees: types)+≡
  type :: phs_tree_t
  private
    integer :: n_branches, n externals, n_in, n_msq, n_angles
    integer(TC) :: n_branches_tot, n_branches_out
    integer(TC) :: mask, mask_in, mask_out
    type(phs_branch_t), dimension(:), allocatable :: branch
    type(mapping_t), dimension(:), allocatable :: mapping
    real(default), dimension(:), allocatable :: mass_sum

```

```

    real(default), dimension(:), allocatable :: effective_mass
    real(default), dimension(:), allocatable :: effective_width
    logical :: real_phsp = .false.
    integer, dimension(:), allocatable :: momentum_link
contains
  <PHS trees: phs tree: TBP>
end type phs_tree_t

```

The maximum number of external particles that can be represented is related to the bit size of the integer that stores binary codes. With the default integer of 32 bit on common machines, this is more than enough space. If TC is actually the default integer kind, there is no need to keep it separate, but doing so marks this as a special type of integer. So, just state that the maximum number is 32:

```

<Limits: public parameters>≡
  integer, parameter, public :: MAX_EXTERNAL = 32

```

Constructor and destructor

Allocate memory for a phase-space tree with given number of externals and incoming. The number of allocated branches can easily become large, but appears manageable for realistic cases, e.g., for $n_{in}=2$ and $n_{out}=8$ we get $2^{10} - 1 = 1023$. Here we set the masks for incoming and for all externals.

```

<PHS trees: phs tree: TBP>≡
  procedure :: init => phs_tree_init
  procedure :: final => phs_tree_final

<PHS trees: sub interfaces>+≡
  elemental module subroutine phs_tree_init &
    (tree, n_in, n_out, n_masses, n_angles)
    class(phs_tree_t), intent(inout) :: tree
    integer, intent(in) :: n_in, n_out, n_masses, n_angles
  end subroutine phs_tree_init
  elemental module subroutine phs_tree_final (tree)
    class(phs_tree_t), intent(inout) :: tree
  end subroutine phs_tree_final

<PHS trees: procedures>+≡
  elemental module subroutine phs_tree_init &
    (tree, n_in, n_out, n_masses, n_angles)
    class(phs_tree_t), intent(inout) :: tree
    integer, intent(in) :: n_in, n_out, n_masses, n_angles
    integer(TC) :: i
    tree%n_externals = n_in + n_out
    tree%n_branches_tot = 2**(n_in+n_out) - 1
    tree%n_branches_out = 2**n_out - 1
    tree%mask = 0
    do i = 0, n_in + n_out - 1
      tree%mask = ibset (tree%mask, i)
    end do
    tree%n_in = n_in
    tree%mask_in = 0
    do i = n_out, n_in + n_out - 1
      tree%mask_in = ibset (tree%mask_in, i)
    end do
  end subroutine phs_tree_init

```

```

end do
tree%mask_out = ieor (tree%mask, tree%mask_in)
tree%n_msq = n_masses
tree%n_angles = n_angles
allocate (tree%branch (tree%n_branches_tot))
tree%n_branches = 0
allocate (tree%mapping (tree%n_branches_out))
allocate (tree%mass_sum (tree%n_branches_out))
allocate (tree%effective_mass (tree%n_branches_out))
allocate (tree%effective_width (tree%n_branches_out))
end subroutine phs_tree_init

elemental module subroutine phs_tree_final (tree)
class(phs_tree_t), intent(inout) :: tree
deallocate (tree%branch)
deallocate (tree%mapping)
deallocate (tree%mass_sum)
deallocate (tree%effective_mass)
deallocate (tree%effective_width)
end subroutine phs_tree_final

```

Screen output

Write only the branches that are set:

```

<PHS trees: phs tree: TBP>+≡
  procedure :: write => phs_tree_write

<PHS trees: sub interfaces>+≡
  module subroutine phs_tree_write (tree, unit)
    class(phs_tree_t), intent(in) :: tree
    integer, intent(in), optional :: unit
  end subroutine phs_tree_write

<PHS trees: procedures>+≡
module subroutine phs_tree_write (tree, unit)
  class(phs_tree_t), intent(in) :: tree
  integer, intent(in), optional :: unit
  integer :: u
  integer(TC) :: k
  u = given_output_unit (unit); if (u < 0) return
  write (u, '(3X,A,1x,I0,5X,A,I3)') &
    'External:', tree%n_externals, 'Mask:', tree%mask
  write (u, '(3X,A,1x,I0,5X,A,I3)') &
    'Incoming:', tree%n_in, 'Mask:', tree%mask_in
  write (u, '(3X,A,1x,I0,5X,A,I3)') &
    'Branches:', tree%n_branches
  do k = size (tree%branch), 1, -1
    if (tree%branch(k)%set) &
      call phs_branch_write (tree%branch(k), unit=unit, kval=k)
  end do
  do k = 1, size (tree%mapping)
    call tree%mapping (k)%write (unit, verbose=.true.)
  end do
  write (u, "(3x,A)") "Arrays: mass_sum, effective_mass, effective_width"

```

```

do k = 1, size (tree%mass_sum)
  if (tree%branch(k)%set) then
    write (u, "(5x,I0,3(2x," // FMT_19 // ")") k, tree%mass_sum(k), &
      tree%effective_mass(k), tree%effective_width(k)
  end if
end do
end subroutine phs_tree_write

subroutine phs_branch_write (b, unit, kval)
  type(phs_branch_t), intent(in) :: b
  integer, intent(in), optional :: unit
  integer(TC), intent(in), optional :: kval
  integer :: u
  integer(TC) :: k
  character(len=6) :: tmp
  character(len=1) :: firstborn(2), sign_decay, sign_axis
  integer :: i
  u = given_output_unit (unit); if (u < 0) return
  k = 0; if (present (kval)) k = kval
  if (b%origin /= 0) then
    write(tmp, '(A,I4,A)') '(', b%origin, ')'
  else
    tmp = ' '
  end if
  do i=1, 2
    if (b%firstborn == i) then
      firstborn(i) = "*"
    else
      firstborn(i) = " "
    end if
  end do
  if (b%inverted_decay) then
    sign_decay = "-"
  else
    sign_decay = "+"
  end if
  if (b%inverted_axis) then
    sign_axis = "-"
  else
    sign_axis = "+"
  end if
  if (b%has_children) then
    if (b%has_friend) then
      write(u, '(4X,A1,I0,3x,A,1X,A,I0,A1,1x,I0,A1,1X,A1,1X,A,1x,I0)') &
        & ' ', k, tmp, &
        & 'Daughters: ', &
        & b%daughter(1), firstborn(1), &
        & b%daughter(2), firstborn(2), sign_decay, &
        & 'Friend: ', b%friend
    else
      write(u, '(4X,A1,I0,3x,A,1X,A,I0,A1,1x,I0,A1,1X,A1,1X,A)') &
        & ' ', k, tmp, &
        & 'Daughters: ', &
        & b%daughter(1), firstborn(1), &

```



```

&    b%daughter(2), firstborn(2), sign_decay, &
&    '(axis '//sign_axis//)'
end if
else
write(u,'(5X,I0)') k
end if
end subroutine phs_branch_write

```

19.7.3 PHS tree setup

Transformation into an array of branch codes and back

Assume that the tree/array has been created before with the appropriate length and is empty.

```

<PHS trees: public>+≡
public :: phs_tree_from_array

<PHS trees: phs tree: TBP>+≡
procedure :: from_array => phs_tree_from_array

<PHS trees: sub interfaces>+≡
module subroutine phs_tree_from_array (tree, a)
class(phs_tree_t), intent(inout) :: tree
integer(TC), dimension(:), intent(in) :: a
end subroutine phs_tree_from_array

<PHS trees: procedures>+≡
module subroutine phs_tree_from_array (tree, a)
class(phs_tree_t), intent(inout) :: tree
integer(TC), dimension(:), intent(in) :: a
integer :: i
integer(TC) :: k
<Set branches from array a>
<Set external branches if necessary>
<Check number of branches>
<Determine the connections>
contains
<Subroutine: set relatives>
end subroutine phs_tree_from_array

```

First, set all branches specified by the user. If all IN-bits are set, we invert the branch code.

```

<Set branches from array a>+≡
do i=1, size(a)
k = a(i)
if (iand(k, tree%mask_in) == tree%mask_in) k = ieor(tree%mask, k)
tree%branch(k)%set = .true.
tree%n_branches = tree%n_branches+1
end do

```

The external branches are understood, so set them now if not yet done. In all cases ensure that the representative with one bit set is used, except for decays where the in-particle is represented by all OUT-bits set instead.

```

<Set external branches if necessary>+≡

```

```

do i=0, tree%n_externals-1
  k = ibset(0,i)
  if (iand(k, tree%mask_in) == tree%mask_in) k = ieor(tree%mask, k)
  if (tree%branch(ieor(tree%mask, k))%set) then
    tree%branch(ieor(tree%mask, k))%set = .false.
    tree%branch(k)%set = .true.
  else if (.not.tree%branch(k)%set) then
    tree%branch(k)%set = .true.
    tree%n_branches = tree%n_branches+1
  end if
end do

```

Now the number of branches set can be checked. Here we assume that the tree is binary. For three externals there are three branches in total, and for each additional external branch we get another internal one.

```

<Check number of branches>≡
  if (tree%n_branches /= tree%n_externals*2-3) then
    call phs_tree_write (tree)
    call msg_bug &
      & (" Wrong number of branches set in phase space tree")
  end if

```

For all branches that are set, except for the externals, we try to find the daughter branches:

```

<Determine the connections>≡
  do k=1, size (tree%branch)
    if (tree%branch(k)%set .and. tc_decay_level (k) /= 1) then
      call branch_set_relatives(k)
    end if
  end do

```

To this end, we scan all codes less than the current code, whether we can find two branches which are set and which together give the current code. After that, the tree may still not be connected, but at least we know if a branch does not have daughters: This indicates some inconsistency.

The algorithm ensures that, at this stage, the first daughter has a smaller code value than the second one.

```

<Subroutine: set relatives>≡
  subroutine branch_set_relatives (k)
    integer(TC), intent(in) :: k
    integer(TC) :: m,n
    do m=1, k-1
      if (iand(k,m)==m) then
        n = ieor(k,m)
        if ( tree%branch(m)%set .and. tree%branch(n)%set ) then
          tree%branch(k)%daughter(1) = m; tree%branch(k)%daughter(2) = n
          tree%branch(m)%mother      = k; tree%branch(n)%mother      = k
          tree%branch(m)%sibling     = n; tree%branch(n)%sibling     = m
          tree%branch(k)%has_children = .true.
        return
      end if
    end if
  end do
  call phs_tree_write (tree)
  call msg_bug &

```

```

        & (" Missing daughter branch(es) in phase space tree")
    end subroutine branch_set_relatives

```

The inverse: this is trivial, fortunately.

Flip t -channel into s -channel

Flipping the tree is done upwards, beginning from the decay products. First we select a t -channel branch k : one which is set, which does have an IN-bit, and which is not an external particle.

Next, we determine the adjacent in-particle (called the 'friend' f here, since it will provide the reference axis for the angular integration). In addition, we look for the 'mother' and 'sibling' of this particle. If the latter field is empty, we select the (unique) other out-particle which has no mother, calling the internal subroutine `find_orphan`.

The flip is done as follows: We assume that the first daughter d is an s -channel line, which is true if the daughters are sorted. This will stay the first daughter. The second one is a t -channel line; it is exchanged with the 'sibling' s . The new line which replaces the branch k is just the sum of s and d . In addition, we have to rearrange the relatives of s and d , as well of f .

Finally, we flip 'sibling' and 'friend' and set the new s -channel branch n which replaces the t -channel branch k . After this is complete, we are ready to execute another flip.

[Although the friend is not needed for the final flip, since it would be an initial particle anyway, we need to know whether we have t - or u -channel.]

```

<PHS trees: phs tree: TBP>+=
    procedure :: flip_t_to_s_channel => phs_tree_flip_t_to_s_channel

<PHS trees: sub interfaces>+=
    module subroutine phs_tree_flip_t_to_s_channel (tree)
        class(phs_tree_t), intent(inout) :: tree
        end subroutine phs_tree_flip_t_to_s_channel

<PHS trees: procedures>+=
    module subroutine phs_tree_flip_t_to_s_channel (tree)
        class(phs_tree_t), intent(inout) :: tree
        integer(TC) :: k, f, m, n, d, s
        if (tree%n_in == 2) then
            FLIP: do k=3, tree%mask-1
                if (.not. tree%branch(k)%set) cycle FLIP
                f = iand(k,tree%mask_in)
                if (f==0 .or. f==k) cycle FLIP
                m = tree%branch(k)%mother
                s = tree%branch(k)%sibling
                if (s==0) call find_orphan(s)
                d = tree%branch(k)%daughter(1)
                n = ior(d,s)
                tree%branch(k)%set = .false.
                tree%branch(n)%set = .true.
                tree%branch(n)%origin = k
                tree%branch(n)%daughter(1) = d; tree%branch(d)%mother = n
                tree%branch(n)%daughter(2) = s; tree%branch(s)%mother = n
                tree%branch(n)%has_children = .true.
            end do
        end if
    end subroutine

```

```

        tree%branch(d)%sibling = s; tree%branch(s)%sibling = d
        tree%branch(n)%sibling = f; tree%branch(f)%sibling = n
        tree%branch(n)%mother   = m
        tree%branch(f)%mother   = m
        if (m/=0) then
            tree%branch(m)%daughter(1) = n
            tree%branch(m)%daughter(2) = f
        end if
        tree%branch(n)%friend = f
        tree%branch(n)%has_friend = .true.
        tree%branch(n)%firstborn = 2
    end do FLIP
end if
contains
    subroutine find_orphan(s)
        integer(TC) :: s
        do s=1, tree%mask_out
            if (tree%branch(s)%set .and. tree%branch(s)%mother==0) return
        end do
        call phs_tree_write (tree)
        call msg_bug (" Can't flip phase space tree to channel")
    end subroutine find_orphan
end subroutine phs_tree_flip_t_to_s_channel

```

After the tree has been flipped, one may need to determine what has become of a particular *t*-channel branch. This function gives the bincode of the flipped tree. If the original bincode does not contain IN-bits, we leave it as it is.

(PHS trees: procedures)+≡

```

function tc_flipped (tree, kt) result (ks)
    type(phs_tree_t), intent(in) :: tree
    integer(TC), intent(in) :: kt
    integer(TC) :: ks
    if (iand (kt, tree%mask_in) == 0) then
        ks = kt
    else
        ks = tree%branch(iand (kt, tree%mask_out))%mother
    end if
end function tc_flipped

```

Scan a tree and make sure that the first daughter has always a smaller code than the second one. Furthermore, delete any `friend` entry in the root branch – this branching has the incoming particle direction as axis anyway. Keep track of reordering by updating `inverted_axis`, `inverted_decay` and `firstborn`.

(PHS trees: phs tree: TBP)+≡

```

procedure :: canonicalize => phs_tree_canonicalize

```

(PHS trees: sub interfaces)+≡

```

module subroutine phs_tree_canonicalize (tree)
    class(phs_tree_t), intent(inout) :: tree
    end subroutine phs_tree_canonicalize

```

(PHS trees: procedures)+≡

```

module subroutine phs_tree_canonicalize (tree)
    class(phs_tree_t), intent(inout) :: tree

```

```

integer :: n_out
integer(TC) :: k_out
call branch_canonicalize (tree%branch(tree%mask_out))
n_out = tree%n_externals - tree%n_in
k_out = tree%mask_out
if (tree%branch(k_out)%has_friend &
    & .and. tree%branch(k_out)%friend == ibset (0, n_out)) then
    tree%branch(k_out)%inverted_axis = .not.tree%branch(k_out)%inverted_axis
end if
tree%branch(k_out)%has_friend = .false.
tree%branch(k_out)%friend = 0
contains
recursive subroutine branch_canonicalize (b)
type(phs_branch_t), intent(inout) :: b
integer(TC) :: d1, d2
if (b%has_children) then
    d1 = b%daughter(1)
    d2 = b%daughter(2)
    if (d1 > d2) then
        b%daughter(1) = d2
        b%daughter(2) = d1
        b%inverted_decay = .not.b%inverted_decay
        if (b%firstborn /= 0) b%firstborn = 3 - b%firstborn
    end if
    call branch_canonicalize (tree%branch(b%daughter(1)))
    call branch_canonicalize (tree%branch(b%daughter(2)))
end if
end subroutine branch_canonicalize
end subroutine phs_tree_canonicalize

```

Mappings

Initialize a mapping for the current tree. This is done while reading from file, so the mapping parameters are read, but applied to the flipped tree. Thus, the size of the array of mappings is given by the number of outgoing particles only.

(PHS trees: phs tree: TBP)+≡

```
procedure :: init_mapping => phs_tree_init_mapping
```

(PHS trees: sub interfaces)+≡

```

module subroutine phs_tree_init_mapping (tree, k, type, pdg, model)
class(phs_tree_t), intent(inout) :: tree
integer(TC), intent(in) :: k
type(string_t), intent(in) :: type
integer, intent(in) :: pdg
class(model_data_t), intent(in), target :: model
end subroutine phs_tree_init_mapping

```

(PHS trees: procedures)+≡

```

module subroutine phs_tree_init_mapping (tree, k, type, pdg, model)
class(phs_tree_t), intent(inout) :: tree
integer(TC), intent(in) :: k
type(string_t), intent(in) :: type
integer, intent(in) :: pdg

```

```

class(model_data_t), intent(in), target :: model
integer(TC) :: kk
kk = tc_flipped (tree, k)
call tree%mapping(kk)%init (kk, type, pdg, model)
end subroutine phs_tree_init_mapping

```

Set the physical parameters for the mapping, using a specific parameter set.
Also set the mass sum array.

```

<PHS trees: phs tree: TBP>+≡
  procedure :: set_mapping_parameters => phs_tree_set_mapping_parameters

<PHS trees: sub interfaces>+≡
  module subroutine phs_tree_set_mapping_parameters &
    (tree, mapping_defaults, variable_limits)
    class(phs_tree_t), intent(inout) :: tree
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    logical, intent(in) :: variable_limits
  end subroutine phs_tree_set_mapping_parameters

<PHS trees: procedures>+≡
  module subroutine phs_tree_set_mapping_parameters &
    (tree, mapping_defaults, variable_limits)
    class(phs_tree_t), intent(inout) :: tree
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    logical, intent(in) :: variable_limits
    integer(TC) :: k
    do k = 1, tree%n_branches_out
      call tree%mapping(k)%set_parameters (mapping_defaults, variable_limits)
    end do
  end subroutine phs_tree_set_mapping_parameters

```

Return the mapping for the sum of all outgoing particles. This should either be no mapping or a global s-channel mapping.

```

<PHS trees: phs tree: TBP>+≡
  procedure :: assign_s_mapping => phs_tree_assign_s_mapping

<PHS trees: sub interfaces>+≡
  module subroutine phs_tree_assign_s_mapping (tree, mapping)
    class(phs_tree_t), intent(in) :: tree
    type(mapping_t), intent(out) :: mapping
  end subroutine phs_tree_assign_s_mapping

<PHS trees: procedures>+≡
  module subroutine phs_tree_assign_s_mapping (tree, mapping)
    class(phs_tree_t), intent(in) :: tree
    type(mapping_t), intent(out) :: mapping
    mapping = tree%mapping(tree%mask_out)
  end subroutine phs_tree_assign_s_mapping

```

Kinematics

Fill the mass sum array, starting from the external particles and working down to the tree root. For each bincode k we scan the bits in k ; if only one is set, we

take the physical mass of the corresponding external particle; if more then one is set, we sum up the two masses (which we know have already been set).

```

<PHS trees: phs tree: TBP>+=
  procedure :: set_mass_sum => phs_tree_set_mass_sum

<PHS trees: sub interfaces>+=
  module subroutine phs_tree_set_mass_sum (tree, flv)
    class(phs_tree_t), intent(inout) :: tree
    type(flavor_t), dimension(:), intent(in) :: flv
  end subroutine phs_tree_set_mass_sum

<PHS trees: procedures>+=
  module subroutine phs_tree_set_mass_sum (tree, flv)
    class(phs_tree_t), intent(inout) :: tree
    type(flavor_t), dimension(:), intent(in) :: flv
    integer(TC) :: k
    integer :: i
    tree%mass_sum = 0
    do k = 1, tree%n_branches_out
      do i = 0, size (flv) - 1
        if (btest(k,i)) then
          if (ibclr(k,i) == 0) then
            tree%mass_sum(k) = flv(i+1)%get_mass ()
          else
            tree%mass_sum(k) = &
              tree%mass_sum(ibclr(k,i)) + tree%mass_sum(ibset(0,i))
          end if
          exit
        end if
      end do
    end do
  end subroutine phs_tree_set_mass_sum

```

Set the effective masses and widths. For each non-resonant branch in a tree, the effective mass is equal to the sum of the effective masses of the children (and analogous for the width). External particles have their real mass and width zero. For resonant branches, we insert mass and width from the corresponding mapping.

This routine has `phs_tree_set_mass_sum` and `phs_tree_set_mapping_parameters` as prerequisites.

```

<PHS trees: phs tree: TBP>+=
  procedure :: set_effective_masses => phs_tree_set_effective_masses

<PHS trees: sub interfaces>+=
  module subroutine phs_tree_set_effective_masses (tree)
    class(phs_tree_t), intent(inout) :: tree
  end subroutine phs_tree_set_effective_masses

<PHS trees: procedures>+=
  module subroutine phs_tree_set_effective_masses (tree)
    class(phs_tree_t), intent(inout) :: tree
    tree%effective_mass = 0
    tree%effective_width = 0
    call set_masses_x (tree%mask_out)
  contains

```

```

recursive subroutine set_masses_x (k)
  integer(TC), intent(in) :: k
  integer(TC) :: k1, k2
  if (tree%branch(k)%has_children) then
    k1 = tree%branch(k)%daughter(1)
    k2 = tree%branch(k)%daughter(2)
    call set_masses_x (k1)
    call set_masses_x (k2)
    if (tree%mapping(k)%is_s_channel ()) then
      tree%effective_mass(k) = tree%mapping(k)%get_mass ()
      tree%effective_width(k) = tree%mapping(k)%get_width ()
    else
      tree%effective_mass(k) = &
        tree%effective_mass(k1) + tree%effective_mass(k2)
      tree%effective_width(k) = &
        tree%effective_width(k1) + tree%effective_width(k2)
    end if
  else
    tree%effective_mass(k) = tree%mass_sum(k)
  end if
end subroutine set_masses_x
end subroutine phs_tree_set_effective_masses

```

Define step mappings, recursively, for the decay products of all intermediate resonances. Step mappings account for the fact that a branch may originate from a resonance, which almost replaces the upper limit on the possible invariant mass. The step mapping implements a smooth cutoff that interpolates between the resonance and the real kinematic limit. The mapping width determines the sharpness of the cutoff.

Step mappings are inserted only for branches that are not mapped otherwise.

At each branch, we record the mass that is effectively available for phase space, by taking the previous limit and subtracting the effective mass of the sibling branch. Widths are added, not subtracted.

If we encounter a resonance decay, we discard the previous limit and replace it by the mass and width of the resonance, also subtracting the sibling branch.

Initially, the limit is zero, so it becomes negative at any branch. Only if there is a resonance, the limit becomes positive. Whenever the limit is positive, and the current branch decays, we activate a step mapping for the current branch.

As a result, step mappings are implemented for all internal lines that originate from an intermediate resonance decay.

The flag `variable_limits` applies to the ultimate limit from the available energy, not to the intermediate resonances whose masses are always fixed.

This routine requires `phs_tree_set_effective_masses`

(PHS trees: phs tree: TBP)+≡

```

procedure :: set_step_mappings => phs_tree_set_step_mappings

```

(PHS trees: sub interfaces)+≡

```

module subroutine phs_tree_set_step_mappings &
  (tree, exp_type, variable_limits)
  class(phs_tree_t), intent(inout) :: tree
  logical, intent(in) :: exp_type
  logical, intent(in) :: variable_limits

```



```

end subroutine phs_tree_set_step_mappings
<PHS trees: procedures>+=
module subroutine phs_tree_set_step_mappings &
  (tree, exp_type, variable_limits)
class(phs_tree_t), intent(inout) :: tree
logical, intent(in) :: exp_type
logical, intent(in) :: variable_limits
type(string_t) :: map_str
integer(TC) :: k
if (exp_type) then
  map_str = "step_exp"
else
  map_str = "step_hyp"
end if
k = tree%mask_out
call set_step_mappings_x (k, 0._default, 0._default)
contains
recursive subroutine set_step_mappings_x (k, m_limit, w_limit)
integer(TC), intent(in) :: k
real(default), intent(in) :: m_limit, w_limit
integer(TC), dimension(2) :: kk
real(default), dimension(2) :: m, w
if (tree%branch(k)%has_children) then
  if (m_limit > 0) then
    if (.not. tree%mapping(k)%is_set ()) then
      call tree%mapping(k)%init (k, map_str)
      call tree%mapping(k)%set_step_mapping_parameters (m_limit, &
        w_limit, variable_limits)
    end if
  end if
  kk = tree%branch(k)%daughter
  m = tree%effective_mass(kk)
  w = tree%effective_width(kk)
  if (tree%mapping(k)%is_s_channel ()) then
    call set_step_mappings_x (kk(1), &
      tree%mapping(k)%get_mass () - m(2), &
      tree%mapping(k)%get_width () + w(2))
    call set_step_mappings_x (kk(2), &
      tree%mapping(k)%get_mass () - m(1), &
      tree%mapping(k)%get_width () + w(1))
  else if (m_limit > 0) then
    call set_step_mappings_x (kk(1), &
      m_limit - m(2), &
      w_limit + w(2))
    call set_step_mappings_x (kk(2), &
      m_limit - m(1), &
      w_limit + w(1))
  else
    call set_step_mappings_x (kk(1), &
      - m(2), &
      + w(2))
    call set_step_mappings_x (kk(2), &
      - m(1), &
      + w(1))
  end if
end if
end subroutine

```

```

        end if
    end if
end subroutine set_step_mappings_x
end subroutine phs_tree_set_step_mappings

```

Resonance structure

We identify the resonances within a tree as the set of s-channel mappings. The `resonance_history_t` type serves as the result container.

```

<PHS trees: phs tree: TBP>+≡
    procedure :: extract_resonance_history => phs_tree_extract_resonance_history

<PHS trees: sub interfaces>+≡
    module subroutine phs_tree_extract_resonance_history (tree, res_history)
        class(phs_tree_t), intent(in) :: tree
        type(resonance_history_t), intent(out) :: res_history
    end subroutine phs_tree_extract_resonance_history

<PHS trees: procedures>+≡
    module subroutine phs_tree_extract_resonance_history (tree, res_history)
        class(phs_tree_t), intent(in) :: tree
        type(resonance_history_t), intent(out) :: res_history
        type(resonance_info_t) :: res_info
        integer :: i
        if (allocated (tree%mapping)) then
            do i = 1, size (tree%mapping)
                associate (mapping => tree%mapping(i))
                    if (mapping%is_s_channel ()) then
                        call res_info%init (mapping%get_bincode (), mapping%get_flv (), &
                            n_out = tree%n_externals - tree%n_in)
                        call res_history%add_resonance (res_info)
                    end if
                end associate
            end do
        end if
    end subroutine phs_tree_extract_resonance_history

```

Structural comparison

This function allows to check whether one tree is the permutation of another one. The permutation is applied to the second tree in the argument list. We do not make up a temporary permuted tree, but compare the two trees directly. The branches are scanned recursively, where for each daughter we check the friend and the mapping as well. Once a discrepancy is found, the recursion is exited immediately.

```

<PHS trees: public>+≡
    public :: phs_tree_equivalent

<PHS trees: sub interfaces>+≡
    module function phs_tree_equivalent (t1, t2, perm) result (is_equal)
        type(phs_tree_t), intent(in) :: t1, t2
        type(permutation_t), intent(in) :: perm
    end function phs_tree_equivalent

```

```

        logical :: equal, is_equal
    end function phs_tree_equivalent

(PHS trees: procedures) +=
module function phs_tree_equivalent (t1, t2, perm) result (is_equal)
    type(phs_tree_t), intent(in) :: t1, t2
    type(permutation_t), intent(in) :: perm
    logical :: equal, is_equal
    integer(TC) :: k1, k2, mask_in
    k1 = t1%mask_out
    k2 = t2%mask_out
    mask_in = t1%mask_in
    equal = .true.
    call check (t1%branch(k1), t2%branch(k2), k1, k2)
    is_equal = equal
contains
    recursive subroutine check (b1, b2, k1, k2)
        type(phs_branch_t), intent(in) :: b1, b2
        integer(TC), intent(in) :: k1, k2
        integer(TC), dimension(2) :: d1, d2, pd2
        integer :: i
        if (.not.b1%has_friend .and. .not.b2%has_friend) then
            equal = .true.
        else if (b1%has_friend .and. b2%has_friend) then
            equal = (b1%friend == tc_permute (b2%friend, perm, mask_in))
        end if
        if (equal) then
            if (b1%has_children .and. b2%has_children) then
                d1 = b1%daughter
                d2 = b2%daughter
                do i=1, 2
                    pd2(i) = tc_permute (d2(i), perm, mask_in)
                end do
                if (d1(1)==pd2(1) .and. d1(2)==pd2(2)) then
                    equal = (b1%firstborn == b2%firstborn)
                    if (equal) call check &
                        & (t1%branch(d1(1)), t2%branch(d2(1)), d1(1), d2(1))
                    if (equal) call check &
                        & (t1%branch(d1(2)), t2%branch(d2(2)), d1(2), d2(2))
                else if (d1(1)==pd2(2) .and. d1(2)==pd2(1)) then
                    equal = ( (b1%firstborn == 0 .and. b2%firstborn == 0) &
                        & .or. (b1%firstborn == 3 - b2%firstborn) )
                    if (equal) call check &
                        & (t1%branch(d1(1)), t2%branch(d2(2)), d1(1), d2(2))
                    if (equal) call check &
                        & (t1%branch(d1(2)), t2%branch(d2(1)), d1(2), d2(1))
                else
                    equal = .false.
                end if
            end if
        end if
        if (equal) then
            equal = (t1%mapping(k1) == t2%mapping(k2))
        end if
    end subroutine check

```

```
end function phs_tree_equivalent
```

Scan two decay trees and determine the correspondence of mass variables, i.e., the permutation that transfers the ordered list of mass variables belonging to the second tree into the first one. Mass variables are assigned beginning from branches and ending at the root.

```
<PHS trees: public>+≡
```

```
public :: phs_tree_find_msq_permutation
```

```
<PHS trees: sub interfaces>+≡
```

```
module subroutine phs_tree_find_msq_permutation &
  (tree1, tree2, perm2, msq_perm)
  type(phs_tree_t), intent(in) :: tree1, tree2
  type(permutation_t), intent(in) :: perm2
  type(permutation_t), intent(out) :: msq_perm
end subroutine phs_tree_find_msq_permutation
```

```
<PHS trees: procedures>+≡
```

```
module subroutine phs_tree_find_msq_permutation &
  (tree1, tree2, perm2, msq_perm)
  type(phs_tree_t), intent(in) :: tree1, tree2
  type(permutation_t), intent(in) :: perm2
  type(permutation_t), intent(out) :: msq_perm
  type(permutation_t) :: perm1
  integer(TC) :: mask_in, root
  integer(TC), dimension(:), allocatable :: index1, index2
  integer :: i
  allocate (index1 (tree1%n_msq), index2 (tree2%n_msq))
  call permutation_init (perm1, permutation_size (perm2))
  mask_in = tree1%mask_in
  root = tree1%mask_out
  i = 0
  call tree_scan (tree1, root, perm1, index1)
  i = 0
  call tree_scan (tree2, root, perm2, index2)
  call permutation_find (msq_perm, index1, index2)
contains
  recursive subroutine tree_scan (tree, k, perm, index)
    type(phs_tree_t), intent(in) :: tree
    integer(TC), intent(in) :: k
    type(permutation_t), intent(in) :: perm
    integer, dimension(:), intent(inout) :: index
    if (tree%branch(k)%has_children) then
      call tree_scan (tree, tree%branch(k)%daughter(1), perm, index)
      call tree_scan (tree, tree%branch(k)%daughter(2), perm, index)
      i = i + 1
      if (i <= size (index)) index(i) = tc_permute (k, perm, mask_in)
    end if
  end subroutine tree_scan
end subroutine phs_tree_find_msq_permutation
```

```
<PHS trees: public>+≡
```

```
public :: phs_tree_find_angle_permutation
```

(PHS trees: sub interfaces)+≡

```

module subroutine phs_tree_find_angle_permutation &
  (tree1, tree2, perm2, angle_perm, sig2)
  type(phs_tree_t), intent(in) :: tree1, tree2
  type(permutation_t), intent(in) :: perm2
  type(permutation_t), intent(out) :: angle_perm
  logical, dimension(:), allocatable, intent(out) :: sig2
end subroutine phs_tree_find_angle_permutation

```

(PHS trees: procedures)+≡

```

module subroutine phs_tree_find_angle_permutation &
  (tree1, tree2, perm2, angle_perm, sig2)
  type(phs_tree_t), intent(in) :: tree1, tree2
  type(permutation_t), intent(in) :: perm2
  type(permutation_t), intent(out) :: angle_perm
  logical, dimension(:), allocatable, intent(out) :: sig2
  type(permutation_t) :: perm1
  integer(TC) :: mask_in, root
  integer(TC), dimension(:), allocatable :: index1, index2
  logical, dimension(:), allocatable :: sig1
  integer :: i
  allocate (index1 (tree1%n_angles), index2 (tree2%n_angles))
  allocate (sig1 (tree1%n_angles), sig2 (tree2%n_angles))
  call permutation_init (perm1, permutation_size (perm2))
  mask_in = tree1%mask_in
  root = tree1%mask_out
  i = 0
  call tree_scan (tree1, root, perm1, index1, sig1)
  i = 0
  call tree_scan (tree2, root, perm2, index2, sig2)
  call permutation_find (angle_perm, index1, index2)
contains
  recursive subroutine tree_scan (tree, k, perm, index, sig)
    type(phs_tree_t), intent(in) :: tree
    integer(TC), intent(in) :: k
    type(permutation_t), intent(in) :: perm
    integer, dimension(:), intent(inout) :: index
    logical, dimension(:), intent(inout) :: sig
    integer(TC) :: k1, k2, kp
    logical :: s
    if (tree%branch(k)%has_children) then
      k1 = tree%branch(k)%daughter(1)
      k2 = tree%branch(k)%daughter(2)
      s = (tc_permute(k1, perm, mask_in) < tc_permute(k2, perm, mask_in))
      kp = tc_permute (k, perm, mask_in)
      i = i + 1
      index(i) = kp
      sig(i) = s
      i = i + 1
      index(i) = - kp
      sig(i) = s
      call tree_scan (tree, k1, perm, index, sig)
      call tree_scan (tree, k2, perm, index, sig)
    end if
  end subroutine tree_scan

```

```
end subroutine phs_tree_find_angle_permutation
```

19.7.4 Phase-space evaluation

Phase-space volume

We compute the phase-space volume recursively, following the same path as for computing other kinematical variables. However, the volume depends just on $\sqrt{\hat{s}}$, not on the momentum configuration.

Note: counting branches, we may replace this by a simple formula.

```
<PHS trees: phs tree: TBP>+≡
  procedure :: compute_volume => phs_tree_compute_volume

<PHS trees: sub interfaces>+≡
  module subroutine phs_tree_compute_volume (tree, sqrts, volume)
    class(phs_tree_t), intent(in) :: tree
    real(default), intent(in) :: sqrts
    real(default), intent(out) :: volume
  end subroutine phs_tree_compute_volume

<PHS trees: procedures>+≡
  module subroutine phs_tree_compute_volume (tree, sqrts, volume)
    class(phs_tree_t), intent(in) :: tree
    real(default), intent(in) :: sqrts
    real(default), intent(out) :: volume
    integer(TC) :: k
    k = tree%mask_out
    if (tree%branch(k)%has_children) then
      call compute_volume_x (tree%branch(k), k, volume, .true.)
    else
      volume = 1
    end if
  contains
    recursive subroutine compute_volume_x (b, k, volume, initial)
      type(phs_branch_t), intent(in) :: b
      integer(TC), intent(in) :: k
      real(default), intent(out) :: volume
      logical, intent(in) :: initial
      integer(TC) :: k1, k2
      real(default) :: v1, v2
      k1 = b%daughter(1); k2 = b%daughter(2)
      if (tree%branch(k1)%has_children) then
        call compute_volume_x (tree%branch(k1), k1, v1, .false.)
      else
        v1 = 1
      end if
      if (tree%branch(k2)%has_children) then
        call compute_volume_x (tree%branch(k2), k2, v2, .false.)
      else
        v2 = 1
      end if
      if (initial) then
        volume = v1 * v2 / (4 * twopi5)
```

```

        else
            volume = v1 * v2 * sqrts**2 / (4 * twopi2)
        end if
    end subroutine compute_volume_x
end subroutine phs_tree_compute_volume

```

Determine momenta

This is done in two steps: First the masses are determined. This step may fail, in which case `ok` is set to false. If successful, we generate angles and the actual momenta. The array `decay_p` serves for transferring the individual three-momenta of the daughter particles in their mother rest frame from the mass generation to the momentum generation step.

(PHS trees: phs tree: TBP)+≡

```

    procedure :: compute_momenta_from_x => phs_tree_compute_momenta_from_x

```

(PHS trees: sub interfaces)+≡

```

    module subroutine phs_tree_compute_momenta_from_x &
        (tree, prt, factor, volume, sqrts, x, ok)
        class(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(inout) :: prt
        real(default), intent(out) :: factor, volume
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(in) :: x
        logical, intent(out) :: ok
    end subroutine phs_tree_compute_momenta_from_x

```

(PHS trees: procedures)+≡

```

    module subroutine phs_tree_compute_momenta_from_x &
        (tree, prt, factor, volume, sqrts, x, ok)
        class(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(inout) :: prt
        real(default), intent(out) :: factor, volume
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(in) :: x
        logical, intent(out) :: ok
        real(default), dimension(tree%mask_out) :: decay_p
        integer :: n1, n2
        integer :: n_out
        if (tree%real_phsp) then
            n_out = tree%n_externals - tree%n_in - 1
            n1 = max (n_out-2, 0)
            n2 = n1 + max (2*n_out, 0)
        else
            n1 = tree%n_msq
            n2 = n1 + tree%n_angles
        end if
        call phs_tree_set_msq &
            (tree, prt, factor, volume, decay_p, sqrts, x(1:n1), ok)
        if (ok) call phs_tree_set_angles &
            (tree, prt, factor, decay_p, sqrts, x(n1+1:n2))
    end subroutine phs_tree_compute_momenta_from_x

```

Mass generation is done recursively. The `ok` flag causes the filled tree to be discarded if set to `.false.` This happens if a three-momentum turns out to be imaginary, indicating impossible kinematics. The index `ix` tells us how far we have used up the input array `x`.

(PHS trees: procedures)+≡

```

subroutine phs_tree_set_msq &
  (tree, prt, factor, volume, decay_p, sqrts, x, ok)
  type(phs_tree_t), intent(inout) :: tree
  type(phs_prt_t), dimension(:), intent(inout) :: prt
  real(default), intent(out) :: factor, volume
  real(default), dimension(:), intent(out) :: decay_p
  real(default), intent(in) :: sqrts
  real(default), dimension(:), intent(in) :: x
  logical, intent(out) :: ok
  integer :: ix
  integer(TC) :: k
  real(default) :: m_tot
  ok = .true.
  ix = 1
  k = tree%mask_out
  m_tot = tree%mass_sum(k)
  decay_p(k) = 0.
  if (m_tot < sqrts .or. k == 1) then
    if (tree%branch(k)%has_children) then
      call set_msq_x (tree%branch(k), k, factor, volume, .true.)
    else
      factor = 1
      volume = 1
    end if
  else
    ok = .false.
  end if
contains
recursive subroutine set_msq_x (b, k, factor, volume, initial)
  type(phs_branch_t), intent(in) :: b
  integer(TC), intent(in) :: k
  real(default), intent(out) :: factor, volume
  logical, intent(in) :: initial
  real(default) :: msq, m, m_min, m_max, m1, m2, msq1, msq2, lda, rlda
  integer(TC) :: k1, k2
  real(default) :: f1, f2, v1, v2
  k1 = b%daughter(1); k2 = b%daughter(2)
  if (tree%branch(k1)%has_children) then
    call set_msq_x (tree%branch(k1), k1, f1, v1, .false.)
    if (.not.ok) return
  else
    f1 = 1; v1 = 1
  end if
  if (tree%branch(k2)%has_children) then
    call set_msq_x (tree%branch(k2), k2, f2, v2, .false.)
    if (.not.ok) return
  else
    f2 = 1; v2 = 1
  end if

```



```

m_min = tree%mass_sum(k)
if (initial) then
  msq = sqrts**2
  m = sqrts
  m_max = sqrts
  factor = f1 * f2
  volume = v1 * v2 / (4 * twopi5)
else
  m_max = sqrts - m_tot + m_min
  call tree%mapping(k)%compute_msq_from_x (sqrts**2, m_min**2, &
    m_max**2, msq, factor, x(ix)); ix = ix + 1
  if (msq >= 0) then
    m = sqrt (msq)
    factor = f1 * f2 * factor
    volume = v1 * v2 * sqrts**2 / (4 * twopi2)
    call prt(k)%set_msq (msq)
    call prt(k)%set_defined ()
  else
    ok = .false.
  end if
end if
if (ok) then
  msq1 = prt(k1)%get_msq (); m1 = sqrt (msq1)
  msq2 = prt(k2)%get_msq (); m2 = sqrt (msq2)
  lda = lambda (msq, msq1, msq2)
  if (lda > 0 .and. m > m1 + m2 .and. m <= m_max) then
    rlda = sqrt (lda)
    decay_p(k1) = rlda / (2*m)
    decay_p(k2) = - decay_p(k1)
    factor = rlda / msq * factor
  else
    ok = .false.
  end if
end if
end subroutine set_msq_x

end subroutine phs_tree_set_msq

```

The heart of phase space generation: Now we have the invariant masses, let us generate angles. At each branch, we take a Lorentz transformation and augment it by a boost to the current particle rest frame, and by rotations ϕ and θ around the z and y axis, respectively. This transformation is passed down to the daughter particles, if present.

(PHS trees: procedures) +≡

```

subroutine phs_tree_set_angles (tree, prt, factor, decay_p, sqrts, x)
  type(phs_tree_t), intent(inout) :: tree
  type(phs_prt_t), dimension(:), intent(inout) :: prt
  real(default), intent(inout) :: factor
  real(default), dimension(:), intent(in) :: decay_p
  real(default), intent(in) :: sqrts
  real(default), dimension(:), intent(in) :: x
  integer :: ix
  integer(TC) :: k

```

```

ix = 1
k = tree%mask_out
call set_angles_x (tree%branch(k), k)
contains
recursive subroutine set_angles_x (b, k, L0)
  type(phs_branch_t), intent(in) :: b
  integer(TC), intent(in) :: k
  type(lorentz_transformation_t), intent(in), optional :: L0
  real(default) :: m, msq, ct, st, phi, f, E, p, bg
  type(lorentz_transformation_t) :: L, LL
  integer(TC) :: k1, k2
  type(vector3_t) :: axis
  p = decay_p(k)
  msq = prt(k)%get_msq (); m = sqrt (msq)
  E = sqrt (msq + p**2)
  if (present (L0)) then
    call prt(k)%set_momentum (L0 * vector4_moving (E,p,3))
  else
    call prt(k)%set_momentum (vector4_moving (E,p,3))
  end if
  call prt(k)%set_defined ()
  if (b%has_children) then
    k1 = b%daughter(1)
    k2 = b%daughter(2)
    if (m > 0) then
      bg = p / m
    else
      bg = 0
    end if
    phi = x(ix) * twopi; ix = ix + 1
    call tree%mapping(k)%compute_ct_from_x (sqrt2**2, ct, st, f, &
      x(ix)); ix = ix + 1
    factor = factor * f
    if (.not. b%has_friend) then
      L = LT_compose_r2_r3_b3 (ct, st, cos(phi), sin(phi), bg)
      !!! The function above is equivalent to:
      ! L = boost (bg,3) * rotation (phi,3) * rotation (ct,st,2)
    else
      LL = boost (-bg,3); if (present (L0)) LL = LL * inverse(L0)
      axis = space_part ( &
        LL * prt(tree%branch(k)%friend)%get_momentum () )
      L = boost(bg,3) * rotation_to_2nd (vector3_canonical(3), axis) &
        * LT_compose_r2_r3_b3 (ct, st, cos(phi), sin(phi), 0._default)
    end if
    if (present (L0)) L = L0 * L
    call set_angles_x (tree%branch(k1), k1, L)
    call set_angles_x (tree%branch(k2), k2, L)
  end if
end subroutine set_angles_x

end subroutine phs_tree_set_angles

```

Recover random numbers

For the other channels we want to compute the random numbers that would have generated the momenta that we already know.

```

(PHS trees: phs tree: TBP)+≡
    procedure :: compute_x_from_momenta => phs_tree_compute_x_from_momenta

(PHS trees: sub interfaces)+≡
    module subroutine phs_tree_compute_x_from_momenta &
        (tree, prt, factor, sqrts, x)
        class(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(in) :: prt
        real(default), intent(out) :: factor
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(inout) :: x
    end subroutine phs_tree_compute_x_from_momenta

(PHS trees: procedures)+≡
    module subroutine phs_tree_compute_x_from_momenta &
        (tree, prt, factor, sqrts, x)
        class(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(in) :: prt
        real(default), intent(out) :: factor
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(inout) :: x
        real(default), dimension(tree%mask_out) :: decay_p
        integer :: n1, n2
        n1 = tree%n_msq
        n2 = n1 + tree%n_angles
        call phs_tree_get_msq &
            (tree, prt, factor, decay_p, sqrts, x(1:n1))
        call phs_tree_get_angles &
            (tree, prt, factor, decay_p, sqrts, x(n1+1:n2))
    end subroutine phs_tree_compute_x_from_momenta

```

The inverse operation follows exactly the same steps. The tree is `inout` because it contains mappings whose parameters can be reset when the mapping is applied.

```

(PHS trees: procedures)+≡
    subroutine phs_tree_get_msq (tree, prt, factor, decay_p, sqrts, x)
        type(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(in) :: prt
        real(default), intent(out) :: factor
        real(default), dimension(:), intent(out) :: decay_p
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(inout) :: x
        integer :: ix
        integer(TC) :: k
        real(default) :: m_tot
        ix = 1
        k = tree%mask_out
        m_tot = tree%mass_sum(k)
        decay_p(k) = 0.
        if (tree%branch(k)%has_children) then

```

```

        call get_msq_x (tree%branch(k), k, factor, .true.)
    else
        factor = 1
    end if
contains
recursive subroutine get_msq_x (b, k, factor, initial)
    type(phas_branch_t), intent(in) :: b
    integer(TC), intent(in) :: k
    real(default), intent(out) :: factor
    logical, intent(in) :: initial
    real(default) :: msq, m, m_min, m_max, msq1, msq2, lda, rlda
    integer(TC) :: k1, k2
    real(default) :: f1, f2
    k1 = b%daughter(1); k2 = b%daughter(2)
    if (tree%branch(k1)%has_children) then
        call get_msq_x (tree%branch(k1), k1, f1, .false.)
    else
        f1 = 1
    end if
    if (tree%branch(k2)%has_children) then
        call get_msq_x (tree%branch(k2), k2, f2, .false.)
    else
        f2 = 1
    end if
    m_min = tree%mass_sum(k)
    m_max = sqrts - m_tot + m_min
    msq = prt(k)%get_msq (); m = sqrt (msq)
    if (initial) then
        factor = f1 * f2
    else
        call tree%mapping(k)%compute_x_from_msq (sqrts**2, m_min**2, &
            m_max**2, msq, factor, x(ix)); ix = ix + 1
        factor = f1 * f2 * factor
    end if
    msq1 = prt(k1)%get_msq ()
    msq2 = prt(k2)%get_msq ()
    lda = lambda (msq, msq1, msq2)
    if (lda > 0) then
        rlda = sqrt (lda)
        decay_p(k1) = rlda / (2 * m)
        decay_p(k2) = - decay_p(k1)
        factor = rlda / msq * factor
    else
        decay_p(k1) = 0
        decay_p(k2) = 0
        factor = 0
    end if
end subroutine get_msq_x

end subroutine phs_tree_get_msq

```

This subroutine is the most time-critical part of the whole program. Therefore, we do not exactly parallel the angle generation routine above but make sure that things get evaluated only if they are really needed, at the expense of

readability. Particularly important is to have as few multiplications of Lorentz transformations as possible.

(*PHS trees: procedures*) \equiv

```

subroutine phs_tree_get_angles (tree, prt, factor, decay_p, sqrts, x)
  type(phs_tree_t), intent(inout) :: tree
  type(phs_prt_t), dimension(:), intent(in) :: prt
  real(default), intent(inout) :: factor
  real(default), dimension(:), intent(in) :: decay_p
  real(default), intent(in) :: sqrts
  real(default), dimension(:), intent(out) :: x
  integer :: ix
  integer(TC) :: k
  ix = 1
  k = tree%mask_out
  if (tree%branch(k)%has_children) then
    call get_angles_x (tree%branch(k), k)
  end if
contains
  recursive subroutine get_angles_x (b, k, ct0, st0, phi0, L0)
    type(phs_branch_t), intent(in) :: b
    integer(TC), intent(in) :: k
    real(default), intent(in), optional :: ct0, st0, phi0
    type(lorentz_transformation_t), intent(in), optional :: L0
    real(default) :: cp0, sp0, m, msq, ct, st, phi, bg, f
    type(lorentz_transformation_t) :: L, LL
    type(vector4_t) :: p1, pf
    type(vector3_t) :: n, axis
    integer(TC) :: k1, k2, kf
    logical :: has_friend, need_L
    k1 = b%daughter(1)
    k2 = b%daughter(2)
    kf = b%friend
    has_friend = b%has_friend
    if (present(L0)) then
      p1 = L0 * prt(k1)%get_momentum ()
      if (has_friend) pf = L0 * prt(kf)%get_momentum ()
    else
      p1 = prt(k1)%get_momentum ()
      if (has_friend) pf = prt(kf)%get_momentum ()
    end if
    if (present(phi0)) then
      cp0 = cos (phi0)
      sp0 = sin (phi0)
    end if
    msq = prt(k)%get_msq (); m = sqrt (msq)
    if (m > 0) then
      bg = decay_p(k) / m
    else
      bg = 0
    end if
    if (has_friend) then
      if (present (phi0)) then
        axis = axis_from_p_r3_r2_b3 (pf, cp0, -sp0, ct0, -st0, -bg)
        LL = rotation_to_2nd (axis, vector3_canonical (3)) &

```

```

        * LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg)
    else
        axis = axis_from_p_b3 (pf, -bg)
        LL = rotation_to_2nd (axis, vector3_canonical(3))
        if (.not. vanishes (bg)) LL = LL * boost(-bg, 3)
    end if
    n = space_part (LL * p1)
else if (present (phi0)) then
    n = axis_from_p_r3_r2_b3 (p1, cp0, -sp0, ct0, -st0, -bg)
else
    n = axis_from_p_b3 (p1, -bg)
end if
phi = azimuthal_angle (n)
x(ix) = phi / twopi; ix = ix + 1
ct = polar_angle_ct (n)
st = sqrt (1 - ct**2)
call tree%mapping(k)%compute_x_from_ct (sqrt(2), ct, f, &
    x(ix)); ix = ix + 1
factor = factor * f
if (tree%branch(k1)%has_children .or. tree%branch(k2)%has_children) then
    need_L = .true.
    if (has_friend) then
        if (present (L0)) then
            L = LL * L0
        else
            L = LL
        end if
    else if (present (L0)) then
        L = LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg) * L0
    else if (present (phi0)) then
        L = LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg)
    else if (bg /= 0) then
        L = boost(-bg, 3)
    else
        need_L = .false.
    end if
    if (need_L) then
        if (tree%branch(k1)%has_children) &
            call get_angles_x (tree%branch(k1), k1, ct, st, phi, L)
        if (tree%branch(k2)%has_children) &
            call get_angles_x (tree%branch(k2), k2, ct, st, phi, L)
    else
        if (tree%branch(k1)%has_children) &
            call get_angles_x (tree%branch(k1), k1, ct, st, phi)
        if (tree%branch(k2)%has_children) &
            call get_angles_x (tree%branch(k2), k2, ct, st, phi)
    end if
end if
end subroutine get_angles_x
end subroutine phs_tree_get_angles

```

Auxiliary stuff

This calculates all momenta that are not yet known by summing up daughter particle momenta. The external particles must be known. Only composite particles not yet known are calculated.

```
<PHS trees: public>+≡
    public :: phs_tree_combine_particles

<PHS trees: sub interfaces>+≡
    module subroutine phs_tree_combine_particles (tree, prt)
        type(phs_tree_t), intent(in) :: tree
        type(phs_prt_t), dimension(:), intent(inout) :: prt
    end subroutine phs_tree_combine_particles

<PHS trees: procedures>+≡
    module subroutine phs_tree_combine_particles (tree, prt)
        type(phs_tree_t), intent(in) :: tree
        type(phs_prt_t), dimension(:), intent(inout) :: prt
        call combine_particles_x (tree%mask_out)
    contains
        recursive subroutine combine_particles_x (k)
            integer(TC), intent(in) :: k
            integer :: k1, k2
            if (tree%branch(k)%has_children) then
                k1 = tree%branch(k)%daughter(1); k2 = tree%branch(k)%daughter(2)
                call combine_particles_x (k1)
                call combine_particles_x (k2)
                if (.not. prt(k)%defined) then
                    call prt(k)%combine (prt(k1), prt(k2))
                end if
            end if
        end subroutine combine_particles_x
    end subroutine phs_tree_combine_particles
```

The previous routine is to be evaluated at runtime. Instead of scanning trees, we can as well set up a multiplication table. This is generated here. Note that the table is `intent(out)`.

```
<PHS trees: public>+≡
    public :: phs_tree_setup_prt_combinations

<PHS trees: sub interfaces>+≡
    module subroutine phs_tree_setup_prt_combinations (tree, comb)
        type(phs_tree_t), intent(in) :: tree
        integer, dimension(:,:), intent(out) :: comb
    end subroutine phs_tree_setup_prt_combinations

<PHS trees: procedures>+≡
    module subroutine phs_tree_setup_prt_combinations (tree, comb)
        type(phs_tree_t), intent(in) :: tree
        integer, dimension(:,:), intent(out) :: comb
        comb = 0
        call setup_prt_combinations_x (tree%mask_out)
    contains
        recursive subroutine setup_prt_combinations_x (k)
            integer(TC), intent(in) :: k
```

```

integer, dimension(2) :: kk
if (tree%branch(k)%has_children) then
  kk = tree%branch(k)%daughter
  call setup_prt_combinations_x (kk(1))
  call setup_prt_combinations_x (kk(2))
  comb(:,k) = kk
end if
end subroutine setup_prt_combinations_x
end subroutine phs_tree_setup_prt_combinations

```

JRR: 2022-01-22 reshuffle_mappings is commented out, and no longer used,
not clear why?

<PHS trees: phs tree: TBP>+≡

```

procedure :: reshuffle_mappings => phs_tree_reshuffle_mappings

```

<PHS trees: sub interfaces>+≡

```

module subroutine phs_tree_reshuffle_mappings (tree)
  class(phs_tree_t), intent(inout) :: tree
  end subroutine phs_tree_reshuffle_mappings

```

<PHS trees: procedures>+≡

```

module subroutine phs_tree_reshuffle_mappings (tree)
  class(phs_tree_t), intent(inout) :: tree
  integer(TC) :: k0, k_old, k_new, k2
  integer :: i
  type(mapping_t) :: mapping_tmp
  real(default) :: mass_tmp
  do i = 1, size (tree%momentum_link)
    if (i /= tree%momentum_link (i)) then
      k_old = 2**(i-tree%n_in-1)
      k_new = 2**(tree%momentum_link(i)-tree%n_in-1)
      k0 = tree%branch(k_old)%mother
      k2 = k_new + tree%branch(k_old)%sibling
      mapping_tmp = tree%mapping(k0)
      mass_tmp = tree%mass_sum(k0)
      tree%mapping(k0) = tree%mapping(k2)
      tree%mapping(k2) = mapping_tmp
      tree%mass_sum(k0) = tree%mass_sum(k2)
      tree%mass_sum(k2) = mass_tmp
    end if
  end do
end subroutine phs_tree_reshuffle_mappings

```

<PHS trees: public>+≡

```

public :: phs_tree_set_momentum_links

```

<PHS trees: sub interfaces>+≡

```

module subroutine phs_tree_set_momentum_links (tree, list)
  type(phs_tree_t), intent(inout) :: tree
  integer, dimension(:), allocatable :: list
  end subroutine phs_tree_set_momentum_links

```

<PHS trees: procedures>+≡

```

module subroutine phs_tree_set_momentum_links (tree, list)
  type(phs_tree_t), intent(inout) :: tree

```



```

integer, dimension(:), allocatable :: list
tree%momentum_link = list
end subroutine phs_tree_set_momentum_links

```

19.7.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_trees_ut.f90>≡
  <File header>

  module phs_trees_ut
    use unit_tests
    use phs_trees_util

    <Standard module head>

    <PHS trees: public test>

    contains

    <PHS trees: test driver>

  end module phs_trees_ut

<phs_trees_util.f90>≡
  <File header>

  module phs_trees_util

    !!!<Use kinds>
    use kinds, only: TC
    <Use strings>
    use flavors, only: flavor_t
    use model_data, only: model_data_t

    use resonances, only: resonance_history_t
    use mappings, only: mapping_defaults_t

    use phs_trees

    <Standard module head>

    <PHS trees: test declarations>

    contains

    <PHS trees: tests>

  end module phs_trees_util
API: driver for the unit tests below.
<PHS trees: public test>≡
  public :: phs_trees_test

```

```

<PHS trees: test driver>≡
  subroutine phs_trees_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <PHS trees: execute tests>
  end subroutine phs_trees_test

```

Create a simple $2 \rightarrow 3$ PHS tree and display it.

```

<PHS trees: execute tests>≡
  call test (phs_tree_1, "phs_tree_1", &
    "check phs tree setup", &
    u, results)

<PHS trees: test declarations>≡
  public :: phs_tree_1

<PHS trees: tests>≡
  subroutine phs_tree_1 (u)
    integer, intent(in) :: u
    type(phs_tree_t) :: tree
    type(model_data_t), target :: model
    type(flavor_t), dimension(5) :: flv
    integer :: i

    write (u, "(A)")  "* Test output: phs_tree_1"
    write (u, "(A)")  "* Purpose: test PHS tree routines"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* Set up flavors"
    write (u, "(A)")

    call flv%init ([1, -2, 24, 5, -5], model)
    do i = 1, 5
      write (u, "(1x)", advance="no")
      call flv(i)%write (u)
    end do
    write (u, *)

    write (u, "(A)")
    write (u, "(A)")  "* Create tree"
    write (u, "(A)")

    call tree%init (2, 3, 0, 0)
    call tree%from_array ([integer(TC) :: 1, 2, 3, 4, 7, 8, 16])
    call tree%set_mass_sum (flv)
    call tree%set_effective_masses ()

    call tree%write (u)

    write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call tree%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_tree_1"

end subroutine phs_tree_1

```

The analogous tree with resonance (s-channel) mappings.

```

<PHS trees: execute tests>+≡
call test (phs_tree_2, "phs_tree_2", &
  "check phs tree with resonances", &
  u, results)

<PHS trees: test declarations>+≡
public :: phs_tree_2

<PHS trees: tests>+≡
subroutine phs_tree_2 (u)
  integer, intent(in) :: u
  type(phs_tree_t) :: tree
  type(model_data_t), target :: model
  type(mapping_defaults_t) :: mapping_defaults
  type(flavor_t), dimension(5) :: flv
  type(resonance_history_t) :: res_history
  integer :: i

  write (u, "(A)")  "* Test output: phs_tree_2"
  write (u, "(A)")  "* Purpose: test PHS tree with resonances"
  write (u, "(A)")

  write (u, "(A)")  "* Read model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* Set up flavors"
  write (u, "(A)")

  call flv%init ([1, -2, 24, 5, -5], model)
  do i = 1, 5
    write (u, "(1x)", advance="no")
    call flv(i)%write (u)
  end do
  write (u, *)

  write (u, "(A)")
  write (u, "(A)")  "* Create tree with mappings"
  write (u, "(A)")

  call tree%init (2, 3, 0, 0)
  call tree%from_array ([integer(TC) :: 1, 2, 3, 4, 7, 8, 16])
  call tree%set_mass_sum (flv)

```

```

call tree%init_mapping (3_TC, var_str ("s_channel"), -24, model)
call tree%init_mapping (7_TC, var_str ("s_channel"), 23, model)

call tree%set_mapping_parameters (mapping_defaults, variable_limits=.false.)
call tree%set_effective_masses ()

call tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract resonances from mappings"
write (u, "(A)")

call tree%extract_resonance_history (res_history)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call tree%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_tree_2"

end subroutine phs_tree_2

```

19.8 The phase-space forest

Simply stated, a phase-space forest is a collection of phase-space trees. More precisely, a `phs_forest` object contains all parameterizations of phase space that WHIZARD will use for a single hard process, prepared in the form of `phs_tree` objects. This is suitable for evaluation by the VAMP integration package: each parameterization (tree) is a valid channel in the multi-channel adaptive integration, and each variable in a tree corresponds to an integration dimension, defined by an appropriate mapping of the $(0, 1)$ interval to the allowed range of the integration variable.

The trees are grouped in groves. The trees (integration channels) within a grove share a common weight, assuming that they are related by some approximate symmetry.

Trees/channels that are related by an exact symmetry are connected by an array of equivalences; each equivalence object holds the data that relate one channel to another.

The phase-space setup, i.e., the detailed structure of trees and forest, are read from a file. Therefore, this module also contains the syntax definition and the parser needed for interpreting this file.

```
<phs_forests.f90>≡  
<File header>
```

```
module phs_forests
```

```
<Use kinds>
```

```
  use kinds, only: TC
```

```
<Use strings>
```

```
  use lorentz
```

```
  use permutations
```

```
  use syntax_rules
```

```
  use parser
```

```
  use model_data
```

```
  use flavors
```

```
  use interactions
```

```
  use phs_base
```

```
  use resonances, only: resonance_history_t
```

```
  use resonances, only: resonance_history_set_t
```

```
  use mappings
```

```
  use phs_trees
```

```
<Standard module head>
```

```
<PHS forests: public>
```

```
<PHS forests: types>
```

```
<PHS forests: interfaces>
```

```
<PHS forests: variables>
```

```
  interface
```

```

    <PHS forests: sub interfaces>
    end interface

contains

    <PHS forests: main procedures>

end module phs_forests
<phs_forests_sub.f90>≡
    <File header>

submodule (phs_forests) phs_forests_s

    use io_units
    use format_defs, only: FMT_19
    use diagnostics
    use numeric_utils
    use ifiles
    use lexers

    implicit none

contains

    <PHS forests: procedures>

end submodule phs_forests_s

```

19.8.1 Phase-space setup parameters

This transparent container holds the parameters that the algorithm needs for phase-space setup, with reasonable defaults.

The threshold mass (for considering a particle as effectively massless) is specified separately for s- and t-channel. The default is to treat W and Z bosons as massive in the s-channel, but as massless in the t-channel. The b -quark is treated always massless, the t -quark always massive.

```

<PHS forests: public>≡
    public :: phs_parameters_t

<PHS forests: types>≡
    type :: phs_parameters_t
        real(default) :: sqrts = 0
        real(default) :: m_threshold_s = 50._default
        real(default) :: m_threshold_t = 100._default
        integer :: off_shell = 1
        integer :: t_channel = 2
        logical :: keep_nonresonant = .true.
    contains
        <PHS forests: phs parameters: TBP>
    end type phs_parameters_t

```

Write phase-space parameters to file.

<PHS forests: phs parameters: TBP>≡

```
procedure :: write => phs_parameters_write
```

<PHS forests: sub interfaces>≡

```
module subroutine phs_parameters_write (phs_par, unit)
  class(phs_parameters_t), intent(in) :: phs_par
  integer, intent(in), optional :: unit
end subroutine phs_parameters_write
```

<PHS forests: procedures>≡

```
module subroutine phs_parameters_write (phs_par, unit)
  class(phs_parameters_t), intent(in) :: phs_par
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(3x,A," // FMT_19 // ")") "sqrts          = ", phs_par%sqrts
  write (u, "(3x,A," // FMT_19 // ")") "m_threshold_s = ", phs_par%m_threshold_s
  write (u, "(3x,A," // FMT_19 // ")") "m_threshold_t = ", phs_par%m_threshold_t
  write (u, "(3x,A,I0)") "off_shell = ", phs_par%off_shell
  write (u, "(3x,A,I0)") "t_channel = ", phs_par%t_channel
  write (u, "(3x,A,L1)") "keep_nonresonant = ", phs_par%keep_nonresonant
end subroutine phs_parameters_write
```

Read phase-space parameters from file.

<PHS forests: phs parameters: TBP>+≡

```
procedure :: read => phs_parameters_read
```

<PHS forests: sub interfaces>+≡

```
module subroutine phs_parameters_read (phs_par, unit)
  class(phs_parameters_t), intent(out) :: phs_par
  integer, intent(in) :: unit
end subroutine phs_parameters_read
```

<PHS forests: procedures>+≡

```
module subroutine phs_parameters_read (phs_par, unit)
  class(phs_parameters_t), intent(out) :: phs_par
  integer, intent(in) :: unit
  character(20) :: dummy
  character :: equals
  read (unit, *) dummy, equals, phs_par%sqrts
  read (unit, *) dummy, equals, phs_par%m_threshold_s
  read (unit, *) dummy, equals, phs_par%m_threshold_t
  read (unit, *) dummy, equals, phs_par%off_shell
  read (unit, *) dummy, equals, phs_par%t_channel
  read (unit, *) dummy, equals, phs_par%keep_nonresonant
end subroutine phs_parameters_read
```

Comparison.

<PHS forests: interfaces>≡

```
interface operator(==)
  module procedure phs_parameters_eq
end interface
interface operator(/=)
  module procedure phs_parameters_ne
end interface
```

```

<PHS forests: sub interfaces>+≡
  module function phs_parameters_eq (phs_par1, phs_par2) result (equal)
    logical :: equal
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
  end function phs_parameters_eq
  module function phs_parameters_ne (phs_par1, phs_par2) result (ne)
    logical :: ne
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
  end function phs_parameters_ne

<PHS forests: procedures>+≡
  module function phs_parameters_eq (phs_par1, phs_par2) result (equal)
    logical :: equal
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
    equal = phs_par1%sqrts == phs_par2%sqrts &
      .and. phs_par1%m_threshold_s == phs_par2%m_threshold_s &
      .and. phs_par1%m_threshold_t == phs_par2%m_threshold_t &
      .and. phs_par1%off_shell == phs_par2%off_shell &
      .and. phs_par1%t_channel == phs_par2%t_channel &
      .and.(phs_par1%keep_nonresonant .eqv. phs_par2%keep_nonresonant)
  end function phs_parameters_eq

  module function phs_parameters_ne (phs_par1, phs_par2) result (ne)
    logical :: ne
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
    ne = phs_par1%sqrts /= phs_par2%sqrts &
      .or. phs_par1%m_threshold_s /= phs_par2%m_threshold_s &
      .or. phs_par1%m_threshold_t /= phs_par2%m_threshold_t &
      .or. phs_par1%off_shell /= phs_par2%off_shell &
      .or. phs_par1%t_channel /= phs_par2%t_channel &
      .or.(phs_par1%keep_nonresonant .neqv. phs_par2%keep_nonresonant)
  end function phs_parameters_ne

```

19.8.2 Equivalences

This type holds information about equivalences between phase-space trees. We make a linked list, where each node contains the two trees which are equivalent and the corresponding permutation of external particles. Two more arrays are to be filled: The permutation of mass variables and the permutation of angular variables, where the signature indicates a necessary exchange of daughter branches.

```

<PHS forests: types>+≡
  type :: equivalence_t
  private
  integer :: left, right
  type(permutation_t) :: perm
  type(permutation_t) :: msq_perm, angle_perm
  logical, dimension(:), allocatable :: angle_sig
  type(equivalence_t), pointer :: next => null ()
end type equivalence_t

```



```

<PHS forests: types>+≡
  type :: equivalence_list_t
  private
    integer :: length = 0
    type(equivalence_t), pointer :: first => null ()
    type(equivalence_t), pointer :: last => null ()
  end type equivalence_list_t

```

Append an equivalence to the list

```

<PHS forests: procedures>+≡
  subroutine equivalence_list_add (eql, left, right, perm)
    type(equivalence_list_t), intent(inout) :: eql
    integer, intent(in) :: left, right
    type(permutation_t), intent(in) :: perm
    type(equivalence_t), pointer :: eq
    allocate (eq)
    eq%left = left
    eq%right = right
    eq%perm = perm
    if (associated (eql%last)) then
      eql%last%next => eq
    else
      eql%first => eq
    end if
    eql%last => eq
    eql%length = eql%length + 1
  end subroutine equivalence_list_add

```

Delete the list contents. Has to be pure because it is called from an elemental subroutine.

```

<PHS forests: procedures>+≡
  pure subroutine equivalence_list_final (eql)
    type(equivalence_list_t), intent(inout) :: eql
    type(equivalence_t), pointer :: eq
    do while (associated (eql%first))
      eq => eql%first
      eql%first => eql%first%next
      deallocate (eq)
    end do
    eql%last => null ()
    eql%length = 0
  end subroutine equivalence_list_final

```

Make a deep copy of the equivalence list. This allows for deep copies of groves and forests.

```

<PHS forests: interfaces>+≡
  interface assignment(=)
    module procedure equivalence_list_assign
  end interface

```

```

<PHS forests: main procedures>≡
  subroutine equivalence_list_assign (eql_out, eql_in)

```

```

type(equivalence_list_t), intent(out) :: eql_out
type(equivalence_list_t), intent(in) :: eql_in
type(equivalence_t), pointer :: eq, eq_copy
eq => eql_in%first
do while (associated (eq))
    allocate (eq_copy)
    eq_copy = eq
    eq_copy%next => null ()
    if (associated (eql_out%first)) then
        eql_out%last%next => eq_copy
    else
        eql_out%first => eq_copy
    end if
    eql_out%last => eq_copy
    eq => eq%next
end do
end subroutine equivalence_list_assign

```

The number of list entries

```

(PHS forests: procedures)+≡
elemental function equivalence_list_length (eql) result (length)
    integer :: length
    type(equivalence_list_t), intent(in) :: eql
    length = eql%length
end function equivalence_list_length

```

Recursively write the equivalences list

```

(PHS forests: procedures)+≡
subroutine equivalence_list_write (eql, unit)
    type(equivalence_list_t), intent(in) :: eql
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    if (associated (eql%first)) then
        call equivalence_write_rec (eql%first, u)
    else
        write (u, *) " [empty]"
    end if
contains
recursive subroutine equivalence_write_rec (eq, u)
    type(equivalence_t), intent(in) :: eq
    integer, intent(in) :: u
    integer :: i
    write (u, "(3x,A,1x,I0,1x,I0,2x,A)", advance="no") &
        "Equivalence:", eq%left, eq%right, "Final state permutation:"
    call permutation_write (eq%perm, u)
    write (u, "(1x,12x,1x,A,1x)", advance="no") &
        "      msq permutation: "
    call permutation_write (eq%msq_perm, u)
    write (u, "(1x,12x,1x,A,1x)", advance="no") &
        "      angle permutation:"
    call permutation_write (eq%angle_perm, u)
    write (u, "(1x,12x,1x,26x)", advance="no")

```

```

do i = 1, size (eq%angle_sig)
  if (eq%angle_sig(i)) then
    write (u, "(1x,A)", advance="no") "+"
  else
    write (u, "(1x,A)", advance="no") "-"
  end if
end do
write (u, *)
if (associated (eq%next)) call equivalence_write_rec (eq%next, u)
end subroutine equivalence_write_rec
end subroutine equivalence_list_write

```

19.8.3 Groves

A grove is a group of trees (phase-space channels) that share a common weight in the integration. Within a grove, channels can be declared equivalent, so they also share their integration grids (up to symmetries). The grove contains a list of equivalences. The `tree_count_offset` is the total number of trees of the preceding groves; when the trees are counted per forest (integration channels), the offset has to be added to all tree indices.

```

<PHS forests: types>+≡
type :: phs_grove_t
private
integer :: tree_count_offset
type(phs_tree_t), dimension(:), allocatable :: tree
type(equivalence_list_t) :: equivalence_list
end type phs_grove_t

```

Call `phs_tree_init` which is also elemental:

```

<PHS forests: procedures>+≡
elemental subroutine phs_grove_init &
  (grove, n_trees, n_in, n_out, n_masses, n_angles)
type(phs_grove_t), intent(inout) :: grove
integer, intent(in) :: n_trees, n_in, n_out, n_masses, n_angles
grove%tree_count_offset = 0
allocate (grove%tree (n_trees))
call grove%tree%init (n_in, n_out, n_masses, n_angles)
end subroutine phs_grove_init

```

The trees do not have pointer components, thus no call to `phs_tree_final`:

```

<PHS forests: procedures>+≡
elemental subroutine phs_grove_final (grove)
type(phs_grove_t), intent(inout) :: grove
deallocate (grove%tree)
call equivalence_list_final (grove%equivalence_list)
end subroutine phs_grove_final

```

Deep copy. This triggers double free corruption with the Intel compiler and hence has to remain in the main module.

```

<PHS forests: interfaces>+≡

```

```

interface assignment(=)
  module procedure phs_grove_assign0
  module procedure phs_grove_assign1
end interface

```

(PHS forests: main procedures)+≡

```

subroutine phs_grove_assign0 (grove_out, grove_in)
  type(phs_grove_t), intent(out) :: grove_out
  type(phs_grove_t), intent(in) :: grove_in
  grove_out%tree_count_offset = grove_in%tree_count_offset
  if (allocated (grove_in%tree)) then
    allocate (grove_out%tree (size (grove_in%tree)))
    grove_out%tree = grove_in%tree
  end if
  grove_out%equivalence_list = grove_in%equivalence_list
end subroutine phs_grove_assign0

subroutine phs_grove_assign1 (grove_out, grove_in)
  type(phs_grove_t), dimension(:), intent(out) :: grove_out
  type(phs_grove_t), dimension(:), intent(in) :: grove_in
  integer :: i
  do i = 1, size (grove_in)
    call phs_grove_assign0 (grove_out(i), grove_in(i))
  end do
end subroutine phs_grove_assign1

```

Get the global (s-channel) mappings. Implemented as a subroutine which returns an array (slice).

(PHS forests: procedures)+≡

```

subroutine phs_grove_assign_s_mappings (grove, mapping)
  type(phs_grove_t), intent(in) :: grove
  type(mapping_t), dimension(:), intent(out) :: mapping
  integer :: i
  if (size (mapping) == size (grove%tree)) then
    do i = 1, size (mapping)
      call grove%tree(i)%assign_s_mapping (mapping(i))
    end do
  else
    call msg_bug ("phs_grove_assign_s_mappings: array size mismatch")
  end if
end subroutine phs_grove_assign_s_mappings

```

19.8.4 The forest type

This is a collection of trees and associated particles. In a given tree, each branch code corresponds to a particle in the `prt` array. Furthermore, we have an array of mass sums which is independent of the decay tree and of the particular event. The mappings directly correspond to the decay trees, and the decay groves collect the trees in classes. The permutation list consists of all permutations of outgoing particles that map the decay forest onto itself.

The particle codes `flv` (one for each external particle) are needed for determining masses and such. The trees and associated information are collected in the `grove` array, together with a lookup table that associates tree indices to groves. Finally, the `prt` array serves as workspace for phase-space evaluation.

The `prt_combination` is a list of index pairs, namely the particle momenta pairs that need to be combined in order to provide all momentum combinations that the phase-space trees need to know.

```

<PHS forests: public>+≡
  public :: phs_forest_t

<PHS forests: types>+≡
  type :: phs_forest_t
    private
    integer :: n_in, n_out, n_tot
    integer :: n_masses, n_angles, n_dimensions
    integer :: n_trees, n_equivalences
    type(flavor_t), dimension(:), allocatable :: flv
    type(phs_grove_t), dimension(:), allocatable :: grove
    integer, dimension(:), allocatable :: grove_lookup
    type(phs_prt_t), dimension(:), allocatable :: prt_in
    type(phs_prt_t), dimension(:), allocatable :: prt_out
    type(phs_prt_t), dimension(:), allocatable :: prt
    integer(TC), dimension(:,:), allocatable :: prt_combination
    type(mapping_t), dimension(:), allocatable :: s_mapping
  contains
    <PHS forests: phs forest: TBP>
  end type phs_forest_t

```

The initialization merely allocates memory. We have to know how many trees there are in each grove, so we can initialize everything. The number of groves is the size of the `n_tree` array.

In the `grove_lookup` table we store the grove index that belongs to each absolute tree index. The difference between the absolute index and the relative (to the grove) index is stored, for each grove, as `tree_count_offset`.

The particle array is allocated according to the total number of branches each tree has, but not filled.

```

<PHS forests: phs forest: TBP>≡
  procedure :: init => phs_forest_init

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_init (forest, n_tree, n_in, n_out)
    class(phs_forest_t), intent(inout) :: forest
    integer, dimension(:), intent(in) :: n_tree
    integer, intent(in) :: n_in, n_out
  end subroutine phs_forest_init

<PHS forests: procedures>+≡
  module subroutine phs_forest_init (forest, n_tree, n_in, n_out)
    class(phs_forest_t), intent(inout) :: forest
    integer, dimension(:), intent(in) :: n_tree
    integer, intent(in) :: n_in, n_out
    integer :: g, count, k_root
    forest%n_in = n_in
    forest%n_out = n_out

```

```

forest%n_tot = n_in + n_out
forest%n_masses = max (n_out - 2, 0)
forest%n_angles = max (2*n_out - 2, 0)
forest%n_dimensions = forest%n_masses + forest%n_angles
forest%n_trees = sum (n_tree)
forest%n_equivalences = 0
allocate (forest%grove (size (n_tree)))
call phs_grove_init &
    (forest%grove, n_tree, n_in, n_out, forest%n_masses, &
    forest%n_angles)
allocate (forest%grove_lookup (forest%n_trees))
count = 0
do g = 1, size (forest%grove)
    forest%grove(g)%tree_count_offset = count
    forest%grove_lookup (count+1:count+n_tree(g)) = g
    count = count + n_tree(g)
end do
allocate (forest%prt_in (n_in))
allocate (forest%prt_out (forest%n_out))
k_root = 2**forest%n_tot - 1
allocate (forest%prt (k_root))
allocate (forest%prt_combination (2, k_root))
allocate (forest%s_mapping (forest%n_trees))
end subroutine phs_forest_init

```

Assign the global (s-channel) mappings.

```

<PHS forests: phs forest: TBP>+≡
    procedure :: set_s_mappings => phs_forest_set_s_mappings

<PHS forests: sub interfaces>+≡
    module subroutine phs_forest_set_s_mappings (forest)
        class(phs_forest_t), intent(inout) :: forest
    end subroutine phs_forest_set_s_mappings

<PHS forests: procedures>+≡
    module subroutine phs_forest_set_s_mappings (forest)
        class(phs_forest_t), intent(inout) :: forest
        integer :: g, i0, i1, n
        do g = 1, size (forest%grove)
            call forest%get_grove_bounds (g, i0, i1, n)
            call phs_grove_assign_s_mappings &
                (forest%grove(g), forest%s_mapping(i0:i1))
        end do
    end subroutine phs_forest_set_s_mappings

```

The grove finalizer is called because it contains the equivalence list:

```

<PHS forests: phs forest: TBP>+≡
    procedure :: final => phs_forest_final

<PHS forests: sub interfaces>+≡
    module subroutine phs_forest_final (forest)
        class(phs_forest_t), intent(inout) :: forest
    end subroutine phs_forest_final

```

```

<PHS forests: procedures>+≡
module subroutine phs_forest_final (forest)
  class(phs_forest_t), intent(inout) :: forest
  if (allocated (forest%grove)) then
    call phs_grove_final (forest%grove)
    deallocate (forest%grove)
  end if
  if (allocated (forest%grove_lookup)) deallocate (forest%grove_lookup)
  if (allocated (forest%prt)) deallocate (forest%prt)
  if (allocated (forest%s_mapping)) deallocate (forest%s_mapping)
end subroutine phs_forest_final

```

19.8.5 Screen output

Write the particles that are non-null, then the trees which point to them:

```

<PHS forests: phs forest: TBP>+≡
  procedure :: write => phs_forest_write

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_write (forest, unit)
    class(phs_forest_t), intent(in) :: forest
    integer, intent(in), optional :: unit
  end subroutine phs_forest_write

<PHS forests: procedures>+≡
module subroutine phs_forest_write (forest, unit)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in), optional :: unit
  integer :: u
  integer :: i, g, k
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "Phase space forest:"
  write (u, "(3x,A,I0)") "n_in = ", forest%n_in
  write (u, "(3x,A,I0)") "n_out = ", forest%n_out
  write (u, "(3x,A,I0)") "n_tot = ", forest%n_tot
  write (u, "(3x,A,I0)") "n_masses = ", forest%n_masses
  write (u, "(3x,A,I0)") "n_angles = ", forest%n_angles
  write (u, "(3x,A,I0)") "n_dim = ", forest%n_dimensions
  write (u, "(3x,A,I0)") "n_trees = ", forest%n_trees
  write (u, "(3x,A,I0)") "n_equiv = ", forest%n_equivalences
  write (u, "(3x,A)", advance="no") "flavors ="
  if (allocated (forest%flv)) then
    do i = 1, size (forest%flv)
      write (u, "(1x,I0)", advance="no") forest%flv(i)%get_pdg ()
    end do
    write (u, "(A)")
  else
    write (u, "(1x,A)") "[empty]"
  end if
  write (u, "(1x,A)") "Particle combinations:"
  if (allocated (forest%prt_combination)) then
    do k = 1, size (forest%prt_combination, 2)
      if (forest%prt_combination(1, k) /= 0) then

```

```

        write (u, "(3x,I0,1x,'<=',1x,I0,1x,'+',1x,I0)") &
            k, forest%prt_combination(:,k)
    end if
end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(1x,A)") "Groves and trees:"
if (allocated (forest%grove)) then
    do g = 1, size (forest%grove)
        write (u, "(3x,A,1x,I0)") "Grove    ", g
        call phs_grove_write (forest%grove(g), unit)
    end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(1x,A,I0)") "Total number of equivalences: ", &
    forest%n_equivalences
write (u, "(A)")
write (u, "(1x,A)") "Global s-channel mappings:"
if (allocated (forest%s_mapping)) then
    do i = 1, size (forest%s_mapping)
        associate (mapping => forest%s_mapping(i))
            if (mapping%is_s_channel () .or. mapping%is_on_shell ()) then
                write (u, "(1x,I0,':',1x)", advance="no") i
                call forest%s_mapping(i)%write (unit)
            end if
        end associate
    end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)") "Incoming particles:"
if (allocated (forest%prt_in)) then
    if (any (forest%prt_in%is_defined ())) then
        do i = 1, size (forest%prt_in)
            if (forest%prt_in(i)%is_defined ()) then
                write (u, "(1x,A,1x,I0)") "Particle", i
                call forest%prt_in(i)%write (u)
            end if
        end do
    else
        write (u, "(3x,A)") "[all undefined]"
    end if
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)") "Outgoing particles:"
if (allocated (forest%prt_out)) then
    if (any (forest%prt_out%is_defined ())) then
        do i = 1, size (forest%prt_out)
            if (forest%prt_out(i)%is_defined ()) then

```



```

        write (u, "(1x,A,1x,I0)") "Particle", i
        call forest%prt_out(i)%write (u)
    end if
end do
else
    write (u, "(3x,A)") "[all undefined]"
end if
else
    write (u, "(1x,A)") " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)") "Tree particles:"
if (allocated (forest%prt)) then
    if (any (forest%prt%is_defined ())) then
        do i = 1, size (forest%prt)
            if (forest%prt(i)%is_defined ()) then
                write (u, "(1x,A,1x,I0)") "Particle", i
                call forest%prt(i)%write (u)
            end if
        end do
    else
        write (u, "(3x,A)") "[all undefined]"
    end if
else
    write (u, "(3x,A)") " [empty]"
end if
end subroutine phs_forest_write

subroutine phs_grove_write (grove, unit)
    type(phs_grove_t), intent(in) :: grove
    integer, intent(in), optional :: unit
    integer :: u
    integer :: t
    u = given_output_unit (unit); if (u < 0) return
    do t = 1, size (grove%tree)
        write (u, "(3x,A,I0)") "Tree      ", t
        call grove%tree(t)%write (unit)
    end do
    write (u, "(1x,A)") "Equivalence list:"
    call equivalence_list_write (grove%equivalence_list, unit)
end subroutine phs_grove_write

```

Deep copy.

<PHS forests: public>+≡

```
public :: assignment(=)
```

<PHS forests: interfaces>+≡

```
interface assignment(=)
```

```
    module procedure phs_forest_assign
```

```
end interface
```

<PHS forests: sub interfaces>+≡

```
module subroutine phs_forest_assign (forest_out, forest_in)
```

```
    type(phs_forest_t), intent(out) :: forest_out
```

```

        type(phs_forest_t), intent(in) :: forest_in
    end subroutine phs_forest_assign
(PHS forests: procedures)+≡
module subroutine phs_forest_assign (forest_out, forest_in)
    type(phs_forest_t), intent(out) :: forest_out
    type(phs_forest_t), intent(in) :: forest_in
    forest_out%n_in = forest_in%n_in
    forest_out%n_out = forest_in%n_out
    forest_out%n_tot = forest_in%n_tot
    forest_out%n_masses = forest_in%n_masses
    forest_out%n_angles = forest_in%n_angles
    forest_out%n_dimensions = forest_in%n_dimensions
    forest_out%n_trees = forest_in%n_trees
    forest_out%n_equivalences = forest_in%n_equivalences
    if (allocated (forest_in%flv)) then
        allocate (forest_out%flv (size (forest_in%flv)))
        forest_out%flv = forest_in%flv
    end if
    if (allocated (forest_in%grove)) then
        allocate (forest_out%grove (size (forest_in%grove)))
        forest_out%grove = forest_in%grove
    end if
    if (allocated (forest_in%grove_lookup)) then
        allocate (forest_out%grove_lookup (size (forest_in%grove_lookup)))
        forest_out%grove_lookup = forest_in%grove_lookup
    end if
    if (allocated (forest_in%prt_in)) then
        allocate (forest_out%prt_in (size (forest_in%prt_in)))
        forest_out%prt_in = forest_in%prt_in
    end if
    if (allocated (forest_in%prt_out)) then
        allocate (forest_out%prt_out (size (forest_in%prt_out)))
        forest_out%prt_out = forest_in%prt_out
    end if
    if (allocated (forest_in%prt)) then
        allocate (forest_out%prt (size (forest_in%prt)))
        forest_out%prt = forest_in%prt
    end if
    if (allocated (forest_in%s_mapping)) then
        allocate (forest_out%s_mapping (size (forest_in%s_mapping)))
        forest_out%s_mapping = forest_in%s_mapping
    end if
    if (allocated (forest_in%prt_combination)) then
        allocate (forest_out%prt_combination &
            (2, size (forest_in%prt_combination, 2)))
        forest_out%prt_combination = forest_in%prt_combination
    end if
end subroutine phs_forest_assign

```

19.8.6 Accessing contents

Get the number of integration parameters

```

<PHS forests: phs forest: TBP>+≡
  procedure :: get_n_parameters => phs_forest_get_n_parameters

<PHS forests: sub interfaces>+≡
  module function phs_forest_get_n_parameters (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
  end function phs_forest_get_n_parameters

<PHS forests: procedures>+≡
  module function phs_forest_get_n_parameters (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
    n = forest%n_dimensions
  end function phs_forest_get_n_parameters

```

Get the number of integration channels

```

<PHS forests: phs forest: TBP>+≡
  procedure :: get_n_channels => phs_forest_get_n_channels

<PHS forests: sub interfaces>+≡
  module function phs_forest_get_n_channels (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
  end function phs_forest_get_n_channels

<PHS forests: procedures>+≡
  module function phs_forest_get_n_channels (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
    n = forest%n_trees
  end function phs_forest_get_n_channels

```

Get the number of groves

```

<PHS forests: phs forest: TBP>+≡
  procedure :: get_n_groves => phs_forest_get_n_groves

<PHS forests: sub interfaces>+≡
  module function phs_forest_get_n_groves (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
  end function phs_forest_get_n_groves

<PHS forests: procedures>+≡
  module function phs_forest_get_n_groves (forest) result (n)
    integer :: n
    class(phs_forest_t), intent(in) :: forest
    n = size (forest%grove)
  end function phs_forest_get_n_groves

```

Get the index bounds for a specific grove.

```

<PHS forests: phs forest: TBP>+≡
  procedure :: get_grove_bounds => phs_forest_get_grove_bounds

```

<PHS forests: sub interfaces>+≡

```

module subroutine phs_forest_get_grove_bounds (forest, g, i0, i1, n)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: g
  integer, intent(out) :: i0, i1, n
end subroutine phs_forest_get_grove_bounds

```

<PHS forests: procedures>+≡

```

module subroutine phs_forest_get_grove_bounds (forest, g, i0, i1, n)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: g
  integer, intent(out) :: i0, i1, n
  n = size (forest%grove(g)%tree)
  i0 = forest%grove(g)%tree_count_offset + 1
  i1 = forest%grove(g)%tree_count_offset + n
end subroutine phs_forest_get_grove_bounds

```

Get the number of equivalences

<PHS forests: phs forest: TBP>+≡

```

procedure :: get_n_equivalences => phs_forest_get_n_equivalences

```

<PHS forests: sub interfaces>+≡

```

module function phs_forest_get_n_equivalences (forest) result (n)
  integer :: n
  class(phs_forest_t), intent(in) :: forest
end function phs_forest_get_n_equivalences

```

<PHS forests: procedures>+≡

```

module function phs_forest_get_n_equivalences (forest) result (n)
  integer :: n
  class(phs_forest_t), intent(in) :: forest
  n = forest%n_equivalences
end function phs_forest_get_n_equivalences

```

Return true if a particular channel has a global (s-channel) mapping; also return the resonance mass and width for this mapping.

<PHS forests: phs forest: TBP>+≡

```

procedure :: get_s_mapping => phs_forest_get_s_mapping
procedure :: get_on_shell => phs_forest_get_on_shell

```

<PHS forests: sub interfaces>+≡

```

module subroutine phs_forest_get_s_mapping &
  (forest, channel, flag, mass, width)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: channel
  logical, intent(out) :: flag
  real(default), intent(out) :: mass, width
end subroutine phs_forest_get_s_mapping
module subroutine phs_forest_get_on_shell (forest, channel, flag, mass)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: channel
  logical, intent(out) :: flag
  real(default), intent(out) :: mass
end subroutine phs_forest_get_on_shell

```

```

(PHS forests: procedures)+≡
module subroutine phs_forest_get_s_mapping &
  (forest, channel, flag, mass, width)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: channel
  logical, intent(out) :: flag
  real(default), intent(out) :: mass, width
  flag = forest%s_mapping(channel)%is_s_channel ()
  if (flag) then
    mass = forest%s_mapping(channel)%get_mass ()
    width = forest%s_mapping(channel)%get_width ()
  else
    mass = 0
    width = 0
  end if
end subroutine phs_forest_get_s_mapping

module subroutine phs_forest_get_on_shell (forest, channel, flag, mass)
  class(phs_forest_t), intent(in) :: forest
  integer, intent(in) :: channel
  logical, intent(out) :: flag
  real(default), intent(out) :: mass
  flag = forest%s_mapping(channel)%is_on_shell ()
  if (flag) then
    mass = forest%s_mapping(channel)%get_mass ()
  else
    mass = 0
  end if
end subroutine phs_forest_get_on_shell

```

Extract the set of unique resonance histories, in form of an array.

```

(PHS forests: phs forest: TBP)+≡
procedure :: extract_resonance_history_set &
  => phs_forest_extract_resonance_history_set

(PHS forests: sub interfaces)+≡
module subroutine phs_forest_extract_resonance_history_set &
  (forest, res_set, include_trivial)
  class(phs_forest_t), intent(in) :: forest
  type(resonance_history_set_t), intent(out) :: res_set
  logical, intent(in), optional :: include_trivial
end subroutine phs_forest_extract_resonance_history_set

(PHS forests: procedures)+≡
module subroutine phs_forest_extract_resonance_history_set &
  (forest, res_set, include_trivial)
  class(phs_forest_t), intent(in) :: forest
  type(resonance_history_set_t), intent(out) :: res_set
  logical, intent(in), optional :: include_trivial
  type(resonance_history_t) :: rh
  integer :: g, t
  logical :: triv
  triv = .false.; if (present (include_trivial)) triv = include_trivial
  call res_set%init ()
  do g = 1, size (forest%grove)

```

```

        associate (grove => forest%grove(g))
        do t = 1, size (grove%tree)
            call grove%tree(t)%extract_resonance_history (rh)
            call res_set%enter (rh, include_trivial)
        end do
    end associate
end do
call res_set%freeze ()
end subroutine phs_forest_extract_resonance_history_set

```

19.8.7 Read the phase space setup from file

The phase space setup is stored in a file. The file may be generated by the `cascades` module below, or by other means. This file has to be read and parsed to create the PHS forest as the internal phase-space representation.

Create lexer and syntax:

```

(PHS forests: procedures)+≡
subroutine define_phs_forest_syntax (ifile)
    type(ifile_t) :: ifile
    call ifile_append (ifile, "SEQ phase_space_list = process_phase_space*")
    call ifile_append (ifile, "SEQ process_phase_space = " &
        // "process_def process_header phase_space")
    call ifile_append (ifile, "SEQ process_def = process process_list")
    call ifile_append (ifile, "KEY process")
    call ifile_append (ifile, "LIS process_list = process_tag*")
    call ifile_append (ifile, "IDE process_tag")
    call ifile_append (ifile, "SEQ process_header = " &
        // "md5sum_process = md5sum " &
        // "md5sum_model_par = md5sum " &
        // "md5sum_phs_config = md5sum " &
        // "sqrts = real " &
        // "m_threshold_s = real " &
        // "m_threshold_t = real " &
        // "off_shell = integer " &
        // "t_channel = integer " &
        // "keep_nonresonant = logical")
    call ifile_append (ifile, "KEY '='")
    call ifile_append (ifile, "KEY '-'")
    call ifile_append (ifile, "KEY md5sum_process")
    call ifile_append (ifile, "KEY md5sum_model_par")
    call ifile_append (ifile, "KEY md5sum_phs_config")
    call ifile_append (ifile, "KEY sqrts")
    call ifile_append (ifile, "KEY m_threshold_s")
    call ifile_append (ifile, "KEY m_threshold_t")
    call ifile_append (ifile, "KEY off_shell")
    call ifile_append (ifile, "KEY t_channel")
    call ifile_append (ifile, "KEY keep_nonresonant")
    call ifile_append (ifile, "QUO md5sum = '""' ... '""'")
    call ifile_append (ifile, "REA real")
    call ifile_append (ifile, "INT integer")
    call ifile_append (ifile, "IDE logical")
    call ifile_append (ifile, "SEQ phase_space = grove_def+")
end subroutine

```

```

call ifile_append (ifile, "SEQ grove_def = grove tree_def+")
call ifile_append (ifile, "KEY grove")
call ifile_append (ifile, "SEQ tree_def = tree bincodes mapping*")
call ifile_append (ifile, "KEY tree")
call ifile_append (ifile, "SEQ bincodes = bincodes*")
call ifile_append (ifile, "INT bincodes")
call ifile_append (ifile, "SEQ mapping = map bincodes channel signed_pdg")
call ifile_append (ifile, "KEY map")
call ifile_append (ifile, "ALT channel = &
    &s_channel | t_channel | u_channel | &
    &collinear | infrared | radiation | on_shell")
call ifile_append (ifile, "KEY s_channel")
! call ifile_append (ifile, "KEY t_channel")    !!! Key already exists
call ifile_append (ifile, "KEY u_channel")
call ifile_append (ifile, "KEY collinear")
call ifile_append (ifile, "KEY infrared")
call ifile_append (ifile, "KEY radiation")
call ifile_append (ifile, "KEY on_shell")
call ifile_append (ifile, "ALT signed_pdg = &
    &pdg | negative_pdg")
call ifile_append (ifile, "SEQ negative_pdg = '-' pdg")
call ifile_append (ifile, "INT pdg")
end subroutine define_phs_forest_syntax

```

The model-file syntax and lexer are fixed, therefore stored as module variables:

(PHS forests: variables)≡

```

type(syntax_t), target, save :: syntax_phs_forest

```

(PHS forests: public)+≡

```

public :: syntax_phs_forest_init

```

(PHS forests: sub interfaces)+≡

```

module subroutine syntax_phs_forest_init ()
end subroutine syntax_phs_forest_init

```

(PHS forests: procedures)+≡

```

module subroutine syntax_phs_forest_init ()
type(ifile_t) :: ifile
call define_phs_forest_syntax (ifile)
call syntax_init (syntax_phs_forest, ifile)
call ifile_final (ifile)
end subroutine syntax_phs_forest_init

```

(PHS forests: procedures)+≡

```

subroutine lexer_init_phs_forest (lexer)
type(lexer_t), intent(out) :: lexer
call lexer_init (lexer, &
    comment_chars = "#!", &
    quote_chars = "'", &
    quote_match = '"', &
    single_chars = "-", &
    special_class = ["="] , &
    keyword_list = syntax_get_keyword_list_ptr (syntax_phs_forest))
end subroutine lexer_init_phs_forest

```

```

<PHS forests: public>+≡
    public :: syntax_phs_forest_final

<PHS forests: sub interfaces>+≡
    module subroutine syntax_phs_forest_final ()
        end subroutine syntax_phs_forest_final

<PHS forests: procedures>+≡
    module subroutine syntax_phs_forest_final ()
        call syntax_final (syntax_phs_forest)
    end subroutine syntax_phs_forest_final

<PHS forests: public>+≡
    public :: syntax_phs_forest_write

<PHS forests: sub interfaces>+≡
    module subroutine syntax_phs_forest_write (unit)
        integer, intent(in), optional :: unit
    end subroutine syntax_phs_forest_write

<PHS forests: procedures>+≡
    module subroutine syntax_phs_forest_write (unit)
        integer, intent(in), optional :: unit
        call syntax_write (syntax_phs_forest, unit)
    end subroutine syntax_phs_forest_write

```

The concrete parser and interpreter. Generate an input stream for the external `unit`, read the parse tree (with given `syntax` and `lexer`) from this stream, and transfer the contents of the parse tree to the PHS forest.

We look for the matching `process` tag, count groves and trees for initializing the forest, and fill the trees.

If the optional parameters are set, compare the parameters stored in the file to those. Set `match` true if everything agrees.

```

<PHS forests: phs forest: TBP>+≡
    generic :: read => read_file, read_unit, read_parse_tree
    procedure :: read_file => phs_forest_read_file
    procedure :: read_unit => phs_forest_read_unit
    procedure :: read_parse_tree => phs_forest_read_parse_tree

<PHS forests: sub interfaces>+≡
    module subroutine phs_forest_read_file &
        (forest, filename, process_id, n_in, n_out, model, found, &
         md5sum_process, md5sum_model_par, &
         md5sum_phs_config, phs_par, match)
        class(phs_forest_t), intent(out) :: forest
        type(string_t), intent(in) :: filename
        type(string_t), intent(in) :: process_id
        integer, intent(in) :: n_in, n_out
        class(model_data_t), intent(in), target :: model
        logical, intent(out) :: found
        character(32), intent(in), optional :: &
            md5sum_process, md5sum_model_par, md5sum_phs_config
        type(phs_parameters_t), intent(in), optional :: phs_par
        logical, intent(out), optional :: match
    end subroutine phs_forest_read_file

```



```

end subroutine phs_forest_read_file
module subroutine phs_forest_read_unit &
    (forest, unit, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
class(phs_forest_t), intent(out) :: forest
integer, intent(in) :: unit
type(string_t), intent(in) :: process_id
integer, intent(in) :: n_in, n_out
class(model_data_t), intent(in), target :: model
logical, intent(out) :: found
character(32), intent(in), optional :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
type(phs_parameters_t), intent(in), optional :: phs_par
logical, intent(out), optional :: match
end subroutine phs_forest_read_unit
module subroutine phs_forest_read_parse_tree &
    (forest, parse_tree, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
class(phs_forest_t), intent(out) :: forest
type(parse_tree_t), intent(in), target :: parse_tree
type(string_t), intent(in) :: process_id
integer, intent(in) :: n_in, n_out
class(model_data_t), intent(in), target :: model
logical, intent(out) :: found
character(32), intent(in), optional :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
type(phs_parameters_t), intent(in), optional :: phs_par
logical, intent(out), optional :: match
end subroutine phs_forest_read_parse_tree

```

(*PHS forests: procedures*)+≡

```

module subroutine phs_forest_read_file &
    (forest, filename, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, &
     md5sum_phs_config, phs_par, match)
class(phs_forest_t), intent(out) :: forest
type(string_t), intent(in) :: filename
type(string_t), intent(in) :: process_id
integer, intent(in) :: n_in, n_out
class(model_data_t), intent(in), target :: model
logical, intent(out) :: found
character(32), intent(in), optional :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
type(phs_parameters_t), intent(in), optional :: phs_par
logical, intent(out), optional :: match
type(parse_tree_t), target :: parse_tree
type(stream_t), target :: stream
type(lexer_t) :: lexer
call lexer_init_phs_forest (lexer)
call stream_init (stream, char (filename))
call lexer_assign_stream (lexer, stream)
call parse_tree_init (parse_tree, syntax_phs_forest, lexer)
call phs_forest_read_parse_tree (forest, parse_tree, &

```

```

        process_id, n_in, n_out, model, found, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
    call stream_final (stream)
    call lexer_final (lexer)
    call parse_tree_final (parse_tree)
end subroutine phs_forest_read_file

module subroutine phs_forest_read_unit &
    (forest, unit, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
    class(phs_forest_t), intent(out) :: forest
    integer, intent(in) :: unit
    type(string_t), intent(in) :: process_id
    integer, intent(in) :: n_in, n_out
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: found
    character(32), intent(in), optional :: &
        md5sum_process, md5sum_model_par, md5sum_phs_config
    type(phs_parameters_t), intent(in), optional :: phs_par
    logical, intent(out), optional :: match
    type(parse_tree_t), target :: parse_tree
    type(stream_t), target :: stream
    type(lexer_t) :: lexer
    call lexer_init_phs_forest (lexer)
    call stream_init (stream, unit)
    call lexer_assign_stream (lexer, stream)
    call parse_tree_init (parse_tree, syntax_phs_forest, lexer)
    call phs_forest_read_parse_tree (forest, parse_tree, &
        process_id, n_in, n_out, model, found, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, &
        phs_par, match)
    call stream_final (stream)
    call lexer_final (lexer)
    call parse_tree_final (parse_tree)
end subroutine phs_forest_read_unit

module subroutine phs_forest_read_parse_tree &
    (forest, parse_tree, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
    class(phs_forest_t), intent(out) :: forest
    type(parse_tree_t), intent(in), target :: parse_tree
    type(string_t), intent(in) :: process_id
    integer, intent(in) :: n_in, n_out
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: found
    character(32), intent(in), optional :: &
        md5sum_process, md5sum_model_par, md5sum_phs_config
    type(phs_parameters_t), intent(in), optional :: phs_par
    logical, intent(out), optional :: match
    type(parse_node_t), pointer :: node_header, node_phs, node_grove
    integer :: n_grove, g
    integer, dimension(:), allocatable :: n_tree

```

```

integer :: t
node_header => parse_tree_get_process_ptr (parse_tree, process_id)
found = associated (node_header); if (.not. found) return
if (present (match)) then
    call phs_forest_check_input (node_header, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
    if (.not. match) return
end if
node_phs => parse_node_get_next_ptr (node_header)
n_grove = parse_node_get_n_sub (node_phs)
allocate (n_tree (n_grove))
do g = 1, n_grove
    node_grove => parse_node_get_sub_ptr (node_phs, g)
    n_tree(g) = parse_node_get_n_sub (node_grove) - 1
end do
call forest%init (n_tree, n_in, n_out)
do g = 1, n_grove
    node_grove => parse_node_get_sub_ptr (node_phs, g)
    do t = 1, n_tree(g)
        call phs_tree_set (forest%grove(g)%tree(t), &
            parse_node_get_sub_ptr (node_grove, t+1), model)
    end do
end do
end subroutine phs_forest_read_parse_tree

```

Check the input for consistency. If any MD5 sum or phase-space parameter disagrees, the phase-space file cannot be used. The MD5 sum checks are skipped if the stored MD5 sum is empty.

(*PHS forests: procedures*) +=

```

subroutine phs_forest_check_input (pn_header, &
    md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
type(parse_node_t), intent(in), target :: pn_header
character(32), intent(in) :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
type(phs_parameters_t), intent(in), optional :: phs_par
logical, intent(out) :: match
type(parse_node_t), pointer :: pn_md5sum, pn_rval, pn_ival, pn_lval
character(32) :: md5sum
type(phs_parameters_t) :: phs_par_old
character(1) :: lstr
pn_md5sum => parse_node_get_sub_ptr (pn_header, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_process) then
    call msg_message ("Phase space: discarding old configuration &
        &(process changed)")
    match = .false.; return
end if
pn_md5sum => parse_node_get_next_ptr (pn_md5sum, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_model_par) then
    call msg_message ("Phase space: discarding old configuration &
        &(model parameters changed)")
    match = .false.; return

```

```

end if
pn_md5sum => parse_node_get_next_ptr (pn_md5sum, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_phs_config) then
    call msg_message ("Phase space: discarding old configuration &
        &(configuration parameters changed)")
    match = .false.; return
end if
if (present (phs_par)) then
    pn_rval => parse_node_get_next_ptr (pn_md5sum, 3)
    phs_par_old%sqrts = parse_node_get_real (pn_rval)
    pn_rval => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%m_threshold_s = parse_node_get_real (pn_rval)
    pn_rval => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%m_threshold_t = parse_node_get_real (pn_rval)
    pn_ival => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%off_shell = parse_node_get_integer (pn_ival)
    pn_ival => parse_node_get_next_ptr (pn_ival, 3)
    phs_par_old%t_channel = parse_node_get_integer (pn_ival)
    pn_lval => parse_node_get_next_ptr (pn_ival, 3)
    lstr = parse_node_get_string (pn_lval)
    read (lstr, "(L1)") phs_par_old%keep_nonresonant
    if (phs_par_old /= phs_par) then
        call msg_message &
            ("Phase space: discarding old configuration &
                &(configuration parameters changed)")
        match = .false.; return
    end if
end if
match = .true.
end subroutine phs_forest_check_input

```

Initialize a specific tree in the forest, using the contents of the 'tree' node. First, count the bincodes, allocate an array and read them in, and make the tree. Each *t*-channel tree is flipped to *s*-channel. Then, find mappings and initialize them.

(*PHS forests: procedures*) +=

```

subroutine phs_tree_set (tree, node, model)
    type(phs_tree_t), intent(inout) :: tree
    type(parse_node_t), intent(in), target :: node
    class(model_data_t), intent(in), target :: model
    type(parse_node_t), pointer :: node_bincodes, node_mapping, pn_pdg
    integer :: n_bincodes, offset
    integer(TC), dimension(:), allocatable :: bincodes
    integer :: b, n_mappings, m
    integer(TC) :: k
    type(string_t) :: type
    integer :: pdg
    node_bincodes => parse_node_get_sub_ptr (node, 2)
    if (associated (node_bincodes)) then
        select case (char (parse_node_get_rule_key (node_bincodes)))
        case ("bincodes")
            n_bincodes = parse_node_get_n_sub (node_bincodes)
            offset = 2

```

```

        case default
            n_bincodes = 0
            offset = 1
        end select
    else
        n_bincodes = 0
        offset = 2
    end if
    allocate (bincode (n_bincodes))
    do b = 1, n_bincodes
        bincode(b) = parse_node_get_integer &
            (parse_node_get_sub_ptr (node_bincodes, b))
    end do
    call phs_tree_from_array (tree, bincode)
    call tree%flip_t_to_s_channel ()
    call tree%canonicalize ()
    n_mappings = parse_node_get_n_sub (node) - offset
    do m = 1, n_mappings
        node_mapping => parse_node_get_sub_ptr (node, m + offset)
        k = parse_node_get_integer &
            (parse_node_get_sub_ptr (node_mapping, 2))
        type = parse_node_get_key &
            (parse_node_get_sub_ptr (node_mapping, 3))
        pn_pdg => parse_node_get_sub_ptr (node_mapping, 4)
        select case (char (pn_pdg%get_rule_key ()))
            case ("pdg")
                pdg = pn_pdg%get_integer ()
            case ("negative_pdg")
                pdg = - parse_node_get_integer (pn_pdg%get_sub_ptr (2))
            end select
        call tree%init_mapping (k, type, pdg, model)
    end do
end subroutine phs_tree_set

```

19.8.8 Preparation

The trees that we read from file do not carry flavor information. This is set separately:

The flavor list must be unique for a unique set of masses; if a given particle can have different flavor, the mass must be degenerate, so we can choose one of the possible flavor combinations.

(PHS forests: phs forest: TBP)+≡

```
procedure :: set_flavors => phs_forest_set_flavors
```

(PHS forests: sub interfaces)+≡

```

module subroutine phs_forest_set_flavors (forest, flv, reshuffle, flv_extra)
    class(phs_forest_t), intent(inout) :: forest
    type(flavor_t), dimension(:), intent(in) :: flv
    integer, intent(in), dimension(:), allocatable, optional :: reshuffle
    type(flavor_t), intent(in), optional :: flv_extra
end subroutine phs_forest_set_flavors

```

<PHS forests: procedures>+≡

```

module subroutine phs_forest_set_flavors (forest, flv, reshuffle, flv_extra)
  class(phs_forest_t), intent(inout) :: forest
  type(flavor_t), dimension(:), intent(in) :: flv
  integer, intent(in), dimension(:), allocatable, optional :: reshuffle
  type(flavor_t), intent(in), optional :: flv_extra
  integer :: i, n_flv0
  if (present (reshuffle) .and. present (flv_extra)) then
    n_flv0 = size (flv)
    do i = 1, n_flv0
      if (reshuffle(i) <= n_flv0) then
        forest%flv(i) = flv (reshuffle(i))
      else
        forest%flv(i) = flv_extra
      end if
    end do
  else
    allocate (forest%flv (size (flv)))
    forest%flv = flv
  end if
end subroutine phs_forest_set_flavors

```

<PHS forests: phs forest: TBP>+≡

```

procedure :: set_momentum_links => phs_forest_set_momentum_links

```

<PHS forests: sub interfaces>+≡

```

module subroutine phs_forest_set_momentum_links (forest, list)
  class(phs_forest_t), intent(inout) :: forest
  integer, intent(in), dimension(:), allocatable :: list
end subroutine phs_forest_set_momentum_links

```

<PHS forests: procedures>+≡

```

module subroutine phs_forest_set_momentum_links (forest, list)
  class(phs_forest_t), intent(inout) :: forest
  integer, intent(in), dimension(:), allocatable :: list
  integer :: g, t
  do g = 1, size (forest%grove)
    do t = 1, size (forest%grove(g)%tree)
      associate (tree => forest%grove(g)%tree(t))
        call phs_tree_set_momentum_links (tree, list)
        !!! call tree%reshuffle_mappings ()
      end associate
    end do
  end do
end subroutine phs_forest_set_momentum_links

```

Once the parameter set is fixed, the masses and the widths of the particles are known and the `mass_sum` arrays as well as the mapping parameters can be computed. Note that order is important: we first compute the mass sums, then the ordinary mappings. The resonances obtained here determine the effective masses, which in turn are used to implement step mappings for resonance decay products that are not mapped otherwise.

<PHS forests: phs forest: TBP>+≡

```

procedure :: set_parameters => phs_forest_set_parameters

```

```

(PHS forests: sub interfaces)+≡
  module subroutine phs_forest_set_parameters &
    (forest, mapping_defaults, variable_limits)
    class(phs_forest_t), intent(inout) :: forest
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    logical, intent(in) :: variable_limits
  end subroutine phs_forest_set_parameters

(PHS forests: procedures)+≡
  module subroutine phs_forest_set_parameters &
    (forest, mapping_defaults, variable_limits)
    class(phs_forest_t), intent(inout) :: forest
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    logical, intent(in) :: variable_limits
    integer :: g, t
    do g = 1, size (forest%grove)
      do t = 1, size (forest%grove(g)%tree)
        call forest%grove(g)%tree(t)%set_mass_sum (forest%flv(forest%n_in+1:))
        call forest%grove(g)%tree(t)%set_mapping_parameters &
          (mapping_defaults, variable_limits)
        call forest%grove(g)%tree(t)%set_effective_masses ( )
        if (mapping_defaults%step_mapping) then
          call forest%grove(g)%tree(t)%set_step_mappings &
            (mapping_defaults%step_mapping_exp, variable_limits)
        end if
      end do
    end do
  end subroutine phs_forest_set_parameters

```

Generate the particle combination table. Scan all trees and merge their individual combination tables. At the end, valid entries are non-zero, and they indicate the indices of a pair of particles to be combined to a new particle. If a particle is accessible by more than one tree (this is usual), only keep the first possibility.

```

(PHS forests: phs forest: TBP)+≡
  procedure :: setup_prt_combinations => phs_forest_setup_prt_combinations

(PHS forests: sub interfaces)+≡
  module subroutine phs_forest_setup_prt_combinations (forest)
    class(phs_forest_t), intent(inout) :: forest
  end subroutine phs_forest_setup_prt_combinations

(PHS forests: procedures)+≡
  module subroutine phs_forest_setup_prt_combinations (forest)
    class(phs_forest_t), intent(inout) :: forest
    integer :: g, t
    integer, dimension(:,,:), allocatable :: tree_prt_combination
    forest%prt_combination = 0
    allocate (tree_prt_combination (2, size (forest%prt_combination, 2)))
    do g = 1, size (forest%grove)
      do t = 1, size (forest%grove(g)%tree)
        call phs_tree_setup_prt_combinations &
          (forest%grove(g)%tree(t), tree_prt_combination)
        where (tree_prt_combination /= 0 .and. forest%prt_combination == 0)
          forest%prt_combination = tree_prt_combination
        end where
      end do
    end do
  end subroutine phs_forest_setup_prt_combinations

```

```

        end do
    end do
end subroutine phs_forest_setup_prt_combinations

```

19.8.9 Accessing the particle arrays

Set the incoming particles from the contents of an interaction.

```

<PHS forests: phs forest: TBP>+≡
    generic :: set_prt_in => set_prt_in_int, set_prt_in_mom
    procedure :: set_prt_in_int => phs_forest_set_prt_in_int
    procedure :: set_prt_in_mom => phs_forest_set_prt_in_mom

<PHS forests: sub interfaces>+≡
    module subroutine phs_forest_set_prt_in_int (forest, int, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    end subroutine phs_forest_set_prt_in_int
    module subroutine phs_forest_set_prt_in_mom (forest, mom, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(vector4_t), dimension(size (forest%prt_in)), intent(in) :: mom
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    end subroutine phs_forest_set_prt_in_mom

<PHS forests: procedures>+≡
    module subroutine phs_forest_set_prt_in_int (forest, int, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call forest%prt_in%set_momentum (inverse (lt_cm_to_lab) * &
                int%get_momenta (outgoing=.false.))
        else
            call forest%prt_in%set_momentum (int%get_momenta (outgoing=.false.))
        end if
        associate (m_in => forest%flv(:forest%n_in)%get_mass ())
            call forest%prt_in%set_msq (m_in ** 2)
        end associate
        call forest%prt_in%set_defined ()
    end subroutine phs_forest_set_prt_in_int

    module subroutine phs_forest_set_prt_in_mom (forest, mom, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(vector4_t), dimension(size (forest%prt_in)), intent(in) :: mom
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call forest%prt_in%set_momentum (inverse (lt_cm_to_lab) * mom)
        else
            call forest%prt_in%set_momentum (mom)
        end if
        associate (m_in => forest%flv(:forest%n_in)%get_mass ())
            call forest%prt_in%set_msq (m_in ** 2)
        end associate
    end subroutine phs_forest_set_prt_in_mom

```



```

    call forest%prt_in%set_defined ()
end subroutine phs_forest_set_prt_in_mom

```

Set the outgoing particles from the contents of an interaction.

```

(PHS forests: phs forest: TBP)+≡
    generic :: set_prt_out => set_prt_out_int, set_prt_out_mom
    procedure :: set_prt_out_int => phs_forest_set_prt_out_int
    procedure :: set_prt_out_mom => phs_forest_set_prt_out_mom

(PHS forests: sub interfaces)+≡
    module subroutine phs_forest_set_prt_out_int (forest, int, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    end subroutine phs_forest_set_prt_out_int
    module subroutine phs_forest_set_prt_out_mom (forest, mom, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(vector4_t), dimension(size (forest%prt_out)), intent(in) :: mom
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    end subroutine phs_forest_set_prt_out_mom

(PHS forests: procedures)+≡
    module subroutine phs_forest_set_prt_out_int (forest, int, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call forest%prt_out%set_momentum (inverse (lt_cm_to_lab) * &
                int%get_momenta (outgoing=.true.))
        else
            call forest%prt_out%set_momentum (int%get_momenta (outgoing=.true.))
        end if
        associate (m_out => forest%flv(forest%n_in+1:)%get_mass ())
            call forest%prt_out%set_msq (m_out ** 2)
        end associate
        call forest%prt_out%set_defined ()
    end subroutine phs_forest_set_prt_out_int

    module subroutine phs_forest_set_prt_out_mom (forest, mom, lt_cm_to_lab)
        class(phs_forest_t), intent(inout) :: forest
        type(vector4_t), dimension(size (forest%prt_out)), intent(in) :: mom
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call forest%prt_out%set_momentum (inverse (lt_cm_to_lab) * mom)
        else
            call forest%prt_out%set_momentum (mom)
        end if
        associate (m_out => forest%flv(forest%n_in+1:)%get_mass ())
            call forest%prt_out%set_msq (m_out ** 2)
        end associate
        call forest%prt_out%set_defined ()
    end subroutine phs_forest_set_prt_out_mom

```

Combine particles as described by the particle combination table. Particle momentum sums will be calculated only if the resulting particle is contained in at least one of the trees in the current forest. The others are kept undefined.

```

(PHS forests: phs forest: TBP)+≡
  procedure :: combine_particles => phs_forest_combine_particles

(PHS forests: sub interfaces)+≡
  module subroutine phs_forest_combine_particles (forest)
    class(phs_forest_t), intent(inout) :: forest
  end subroutine phs_forest_combine_particles

(PHS forests: procedures)+≡
  module subroutine phs_forest_combine_particles (forest)
    class(phs_forest_t), intent(inout) :: forest
    integer :: k
    integer, dimension(2) :: kk
    do k = 1, size (forest%prt_combination, 2)
      kk = forest%prt_combination(:,k)
      if (kk(1) /= 0) then
        call forest%prt(k)%combine (forest%prt(kk(1)), forest%prt(kk(2)))
      end if
    end do
  end subroutine phs_forest_combine_particles

```

Extract the outgoing particles and insert into an interaction.

```

(PHS forests: phs forest: TBP)+≡
  procedure :: get_prt_out => phs_forest_get_prt_out

(PHS forests: sub interfaces)+≡
  module subroutine phs_forest_get_prt_out (forest, int, lt_cm_to_lab)
    class(phs_forest_t), intent(in) :: forest
    type(interaction_t), intent(inout) :: int
    type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
  end subroutine phs_forest_get_prt_out

(PHS forests: procedures)+≡
  module subroutine phs_forest_get_prt_out (forest, int, lt_cm_to_lab)
    class(phs_forest_t), intent(in) :: forest
    type(interaction_t), intent(inout) :: int
    type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    if (present (lt_cm_to_lab)) then
      call int%set_momenta (lt_cm_to_lab * &
        forest%prt_out%get_momentum (), outgoing=.true.)
    else
      call int%set_momenta (forest%prt_out%get_momentum (), &
        outgoing=.true.)
    end if
  end subroutine phs_forest_get_prt_out

```

Extract the outgoing particle momenta

```

(PHS forests: phs forest: TBP)+≡
  procedure :: get_momenta_out => phs_forest_get_momenta_out

```

(PHS forests: sub interfaces)+≡

```

module function phs_forest_get_momenta_out (forest, lt_cm_to_lab) result (p)
  class(phs_forest_t), intent(in) :: forest
  type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
  type(vector4_t), dimension(size (forest%prt_out)) :: p
end function phs_forest_get_momenta_out

```

(PHS forests: procedures)+≡

```

module function phs_forest_get_momenta_out (forest, lt_cm_to_lab) result (p)
  class(phs_forest_t), intent(in) :: forest
  type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
  type(vector4_t), dimension(size (forest%prt_out)) :: p
  p = forest%prt_out%get_momentum ()
  if (present (lt_cm_to_lab)) p = p * lt_cm_to_lab
end function phs_forest_get_momenta_out

```

19.8.10 Find equivalences among phase-space trees

Scan phase space for equivalences. We generate the complete set of unique permutations for the given list of outgoing particles, and use this for scanning equivalences within each grove. We scan all pairs of trees, using all permutations. This implies that trivial equivalences are included, and equivalences between different trees are recorded twice. This is intentional.

(PHS forests: procedures)+≡

```

subroutine phs_grove_set_equivalences (grove, perm_array)
  type(phs_grove_t), intent(inout) :: grove
  type(permutation_t), dimension(:), intent(in) :: perm_array
  type(equivalence_t), pointer :: eq
  integer :: t1, t2, i
  do t1 = 1, size (grove%tree)
    do t2 = 1, size (grove%tree)
      SCAN_PERM: do i = 1, size (perm_array)
        if (phs_tree_equivalent &
            (grove%tree(t1), grove%tree(t2), perm_array(i))) then
          call equivalence_list_add &
            (grove%equivalence_list, t1, t2, perm_array(i))
          eq => grove%equivalence_list%last
          call phs_tree_find_msq_permutation &
            (grove%tree(t1), grove%tree(t2), eq%perm, &
             eq%msq_perm)
          call phs_tree_find_angle_permutation &
            (grove%tree(t1), grove%tree(t2), eq%perm, &
             eq%angle_perm, eq%angle_sig)
        end if
      end do SCAN_PERM
    end do
  end do
end subroutine phs_grove_set_equivalences

```

(PHS forests: phs forest: TBP)+≡

```

procedure :: set_equivalences => phs_forest_set_equivalences

```

```

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_set_equivalences (forest)
    class(phs_forest_t), intent(inout) :: forest
  end subroutine phs_forest_set_equivalences

<PHS forests: procedures>+≡
  module subroutine phs_forest_set_equivalences (forest)
    class(phs_forest_t), intent(inout) :: forest
    type(permutation_t), dimension(:), allocatable :: perm_array
    integer :: i
    call permutation_array_make &
      (perm_array, forest%flv(forest%n_in+1:)%get_pdg ())
    do i = 1, size (forest%grove)
      call phs_grove_set_equivalences (forest%grove(i), perm_array)
    end do
    forest%n_equivalences = sum (forest%grove%equivalence_list%length)
  end subroutine phs_forest_set_equivalences

```

19.8.11 Interface for channel equivalences

Here, we store the equivalence list in the appropriate containers that the `phs_base` module provides. There is one separate list for each channel.

```

<PHS forests: phs forest: TBP>+≡
  procedure :: get_equivalences => phs_forest_get_equivalences

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_get_equivalences &
    (forest, channel, azimuthal_dependence)
    class(phs_forest_t), intent(in) :: forest
    type(phs_channel_t), dimension(:), intent(out) :: channel
    logical, intent(in) :: azimuthal_dependence
  end subroutine phs_forest_get_equivalences

<PHS forests: procedures>+≡
  module subroutine phs_forest_get_equivalences &
    (forest, channel, azimuthal_dependence)
    class(phs_forest_t), intent(in) :: forest
    type(phs_channel_t), dimension(:), intent(out) :: channel
    logical, intent(in) :: azimuthal_dependence
    integer :: n_masses, n_angles
    integer :: mode_azimuthal_angle
    integer, dimension(:), allocatable :: n_eq
    type(equivalence_t), pointer :: eq
    integer, dimension(:), allocatable :: perm, mode
    integer :: g, c, j, left, right
    n_masses = forest%n_masses
    n_angles = forest%n_angles
    allocate (n_eq (forest%n_trees), source = 0)
    allocate (perm (forest%n_dimensions))
    allocate (mode (forest%n_dimensions), source = EQ_IDENTITY)
    do g = 1, size (forest%grove)
      eq => forest%grove(g)%equivalence_list%first
      do while (associated (eq))
        left = eq%left + forest%grove(g)%tree_count_offset

```

```

        n_eq(left) = n_eq(left) + 1
        eq => eq%next
    end do
end do
do c = 1, size (channel)
    allocate (channel(c)%eq (n_eq(c)))
    do j = 1, n_eq(c)
        call channel(c)%eq(j)%init (forest%n_dimensions)
    end do
end do
n_eq = 0
if (azimuthal_dependence) then
    mode_azimuthal_angle = EQ_IDENTITY
else
    mode_azimuthal_angle = EQ_INVARIANT
end if
do g = 1, size (forest%grove)
    eq => forest%grove(g)%equivalence_list%first
    do while (associated (eq))
        left = eq%left + forest%grove(g)%tree_count_offset
        right = eq%right + forest%grove(g)%tree_count_offset
        do j = 1, n_masses
            perm(j) = permute (j, eq%msq_perm)
            mode(j) = EQ_IDENTITY
        end do
        do j = 1, n_angles
            perm(n_masses+j) = n_masses + permute (j, eq%angle_perm)
            if (j == 1) then
                mode(n_masses+j) = mode_azimuthal_angle    ! first az. angle
            else if (mod(j,2) == 1) then
                mode(n_masses+j) = EQ_SYMMETRIC            ! other az. angles
            else if (eq%angle_sig(j)) then
                mode(n_masses+j) = EQ_IDENTITY            ! polar angle +
            else
                mode(n_masses+j) = EQ_INVERT                ! polar angle -
            end if
        end do
        n_eq(left) = n_eq(left) + 1
        associate (eq_cur => channel(left)%eq(n_eq(left)))
            eq_cur%c = right
            eq_cur%perm = perm
            eq_cur%mode = mode
        end associate
        eq => eq%next
    end do
end do
end subroutine phs_forest_get_equivalences

```

19.8.12 Phase-space evaluation

Given one row of the **x** parameter array and the corresponding channel index, compute first all relevant momenta and then recover the remainder of the **x**

array, the Jacobians `phs_factor`, and the phase-space volume.

The output argument `ok` indicates whether this was successful.

(PHS forests: phs forest: TBP)+≡

```
procedure :: evaluate_selected_channel => phs_forest_evaluate_selected_channel
```

(PHS forests: sub interfaces)+≡

```
module subroutine phs_forest_evaluate_selected_channel &
  (forest, channel, active, sqrts, x, phs_factor, volume, ok)
  class(phs_forest_t), intent(inout) :: forest
  integer, intent(in) :: channel
  logical, dimension(:), intent(in) :: active
  real(default), intent(in) :: sqrts
  real(default), dimension(:,:), intent(inout) :: x
  real(default), dimension(:), intent(out) :: phs_factor
  real(default), intent(out) :: volume
  logical, intent(out) :: ok
end subroutine phs_forest_evaluate_selected_channel
```

(PHS forests: procedures)+≡

```
module subroutine phs_forest_evaluate_selected_channel &
  (forest, channel, active, sqrts, x, phs_factor, volume, ok)
  class(phs_forest_t), intent(inout) :: forest
  integer, intent(in) :: channel
  logical, dimension(:), intent(in) :: active
  real(default), intent(in) :: sqrts
  real(default), dimension(:,:), intent(inout) :: x
  real(default), dimension(:), intent(out) :: phs_factor
  real(default), intent(out) :: volume
  logical, intent(out) :: ok
  integer :: g, t
  integer(TC) :: k, k_root, k_in

  g = forest%grove_lookup (channel)
  t = channel - forest%grove(g)%tree_count_offset
  call forest%prt%set_undefined ()
  call forest%prt_out%set_undefined ()
  k_in = forest%n_tot

  do k = 1, forest%n_in
    forest%prt(ibset(0, k_in - k)) = forest%prt_in(k)
  end do

  do k = 1, forest%n_out
    call forest%prt(ibset(0, k - 1))%set_msq &
      (forest%flv(forest%n_in + k)%get_mass () ** 2)
  end do

  k_root = 2**forest%n_out - 1
  select case (forest%n_in)
  case (1)
    forest%prt(k_root) = forest%prt_in(1)
  case (2)
    call forest%prt(k_root)%combine (forest%prt_in(1), forest%prt_in(2))
  end select
```

```

call forest%grove(g)%tree(t)%compute_momenta_from_x (forest%prt, &
  phs_factor(channel), volume, sqrts, x(:,channel), ok)
if (ok) then
  do k = 1, forest%n_out
    forest%prt_out(k) = forest%prt(ibset(0,k-1))
  end do
end if
end subroutine phs_forest_evaluate_selected_channel

```

The remainder: recover x values for all channels except for the current channel.

NOTE: OpenMP not used for the first loop. `combine_particles` is not a channel-local operation.

```

<PHS forests: phs_forest: TBP>+≡
  procedure :: evaluate_other_channels => phs_forest_evaluate_other_channels

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_evaluate_other_channels &
    (forest, channel, active, sqrts, x, phs_factor, combine)
    class(phs_forest_t), intent(inout) :: forest
    integer, intent(in) :: channel
    logical, dimension(:), intent(in) :: active
    real(default), intent(in) :: sqrts
    real(default), dimension(:,:), intent(inout) :: x
    real(default), dimension(:), intent(inout) :: phs_factor
    logical, intent(in) :: combine
  end subroutine phs_forest_evaluate_other_channels

<PHS forests: procedures>+≡
  module subroutine phs_forest_evaluate_other_channels &
    (forest, channel, active, sqrts, x, phs_factor, combine)
    class(phs_forest_t), intent(inout) :: forest
    integer, intent(in) :: channel
    logical, dimension(:), intent(in) :: active
    real(default), intent(in) :: sqrts
    real(default), dimension(:,:), intent(inout) :: x
    real(default), dimension(:), intent(inout) :: phs_factor
    logical, intent(in) :: combine
    integer :: g, t, ch, n_channel

    g = forest%grove_lookup (channel)
    t = channel - forest%grove(g)%tree_count_offset

    n_channel = forest%n_trees
    if (combine) then
      do ch = 1, n_channel
        if (ch == channel) cycle
        if (active(ch)) then
          g = forest%grove_lookup(ch)
          t = ch - forest%grove(g)%tree_count_offset
          call phs_tree_combine_particles &
            (forest%grove(g)%tree(t), forest%prt)
        end if
      end do
    end if
  end subroutine

```

```

!OMP PARALLEL PRIVATE (g,t,ch) SHARED(active,forest,sqrts,x,channel)
!OMP DO SCHEDULE(STATIC)
do ch = 1, n_channel
  if (ch == channel) cycle
  if (active(ch)) then
    g = forest%grove_lookup(ch)
    t = ch - forest%grove(g)%tree_count_offset
    call forest%grove(g)%tree(t)%compute_x_from_momenta (forest%prt, &
      phs_factor(ch), sqrts, x(:,ch))
  end if
end do
!OMP END DO
!OMP END PARALLEL

end subroutine phs_forest_evaluate_other_channels

```

The complement: recover one row of the x array and the associated Jacobian entry, corresponding to `channel`, from incoming and outgoing momenta. Also compute the phase-space volume.

```

<PHS forests: phs forest: TBP>+≡
  procedure :: recover_channel => phs_forest_recover_channel

<PHS forests: sub interfaces>+≡
  module subroutine phs_forest_recover_channel &
    (forest, channel, sqrts, x, phs_factor, volume)
    class(phs_forest_t), intent(inout) :: forest
    integer, intent(in) :: channel
    real(default), intent(in) :: sqrts
    real(default), dimension(:,:), intent(inout) :: x
    real(default), dimension(:), intent(inout) :: phs_factor
    real(default), intent(out) :: volume
  end subroutine phs_forest_recover_channel

<PHS forests: procedures>+≡
  module subroutine phs_forest_recover_channel &
    (forest, channel, sqrts, x, phs_factor, volume)
    class(phs_forest_t), intent(inout) :: forest
    integer, intent(in) :: channel
    real(default), intent(in) :: sqrts
    real(default), dimension(:,:), intent(inout) :: x
    real(default), dimension(:), intent(inout) :: phs_factor
    real(default), intent(out) :: volume
    integer :: g, t
    integer(TC) :: k, k_in
    g = forest%grove_lookup (channel)
    t = channel - forest%grove(g)%tree_count_offset
    call forest%prt%set_undefined ()
    k_in = forest%n_tot
    forall (k = 1:forest%n_in)
      forest%prt(ibset(0,k_in-k)) = forest%prt_in(k)
    end forall
    forall (k = 1:forest%n_out)
      forest%prt(ibset(0,k-1)) = forest%prt_out(k)
    end forall
  end subroutine

```



```

end forall
call forest%combine_particles ()
call forest%grove(g)%tree(t)%compute_volume (sqrts, volume)
call forest%grove(g)%tree(t)%compute_x_from_momenta (forest%prt, &
    phs_factor(channel), sqrts, x(:,channel))
end subroutine phs_forest_recover_channel

```

19.8.13 Unit tests

Test module, followed by the corresponding implementation module.

```

(phs_forests_ut.f90)≡
  ⟨File header⟩

```

```

module phs_forests_ut
  use unit_tests
  use phs_forests_uti

```

⟨Standard module head⟩

⟨PHS forests: public test⟩

contains

⟨PHS forests: test driver⟩

```

end module phs_forests_ut

```

```

(phs_forests_uti.f90)≡
  ⟨File header⟩

```

```

module phs_forests_uti

```

⟨Use kinds⟩

⟨Use strings⟩

```

  use io_units
  use format_defs, only: FMT_12
  use lorentz
  use flavors
  use interactions
  use model_data
  use mappings
  use phs_base
  use resonances, only: resonance_history_set_t

```

```

  use phs_forests

```

⟨Standard module head⟩

⟨PHS forests: test declarations⟩

contains

⟨PHS forests: tests⟩

```

end module phs_forests_util
API: driver for the unit tests below.
<PHS forests: public test>≡
    public :: phs_forests_test
<PHS forests: test driver>≡
    subroutine phs_forests_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS forests: execute tests>
    end subroutine phs_forests_test

```

Basic universal test

Write a possible phase-space file for a $2 \rightarrow 3$ process and make the corresponding forest, print the forest. Choose some in-particle momenta and a random-number array and evaluate out-particles and phase-space factors.

```

<PHS forests: execute tests>≡
    call test (phs_forest_1, "phs_forest_1", &
        "check phs forest setup", &
        u, results)
<PHS forests: test declarations>≡
    public :: phs_forest_1
<PHS forests: tests>≡
    subroutine phs_forest_1 (u)
        use os_interface
        integer, intent(in) :: u
        type(phs_forest_t) :: forest
        type(phs_channel_t), dimension(:), allocatable :: channel
        type(model_data_t), target :: model
        type(string_t) :: process_id
        type(flavor_t), dimension(5) :: flv
        type(string_t) :: filename
        type(interaction_t) :: int
        integer :: unit_fix
        type(mapping_defaults_t) :: mapping_defaults
        logical :: found_process, ok
        integer :: n_channel, ch, i
        logical, dimension(4) :: active = .true.
        real(default) :: sqrts = 1000
        real(default), dimension(5,4) :: x
        real(default), dimension(4) :: factor
        real(default) :: volume

        write (u, "(A)")  "* Test output: PHS forest"
        write (u, "(A)")  "* Purpose: test PHS forest routines"
        write (u, "(A)")

        write (u, "(A)")  "* Reading model file"
    end subroutine phs_forest_1

```

```

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Create phase-space file 'phs_forest_test.phs'"
write (u, "(A)")

call flv%init ([11, -11, 11, -11, 22], model)
unit_fix = free_unit ()
open (file="phs_forest_test.phs", unit=unit_fix, action="write")
write (unit_fix, *) "process foo"
write (unit_fix, *) 'md5sum_process      = "6ABA33BC2927925D0F073B1C1170780A"'
write (unit_fix, *) 'md5sum_model_par   = "1A0B151EE6E2DEB92D880320355A3EAB"'
write (unit_fix, *) 'md5sum_phs_config = "B6A8877058809A8BDD54753CDAB83ACE"'
write (unit_fix, *) "sqrts              = 100.00000000000000"
write (unit_fix, *) "m_threshold_s      = 50.00000000000000"
write (unit_fix, *) "m_threshold_t      = 100.00000000000000"
write (unit_fix, *) "off_shell         = 2"
write (unit_fix, *) "t_channel         = 6"
write (unit_fix, *) "keep_nonresonant = F"
write (unit_fix, *) ""
write (unit_fix, *) "  grove"
write (unit_fix, *) "    tree 3 7"
write (unit_fix, *) "      map 3 s_channel 23"
write (unit_fix, *) "    tree 5 7"
write (unit_fix, *) "    tree 6 7"
write (unit_fix, *) "  grove"
write (unit_fix, *) "    tree 9 11"
write (unit_fix, *) "      map 9 t_channel 22"
close (unit_fix)

write (u, "(A)")
write (u, "(A)")  "* Read phase-space file 'phs_forest_test.phs'"

call syntax_phs_forest_init ()
process_id = "foo"
filename = "phs_forest_test.phs"
call forest%read (filename, process_id, 2, 3, model, found_process)

write (u, "(A)")
write (u, "(A)")  "* Set parameters, flavors, equiv, momenta"
write (u, "(A)")

call forest%set_flavors (flv)
call forest%set_parameters (mapping_defaults, .false.)
call forest%setup_prt_combinations ()
call forest%set_equivalences ()
call int%basic_init (2, 0, 3)
call int%set_momentum &
  (vector4_moving (500._default, 500._default, 3), 1)
call int%set_momentum &
  (vector4_moving (500._default, -500._default, 3), 2)
call forest%set_prt_in (int)
n_channel = 2
x = 0

```

```

x(:,n_channel) = [0.3, 0.4, 0.1, 0.9, 0.6]
write (u, "(A)") "   Input values:"
write (u, "(3x,5(1x," // FMT_12 // "))") x(:,n_channel)

write (u, "(A)")
write (u, "(A)")  "* Evaluating phase space"

call forest%evaluate_selected_channel (n_channel, active, sqrts, &
    x, factor, volume, ok)
call forest%evaluate_other_channels (n_channel, active, sqrts, &
    x, factor, combine=.true.)
call forest%get_prt_out (int)
write (u, "(A)") "   Output values:"
do ch = 1, 4
    write (u, "(3x,5(1x," // FMT_12 // "))") x(:,ch)
end do
call int%basic_write (u)
write (u, "(A)") "   Factors:"
write (u, "(3x,5(1x," // FMT_12 // "))") factor
write (u, "(A)") "   Volume:"
write (u, "(3x,5(1x," // FMT_12 // "))") volume
call forest%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute equivalences"

n_channel = 4
allocate (channel (n_channel))
call forest%get_equivalences (channel, .true.)
do i = 1, n_channel
    write (u, "(1x,I0,':')", advance = "no") ch
    call channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()
call forest%final ()
call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_forest_1"

end subroutine phs_forest_1

```

Resonance histories

Read a suitably nontrivial forest from file and recover the set of resonance histories.

```

<PHS forests: execute tests>+≡
    call test (phs_forest_2, "phs_forest_2", &

```

```

        "handle phs forest resonance content", &
        u, results)

<PHS forests: test declarations>+=
    public :: phs_forest_2

<PHS forests: tests>+=
    subroutine phs_forest_2 (u)
        use os_interface
        integer, intent(in) :: u
        integer :: unit_fix
        type(phs_forest_t) :: forest
        type(model_data_t), target :: model
        type(string_t) :: process_id
        type(string_t) :: filename
        logical :: found_process
        type(resonance_history_set_t) :: res_set
        integer :: i

        write (u, "(A)")  "* Test output: phs_forest_2"
        write (u, "(A)")  "* Purpose: test PHS forest routines"
        write (u, "(A)")

        write (u, "(A)")  "* Reading model file"

        call model%init_sm_test ()

        write (u, "(A)")
        write (u, "(A)")  "* Create phase-space file 'phs_forest_2.phs'"
        write (u, "(A)")

        unit_fix = free_unit ()
        open (file="phs_forest_2.phs", unit=unit_fix, action="write")
        write (unit_fix, *) "process foo"
        write (unit_fix, *) 'md5sum_process      = "XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX"'
        write (unit_fix, *) 'md5sum_model_par   = "1A0B151EE6E2DEB92D880320355A3EAB"'
        write (unit_fix, *) 'md5sum_phs_config = "XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX"'
        write (unit_fix, *) "sqrts              = 100.00000000000000"
        write (unit_fix, *) "m_threshold_s   = 50.00000000000000"
        write (unit_fix, *) "m_threshold_t   = 100.00000000000000"
        write (unit_fix, *) "off_shell      = 2"
        write (unit_fix, *) "t_channel      = 6"
        write (unit_fix, *) "keep_nonresonant = F"
        write (unit_fix, *) ""
        write (unit_fix, *) "  grove"
        write (unit_fix, *) "    tree 3 7"
        write (unit_fix, *) "    tree 3 7"
        write (unit_fix, *) "      map 3 s_channel -24"
        write (unit_fix, *) "    tree 5 7"
        write (unit_fix, *) "    tree 3 7"
        write (unit_fix, *) "      map 3 s_channel -24"
        write (unit_fix, *) "      map 7 s_channel 23"
        write (unit_fix, *) "    tree 5 7"
        write (unit_fix, *) "      map 7 s_channel 25"
        write (unit_fix, *) "    tree 3 11"

```

```

write (unit_fix, *) "          map 3 s_channel -24"
close (unit_fix)

write (u, "(A)")  "* Read phase-space file 'phs_forest_2.phs'"

call syntax_phs_forest_init ()
process_id = "foo"
filename = "phs_forest_2.phs"
call forest%read (filename, process_id, 2, 3, model, found_process)

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call forest%extract_resonance_history_set (res_set)
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()
call forest%final ()
call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_forest_2"

end subroutine phs_forest_2

```

19.9 Finding phase space parameterizations

If the phase space configuration is not found in the appropriate file, we should generate one.

The idea is to construct all Feynman diagrams subject to certain constraints which eliminate everything that is probably irrelevant for the integration. These Feynman diagrams (cascades) are grouped in groves by finding equivalence classes related by symmetry and ordered with respect to their importance (resonances). Finally, the result (or part of it) is written to file and used for the integration.

This module may eventually disappear and be replaced by CAML code. In particular, we need here a set of Feynman rules (vertices with particle codes, but not the factors). Thus, the module works for the Standard Model only.

Note that this module is stand-alone, it communicates to the main program only via the generated ASCII phase-space configuration file.

```

<cascades.f90>≡
  <File header>

  module cascades

    <Use kinds>

```

```

    use kinds, only: TC, i8, i32
    <Use strings>
    <Use debug>
    use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
    use physics_defs, only: UNDEFINED
    use model_data
    use flavors

    use resonances, only: resonance_info_t
    use resonances, only: resonance_history_t
    use resonances, only: resonance_history_set_t
    use phs_forests

    <Standard module head>

    <Cascades: public>

    <Cascades: parameters>

    <Cascades: types>

    <Cascades: interfaces>

    interface
    <Cascades: sub interfaces>
    end interface

end module cascades
<cascades_sub.f90>≡
<File header>

submodule (cascades) cascades_s

    use io_units
    use constants, only: one
    use format_defs, only: FMT_12, FMT_19
    use numeric_utils
    use diagnostics
    use hashes
    use sorting
    use lorentz

    implicit none

contains

    <Cascades: procedures>

end submodule cascades_s

```

19.9.1 The mapping modes

The valid mapping modes, to be used below. We will make use of the convention that mappings of internal particles have a positive value. Only for positive values, the flavor code is propagated when combining cascades.

```

⟨Mapping modes⟩≡
    integer, parameter :: &
        & EXTERNAL_PRT = -1, &
        & NO_MAPPING = 0, S_CHANNEL = 1, T_CHANNEL = 2, U_CHANNEL = 3, &
        & RADIATION = 4, COLLINEAR = 5, INFRARED = 6, &
        & STEP_MAPPING_E = 11, STEP_MAPPING_H = 12, &
        & ON_SHELL = 99

⟨Cascades: parameters⟩≡
    ⟨Mapping modes⟩

```

19.9.2 The cascade type

A cascade is essentially the same as a decay tree (both definitions may be merged in a later version). It contains a linked tree of nodes, each of which representing an internal particle. In contrast to decay trees, each node has a definite particle code. These nodes need not be modified, therefore we can use pointers and do not have to copy them. Thus, physically each cascades has only a single node, the mother particle. However, to be able to compare trees quickly, we store in addition an array of binary codes which is always sorted in ascending order. This is accompanied by a corresponding list of particle codes. The index is the location of the corresponding cascade in the cascade set, this may be used to access the daughters directly.

The real mass is the particle mass belonging to the particle code. The minimal mass is the sum of the real masses of all its daughters; this is the kinematical cutoff. The effective mass may be zero if the particle mass is below a certain threshold; it may be the real mass if the particle is resonant; or it may be some other value.

The logical `t_channel` is set if this a t -channel line, while `initial` is true only for an initial particle. Note that both initial particles are also `t_channel` by definition, and that they are distinguished by the direction of the tree: One of them decays and is the root of the tree, while the other one is one of the leaves.

The cascade is a list of nodes (particles) which are linked via the `daughter` entries. The node is the mother particle of the decay cascade. Much of the information in the nodes is repeated in arrays, to be accessible more easily. The arrays will be kept sorted by binary codes.

The counter `n_off_shell` is increased for each internal line that is neither resonant nor log-enhanced. It is set to zero if the current line is resonant, since this implies on-shell particle production and subsequent decay.

The counter `n_t_channel` is non-negative once an initial particle is included in the tree: then, it counts the number of t -channel lines.

The `multiplicity` is the number of branchings to follow until all daughters are on-shell. A resonant or non-decaying particle has multiplicity one. Merging nodes, the multiplicities add unless the mother is a resonance. An initial or final node has multiplicity zero.

The arrays correspond to the subnode tree **tree** of the current cascade. PDG codes are stored only for those positions which are resonant, with the exception of the last entry, i.e., the current node. Other positions, in particular external legs, are assigned undefined PDG code.

A cascade is uniquely identified by its tree, the tree of PDG codes, and the tree of mappings. The tree of resonances is kept only to mask the PDG tree as described above.

```

<Cascades: types>≡
  type :: cascade_t
    private
    ! counters
    integer :: index = 0
    integer :: grove = 0
    ! status
    logical :: active = .false.
    logical :: complete = .false.
    logical :: incoming = .false.
    ! this node
    integer(TC) :: bincode = 0
    type(flavor_t) :: flv
    integer :: pdg = UNDEFINED
    logical :: is_vector = .false.
    real(default) :: m_min = 0
    real(default) :: m_rea = 0
    real(default) :: m_eff = 0
    integer :: mapping = NO_MAPPING
    logical :: on_shell = .false.
    logical :: resonant = .false.
    logical :: log_enhanced = .false.
    logical :: t_channel = .false.
    ! global tree properties
    integer :: multiplicity = 0
    integer :: internal = 0
    integer :: n_off_shell = 0
    integer :: n_resonances = 0
    integer :: n_log_enhanced = 0
    integer :: n_t_channel = 0
    integer :: res_hash = 0
    ! the sub-node tree
    integer :: depth = 0
    integer(TC), dimension(:), allocatable :: tree
    integer, dimension(:), allocatable :: tree_pdg
    integer, dimension(:), allocatable :: tree_mapping
    logical, dimension(:), allocatable :: tree_resonant
    ! branch connections
    logical :: has_children = .false.
    type(cascade_t), pointer :: daughter1 => null ()
    type(cascade_t), pointer :: daughter2 => null ()
    type(cascade_t), pointer :: mother => null ()
    ! next in list
    type(cascade_t), pointer :: next => null ()
contains
  <Cascades: cascade: TBP>

```

```
end type cascade_t
```

```
(Cascades: procedures)≡
subroutine cascade_init (cascade, depth)
  type(cascade_t), intent(out) :: cascade
  integer, intent(in) :: depth
  integer, save :: index = 0
  index = cascade_index ()
  cascade%index = index
  cascade%depth = depth
  cascade%active = .true.
  allocate (cascade%tree (depth))
  allocate (cascade%tree_pdg (depth))
  allocate (cascade%tree_mapping (depth))
  allocate (cascade%tree_resonant (depth))
end subroutine cascade_init
```

Keep and increment a global index

```
(Cascades: procedures)+=≡
function cascade_index (seed) result (index)
  integer :: index
  integer, intent(in), optional :: seed
  integer, save :: i = 0
  if (present (seed)) i = seed
  i = i + 1
  index = i
end function cascade_index
```

We need three versions of writing cascades. This goes to the phase-space file.

For t/u channel mappings, we use the absolute value of the PDG code.

```
(Cascades: procedures)+=≡
subroutine cascade_write_file_format (cascade, model, unit)
  type(cascade_t), intent(in) :: cascade
  class(model_data_t), intent(in), target :: model
  integer, intent(in), optional :: unit
  type(flavor_t) :: flv
  integer :: u, i
2  format(3x,A,1x,I3,1x,A,1x,I9,1x,'!',1x,A)
  u = given_output_unit (unit); if (u < 0) return
  call write_reduced(cascade%tree, u)
  write (u, "(A)")
  do i = 1, cascade%depth
    call flv%init (cascade%tree_pdg(i), model)
    select case (cascade%tree_mapping(i))
    case (NO_MAPPING, EXTERNAL_PRT)
    case (S_CHANNEL)
      write(u,2) 'map', &
        cascade%tree(i), 's_channel', cascade%tree_pdg(i), &
        char (flv%get_name ())
    case (T_CHANNEL)
      write(u,2) 'map', &
        cascade%tree(i), 't_channel', abs (cascade%tree_pdg(i)), &
        char (flv%get_name ())
```

```

case (U_CHANNEL)
  write(u,2) 'map', &
    cascade%tree(i), 'u_channel', abs (cascade%tree_pdg(i)), &
    char (flv%get_name ())
case (RADIATION)
  write(u,2) 'map', &
    cascade%tree(i), 'radiation', cascade%tree_pdg(i), &
    char (flv%get_name ())
case (COLLINEAR)
  write(u,2) 'map', &
    cascade%tree(i), 'collinear', cascade%tree_pdg(i), &
    char (flv%get_name ())
case (INFRARED)
  write(u,2) 'map', &
    cascade%tree(i), 'infrared ', cascade%tree_pdg(i), &
    char (flv%get_name ())
case (ON_SHELL)
  write(u,2) 'map', &
    cascade%tree(i), 'on_shell ', cascade%tree_pdg(i), &
    char (flv%get_name ())
case default
  call msg_bug (" Impossible mapping mode encountered")
end select
end do
contains
subroutine write_reduced (array, unit)
  integer(TC), dimension(:), intent(in) :: array
  integer, intent(in) :: unit
  integer :: i
  write (u, "(3x,A,1x)", advance="no") "tree"
  do i = 1, size (array)
    if (decay_level (array(i)) > 1) then
      write (u, "(1x,I0)", advance="no") array(i)
    end if
  end do
end subroutine write_reduced

elemental function decay_level (k) result (l)
  integer(TC), intent(in) :: k
  integer :: l
  integer :: i
  l = 0
  do i = 0, bit_size(k) - 1
    if (btest(k,i)) l = l + 1
  end do
end function decay_level
subroutine start_comment (u)
  integer, intent(in) :: u
  write(u, '(1x,A)', advance='no') '!'
end subroutine start_comment
end subroutine cascade_write_file_format

```

This creates metapost source for graphical display:

<Cascades: procedures>+≡

```

subroutine cascade_write_graph_format (cascade, count, unit)
  type(cascade_t), intent(in) :: cascade
  integer, intent(in) :: count
  integer, intent(in), optional :: unit
  integer :: u
  integer(TC) :: mask
  type(string_t) :: left_str, right_str
  u = given_output_unit (unit); if (u < 0) return
  mask = 2**((cascade%depth+3)/2) - 1
  left_str = ""
  right_str = ""
  write (u, '(A)') "\begin{minipage}{105pt}"
  write (u, '(A)') "\vspace{30pt}"
  write (u, '(A)') "\begin{center}"
  write (u, '(A)') "\begin{fmfgraph*}(55,55)"
  call graph_write (cascade, mask)
  write (u, '(A)') "\fmfleft{" // char (extract (left_str, 2)) // "}"
  write (u, '(A)') "\fmfright{" // char (extract (right_str, 2)) // "}"
  write (u, '(A)') "\end{fmfgraph*}\\"
  write (u, '(A,I5,A)') "\fbox{$", count, "$"
  write (u, '(A)') "\end{center}"
  write (u, '(A)') "\end{minipage}"
  write (u, '(A)') "%"
contains
  recursive subroutine graph_write (cascade, mask, reverse)
    type(cascade_t), intent(in) :: cascade
    integer(TC), intent(in) :: mask
    logical, intent(in), optional :: reverse
    type(flavor_t) :: anti
    logical :: rev
    rev = .false.; if (present(reverse)) rev = reverse
    if (cascade%has_children) then
      if (.not.rev) then
        call vertex_write (cascade, cascade%daughter1, mask)
        call vertex_write (cascade, cascade%daughter2, mask)
      else
        call vertex_write (cascade, cascade%daughter2, mask, .true.)
        call vertex_write (cascade, cascade%daughter1, mask, .true.)
      end if
      if (cascade%complete) then
        call vertex_write (cascade, cascade%mother, mask, .true.)
        write (u, '(A,I0,A)') "\fmfv{d.shape=square}{v0}"
      end if
    else
      if (cascade%incoming) then
        anti = cascade%flv%anti ()
        call external_write (cascade%bincode, anti%get_tex_name (), &
          left_str)
      else
        call external_write (cascade%bincode, cascade%flv%get_tex_name (), &
          right_str)
      end if
    end if
  end subroutine graph_write

```

```

recursive subroutine vertex_write (cascade, daughter, mask, reverse)
  type(cascade_t), intent(in) :: cascade, daughter
  integer(TC), intent(in) :: mask
  logical, intent(in), optional :: reverse
  integer :: bincode
  if (cascade%complete) then
    bincode = 0
  else
    bincode = cascade%bincode
  end if
  call graph_write (daughter, mask, reverse)
  if (daughter%has_children) then
    call line_write (bincode, daughter%bincode, daughter%flv, &
      mapping=daughter%mapping)
  else
    call line_write (bincode, daughter%bincode, daughter%flv)
  end if
end subroutine vertex_write
subroutine line_write (i1, i2, flv, mapping)
  integer(TC), intent(in) :: i1, i2
  type(flavor_t), intent(in) :: flv
  integer, intent(in), optional :: mapping
  integer :: k1, k2
  type(string_t) :: prt_type
  select case (flv%get_spin_type ())
  case (SCALAR);      prt_type = "plain"
  case (SPINOR);      prt_type = "fermion"
  case (VECTOR);      prt_type = "boson"
  case (VECTORSPINOR); prt_type = "fermion"
  case (TENSOR);      prt_type = "dbl_wiggly"
  case default;      prt_type = "dashes"
  end select
  if (flv%is_antiparticle ()) then
    k1 = i2; k2 = i1
  else
    k1 = i1; k2 = i2
  end if
  if (present (mapping)) then
    select case (mapping)
    case (S_CHANNEL)
      write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=blue,lab=\sm\blue$" // &
        & char (flv%get_tex_name ()) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (T_CHANNEL, U_CHANNEL)
      write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=cyan,lab=\sm\cyan$" // &
        & char (flv%get_tex_name ()) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (RADIATION)
      write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=green,lab=\sm\green$" // &
        & char (flv%get_tex_name ()) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    end select
  end if
end subroutine line_write

```

```

case (COLLINEAR)
  write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & " ,f=magenta,lab=\sm\magenta$" // &
    & char (flv%get_tex_name ()) // "$}" // &
    & "{v", k1, ",v", k2, "}"
case (INFRARED)
  write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & " ,f=red,lab=\sm\red$" // &
    & char (flv%get_tex_name ()) // "$}" // &
    & "{v", k1, ",v", k2, "}"
case default
  write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & " ,f=black}" // &
    & "{v", k1, ",v", k2, "}"
end select
else
  write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & "}" // &
    & "{v", k1, ",v", k2, "}"
end if
end subroutine line_write
subroutine external_write (bincode, name, ext_str)
  integer(TC), intent(in) :: bincode
  type(string_t), intent(in) :: name
  type(string_t), intent(inout) :: ext_str
  character(len=20) :: str
  write (str, '(A2,I0)') ",v", bincode
  ext_str = ext_str // trim (str)
  write (u, '(A,I0,A,I0,A)') "\fmflabel{\sm$" &
    // char (name) &
    // "\",(" , bincode, ")" &
    // "$}{v", bincode, "}"
end subroutine external_write
end subroutine cascade_write_graph_format

```

This is for screen/debugging output:

<Cascades: procedures>+≡

```

subroutine cascade_write (cascade, unit)
  type(cascade_t), intent(in) :: cascade
  integer, intent(in), optional :: unit
  integer :: u
  character(9) :: depth
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A,(1x,I7))") 'Cascade #', cascade%index
  write (u, "(A,(1x,I7))") ' Grove:      #', cascade%grove
  write (u, "(A,3(1x,L1))") ' act/cmp/inc: ', &
    cascade%active, cascade%complete, cascade%incoming
  write (u, "(A,I0)") ' Brcode:      ', cascade%bincode
  write (u, "(A)", advance="no") ' Flavor:      '
  call cascade%flv%write (unit)
  write (u, "(A,I9)") ' Active flavor:', cascade%pdg
  write (u, "(A,L1)") ' Is vector:   ', cascade%is_vector
  write (u, "(A,3(1x," // FMT_19 // ")") ' Mass (m/r/e): ', &
    cascade%m_min, cascade%m_rea, cascade%m_eff

```

```

write (u, "(A,I1)") ' Mapping: ', cascade%mapping
write (u, "(A,3(1x,L1))") ' res/log/tch: ', &
    cascade%resonant, cascade%log_enhanced, cascade%t_channel
write (u, "(A,(1x,I7))") ' Multiplicity: ', cascade%multiplicity
write (u, "(A,2(1x,I7))") ' n intern/off: ', &
    cascade%internal, cascade%n_off_shell
write (u, "(A,3(1x,I7))") ' n res/log/tch:', &
    cascade%n_resonances, cascade%n_log_enhanced, cascade%n_t_channel
write (u, "(A,I7)") ' Depth: ', cascade%depth
write (depth, "(I7)") cascade%depth
write (u, "(A," // depth // "(1x,I7))") &
    ' Tree: ', cascade%tree
write (u, "(A," // depth // "(1x,I7))") &
    ' Tree(PDG): ', cascade%tree_pdg
write (u, "(A," // depth // "(1x,I7))") &
    ' Tree(mapping):', cascade%tree_mapping
write (u, "(A," // depth // "(1x,L1))") &
    ' Tree(res): ', cascade%tree_resonant
if (cascade%has_children) then
    write (u, "(A,I7,1x,I7)") ' Daughter1/2: ', &
        cascade%daughter1%index, cascade%daughter2%index
end if
if (associated (cascade%mother)) then
    write (u, "(A,I7)") ' Mother: ', cascade%mother%index
end if
end subroutine cascade_write

```

19.9.3 Creating new cascades

This initializes a single-particle cascade (external, final state). The PDG entry in the tree is set undefined because the cascade is not resonant. However, the flavor entry is set, so the cascade flavor is identified nevertheless.

(Cascades: procedures)+≡

```

subroutine cascade_init_outgoing (cascade, flv, pos, m_thr)
    type(cascade_t), intent(out) :: cascade
    type(flavor_t), intent(in) :: flv
    integer, intent(in) :: pos
    real(default), intent(in) :: m_thr
    call cascade_init (cascade, 1)
    cascade%bincode = ibset (0_TC, pos-1)
    cascade%flv = flv
    cascade%pdg = cascade%flv%get_pdg ()
    cascade%is_vector = flv%get_spin_type () == VECTOR
    cascade%m_min = flv%get_mass ()
    cascade%m_rea = cascade%m_min
    if (cascade%m_rea >= m_thr) then
        cascade%m_eff = cascade%m_rea
    end if
    cascade%on_shell = .true.
    cascade%multiplicity = 1
    cascade%tree(1) = cascade%bincode
    cascade%tree_pdg(1) = cascade%pdg

```

```

        cascade%tree_mapping(1) = EXTERNAL_PRT
        cascade%tree_resonant(1) = .false.
    end subroutine cascade_init_outgoing

```

The same for an incoming line:

```

<Cascades: procedures>+=
    subroutine cascade_init_incoming (cascade, flv, pos, m_thr)
        type(cascade_t), intent(out) :: cascade
        type(flavor_t), intent(in) :: flv
        integer, intent(in) :: pos
        real(default), intent(in) :: m_thr
        call cascade_init (cascade, 1)
        cascade%incoming = .true.
        cascade%bincode = ibset (0_TC, pos-1)
        cascade%flv = flv%anti ()
        cascade%pdg = cascade%flv%get_pdg ()
        cascade%is_vector = flv%get_spin_type () == VECTOR
        cascade%m_min = flv%get_mass ()
        cascade%m_rea = cascade%m_min
        if (cascade%m_rea >= m_thr) then
            cascade%m_eff = cascade%m_rea
        end if
        cascade%on_shell = .true.
        cascade%n_t_channel = 0
        cascade%n_off_shell = 0
        cascade%tree(1) = cascade%bincode
        cascade%tree_pdg(1) = cascade%pdg
        cascade%tree_mapping(1) = EXTERNAL_PRT
        cascade%tree_resonant(1) = .false.
    end subroutine cascade_init_incoming

```

19.9.4 Tools

This function returns true if the two cascades share no common external particle. This is a requirement for joining them.

```

<Cascades: interfaces>=
    interface operator(.disjunct.)
        module procedure cascade_disjunct
    end interface

<Cascades: sub interfaces>=
    module function cascade_disjunct (cascade1, cascade2) result (flag)
        logical :: flag
        type(cascade_t), intent(in) :: cascade1, cascade2
    end function cascade_disjunct

<Cascades: procedures>+=
    module function cascade_disjunct (cascade1, cascade2) result (flag)
        logical :: flag
        type(cascade_t), intent(in) :: cascade1, cascade2
        flag = iand (cascade1%bincode, cascade2%bincode) == 0
    end function cascade_disjunct

```


Compute a hash code for the resonance pattern of a cascade. We count the number of times each particle appears as a resonance.

We pack the PDG codes of the resonances in two arrays (s-channel and t-channel), sort them both, concatenate the results, transfer to `i8` integers, and compute the hash code from this byte stream.

For t/u-channel, we remove the sign for antiparticles since this is not well-defined.

```

<Cascades: procedures> +=
  subroutine cascade_assign_resonance_hash (cascade)
    type(cascade_t), intent(inout) :: cascade
    integer(i8), dimension(1) :: mold
    cascade%res_hash = hash (transfer &
      ([sort (pack (cascade%tree_pdg, &
        cascade%tree_resonant)), &
        sort (pack (abs (cascade%tree_pdg), &
          cascade%tree_mapping == T_CHANNEL .or. &
          cascade%tree_mapping == U_CHANNEL))], &
        mold))
  end subroutine cascade_assign_resonance_hash

```

19.9.5 Hash entries for cascades

We will set up a hash array which contains keys of and pointers to cascades. We hold a list of cascade (pointers) within each bucket. This is not for collision resolution, but for keeping similar, but unequal cascades together.

```

<Cascades: types> +=
  type :: cascade_p
    type(cascade_t), pointer :: cascade => null ()
    type(cascade_p), pointer :: next => null ()
  end type cascade_p

```

Here is the bucket or hash entry type:

```

<Cascades: types> +=
  type :: hash_entry_t
    integer(i32) :: hashval = 0
    integer(i8), dimension(:), allocatable :: key
    type(cascade_p), pointer :: first => null ()
    type(cascade_p), pointer :: last => null ()
  end type hash_entry_t

```

```

<Cascades: public> =
  public :: hash_entry_init

```

```

<Cascades: sub interfaces> +=
  module subroutine hash_entry_init (entry, entry_in)
    type(hash_entry_t), intent(out) :: entry
    type(hash_entry_t), intent(in) :: entry_in
  end subroutine hash_entry_init

```

```

<Cascades: procedures>+=
module subroutine hash_entry_init (entry, entry_in)
  type(hash_entry_t), intent(out) :: entry
  type(hash_entry_t), intent(in) :: entry_in
  type(cascade_p), pointer :: casc_iter, casc_copy
  entry%hashval = entry_in%hashval
  entry%key = entry_in%key
  casc_iter => entry_in%first
  do while (associated (casc_iter))
    allocate (casc_copy)
    casc_copy = casc_iter
    casc_copy%next => null ()
    if (associated (entry%first)) then
      entry%last%next => casc_copy
    else
      entry%first => casc_copy
    end if
    entry%last => casc_copy
    casc_iter => casc_iter%next
  end do
end subroutine hash_entry_init

```

Finalize: just deallocate the list; the contents are just pointers.

```

<Cascades: procedures>+=
subroutine hash_entry_final (hash_entry)
  type(hash_entry_t), intent(inout) :: hash_entry
  type(cascade_p), pointer :: current
  do while (associated (hash_entry%first))
    current => hash_entry%first
    hash_entry%first => current%next
    deallocate (current)
  end do
end subroutine hash_entry_final

```

Output: concise format for debugging, just list cascade indices.

```

<Cascades: procedures>+=
subroutine hash_entry_write (hash_entry, unit)
  type(hash_entry_t), intent(in) :: hash_entry
  integer, intent(in), optional :: unit
  type(cascade_p), pointer :: current
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)", advance="no") "Entry:"
  do i = 1, size (hash_entry%key)
    write (u, "(1x,I0)", advance="no") hash_entry%key(i)
  end do
  write (u, "(1x,A)", advance="no") "->"
  current => hash_entry%first
  do while (associated (current))
    write (u, "(1x,I7)", advance="no") current%cascade%index
    current => current%next
  end do
  write (u, *)

```

```
end subroutine hash_entry_write
```

This function adds a cascade pointer to the bucket. If `ok` is present, check first if it is already there and return failure if yes. If `cascade_ptr` is also present, set it to the current cascade if successful. If not, set it to the cascade that is already there.

(Cascades: procedures)+≡

```
subroutine hash_entry_add_cascade_ptr (hash_entry, cascade, ok, cascade_ptr)
  type(hash_entry_t), intent(inout) :: hash_entry
  type(cascade_t), intent(in), target :: cascade
  logical, intent(out), optional :: ok
  type(cascade_t), optional, pointer :: cascade_ptr
  type(cascade_p), pointer :: current
  if (present (ok)) then
    call hash_entry_check_cascade (hash_entry, cascade, ok, cascade_ptr)
    if (.not. ok) return
  end if
  allocate (current)
  current%cascade => cascade
  if (associated (hash_entry%last)) then
    hash_entry%last%next => current
  else
    hash_entry%first => current
  end if
  hash_entry%last => current
end subroutine hash_entry_add_cascade_ptr
```

This function checks whether a cascade is already in the bucket. For incomplete cascades, we look for an exact match. It should suffice to verify the tree, the PDG codes, and the mapping modes. This is the information that is written to the phase space file.

For complete cascades, we ignore the PDG code at positions with mappings infrared, collinear, or t/u-channel. Thus a cascade which is distinguished only by PDG code at such places, is flagged existent. If the convention is followed that light particles come before heavier ones (in the model definition), this ensures that the lightest particle is kept in the appropriate place, corresponding to the strongest peak.

For external cascades (incoming/outgoing) we take the PDG code into account even though it is zeroed in the PDG-code tree.

(Cascades: procedures)+≡

```
subroutine hash_entry_check_cascade (hash_entry, cascade, ok, cascade_ptr)
  type(hash_entry_t), intent(in), target :: hash_entry
  type(cascade_t), intent(in), target :: cascade
  logical, intent(out) :: ok
  type(cascade_t), optional, pointer :: cascade_ptr
  type(cascade_p), pointer :: current
  integer, dimension(:), allocatable :: tree_pdg
  ok = .true.
  allocate (tree_pdg (size (cascade%tree_pdg)))
  if (cascade%complete) then
    where (cascade%tree_mapping == INFRARED .or. &
           cascade%tree_mapping == COLLINEAR .or. &
```

```

        cascade%tree_mapping == T_CHANNEL .or. &
        cascade%tree_mapping == U_CHANNEL)
    tree_pdg = 0
  elsewhere
    tree_pdg = cascade%tree_pdg
  end where
else
  tree_pdg = cascade%tree_pdg
end if
current => hash_entry%first
do while (associated (current))
  if (current%cascade%depth == cascade%depth) then
    if (all (current%cascade%tree == cascade%tree)) then
      if (all (current%cascade%tree_mapping == cascade%tree_mapping)) &
      then
        if (all (current%cascade%tree_pdg .match. tree_pdg)) then
          if (present (cascade_ptr)) cascade_ptr => current%cascade
          ok = .false.; return
        end if
      end if
    end if
  end if
  current => current%next
end do
if (present (cascade_ptr)) cascade_ptr => cascade
end subroutine hash_entry_check_cascade

```

For PDG codes, we specify that the undefined code matches any code. This is already defined for flavor objects, but here we need it for the codes themselves.

```

<Cascades: interfaces>+≡
  interface operator(.match.)
    module procedure pdg_match
  end interface

<Cascades: sub interfaces>+≡
  elemental module function pdg_match (pdg1, pdg2) result (flag)
    logical :: flag
    integer(TC), intent(in) :: pdg1, pdg2
  end function pdg_match

<Cascades: procedures>+≡
  elemental module function pdg_match (pdg1, pdg2) result (flag)
    logical :: flag
    integer(TC), intent(in) :: pdg1, pdg2
    select case (pdg1)
    case (0)
      flag = .true.
    case default
      select case (pdg2)
      case (0)
        flag = .true.
      case default
        flag = pdg1 == pdg2
      end select
    end select
  end function pdg_match

```

```
end function pdg_match
```

19.9.6 The cascade set

The cascade set will later be transformed into the decay forest. It is set up as a linked list. In addition to the usual `first` and `last` pointers, there is a `first_t` pointer which points to the first t-channel cascade (after all s-channel cascades), and a `first_k` pointer which points to the first final cascade (with a keystone).

As an auxiliary device, the object contains a hash array with associated parameters where an additional pointer is stored for each cascade. The keys are made from the relevant cascade data. This hash is used for fast detection (and thus avoidance) of double entries in the cascade list.

```
<Cascades: public>+≡
    public :: cascade_set_t

<Cascades: types>+≡
    type :: cascade_set_t
        private
        class(model_data_t), pointer :: model
        integer :: n_in, n_out, n_tot
        type(flavor_t), dimension(:, :), allocatable :: flv
        integer :: depth_out, depth_tot
        real(default) :: sqrts = 0
        real(default) :: m_threshold_s = 0
        real(default) :: m_threshold_t = 0
        integer :: off_shell = 0
        integer :: t_channel = 0
        logical :: keep_nonresonant
        integer :: n_groves = 0
        ! The cascade list
        type(cascade_t), pointer :: first => null ()
        type(cascade_t), pointer :: last => null ()
        type(cascade_t), pointer :: first_t => null ()
        type(cascade_t), pointer :: first_k => null ()
        ! The hashtable
        integer :: n_entries = 0
        real :: fill_ratio = 0
        integer :: n_entries_max = 0
        integer(i32) :: mask = 0
        logical :: fatal_beam_decay = .true.
        type(hash_entry_t), dimension(:), allocatable :: entry
    end type cascade_set_t

<Cascades: public>+≡
    interface cascade_set_init
        module procedure cascade_set_init_base
        module procedure cascade_set_init_from_cascade
    end interface

This might be broken. Test before using.

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_init_from_cascade &
```

```

        (cascade_set, cascade_set_in)
        type(cascade_set_t), intent(out) :: cascade_set
        type(cascade_set_t), intent(in), target :: cascade_set_in
    end subroutine cascade_set_init_from_cascade
<Cascades: procedures>+≡
    module subroutine cascade_set_init_from_cascade &
        (cascade_set, cascade_set_in)
        type(cascade_set_t), intent(out) :: cascade_set
        type(cascade_set_t), intent(in), target :: cascade_set_in
        type(cascade_t), pointer :: casc_iter, casc_copy
        cascade_set%model => cascade_set_in%model
        cascade_set%n_in = cascade_set_in%n_in
        cascade_set%n_out = cascade_set_in%n_out
        cascade_set%n_tot = cascade_set_in%n_tot
        cascade_set%flv = cascade_set_in%flv
        cascade_set%depth_out = cascade_set_in%depth_out
        cascade_set%depth_tot = cascade_set_in%depth_tot
        cascade_set%sqrts = cascade_set_in%sqrts
        cascade_set%m_threshold_s = cascade_set_in%m_threshold_s
        cascade_set%m_threshold_t = cascade_set_in%m_threshold_t
        cascade_set%off_shell = cascade_set_in%off_shell
        cascade_set%t_channel = cascade_set_in%t_channel
        cascade_set%keep_nonresonant = cascade_set_in%keep_nonresonant
        cascade_set%n_groves = cascade_set_in%n_groves

        casc_iter => cascade_set_in%first
        do while (associated (casc_iter))
            allocate (casc_copy)
            casc_copy = casc_iter
            casc_copy%next => null ()
            if (associated (cascade_set%first)) then
                cascade_set%last%next => casc_copy
            else
                cascade_set%first => casc_copy
            end if
            cascade_set%last => casc_copy
            casc_iter => casc_iter%next
        end do

        cascade_set%n_entries = cascade_set_in%n_entries
        cascade_set%fill_ratio = cascade_set_in%fill_ratio
        cascade_set%n_entries_max = cascade_set_in%n_entries_max
        cascade_set%mask = cascade_set_in%mask
        cascade_set%fatal_beam_decay = cascade_set_in%fatal_beam_decay
        allocate (cascade_set%entry (0:cascade_set%mask))
        cascade_set%entry = cascade_set_in%entry
    end subroutine cascade_set_init_from_cascade

```

Return true if there are cascades which are active and complete, so the phase space file would be nonempty.

```

<Cascades: public>+≡
    public :: cascade_set_is_valid

```

```

<Cascades: sub interfaces>+≡
    module function cascade_set_is_valid (cascade_set) result (flag)
        logical :: flag
        type(cascade_set_t), intent(in) :: cascade_set
    end function cascade_set_is_valid

<Cascades: procedures>+≡
    module function cascade_set_is_valid (cascade_set) result (flag)
        logical :: flag
        type(cascade_set_t), intent(in) :: cascade_set
        type(cascade_t), pointer :: cascade
        flag = .false.
        cascade => cascade_set%first_k
        do while (associated (cascade))
            if (cascade%active .and. cascade%complete) then
                flag = .true.
                return
            end if
            cascade => cascade%next
        end do
    end function cascade_set_is_valid

```

The initializer sets up the hash table with some initial size guessed by looking at the number of external particles. We choose 256 for 3 external particles and a factor of 4 for each additional particle, limited at $2^{30}=1\text{G}$.

```

<Cascades: parameters>+≡
    real, parameter, public :: CASCADE_SET_FILL_RATIO = 0.1

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_init_base (cascade_set, model, &
        n_in, n_out, phs_par, fatal_beam_decay, flv)
        type(cascade_set_t), intent(out) :: cascade_set
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in, n_out
        type(phs_parameters_t), intent(in) :: phs_par
        logical, intent(in) :: fatal_beam_decay
        type(flavor_t), dimension(:, :), intent(in), optional :: flv
    end subroutine cascade_set_init_base

<Cascades: procedures>+≡
    module subroutine cascade_set_init_base (cascade_set, model, &
        n_in, n_out, phs_par, fatal_beam_decay, flv)
        type(cascade_set_t), intent(out) :: cascade_set
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in, n_out
        type(phs_parameters_t), intent(in) :: phs_par
        logical, intent(in) :: fatal_beam_decay
        type(flavor_t), dimension(:, :), intent(in), optional :: flv
        integer :: size_guess
        integer :: i, j
        cascade_set%model => model
        cascade_set%n_in = n_in
        cascade_set%n_out = n_out
        cascade_set%n_tot = n_in + n_out
        if (present (flv)) then

```

```

        allocate (cascade_set%flv (size (flv, 1), size (flv, 2)))
        do i = 1, size (flv, 2)
            do j = 1, size (flv, 1)
                call cascade_set%flv(j,i)%init (flv(j,i)%get_pdg (), model)
            end do
        end do
    end if
    select case (n_in)
    case (1); cascade_set%depth_out = 2 * n_out - 3
    case (2); cascade_set%depth_out = 2 * n_out - 1
    end select
    cascade_set%depth_tot = 2 * cascade_set%n_tot - 3
    cascade_set%sqrts = phs_par%sqrts
    cascade_set%m_threshold_s = phs_par%m_threshold_s
    cascade_set%m_threshold_t = phs_par%m_threshold_t
    cascade_set%off_shell = phs_par%off_shell
    cascade_set%t_channel = phs_par%t_channel
    cascade_set%keep_nonresonant = phs_par%keep_nonresonant
    cascade_set%fill_ratio = CASCADE_SET_FILL_RATIO
    size_guess = ishft (256, min (2 * (cascade_set%n_tot - 3), 22))
    cascade_set%n_entries_max = size_guess * cascade_set%fill_ratio
    cascade_set%mask = size_guess - 1
    allocate (cascade_set%entry (0:cascade_set%mask))
    cascade_set%fatal_beam_decay = fatal_beam_decay
end subroutine cascade_set_init_base

```

The finalizer has to delete both the hash and the list.

```

<Cascades: public>+≡
    public :: cascade_set_final

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_final (cascade_set)
        type(cascade_set_t), intent(inout), target :: cascade_set
    end subroutine cascade_set_final

<Cascades: procedures>+≡
    module subroutine cascade_set_final (cascade_set)
        type(cascade_set_t), intent(inout), target :: cascade_set
        type(cascade_t), pointer :: current
        integer :: i
        if (allocated (cascade_set%entry)) then
            do i = 0, cascade_set%mask
                call hash_entry_final (cascade_set%entry(i))
            end do
            deallocate (cascade_set%entry)
        end if
        do while (associated (cascade_set%first))
            current => cascade_set%first
            cascade_set%first => cascade_set%first%next
            deallocate (current)
        end do
    end subroutine cascade_set_final

```


Write the process in ASCII format, in columns that are headed by the corresponding bincode.

```

<Cascades: public>+≡
    public :: cascade_set_write_process_bincode_format

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_write_process_bincode_format &
        (cascade_set, unit)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: unit
    end subroutine cascade_set_write_process_bincode_format

<Cascades: procedures>+≡
    module subroutine cascade_set_write_process_bincode_format &
        (cascade_set, unit)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: unit
        integer, dimension(:), allocatable :: bincode, field_width
        integer :: n_in, n_out, n_tot, n_flv
        integer :: u, f, i, bc
        character(20) :: str
        type(string_t) :: fmt_head
        type(string_t), dimension(:), allocatable :: fmt_proc
        u = given_output_unit (unit); if (u < 0) return
        if (.not. allocated (cascade_set%flv)) return
        write (u, "('!',1x,A)") "List of subprocesses with particle bincodes:"
        n_in = cascade_set%n_in
        n_out = cascade_set%n_out
        n_tot = cascade_set%n_tot
        n_flv = size (cascade_set%flv, 2)
        allocate (bincode (n_tot), field_width (n_tot), fmt_proc (n_tot))
        bc = 1
        do i = 1, n_out
            bincode(n_in + i) = bc
            bc = 2 * bc
        end do
        do i = n_in, 1, -1
            bincode(i) = bc
            bc = 2 * bc
        end do
        do i = 1, n_tot
            write (str, "(I0)") bincode(i)
            field_width(i) = len_trim (str)
            do f = 1, n_flv
                field_width(i) = max (field_width(i), &
                    len (cascade_set%flv(i,f)%get_name ()))
            end do
        end do
        fmt_head = "('!',1x,A)"
        do i = 1, n_tot
            fmt_head = fmt_head // "1x,"
            fmt_proc(i) = "(1x,"
            write (str, "(I0)") field_width(i)
            fmt_head = fmt_head // "I" // trim(str)
            fmt_proc(i) = fmt_proc(i) // "A" // trim(str)
        end do
    end module

```

```

        if (i == n_in) then
            fmt_head = fmt_head // ",1x,' ' "
        end if
    end do
do i = 1, n_tot
    fmt_proc(i) = fmt_proc(i) // " "
end do
fmt_head = fmt_head // " "
write (u, char (fmt_head)) bincode
do f = 1, n_flv
    write (u, "('!')", advance="no")
    do i = 1, n_tot
        write (u, char (fmt_proc(i)), advance="no") &
            char (cascade_set%flv(i,f)%get_name ())
        if (i == n_in) write (u, "(1x,'=>')", advance="no")
    end do
    write (u, *)
end do
write (u, char (fmt_head)) bincode
end subroutine cascade_set_write_process_bincode_format

```

Write the process as a L^AT_EX expression.

(*Cascades: procedures*)+≡

```

subroutine cascade_set_write_process_tex_format (cascade_set, unit)
    type(cascade_set_t), intent(in), target :: cascade_set
    integer, intent(in), optional :: unit
    integer :: u, f, i
    u = given_output_unit (unit); if (u < 0) return
    if (.not. allocated (cascade_set%flv)) return
    write (u, "(A)" "\begin{align*}")
    do f = 1, size (cascade_set%flv, 2)
        do i = 1, cascade_set%n_in
            if (i > 1) write (u, "(A)", advance="no") "\quad "
            write (u, "(A)", advance="no") &
                char (cascade_set%flv(i,f)%get_tex_name ())
        end do
        write (u, "(A)", advance="no") "\quad &to\quad "
        do i = cascade_set%n_in + 1, cascade_set%n_tot
            if (i > cascade_set%n_in + 1) write (u, "(A)", advance="no") "\quad "
            write (u, "(A)", advance="no") &
                char (cascade_set%flv(i,f)%get_tex_name ())
        end do
        if (f < size (cascade_set%flv, 2)) then
            write (u, "(A)" "\\")
        else
            write (u, "(A)" "")
        end if
    end do
    write (u, "(A)" "\end{align*}")
end subroutine cascade_set_write_process_tex_format

```

Three output routines: phase-space file, graph source code, and screen output.

This version generates the phase space file. It deals only with complete

cascades.

<Cascades: public>+≡

public :: cascade_set_write_file_format

<Cascades: sub interfaces>+≡

```
module subroutine cascade_set_write_file_format (cascade_set, unit)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer, intent(in), optional :: unit
end subroutine cascade_set_write_file_format
```

<Cascades: procedures>+≡

```
module subroutine cascade_set_write_file_format (cascade_set, unit)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer, intent(in), optional :: unit
  type(cascade_t), pointer :: cascade
  integer :: u, grove, count
  logical :: first_in_grove
  u = given_output_unit (unit); if (u < 0) return
  count = 0
  do grove = 1, cascade_set%n_groves
    first_in_grove = .true.
    cascade => cascade_set%first_k
    do while (associated (cascade))
      if (cascade%active .and. cascade%complete) then
        if (cascade%grove == grove) then
          if (first_in_grove) then
            first_in_grove = .false.
            write (u, "(A)")
            write (u, "(1x,'!',1x,A,1x,I0,A)", advance='no') &
              'Multiplicity =', cascade%multiplicity, ", "
            select case (cascade%n_resonances)
            case (0)
              write (u, '(1x,A)', advance='no') 'no resonances, '
            case (1)
              write (u, '(1x,A)', advance='no') '1 resonance, '
            case default
              write (u, '(1x,I0,1x,A)', advance='no') &
                cascade%n_resonances, 'resonances, '
            end select
            write (u, '(1x,I0,1x,A)', advance='no') &
              cascade%n_log_enhanced, 'logs, '
            write (u, '(1x,I0,1x,A)', advance='no') &
              cascade%n_off_shell, 'off-shell, '
            select case (cascade%n_t_channel)
            case (0); write (u, '(1x,A)') 's-channel graph'
            case (1); write (u, '(1x,A)') '1 t-channel line'
            case default
              write(u,'(1x,I0,1x,A)') &
                cascade%n_t_channel, 't-channel lines'
            end select
            write (u, '(1x,A,I0)') 'grove #', grove
          end if
          count = count + 1
          write (u, "(1x,'!',1x,A,I0)") "Channel #", count
          call cascade_write_file_format (cascade, cascade_set%model, u)
        end if
      end while
    end do
  end do
```

```

        end if
    end if
    cascade => cascade%next
end do
end do
end subroutine cascade_set_write_file_format

```

This is the graph output format, the driver-file

```

<Cascades: public>+=
    public :: cascade_set_write_graph_format

<Cascades: sub interfaces>+=
    module subroutine cascade_set_write_graph_format &
        (cascade_set, filename, process_id, unit)
        type(cascade_set_t), intent(in), target :: cascade_set
        type(string_t), intent(in) :: filename, process_id
        integer, intent(in), optional :: unit
    end subroutine cascade_set_write_graph_format

<Cascades: procedures>+=
    module subroutine cascade_set_write_graph_format &
        (cascade_set, filename, process_id, unit)
        type(cascade_set_t), intent(in), target :: cascade_set
        type(string_t), intent(in) :: filename, process_id
        integer, intent(in), optional :: unit
        type(cascade_t), pointer :: cascade
        integer :: u, grove, count, pgcount
        logical :: first_in_grove
        u = given_output_unit (unit); if (u < 0) return
        write (u, '(A)') "\documentclass[10pt]{article}"
        write (u, '(A)') "\usepackage{amsmath}"
        write (u, '(A)') "\usepackage{feynmp}"
        write (u, '(A)') "\usepackage{url}"
        write (u, '(A)') "\usepackage{color}"
        write (u, *)
        write (u, '(A)') "\textwidth 18.5cm"
        write (u, '(A)') "\evensidemargin -1.5cm"
        write (u, '(A)') "\oddsidemargin -1.5cm"
        write (u, *)
        write (u, '(A)') "\newcommand{\blue}{\color{blue}}"
        write (u, '(A)') "\newcommand{\green}{\color{green}}"
        write (u, '(A)') "\newcommand{\red}{\color{red}}"
        write (u, '(A)') "\newcommand{\magenta}{\color{magenta}}"
        write (u, '(A)') "\newcommand{\cyan}{\color{cyan}}"
        write (u, '(A)') "\newcommand{\sm}{\footnotesize}"
        write (u, '(A)') "\setlength{\parindent}{0pt}"
        write (u, '(A)') "\setlength{\parsep}{20pt}"
        write (u, *)
        write (u, '(A)') "\begin{document}"
        write (u, '(A)') "\begin{fmffile}{ // char (filename) // }"
        write (u, '(A)') "\fmfcmd{color magenta; magenta = red + blue;}"
        write (u, '(A)') "\fmfcmd{color cyan; cyan = green + blue;}"
        write (u, '(A)') "\begin{fmfshrink}{0.5}"
        write (u, '(A)') "\begin{flushleft}"
        write (u, *)

```

```

write (u, '(A)') "\noindent" // &
& "\textbf{\large\texttt{WHIZARD} phase space channels}" // &
& "\hfill\today"
write (u, *)
write (u, '(A)') "\vspace{10pt}"
write (u, '(A)') "\noindent" // &
& "\textbf{Process:} \url{" // char (process_id) // "}"
call cascade_set_write_process_tex_format (cascade_set, u)
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Note:} These are pseudo Feynman graphs that "
write (u, '(A)') "visualize phase-space parameterizations " // &
& "('integration channels')."
write (u, '(A)') "They do \emph{not} indicate Feynman graphs used for the " // &
& "matrix element."
write (u, *)
write (u, '(A)') "\textbf{Color code:} " // &
& "{\blue resonance,} " // &
& "{\cyan t-channel,} " // &
& "{\green radiation,} "
write (u, '(A)') "{\red infrared,} " // &
& "{\magenta collinear,} " // &
& "external/off-shell"
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Black square:} Keystone, indicates ordering of " // &
& "phase space parameters."
write (u, *)
write (u, '(A)') "\vspace{-20pt}"
count = 0
pgcount = 0
do grove = 1, cascade_set%n_groves
  first_in_grove = .true.
  cascade => cascade_set%first
  do while (associated (cascade))
    if (cascade%active .and. cascade%complete) then
      if (cascade%grove == grove) then
        if (first_in_grove) then
          first_in_grove = .false.
          write (u, *)
          write (u, '(A)') "\vspace{20pt}"
          write (u, '(A)') "\begin{tabular}{l}"
          write (u, '(A,I5,A)') &
            & "\fbox{\bf Grove \boldmath$, grove, "$} \\\[10pt]"
          write (u, '(A,I1,A)') "Multiplicity: ", &
            cascade%multiplicity, "\\"
          write (u, '(A,I1,A)') "Resonances: ", &
            cascade%n_resonances, "\\"
          write (u, '(A,I1,A)') "Log-enhanced: ", &
            cascade%n_log_enhanced, "\\"
          write (u, '(A,I1,A)') "Off-shell: ", &
            cascade%n_off_shell, "\\"
          write (u, '(A,I1,A)') "t-channel: ", &
            cascade%n_t_channel, ""

```

```

        write (u, '(A)') "\end{tabular}"
    end if
    count = count + 1
    call cascade_write_graph_format (cascade, count, unit)
    if (pgcount >= 250) then
        write (u, '(A)') "\clearpage"
        pgcount = 0
    end if
end if
end if
cascade => cascade%next
end do
end do
write (u, '(A)') "\end{flushleft}"
write (u, '(A)') "\end{fmfshrink}"
write (u, '(A)') "\end{fmffile}"
write (u, '(A)') "\end{document}"
end subroutine cascade_set_write_graph_format

```

This is for screen output and debugging:

```

<Cascades: public>+≡
    public :: cascade_set_write

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_write &
        (cascade_set, unit, active_only, complete_only)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: active_only, complete_only
    end subroutine cascade_set_write

<Cascades: procedures>+≡
    module subroutine cascade_set_write &
        (cascade_set, unit, active_only, complete_only)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: active_only, complete_only
        logical :: active, complete
        type(cascade_t), pointer :: cascade
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        active = .true.; if (present (active_only)) active = active_only
        complete = .false.; if (present (complete_only)) complete = complete_only
        write (u, "(A)") "Cascade set:"
        write (u, "(3x,A)", advance="no") "Model:"
        if (associated (cascade_set%model)) then
            write (u, "(1x,A)") char (cascade_set%model%get_name ())
        else
            write (u, "(1x,A)") "[none]"
        end if
        write (u, "(3x,A)", advance="no") "n_in/out/tot ="
        write (u, "(3(1x,I7))") &
            cascade_set%n_in, cascade_set%n_out, cascade_set%n_tot
        write (u, "(3x,A)", advance="no") "depth_out/tot ="
        write (u, "(2(1x,I7))") cascade_set%depth_out, cascade_set%depth_tot
    end subroutine cascade_set_write

```

```

write (u, "(3x,A)", advance="no") "mass thr(s/t) ="
write (u, "(2(1x," // FMT_19 // "))" &
      cascade_set%m_threshold_s, cascade_set%m_threshold_t
write (u, "(3x,A)", advance="no") "off shell      ="
write (u, "(1x,I7)") cascade_set%off_shell
write (u, "(3x,A)", advance="no") "keep_nonreson ="
write (u, "(1x,L1)") cascade_set%keep_nonresonant
write (u, "(3x,A)", advance="no") "n_groves      ="
write (u, "(1x,I7)") cascade_set%n_groves
write (u, "(A)")
write (u, "(A)") "Cascade list:"
if (associated (cascade_set%first)) then
  cascade => cascade_set%first
  do while (associated (cascade))
    if (active .and. .not. cascade%active) cycle
    if (complete .and. .not. cascade%complete) cycle
    call cascade_write (cascade, unit)
    cascade => cascade%next
  end do
else
  write (u, "(A)") "[empty]"
end if
write (u, "(A)") "Hash array"
write (u, "(3x,A)", advance="no") "n_entries      ="
write (u, "(1x,I7)") cascade_set%n_entries
write (u, "(3x,A)", advance="no") "fill_ratio     ="
write (u, "(1x," // FMT_12 // ")") cascade_set%fill_ratio
write (u, "(3x,A)", advance="no") "n_entries_max ="
write (u, "(1x,I7)") cascade_set%n_entries_max
write (u, "(3x,A)", advance="no") "mask          ="
write (u, "(1x,I0)") cascade_set%mask
do i = 0, ubound (cascade_set%entry, 1)
  if (allocated (cascade_set%entry(i)%key)) then
    write (u, "(1x,I7)") i
    call hash_entry_write (cascade_set%entry(i), u)
  end if
end do
end subroutine cascade_set_write

```

19.9.7 Adding cascades

Add a deep copy of a cascade to the set. The copy has all content of the original, but the pointers are nullified. We do not care whether insertion was successful or not. The pointer argument, if present, is assigned to the input cascade, or to the hash entry if it is already present.

The procedure is recursive: any daughter or mother entries are also deep-copied and added to the cascade set before the current copy is added.

(Cascades: procedures) +=

```

recursive subroutine cascade_set_add_copy &
  (cascade_set, cascade_in, cascade_ptr)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in) :: cascade_in

```

```

type(cascade_t), optional, pointer :: cascade_ptr
type(cascade_t), pointer :: cascade
logical :: ok
allocate (cascade)
cascade = cascade_in
if (associated (cascade_in%daughter1)) call cascade_set_add_copy &
    (cascade_set, cascade_in%daughter1, cascade%daughter1)
if (associated (cascade_in%daughter2)) call cascade_set_add_copy &
    (cascade_set, cascade_in%daughter2, cascade%daughter2)
if (associated (cascade_in%mother)) call cascade_set_add_copy &
    (cascade_set, cascade_in%mother, cascade%mother)
cascade%next => null ()
call cascade_set_add (cascade_set, cascade, ok, cascade_ptr)
if (.not. ok) deallocate (cascade)
end subroutine cascade_set_add_copy

```

Add a cascade to the set. This does not deep-copy. We first try to insert it in the hash array. If successful, add it to the list. Failure indicates that it is already present, and we drop it.

The hash key is built solely from the tree array, so neither particle codes nor resonances count, just topology.

Technically, hash and list receive only pointers, so the cascade can be considered as being in either of both. We treat it as part of the list.

```

<Cascades: procedures>+=
subroutine cascade_set_add (cascade_set, cascade, ok, cascade_ptr)
type(cascade_set_t), intent(inout), target :: cascade_set
type(cascade_t), intent(in), target :: cascade
logical, intent(out) :: ok
type(cascade_t), optional, pointer :: cascade_ptr
integer(i8), dimension(1) :: mold
call cascade_set_hash_insert &
    (cascade_set, transfer (cascade%tree, mold), cascade, ok, cascade_ptr)
if (ok) call cascade_set_list_add (cascade_set, cascade)
end subroutine cascade_set_add

```

Add a new cascade to the list:

```

<Cascades: procedures>+=
subroutine cascade_set_list_add (cascade_set, cascade)
type(cascade_set_t), intent(inout) :: cascade_set
type(cascade_t), intent(in), target :: cascade
if (associated (cascade_set%last)) then
    cascade_set%last%next => cascade
else
    cascade_set%first => cascade
end if
cascade_set%last => cascade
end subroutine cascade_set_list_add

```

Add a cascade entry to the hash array:

```

<Cascades: procedures>+=
subroutine cascade_set_hash_insert &
    (cascade_set, key, cascade, ok, cascade_ptr)

```



```

type(cascade_set_t), intent(inout), target :: cascade_set
integer(i8), dimension(:), intent(in) :: key
type(cascade_t), intent(in), target :: cascade
logical, intent(out) :: ok
type(cascade_t), optional, pointer :: cascade_ptr
integer(i32) :: h
if (cascade_set%n_entries >= cascade_set%n_entries_max) &
    call cascade_set_hash_expand (cascade_set)
h = hash (key)
call cascade_set_hash_insert_rec &
    (cascade_set, h, h, key, cascade, ok, cascade_ptr)
end subroutine cascade_set_hash_insert

```

Double the hashtable size when necessary:

```

<Cascades: procedures>+=
subroutine cascade_set_hash_expand (cascade_set)
type(cascade_set_t), intent(inout), target :: cascade_set
type(hash_entry_t), dimension(:), allocatable, target :: table_tmp
type(cascade_p), pointer :: current
integer :: i, s
allocate (table_tmp (0:cascade_set%mask))
table_tmp = cascade_set%entry
deallocate (cascade_set%entry)
s = 2 * size (table_tmp)
cascade_set%n_entries = 0
cascade_set%n_entries_max = s * cascade_set%fill_ratio
cascade_set%mask = s - 1
allocate (cascade_set%entry (0:cascade_set%mask))
do i = 0, ubound (table_tmp, 1)
    current => table_tmp(i)%first
    do while (associated (current))
        call cascade_set_hash_insert_rec &
            (cascade_set, table_tmp(i)%hashval, table_tmp(i)%hashval, &
                table_tmp(i)%key, current%cascade)
        current => current%next
    end do
end do
end subroutine cascade_set_hash_expand

```

Insert the cascade at the bucket determined by the hash value. If the bucket is filled, check first for a collision (unequal keys). In that case, choose the following bucket and repeat. Otherwise, add the cascade to the bucket.

If the bucket is empty, record the hash value, allocate and store the key, and then add the cascade to the bucket.

If ok is present, before insertion we check whether the cascade is already stored, and return failure if yes.

```

<Cascades: procedures>+=
recursive subroutine cascade_set_hash_insert_rec &
    (cascade_set, h, hashval, key, cascade, ok, cascade_ptr)
type(cascade_set_t), intent(inout) :: cascade_set
integer(i32), intent(in) :: h, hashval
integer(i8), dimension(:), intent(in) :: key

```

```

type(cascade_t), intent(in), target :: cascade
logical, intent(out), optional :: ok
type(cascade_t), optional, pointer :: cascade_ptr
integer(i32) :: i
i = iand (h, cascade_set%mask)
if (allocated (cascade_set%entry(i)%key)) then
  if (size (cascade_set%entry(i)%key) /= size (key)) then
    call cascade_set_hash_insert_rec &
      (cascade_set, h + 1, hashval, key, cascade, ok, cascade_ptr)
  else if (any (cascade_set%entry(i)%key /= key)) then
    call cascade_set_hash_insert_rec &
      (cascade_set, h + 1, hashval, key, cascade, ok, cascade_ptr)
  else
    call hash_entry_add_cascade_ptr &
      (cascade_set%entry(i), cascade, ok, cascade_ptr)
  end if
else
  cascade_set%entry(i)%hashval = hashval
  allocate (cascade_set%entry(i)%key (size (key)))
  cascade_set%entry(i)%key = key
  call hash_entry_add_cascade_ptr &
    (cascade_set%entry(i), cascade, ok, cascade_ptr)
  cascade_set%n_entries = cascade_set%n_entries + 1
end if
end subroutine cascade_set_hash_insert_rec

```

19.9.8 External particles

We want to initialize the cascade set with the outgoing particles. In case of multiple processes, initial cascades are prepared for all of them. The hash array check ensures that no particle appears more than once at the same place.

```

<Cascades: interfaces>+≡
  interface cascade_set_add_outgoing
    module procedure cascade_set_add_outgoing1
    module procedure cascade_set_add_outgoing2
  end interface

<Cascades: sub interfaces>+≡
  module subroutine cascade_set_add_outgoing1 (cascade_set, flv)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(flavor_t), dimension(:), intent(in) :: flv
  end subroutine cascade_set_add_outgoing1
  module subroutine cascade_set_add_outgoing2 (cascade_set, flv)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(flavor_t), dimension(:,,:), intent(in) :: flv
  end subroutine cascade_set_add_outgoing2

<Cascades: procedures>+≡
  module subroutine cascade_set_add_outgoing2 (cascade_set, flv)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(flavor_t), dimension(:,,:), intent(in) :: flv
    integer :: pos, prc, n_out, n_prc

```

```

type(cascade_t), pointer :: cascade
logical :: ok
n_out = size (flv, dim=1)
n_prc = size (flv, dim=2)
do prc = 1, n_prc
  do pos = 1, n_out
    allocate (cascade)
    call cascade_init_outgoing &
      (cascade, flv(pos,prc), pos, cascade_set%m_threshold_s)
    call cascade_set_add (cascade_set, cascade, ok)
    if (.not. ok) then
      deallocate (cascade)
    end if
  end do
end do
end subroutine cascade_set_add_outgoing2

module subroutine cascade_set_add_outgoing1 (cascade_set, flv)
type(cascade_set_t), intent(inout), target :: cascade_set
type(flavor_t), dimension(:), intent(in) :: flv
integer :: pos, n_out
type(cascade_t), pointer :: cascade
logical :: ok
n_out = size (flv, dim=1)
do pos = 1, n_out
  allocate (cascade)
  call cascade_init_outgoing &
    (cascade, flv(pos), pos, cascade_set%m_threshold_s)
  call cascade_set_add (cascade_set, cascade, ok)
  if (.not. ok) then
    deallocate (cascade)
  end if
end do
end subroutine cascade_set_add_outgoing1

```

The incoming particles are added one at a time. Nevertheless, we may have several processes which are looped over. At the first opportunity, we set the pointer `first_t` in the cascade set which should point to the first t-channel cascade.

Return the indices of the first and last cascade generated.

<Cascades: interfaces>+≡

```

interface cascade_set_add_incoming
  module procedure cascade_set_add_incoming0
  module procedure cascade_set_add_incoming1
end interface

```

<Cascades: sub interfaces>+≡

```

module subroutine cascade_set_add_incoming1 (cascade_set, n1, n2, pos, flv)
type(cascade_set_t), intent(inout), target :: cascade_set
integer, intent(out) :: n1, n2
integer, intent(in) :: pos
type(flavor_t), dimension(:), intent(in) :: flv
end subroutine cascade_set_add_incoming1

```

```

module subroutine cascade_set_add_incoming0 (cascade_set, n1, n2, pos, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(out) :: n1, n2
  integer, intent(in) :: pos
  type(flavor_t), intent(in) :: flv
end subroutine cascade_set_add_incoming0

```

(Cascades: procedures)+≡

```

module subroutine cascade_set_add_incoming1 (cascade_set, n1, n2, pos, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(out) :: n1, n2
  integer, intent(in) :: pos
  type(flavor_t), dimension(:), intent(in) :: flv
  integer :: prc, n_prc
  type(cascade_t), pointer :: cascade
  logical :: ok
  n1 = 0
  n2 = 0
  n_prc = size (flv)
  do prc = 1, n_prc
    allocate (cascade)
    call cascade_init_incoming &
      (cascade, flv(prc), pos, cascade_set%m_threshold_t)
    call cascade_set_add (cascade_set, cascade, ok)
    if (ok) then
      if (n1 == 0) n1 = cascade%index
      n2 = cascade%index
      if (.not. associated (cascade_set%first_t)) then
        cascade_set%first_t => cascade
      end if
    else
      deallocate (cascade)
    end if
  end do
end subroutine cascade_set_add_incoming1

```

```

module subroutine cascade_set_add_incoming0 (cascade_set, n1, n2, pos, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(out) :: n1, n2
  integer, intent(in) :: pos
  type(flavor_t), intent(in) :: flv
  type(cascade_t), pointer :: cascade
  logical :: ok
  n1 = 0
  n2 = 0
  allocate (cascade)
  call cascade_init_incoming &
    (cascade, flv, pos, cascade_set%m_threshold_t)
  call cascade_set_add (cascade_set, cascade, ok)
  if (ok) then
    if (n1 == 0) n1 = cascade%index
    n2 = cascade%index
    if (.not. associated (cascade_set%first_t)) then
      cascade_set%first_t => cascade
    end if
  end if

```

```

else
    deallocate (cascade)
end if
end subroutine cascade_set_add_incoming0

```

19.9.9 Cascade combination I: flavor assignment

We have two disjunct cascades, now use the vertex table to determine the possible flavors of the combination cascade. For each possibility, try to generate a new cascade. The total cascade depth has to be one less than the limit, because this is reached by setting the keystone.

```

(Cascades: procedures) +=
subroutine cascade_match_pair (cascade_set, cascade1, cascade2, s_channel)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(cascade_t), intent(in), target :: cascade1, cascade2
    logical, intent(in) :: s_channel
    integer, dimension(:), allocatable :: pdg3
    integer :: i, depth_max
    type(flavor_t) :: flv
    if (s_channel) then
        depth_max = cascade_set%depth_out
    else
        depth_max = cascade_set%depth_tot
    end if
    if (cascade1%depth + cascade2%depth < depth_max) then
        call cascade_set%model%match_vertex ( &
            cascade1%flv%get_pdg (), &
            cascade2%flv%get_pdg (), &
            pdg3)
        do i = 1, size (pdg3)
            call flv%init (pdg3(i), cascade_set%model)
            if (s_channel) then
                call cascade_combine_s (cascade_set, cascade1, cascade2, flv)
            else
                call cascade_combine_t (cascade_set, cascade1, cascade2, flv)
            end if
        end do
        deallocate (pdg3)
    end if
end subroutine cascade_match_pair

```

The triplet version takes a third cascade, and we check whether this triplet has a matching vertex in the database. If yes, we make a keystone cascade.

```

(Cascades: procedures) +=
subroutine cascade_match_triplet &
    (cascade_set, cascade1, cascade2, cascade3, s_channel)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
    logical, intent(in) :: s_channel
    integer :: depth_max
    depth_max = cascade_set%depth_tot

```

```

if (cascade1%depth + cascade2%depth + cascade3%depth == depth_max) then
  if (cascade_set%model%check_vertex ( &
    cascade1%flv%get_pdg (), &
    cascade2%flv%get_pdg (), &
    cascade3%flv%get_pdg ())) then
    call cascade_combine_keystone &
      (cascade_set, cascade1, cascade2, cascade3, s_channel)
  end if
end if
end subroutine cascade_match_triplet

```

19.9.10 Cascade combination II: kinematics setup and check

Having three matching flavors, we start constructing the combination cascade. We look at the mass hierarchies and determine whether the cascade is to be kept. In passing we set mapping modes, resonance properties and such.

If successful, the cascade is finalized. For a resonant cascade, we prepare in addition a copy without the resonance.

```

<Cascades: procedures>+≡
subroutine cascade_combine_s (cascade_set, cascade1, cascade2, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  type(flavor_t), intent(in) :: flv
  type(cascade_t), pointer :: cascade3, cascade4
  real(default) :: width
  logical :: keep
  keep = .false.
  allocate (cascade3)
  call cascade_init (cascade3, cascade1%depth + cascade2%depth + 1)
  cascade3%bincode = ior (cascade1%bincode, cascade2%bincode)
  cascade3%flv = flv%anti ()
  cascade3%pdg = cascade3%flv%get_pdg ()
  cascade3%is_vector = flv%get_spin_type () == VECTOR
  cascade3%m_min = cascade1%m_min + cascade2%m_min
  cascade3%m_rea = flv%get_mass ()
  width = flv%get_width ()
  if (cascade3%m_rea > cascade_set%m_threshold_s) then
    cascade3%m_eff = cascade3%m_rea
  end if
  ! Potentially resonant cases [sqrts = m_rea for on-shell decay]
  if (cascade3%m_rea > cascade3%m_min .and. &
    cascade3%m_rea <= cascade_set%sqrts) then
    if (width /= 0) then
      if (cascade1%on_shell .or. cascade2%on_shell) then
        keep = .true.
        cascade3%mapping = S_CHANNEL
        cascade3%resonant = .true.
      end if
    else
      call warn_decay (flv)
    end if
  end if
  ! Collinear and IR singular cases

```

```

else if (cascade3%m_rea < cascade_set%sqrts) then
  ! Massless splitting
  if (cascade1%m_eff == 0 .and. cascade2%m_eff == 0 &
    .and. cascade3%depth <= 3) then
    keep = .true.
    cascade3%log_enhanced = .true.
    if (cascade3%is_vector) then
      if (cascade1%is_vector .and. cascade2%is_vector) then
        cascade3%mapping = COLLINEAR    ! three-vector-vertex
      else
        cascade3%mapping = INFRARED     ! vector splitting into matter
      end if
    else
      if (cascade1%is_vector .or. cascade2%is_vector) then
        cascade3%mapping = COLLINEAR    ! vector radiation off matter
      else
        cascade3%mapping = INFRARED     ! scalar radiation/splitting
      end if
    end if
    ! IR radiation off massive particle
  else if (cascade3%m_eff > 0 .and. cascade1%m_eff > 0 &
    .and. cascade2%m_eff == 0 &
    .and. (cascade1%on_shell .or. cascade1%mapping == RADIATION) &
    .and. abs (cascade3%m_eff - cascade1%m_eff) &
      < cascade_set%m_threshold_s) &
    then
      keep = .true.
      cascade3%log_enhanced = .true.
      cascade3%mapping = RADIATION
    else if (cascade3%m_eff > 0 .and. cascade2%m_eff > 0 &
      .and. cascade1%m_eff == 0 &
      .and. (cascade2%on_shell .or. cascade2%mapping == RADIATION) &
      .and. abs (cascade3%m_eff - cascade2%m_eff) &
        < cascade_set%m_threshold_s) &
      then
        keep = .true.
        cascade3%log_enhanced = .true.
        cascade3%mapping = RADIATION
      end if
    end if
  ! Non-singular cases, including failed resonances
  if (.not. keep) then
    ! Two on-shell particles from a virtual mother
    if (cascade1%on_shell .or. cascade2%on_shell) then
      keep = .true.
      cascade3%m_eff = max (cascade3%m_min, &
        cascade1%m_eff + cascade2%m_eff)
      if (cascade3%m_eff < cascade_set%m_threshold_s) then
        cascade3%m_eff = 0
      end if
    end if
  end if
end if
! Complete and register the cascade (two in case of resonance)
if (keep) then

```

```

cascade3%on_shell = cascade3%resonant .or. cascade3%log_enhanced
if (cascade3%resonant) then
  cascade3%pdg = cascade3%flv%get_pdg ()
  if (cascade_set%keep_nonresonant) then
    allocate (cascade4)
    cascade4 = cascade3
    cascade4%index = cascade_index ()
    cascade4%pdg = UNDEFINED
    cascade4%mapping = NO_MAPPING
    cascade4%resonant = .false.
    cascade4%on_shell = .false.
  end if
  cascade3%m_min = cascade3%m_rea
  call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
  if (cascade_set%keep_nonresonant) then
    call cascade_fusion (cascade_set, cascade1, cascade2, cascade4)
  end if
else
  call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
end if
else
  deallocate (cascade3)
end if
contains
subroutine warn_decay (flv)
  type(flavor_t), intent(in) :: flv
  integer :: i
  integer, dimension(MAX_WARN_RESONANCE), save :: warned_code = 0
  LOOP_WARNED: do i = 1, MAX_WARN_RESONANCE
    if (warned_code(i) == 0) then
      warned_code(i) = flv%get_pdg ()
      write (msg_buffer, "(A)") &
        & " Intermediate decay of zero-width particle " &
        & // char (flv%get_name ()) &
        & // " may be possible."
      call msg_warning
      exit LOOP_WARNED
    else if (warned_code(i) == flv%get_pdg ()) then
      exit LOOP_WARNED
    end if
  end do LOOP_WARNED
end subroutine warn_decay
end subroutine cascade_combine_s

```

<Cascades: parameters>+≡

```
integer, parameter, public :: MAX_WARN_RESONANCE = 50
```

This is the t-channel version. `cascade1` is t-channel and contains the seed, `cascade2` is s-channel. We check for kinematically allowed beam decay (which is a fatal error), or massless splitting / soft radiation. The cascade is kept in all remaining cases and submitted for registration.

<Cascades: procedures>+≡

```
subroutine cascade_combine_t (cascade_set, cascade1, cascade2, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set

```



```

type(cascade_t), intent(in), target :: cascade1, cascade2
type(flavor_t), intent(in) :: flv
type(cascade_t), pointer :: cascade3
allocate (cascade3)
call cascade_init (cascade3, cascade1%depth + cascade2%depth + 1)
cascade3%bincode = ior (cascade1%bincode, cascade2%bincode)
cascade3%flv = flv%anti ()
cascade3%pdg = abs (cascade3%flv%get_pdg ())
cascade3%is_vector = flv%get_spin_type () == VECTOR
if (cascade1%incoming) then
    cascade3%m_min = cascade2%m_min
else
    cascade3%m_min = cascade1%m_min + cascade2%m_min
end if
cascade3%m_rea = flv%get_mass ()
if (cascade3%m_rea > cascade_set%m_threshold_t) then
    cascade3%m_eff = max (cascade3%m_rea, cascade2%m_eff)
else if (cascade2%m_eff > cascade_set%m_threshold_t) then
    cascade3%m_eff = cascade2%m_eff
else
    cascade3%m_eff = 0
end if
! Allowed decay of beam particle
if (cascade1%incoming &
    .and. cascade1%m_rea > cascade2%m_rea + cascade3%m_rea) then
    call beam_decay (cascade_set%fatal_beam_decay)
! Massless splitting
else if (cascade1%m_eff == 0 &
    .and. cascade2%m_eff < cascade_set%m_threshold_t &
    .and. cascade3%m_eff == 0) then
    cascade3%mapping = U_CHANNEL
    cascade3%log_enhanced = .true.
! IR radiation off massive particle
else if (cascade1%m_eff /= 0 .and. cascade2%m_eff == 0 &
    .and. cascade3%m_eff /= 0 &
    .and. (cascade1%on_shell .or. cascade1%mapping == RADIATION) &
    .and. abs (cascade1%m_eff - cascade3%m_eff) &
        < cascade_set%m_threshold_t) &
    then
        cascade3%pdg = flv%get_pdg ()
        cascade3%log_enhanced = .true.
        cascade3%mapping = RADIATION
    end if
cascade3%t_channel = .true.
call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
contains
subroutine beam_decay (fatal_beam_decay)
    logical, intent(in) :: fatal_beam_decay
    write (msg_buffer, "(1x,A,1x,'->',1x,A,1x,A)") &
        char (cascade1%flv%get_name ()), &
        char (cascade3%flv%get_name ()), &
        char (cascade2%flv%get_name ())
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,')' = ',1x,E17.10)") &

```

```

        char (cascade1%flv%get_name ()), cascade1%m_rea
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,') =' ,1x,E17.10)") &
        char (cascade3%flv%get_name ()), cascade3%m_rea
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,') =' ,1x,E17.10)") &
        char (cascade2%flv%get_name ()), cascade2%m_rea
    call msg_message
    if (fatal_beam_decay) then
        call msg_fatal (" Phase space: Initial beam particle can decay")
    else
        call msg_warning (" Phase space: Initial beam particle can decay")
    end if
end subroutine beam_decay
end subroutine cascade_combine_t

```

Here we complete a decay cascade. The third input is the single-particle cascade for the initial particle. There is no resonance or mapping assignment. The only condition for keeping the cascade is the mass sum of the final state, which must be less than the available energy.

Two modifications are necessary for scattering cascades: a pure s-channel diagram (cascade1 is the incoming particle) do not have a logarithmic mapping at top-level. And in a t-channel diagram, the last line exchanged is mapped t-channel, not u-channel. Finally, we can encounter the case of a $2 \rightarrow 1$ process, where cascade1 is incoming, and cascade2 is the outgoing particle. In all three cases we register a new cascade with the modified mapping.

```

(Cascades: procedures) +=
subroutine cascade_combine_keystone &
    (cascade_set, cascade1, cascade2, cascade3, s_channel)
type(cascade_set_t), intent(inout), target :: cascade_set
type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
logical, intent(in) :: s_channel
type(cascade_t), pointer :: cascade4, cascade0
logical :: keep, ok
keep = .false.
allocate (cascade4)
call cascade_init &
    (cascade4, cascade1%depth + cascade2%depth + cascade3%depth)
cascade4%complete = .true.
if (s_channel) then
    cascade4%bincode = ior (cascade1%bincode, cascade2%bincode)
else
    cascade4%bincode = cascade3%bincode
end if
cascade4%flv = cascade3%flv
cascade4%pdg = cascade3%pdg
cascade4%mapping = EXTERNAL_PRT
cascade4%is_vector = cascade3%is_vector
cascade4%m_min = cascade1%m_min + cascade2%m_min
cascade4%m_rea = cascade3%m_rea
cascade4%m_eff = cascade3%m_rea
if (cascade4%m_min < cascade_set%sqrts) then
    keep = .true.

```

```

end if
if (keep) then
  if (cascade1%incoming .and. cascade2%log_enhanced) then
    allocate (cascade0)
    cascade0 = cascade2
    cascade0%next => null ()
    cascade0%index = cascade_index ()
    cascade0%mapping = NO_MAPPING
    cascade0%log_enhanced = .false.
    cascade0%n_log_enhanced = cascade0%n_log_enhanced - 1
    cascade0%tree_mapping(cascade0%depth) = NO_MAPPING
    call cascade_keystone &
      (cascade_set, cascade1, cascade0, cascade3, cascade4, ok)
    if (ok) then
      call cascade_set_add (cascade_set, cascade0, ok)
    else
      deallocate (cascade0)
    end if
  else if (cascade1%t_channel .and. cascade1%mapping == U_CHANNEL) then
    allocate (cascade0)
    cascade0 = cascade1
    cascade0%next => null ()
    cascade0%index = cascade_index ()
    cascade0%mapping = T_CHANNEL
    cascade0%tree_mapping(cascade0%depth) = T_CHANNEL
    call cascade_keystone &
      (cascade_set, cascade0, cascade2, cascade3, cascade4, ok)
    if (ok) then
      call cascade_set_add (cascade_set, cascade0, ok)
    else
      deallocate (cascade0)
    end if
  else if (cascade1%incoming .and. cascade2%depth == 1) then
    allocate (cascade0)
    cascade0 = cascade2
    cascade0%next => null ()
    cascade0%index = cascade_index ()
    cascade0%mapping = ON_SHELL
    cascade0%tree_mapping(cascade0%depth) = ON_SHELL
    call cascade_keystone &
      (cascade_set, cascade1, cascade0, cascade3, cascade4, ok)
    if (ok) then
      call cascade_set_add (cascade_set, cascade0, ok)
    else
      deallocate (cascade0)
    end if
  else
    call cascade_keystone &
      (cascade_set, cascade1, cascade2, cascade3, cascade4, ok)
  end if
else
  deallocate (cascade4)
end if
end subroutine cascade_combine_keystone

```

19.9.11 Cascade combination III: node connections and tree fusion

Here we assign global tree properties. If the allowed number of off-shell lines is exceeded, discard the new cascade. Otherwise, assign the trees, sort them, and assign connections. Finally, append the cascade to the list. This may fail (because in the hash array there is already an equivalent cascade). On failure, discard the cascade.

(Cascades: procedures) +=

```
subroutine cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  type(cascade_t), pointer :: cascade3
  integer :: i1, i2, i3, i4
  logical :: ok
  cascade3%internal = (cascade3%depth - 3) / 2
  if (cascade3%resonant) then
    cascade3%multiplicity = 1
    cascade3%n_resonances = &
      cascade1%n_resonances + cascade2%n_resonances + 1
  else
    cascade3%multiplicity = cascade1%multiplicity + cascade2%multiplicity
    cascade3%n_resonances = cascade1%n_resonances + cascade2%n_resonances
  end if
  if (cascade3%log_enhanced) then
    cascade3%n_log_enhanced = &
      cascade1%n_log_enhanced + cascade2%n_log_enhanced + 1
  else
    cascade3%n_log_enhanced = &
      cascade1%n_log_enhanced + cascade2%n_log_enhanced
  end if
  if (cascade3%resonant) then
    cascade3%n_off_shell = 0
  else if (cascade3%log_enhanced) then
    cascade3%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell
  else
    cascade3%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell + 1
  end if
  if (cascade3%t_channel) then
    cascade3%n_t_channel = cascade1%n_t_channel + 1
  end if
  if (cascade3%n_off_shell > cascade_set%off_shell) then
    deallocate (cascade3)
  else if (cascade3%n_t_channel > cascade_set%t_channel) then
    deallocate (cascade3)
  else
    i1 = cascade1%depth
    i2 = i1 + 1
    i3 = i1 + cascade2%depth
    i4 = cascade3%depth
    cascade3%tree(:i1) = cascade1%tree
```

```

where (cascade1%tree_mapping > NO_MAPPING)
  cascade3%tree_pdg(:i1) = cascade1%tree_pdg
elsewhere
  cascade3%tree_pdg(:i1) = UNDEFINED
end where
cascade3%tree_mapping(:i1) = cascade1%tree_mapping
cascade3%tree_resonant(:i1) = cascade1%tree_resonant
cascade3%tree(i2:i3) = cascade2%tree
where (cascade2%tree_mapping > NO_MAPPING)
  cascade3%tree_pdg(i2:i3) = cascade2%tree_pdg
elsewhere
  cascade3%tree_pdg(i2:i3) = UNDEFINED
end where
cascade3%tree_mapping(i2:i3) = cascade2%tree_mapping
cascade3%tree_resonant(i2:i3) = cascade2%tree_resonant
cascade3%tree(i4) = cascade3%bincode
cascade3%tree_pdg(i4) = cascade3%pdg
cascade3%tree_mapping(i4) = cascade3%mapping
cascade3%tree_resonant(i4) = cascade3%resonant
call tree_sort (cascade3%tree, &
  cascade3%tree_pdg, cascade3%tree_mapping, cascade3%tree_resonant)
cascade3%has_children = .true.
cascade3%daughter1 => cascade1
cascade3%daughter2 => cascade2
call cascade_set_add (cascade_set, cascade3, ok)
if (.not. ok) deallocate (cascade3)
end if
end subroutine cascade_fusion

```

Here we combine a cascade pair with an incoming particle, i.e., we set a keystone. Otherwise, this is similar. On the first opportunity, we set the `first_k` pointer in the cascade set.

(*Cascades: procedures*) +=

```

subroutine cascade_keystone &
  (cascade_set, cascade1, cascade2, cascade3, cascade4, ok)
type(cascade_set_t), intent(inout), target :: cascade_set
type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
type(cascade_t), pointer :: cascade4
logical, intent(out) :: ok
integer :: i1, i2, i3, i4
cascade4%internal = (cascade4%depth - 3) / 2
cascade4%multiplicity = cascade1%multiplicity + cascade2%multiplicity
cascade4%n_resonances = cascade1%n_resonances + cascade2%n_resonances
cascade4%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell
cascade4%n_log_enhanced = &
  cascade1%n_log_enhanced + cascade2%n_log_enhanced
cascade4%n_t_channel = cascade1%n_t_channel + cascade2%n_t_channel
if (cascade4%n_off_shell > cascade_set%off_shell) then
  deallocate (cascade4)
  ok = .false.
else if (cascade4%n_t_channel > cascade_set%t_channel) then
  deallocate (cascade4)
  ok = .false.

```

```

else
  i1 = cascade1%depth
  i2 = i1 + 1
  i3 = i1 + cascade2%depth
  i4 = cascade4%depth
  cascade4%tree(:i1) = cascade1%tree
  where (cascade1%tree_mapping > NO_MAPPING)
    cascade4%tree_pdg(:i1) = cascade1%tree_pdg
  elsewhere
    cascade4%tree_pdg(:i1) = UNDEFINED
  end where
  cascade4%tree_mapping(:i1) = cascade1%tree_mapping
  cascade4%tree_resonant(:i1) = cascade1%tree_resonant
  cascade4%tree(i2:i3) = cascade2%tree
  where (cascade2%tree_mapping > NO_MAPPING)
    cascade4%tree_pdg(i2:i3) = cascade2%tree_pdg
  elsewhere
    cascade4%tree_pdg(i2:i3) = UNDEFINED
  end where
  cascade4%tree_mapping(i2:i3) = cascade2%tree_mapping
  cascade4%tree_resonant(i2:i3) = cascade2%tree_resonant
  cascade4%tree(i4) = cascade4%bincode
  cascade4%tree_pdg(i4) = UNDEFINED
  cascade4%tree_mapping(i4) = cascade4%mapping
  cascade4%tree_resonant(i4) = .false.
  call tree_sort (cascade4%tree, &
    cascade4%tree_pdg, cascade4%tree_mapping, cascade4%tree_resonant)
  cascade4%has_children = .true.
  cascade4%daughter1 => cascade1
  cascade4%daughter2 => cascade2
  cascade4%mother => cascade3
  call cascade_set_add (cascade_set, cascade4, ok)
  if (ok) then
    if (.not. associated (cascade_set%first_k)) then
      cascade_set%first_k => cascade4
    end if
  else
    deallocate (cascade4)
  end if
end if
end subroutine cascade_keystone

```

Sort a tree (array of binary codes) and particle code array simultaneously, by ascending binary codes. A convenient method is to use the `maxloc` function iteratively, to find and remove the largest entry in the tree array one by one.

(Cascades: procedures)+≡

```

subroutine tree_sort (tree, pdg, mapping, resonant)
  integer(TC), dimension(:), intent(inout) :: tree
  integer, dimension(:), intent(inout) :: pdg, mapping
  logical, dimension(:), intent(inout) :: resonant
  integer(TC), dimension(size(tree)) :: tree_tmp
  integer, dimension(size(pdg)) :: pdg_tmp, mapping_tmp
  logical, dimension(size(resonant)) :: resonant_tmp

```

```

integer, dimension(1) :: pos
integer :: i
tree_tmp = tree
pdg_tmp = pdg
mapping_tmp = mapping
resonant_tmp = resonant
do i = size(tree),1,-1
  pos = maxloc (tree_tmp)
  tree(i) = tree_tmp (pos(1))
  pdg(i) = pdg_tmp (pos(1))
  mapping(i) = mapping_tmp (pos(1))
  resonant(i) = resonant_tmp (pos(1))
  tree_tmp(pos(1)) = 0
end do
end subroutine tree_sort

```

19.9.12 Cascade set generation

These procedures loop over cascades and build up the cascade set. After each iteration of the innermost loop, we set a breakpoint.

s-channel: We use a nested scan to combine all cascades with all other cascades.

```

(Cascades: procedures) +=
  subroutine cascade_set_generate_s (cascade_set)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(cascade_t), pointer :: cascade1, cascade2
    cascade1 => cascade_set%first
    LOOP1: do while (associated (cascade1))
      cascade2 => cascade_set%first
      LOOP2: do while (associated (cascade2))
        if (cascade2%index >= cascade1%index) exit LOOP2
        if (cascade1 .disjunct. cascade2) then
          call cascade_match_pair (cascade_set, cascade1, cascade2, .true.)
        end if
        call terminate_now_if_signal ()
        cascade2 => cascade2%next
      end do LOOP2
      cascade1 => cascade1%next
    end do LOOP1
  end subroutine cascade_set_generate_s

```

The t-channel cascades are directed and have a seed (one of the incoming particles) and a target (the other one). We loop over all possible seeds and targets. Inside this, we loop over all t-channel cascades (*cascade1*) and s-channel cascades (*cascade2*) and try to combine them.

```

(Cascades: procedures) +=
  subroutine cascade_set_generate_t (cascade_set, pos_seed, pos_target)
    type(cascade_set_t), intent(inout), target :: cascade_set
    integer, intent(in) :: pos_seed, pos_target
    type(cascade_t), pointer :: cascade_seed, cascade_target
    type(cascade_t), pointer :: cascade1, cascade2

```

```

integer(TC) :: bc_seed, bc_target
bc_seed = ibset (0_TC, pos_seed-1)
bc_target = ibset (0_TC, pos_target-1)
cascade_seed => cascade_set%first_t
LOOP_SEED: do while (associated (cascade_seed))
  if (cascade_seed%bincode == bc_seed) then
    cascade_target => cascade_set%first_t
    LOOP_TARGET: do while (associated (cascade_target))
      if (cascade_target%bincode == bc_target) then
        cascade1 => cascade_set%first_t
        LOOP_T: do while (associated (cascade1))
          if ((cascade1 .disjunct. cascade_target) &
              .and. .not. (cascade1 .disjunct. cascade_seed)) then
            cascade2 => cascade_set%first
            LOOP_S: do while (associated (cascade2))
              if ((cascade2 .disjunct. cascade_target) &
                  .and. (cascade2 .disjunct. cascade1)) then
                call cascade_match_pair &
                  (cascade_set, cascade1, cascade2, .false.)
              end if
              call terminate_now_if_signal ()
              cascade2 => cascade2%next
            end do LOOP_S
          end if
          call terminate_now_if_signal ()
          cascade1 => cascade1%next
        end do LOOP_T
      end if
      call terminate_now_if_signal ()
      cascade_target => cascade_target%next
    end do LOOP_TARGET
  end if
  call terminate_now_if_signal ()
  cascade_seed => cascade_seed%next
end do LOOP_SEED
end subroutine cascade_set_generate_t

```

This part completes the phase space for decay processes. It is similar to s-channel cascade generation, but combines two cascade with the particular cascade of the incoming particle. This particular cascade is expected to be pointed at by `first_t`.

(Cascades: procedures)+≡

```

subroutine cascade_set_generate_decay (cascade_set)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), pointer :: cascade1, cascade2
  type(cascade_t), pointer :: cascade_in
  cascade_in => cascade_set%first_t
  cascade1 => cascade_set%first
  do while (associated (cascade1))
    if (cascade1 .disjunct. cascade_in) then
      cascade2 => cascade1%next
      do while (associated (cascade2))
        if ((cascade2 .disjunct. cascade1) &

```



```

        .and. (cascade2 .disjunct. cascade_in)) then
        call cascade_match_triplet (cascade_set, &
            cascade1, cascade2, cascade_in, .true.)
        end if
        call terminate_now_if_signal ()
        cascade2 => cascade2%next
    end do
end if
call terminate_now_if_signal ()
cascade1 => cascade1%next
end do
end subroutine cascade_set_generate_decay

```

This part completes the phase space for scattering processes. We combine a t-channel cascade (containing the seed) with a s-channel cascade and the target.

(*Cascades: procedures*)+=

```

subroutine cascade_set_generate_scattering &
    (cascade_set, ns1, ns2, nt1, nt2, pos_seed, pos_target)
type(cascade_set_t), intent(inout), target :: cascade_set
integer, intent(in) :: pos_seed, pos_target
integer, intent(in) :: ns1, ns2, nt1, nt2
type(cascade_t), pointer :: cascade_seed, cascade_target
type(cascade_t), pointer :: cascade1, cascade2
integer(TC) :: bc_seed, bc_target
bc_seed = ibset (0_TC, pos_seed-1)
bc_target = ibset (0_TC, pos_target-1)
cascade_seed => cascade_set%first_t
LOOP_SEED: do while (associated (cascade_seed))
    if (cascade_seed%index < ns1) then
        cascade_seed => cascade_seed%next
        cycle LOOP_SEED
    else if (cascade_seed%index > ns2) then
        exit LOOP_SEED
    else if (cascade_seed%bincode == bc_seed) then
        cascade_target => cascade_set%first_t
        LOOP_TARGET: do while (associated (cascade_target))
            if (cascade_target%index < nt1) then
                cascade_target => cascade_target%next
                cycle LOOP_TARGET
            else if (cascade_target%index > nt2) then
                exit LOOP_TARGET
            else if (cascade_target%bincode == bc_target) then
                cascade1 => cascade_set%first_t
                LOOP_T: do while (associated (cascade1))
                    if ((cascade1 .disjunct. cascade_target) &
                        .and. .not. (cascade1 .disjunct. cascade_seed)) then
                        cascade2 => cascade_set%first
                        LOOP_S: do while (associated (cascade2))
                            if ((cascade2 .disjunct. cascade_target) &
                                .and. (cascade2 .disjunct. cascade1)) then
                                call cascade_match_triplet (cascade_set, &
                                    cascade1, cascade2, cascade_target, .false.)
                            end if
                        end do
                    end if
                end do
            end if
        end do
    end if
end do

```

```

        call terminate_now_if_signal ()
        cascade2 => cascade2%next
    end do LOOP_S
end if
call terminate_now_if_signal ()
cascade1 => cascade1%next
end do LOOP_T
end if
call terminate_now_if_signal ()
cascade_target => cascade_target%next
end do LOOP_TARGET
end if
call terminate_now_if_signal ()
cascade_seed => cascade_seed%next
end do LOOP_SEED
end subroutine cascade_set_generate_scattering

```

19.9.13 Groves

Before assigning groves, assign hashcodes to the resonance patterns, so they can easily be compared.

(Cascades: procedures)+≡

```

subroutine cascade_set_assign_resonance_hash (cascade_set)
    type(cascade_set_t), intent(inout) :: cascade_set
    type(cascade_t), pointer :: cascade
    cascade => cascade_set%first_k
    do while (associated (cascade))
        call cascade_assign_resonance_hash (cascade)
        cascade => cascade%next
    end do
end subroutine cascade_set_assign_resonance_hash

```

After all cascades are recorded, we group the complete cascades in groves. A grove consists of cascades with identical multiplicity, number of resonances, log-enhanced, t-channel lines, and resonance flavors.

(Cascades: procedures)+≡

```

subroutine cascade_set_assign_groves (cascade_set)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(cascade_t), pointer :: cascade1, cascade2
    integer :: multiplicity
    integer :: n_resonances, n_log_enhanced, n_t_channel, n_off_shell
    integer :: res_hash
    integer :: grove
    grove = 0
    cascade1 => cascade_set%first_k
    do while (associated (cascade1))
        if (cascade1%active .and. cascade1%complete &
            .and. cascade1%grove == 0) then
            grove = grove + 1
            cascade1%grove = grove
            multiplicity = cascade1%multiplicity
            n_resonances = cascade1%n_resonances

```

```

n_log_enhanced = cascade1%n_log_enhanced
n_off_shell = cascade1%n_off_shell
n_t_channel = cascade1%n_t_channel
res_hash = cascade1%res_hash
cascade2 => cascade1%next
do while (associated (cascade2))
  if (cascade2%grove == 0) then
    if (cascade2%multiplicity == multiplicity &
        .and. cascade2%n_resonances == n_resonances &
        .and. cascade2%n_log_enhanced == n_log_enhanced &
        .and. cascade2%n_off_shell == n_off_shell &
        .and. cascade2%n_t_channel == n_t_channel &
        .and. cascade2%res_hash == res_hash) then
      cascade2%grove = grove
    end if
  end if
  call terminate_now_if_signal ()
  cascade2 => cascade2%next
end do
end if
call terminate_now_if_signal ()
cascade1 => cascade1%next
end do
cascade_set%n_groves = grove
end subroutine cascade_set_assign_groves

```

19.9.14 Generate the phase space file

Generate a complete phase space configuration.

For each flavor assignment: First, all s-channel graphs that can be built up from the outgoing particles. Then we distinguish (1) decay, where we complete the s-channel graphs by connecting to the input line, and (2) scattering, where we now generate t-channel graphs by introducing an incoming particle, and complete this by connecting to the other incoming particle.

After all cascade sets have been generated, merge them into a common set. This eliminates redundancies between flavor assignments.

```

<Cascades: public>+≡
  public :: cascade_set_generate

<Cascades: sub interfaces>+≡
  module subroutine cascade_set_generate &
    (cascade_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay)
    type(cascade_set_t), intent(out) :: cascade_set
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in, n_out
    type(flavor_t), dimension(:, :), intent(in) :: flv
    type(phs_parameters_t), intent(in) :: phs_par
    logical, intent(in) :: fatal_beam_decay
  end subroutine cascade_set_generate

<Cascades: procedures>+≡
  module subroutine cascade_set_generate &
    (cascade_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay)

```

```

type(cascade_set_t), intent(out) :: cascade_set
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in, n_out
type(flavor_t), dimension(:,:), intent(in) :: flv
type(phs_parameters_t), intent(in) :: phs_par
logical, intent(in) :: fatal_beam_decay
type(cascade_set_t), dimension(:), allocatable :: cset
type(cascade_t), pointer :: cascade
integer :: i
if (phase_space_vanishes (phs_par%sqrts, n_in, flv)) return
call cascade_set_init (cascade_set, model, n_in, n_out, phs_par, &
    fatal_beam_decay, flv)
allocate (cset (size (flv, 2)))
do i = 1, size (cset)
    call cascade_set_generate_single (cset(i), &
        model, n_in, n_out, flv(:,i), phs_par, fatal_beam_decay)
    cascade => cset(i)%first_k
    do while (associated (cascade))
        if (cascade%active .and. cascade%complete) then
            call cascade_set_add_copy (cascade_set, cascade)
        end if
        cascade => cascade%next
    end do
    call cascade_set_final (cset(i))
end do
cascade_set%first_k => cascade_set%first
call cascade_set_assign_resonance_hash (cascade_set)
call cascade_set_assign_groves (cascade_set)
end subroutine cascade_set_generate

```

This generates phase space for a single channel, without assigning groves.

(Cascades: procedures)+≡

```

subroutine cascade_set_generate_single (cascade_set, &
    model, n_in, n_out, flv, phs_par, fatal_beam_decay)
type(cascade_set_t), intent(out) :: cascade_set
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in, n_out
type(flavor_t), dimension(:), intent(in) :: flv
type(phs_parameters_t), intent(in) :: phs_par
logical, intent(in) :: fatal_beam_decay
integer :: n11, n12, n21, n22
call cascade_set_init (cascade_set, model, n_in, n_out, phs_par, &
    fatal_beam_decay)
call cascade_set_add_outgoing (cascade_set, flv(n_in+1:))
call cascade_set_generate_s (cascade_set)
select case (n_in)
case(1)
    call cascade_set_add_incoming &
        (cascade_set, n11, n12, n_out + 1, flv(1))
    call cascade_set_generate_decay (cascade_set)
case(2)
    call cascade_set_add_incoming &
        (cascade_set, n11, n12, n_out + 1, flv(2))

```

```

        call cascade_set_add_incoming &
            (cascade_set, n21, n22, n_out + 2, flv(1))
        call cascade_set_generate_t (cascade_set, n_out + 1, n_out + 2)
        call cascade_set_generate_t (cascade_set, n_out + 2, n_out + 1)
        call cascade_set_generate_scattering &
            (cascade_set, n11, n12, n21, n22, n_out + 1, n_out + 2)
        call cascade_set_generate_scattering &
            (cascade_set, n21, n22, n11, n12, n_out + 2, n_out + 1)
    end select
end subroutine cascade_set_generate_single

```

Sanity check: Before anything else is done, check if there could possibly be any phase space.

```

<Cascades: public>+≡
    public :: phase_space_vanishes

<Cascades: sub interfaces>+≡
    module function phase_space_vanishes (sqrts, n_in, flv) result (flag)
        logical :: flag
        real(default), intent(in) :: sqrts
        integer, intent(in) :: n_in
        type(flavor_t), dimension(:, :), intent(in) :: flv
    end function phase_space_vanishes

<Cascades: procedures>+≡
    module function phase_space_vanishes (sqrts, n_in, flv) result (flag)
        logical :: flag
        real(default), intent(in) :: sqrts
        integer, intent(in) :: n_in
        type(flavor_t), dimension(:, :), intent(in) :: flv
        real(default), dimension(:, :), allocatable :: mass
        real(default), dimension(:), allocatable :: mass_in, mass_out
        integer :: n_prt, n_flv, i, j
        flag = .false.
        if (sqrts <= 0) then
            call msg_error ("Phase space vanishes (sqrts must be positive)")
            flag = .true.; return
        end if
        n_prt = size (flv, 1)
        n_flv = size (flv, 2)
        allocate (mass (n_prt, n_flv), mass_in (n_flv), mass_out (n_flv))
        mass = flv%get_mass ()
        mass_in = sum (mass(:, n_in, :), 1)
        mass_out = sum (mass(n_in+1:, :, 1)
        if (any (mass_in > sqrts)) then
            call msg_error ("Mass sum of incoming particles " &
                // "is more than available energy")
            flag = .true.; return
        end if
        if (any (mass_out > sqrts)) then
            call msg_error ("Mass sum of outgoing particles " &
                // "is more than available energy")
            flag = .true.; return
        end if
    end function phase_space_vanishes

```

19.9.15 Return the resonance histories for subtraction

This appears to be essential (re-export of some imported assignment?!)

<Cascades: public>+≡

public :: assignment(=)

Extract the resonance set from a complete cascade.

<Cascades: cascade: TBP>≡

procedure :: extract_resonance_history => cascade_extract_resonance_history

<Cascades: sub interfaces>+≡

```
module subroutine cascade_extract_resonance_history &
  (cascade, res_hist, model, n_out)
  class(cascade_t), intent(in), target :: cascade
  type(resonance_history_t), intent(out) :: res_hist
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_out
end subroutine cascade_extract_resonance_history
```

<Cascades: procedures>+≡

```
module subroutine cascade_extract_resonance_history &
  (cascade, res_hist, model, n_out)
  class(cascade_t), intent(in), target :: cascade
  type(resonance_history_t), intent(out) :: res_hist
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_out
  type(resonance_info_t) :: resonance
  integer :: i, mom_id, pdg
  if (debug_on) call msg_debug2 (D_PHASESPACE, "cascade_extract_resonance_history")
  if (cascade%n_resonances > 0) then
    if (cascade%has_children) then
      if (debug_on) call msg_debug2 (D_PHASESPACE, "cascade has resonances and children")
      do i = 1, size(cascade%tree_resonant)
        if (cascade%tree_resonant (i)) then
          mom_id = cascade%tree (i)
          pdg = cascade%tree_pdg (i)
          call resonance%init (mom_id, pdg, model, n_out)
          if (debug2_active (D_PHASESPACE)) then
            print *, 'D: Adding resonance'
            call resonance%write ()
          end if
          call res_hist%add_resonance (resonance)
        end if
      end do
    end if
  end if
end subroutine cascade_extract_resonance_history
```

<Cascades: public>+≡

public :: cascade_set_get_n_trees

```

<Cascades: sub interfaces>+≡
    module function cascade_set_get_n_trees (cascade_set) result (n)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer :: n
    end function cascade_set_get_n_trees

<Cascades: procedures>+≡
    module function cascade_set_get_n_trees (cascade_set) result (n)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer :: n
        type(cascade_t), pointer :: cascade
        integer :: grove
        if (debug_on) call msg_debug (D_PHASESPACE, "cascade_set_get_n_trees")
        n = 0
        do grove = 1, cascade_set%n_groves
            cascade => cascade_set%first_k
            do while (associated (cascade))
                if (cascade%active .and. cascade%complete) then
                    if (cascade%grove == grove) then
                        n = n + 1
                    end if
                end if
                cascade => cascade%next
            end do
        end do
        if (debug_on) call msg_debug (D_PHASESPACE, "n", n)
    end function cascade_set_get_n_trees

```

Distill the set of resonance histories from the cascade set. The result is an array which contains each valid history exactly once.

```

<Cascades: public>+≡
    public :: cascade_set_get_resonance_histories

<Cascades: sub interfaces>+≡
    module subroutine cascade_set_get_resonance_histories &
        (cascade_set, n_filter, res_hists)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: n_filter
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
            res_hists
    end subroutine cascade_set_get_resonance_histories

<Cascades: procedures>+≡
    module subroutine cascade_set_get_resonance_histories &
        (cascade_set, n_filter, res_hists)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: n_filter
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
            res_hists
        type(resonance_history_t), dimension(:), allocatable :: tmp
        type(cascade_t), pointer :: cascade
        type(resonance_history_t) :: res_hist
        type(resonance_history_set_t) :: res_hist_set
        integer :: grove, i, n_hists
        logical :: included, add_to_list

```

```

if (debug_on) call msg_debug &
    (D_PHASESPACE, "cascade_set_get_resonance_histories")
call res_hist_set%init (n_filter = n_filter)
do grove = 1, cascade_set%n_groves
    cascade => cascade_set%first_k
    do while (associated (cascade))
        if (cascade%active .and. cascade%complete) then
            if (cascade%grove == grove) then
                if (debug_on) call msg_debug2 (D_PHASESPACE, "grove", grove)
                call cascade%extract_resonance_history &
                    (res_hist, cascade_set%model, cascade_set%n_out)
                call res_hist_set%enter (res_hist)
            end if
        end if
        cascade => cascade%next
    end do
end do
call res_hist_set%freeze ()
call res_hist_set%to_array (res_hists)
end subroutine cascade_set_get_resonance_histories

```

19.9.16 Unit tests

Test module, followed by the corresponding implementation module.

<cascades_ut.f90>≡
<File header>

```

module cascades_ut
    use unit_tests
    use cascades_uti

```

<Standard module head>

<Cascades: public test>

contains

<Cascades: test driver>

```

end module cascades_ut

```

<cascades_uti.f90>≡
<File header>

```

module cascades_uti

```

<Use kinds>

<Use strings>

```

    use numeric_utils

```

```

    use flavors

```

```

    use model_data

```

```

    use phs_forests, only: phs_parameters_t

```

```

    use resonances, only: resonance_history_t

```



```

        use cascades

        <Standard module head>

        <Cascades: test declarations>

contains

        <Cascades: tests>

    end module cascades_uti
API: driver for the unit tests below.
<Cascades: public test>≡
    public :: cascades_test
<Cascades: test driver>≡
    subroutine cascades_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Cascades: execute tests>
    end subroutine cascades_test

```

Check cascade setup

Checking the basic setup up of the phase space cascade parameterizations.

```

<Cascades: execute tests>≡
    call test (cascades_1, "cascades_1", &
        "check cascade setup", &
        u, results)
<Cascades: test declarations>≡
    public :: cascades_1
<Cascades: tests>≡
    subroutine cascades_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t), dimension(5,2) :: flv
        type(cascade_set_t) :: cascade_set
        type(phs_parameters_t) :: phs_par

        write (u, "(A)")  "* Test output: cascades_1"
        write (u, "(A)")  "* Purpose: test cascade phase space functions"
        write (u, "(A)")

        write (u, "(A)")  "* Initializing"
        write (u, "(A)")

        call model%init_sm_test ()

        call flv(1,1)%init ( 2, model)
        call flv(2,1)%init (-2, model)
        call flv(3,1)%init ( 1, model)
    end subroutine cascades_1

```

```

call flv(4,1)%init (-1, model)
call flv(5,1)%init (21, model)
call flv(1,2)%init ( 2, model)
call flv(2,2)%init (-2, model)
call flv(3,2)%init ( 2, model)
call flv(4,2)%init (-2, model)
call flv(5,2)%init (21, model)
phs_par%sqrts = 1000._default
phs_par%off_shell = 2

write (u, "(A)")
write (u, "(A)")  "* Generating the cascades"
write (u, "(A)")

call cascade_set_generate (cascade_set, model, 2, 3, flv, phs_par,.true.)
call cascade_set_write (cascade_set, u)
call cascade_set_write_file_format (cascade_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call cascade_set_final (cascade_set)
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades_1"

end subroutine cascades_1

```

Check resonance history

```

<Cascades: execute tests>+≡
  call test(cascades_2, "cascades_2", &
    "Check resonance history", u, results)

<Cascades: test declarations>+≡
  public :: cascades_2

<Cascades: tests>+≡
  subroutine cascades_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(5,1) :: flv
    type(cascade_set_t) :: cascade_set
    type(phs_parameters_t) :: phs_par
    type(resonance_history_t), dimension(:), allocatable :: res_hists
    integer :: n, i
    write (u, "(A)")  "* Test output: cascades_2"
    write (u, "(A)")  "* Purpose: Check resonance history"
    write (u, "(A)")

    write (u, "(A)")  "* Initializing"
    write (u, "(A)")

```

```

call model%init_sm_test ()

call flv(1,1)%init ( 2, model)
call flv(2,1)%init (-2, model)
call flv(3,1)%init ( 1, model)
call flv(4,1)%init (-1, model)
call flv(5,1)%init (22, model)
phs_par%sqrts = 1000._default
phs_par%off_shell = 2

write (u, "(A)")
write (u, "(A)")  /* Generating the cascades"
write (u, "(A)")

call cascade_set_generate (cascade_set, model, 2, 3, flv, phs_par,.true.)
call cascade_set_get_resonance_histories (cascade_set, res_hists = res_hists)
n = cascade_set_get_n_trees (cascade_set)
call assert_equal (u, n, 24, "Number of trees")
do i = 1, size(res_hists)
    call res_hists(i)%write (u)
    write (u, "(A)")
end do

write (u, "(A)")  /* Cleanup"
write (u, "(A)")

call cascade_set_final (cascade_set)
call model%final ()

write (u, "(A)")
write (u, "(A)")  /* Test output end: cascades_2"
end subroutine cascades_2

```

19.10 A lexer for O’Mega’s phase-space output

This module provides three data types. One of them is the type `dag_string_t` which should contain the information of all Feynman diagrams in the factorized form which is provided by O’Mega in its phase-space outout. This output is translated into a string of tokens (in the form of an a array of the type `dag_token_t`) which have a certain meaning. The purpose of this module is only to identify these tokens correctly and to provide some procedures and interfaces which allow us to use these strings in a similar way as variables of the basic character type or the type `iso_varying_string`. Both `character` and `iso_varying_string` have some disadvantages at least if one wants to keep support for some older compiler versions. These can be circumvented by the `dag_string_t` type. Finally the `dag_chain_t` type is used to create a larger string in several steps without always recreating the string, which is done in the form of a simple linked list. In the end one can create a single `dag_string` out of this list, which is more useful.

(cascades2_lexer.f90)≡

```

    <File header>

module cascades2_lexer

    <Use kinds>
        use kinds, only: TC, i8

    <Standard module head>

    <Cascades2 lexer: public>

    <Cascades2 lexer: parameters>

    <Cascades2 lexer: types>

    <Cascades2 lexer: interfaces>

        interface
    <Cascades2 lexer: sub interfaces>
        end interface

end module cascades2_lexer

<cascades2_lexer_sub.f90>≡
    <File header>

    submodule (cascades2_lexer) cascades2_lexer_s

        implicit none

    contains

    <Cascades2 lexer: procedures>

end submodule cascades2_lexer_s

```

This is the token type. By default the variable `type` is `EMPTY_TK` but can obtain other values corresponding to the parameters defined below. The type of the token corresponds to a particular sequence of characters. When the token corresponds to a node of a tree, i.e. some particle in the Feynman diagram, the type is `NODE_TK` and the `particle_name` variable is holding the name of the particle. O'Megas output contains in addition to the particle name some numbers which indicate the external momenta that are flowing through this line. These numbers are translated into a binary code and saved in the variable `bincode`. In this case the number 1 corresponds to a bit set at position 0, 2 corresponds to a bit set at position 1, etc. Instead of numbers which are composed out of several digits, letters are used, i.e. A instead of 10 (bit at position 9), B instead of 11 (bit at position 10), etc.

When the DAG is reconstructed from a `dag_string` which was built from O'Mega's output, this string is modified such that a substring (a set of tokens) is replaced by a single token where the type variable is one of the three parameters `DAG_NODE_TK`, `DAG_OPTIONS_TK` and `DAG_COMBINATION_TK`. These

parameters correspond to the three types `dag_node_t`, `dag_options_t` and `dag_combination_t` (see `cascades2` for more information. In this case, since these objects are organized in arrays, the `index` variable holds the corresponding position in the array.

In any case, we want to be able to reproduce the character string from which a token (or a string) has been created. The variable `char_len` is the length of this string. For tokens with the type `DAG_NODE_TK`, `DAG_OPTIONS_TK` and `DAG_COMBINATION_TK` we use output of the form `<N23>`, `<O23>` or `<C23>` which is useful for debugging the parser. Here 23 is the `index` and N, O or C obviously corresponds to the `type`.

```

<Cascades2 lexer: parameters>≡
    integer, parameter :: PRT_NAME_LEN = 20

<Cascades2 lexer: public>≡
    public :: dag_token_t

<Cascades2 lexer: types>≡
    type :: dag_token_t
        integer :: type = EMPTY_TK
        integer :: char_len = 0
        integer(TC) :: bincode = 0
        character(len=PRT_NAME_LEN) :: particle_name=""
        integer :: index = 0
    contains
        <Cascades2 lexer: dag token: TBP>
    end type dag_token_t

```

This is the string type. It also holds the number of characters in the corresponding character string. It contains an array of tokens. If the `dag_string` is constructed using the type `dag_chain_t`, which creates a linked list, we also need the pointer `next`.

```

<Cascades2 lexer: public>+≡
    public :: dag_string_t

<Cascades2 lexer: types>+≡
    type :: dag_string_t
        integer :: char_len = 0
        type(dag_token_t), dimension(:), allocatable :: t
        type(dag_string_t), pointer :: next => null ()
    contains
        <Cascades2 lexer: dag string: TBP>
    end type dag_string_t

```

This is the chain of `dag_strings`. It allows us to construct a large string by appending new strings to the linked list, which can later be merged to a single string. This is very useful because the file written by O'Mega contains large strings where each string contains all Feynman diagrams in a factorized form, but these large strings are cut into several pieces and distributed over many lines. As the file can become large, rewriting a new `dag_string` (or `iso_varying_string`) would consume more and more time with each additional line. For recreating a single `dag_string` out of this chain, we need the total character length and the sum of all sizes of the `dag_token` arrays `t`.

```

<Cascades2 lexer: public>+≡

```

```

    public :: dag_chain_t
  <Cascades2 lexer: types>+≡
    type :: dag_chain_t
      integer :: char_len = 0
      integer :: t_size = 0
      type(dag_string_t), pointer :: first => null ()
      type(dag_string_t), pointer :: last => null ()
    contains
      <Cascades2 lexer: dag chain: TBP>
    end type dag_chain_t

```

We define two parameters holding the characters corresponding to a backslash and a blanc space.

```

  <Cascades2 lexer: parameters>+≡
    character(len=1), parameter, public :: BACKSLASH_CHAR = "\"
    character(len=1), parameter :: BLANC_CHAR = " "

```

These are the parameters which correspond to meaningful types of token.

```

  <Cascades2 lexer: parameters>+≡
    integer, parameter, public :: NEW_LINE_TK = -2
    integer, parameter :: BLANC_SPACE_TK = -1
    integer, parameter :: EMPTY_TK = 0
    integer, parameter, public :: NODE_TK = 1
    integer, parameter, public :: DAG_NODE_TK = 2
    integer, parameter, public :: DAG_OPTIONS_TK = 3
    integer, parameter, public :: DAG_COMBINATION_TK = 4
    integer, parameter, public :: COLON_TK = 11
    integer, parameter, public :: COMMA_TK = 12
    integer, parameter, public :: VERTICAL_BAR_TK = 13
    integer, parameter, public :: OPEN_PAR_TK = 21
    integer, parameter, public :: CLOSED_PAR_TK = 22
    integer, parameter, public :: OPEN_CURLY_TK = 31
    integer, parameter, public :: CLOSED_CURLY_TK = 32

```

Different sorts of assignment. This contains the conversion of a character variable into a dag_token or dag_string.

```

  <Cascades2 lexer: public>+≡
    public :: assignment (=)

  <Cascades2 lexer: interfaces>≡
    interface assignment (=)
      module procedure dag_token_assign_from_char_string
      module procedure dag_token_assign_from_dag_token
      module procedure dag_string_assign_from_dag_token
      module procedure dag_string_assign_from_char_string
      module procedure dag_string_assign_from_dag_string
      module procedure dag_string_assign_from_dag_token_array
    end interface assignment (=)

  <Cascades2 lexer: dag token: TBP>≡
    procedure :: init_dag_object_token => dag_token_init_dag_object_token

```

```

<Cascades2 lexer: sub interfaces>≡
  module subroutine dag_token_init_dag_object_token (dag_token, type, index)
    class(dag_token_t), intent(out) :: dag_token
    integer, intent(in) :: index
    integer :: type
  end subroutine dag_token_init_dag_object_token

```

```

<Cascades2 lexer: procedures>≡
  module subroutine dag_token_init_dag_object_token (dag_token, type, index)
    class(dag_token_t), intent(out) :: dag_token
    integer, intent(in) :: index
    integer :: type
    dag_token%type = type
    dag_token%char_len = integer_n_dec_digits (index) + 3
    dag_token%index = index
  contains
    function integer_n_dec_digits (number) result (n_digits)
      integer, intent(in) :: number
      integer :: n_digits
      integer :: div_number
      n_digits = 0
      div_number = number
      do
        div_number = div_number / 10
        n_digits = n_digits + 1
        if (div_number == 0) exit
      end do
    end function integer_n_dec_digits
  end subroutine dag_token_init_dag_object_token

```

```

<Cascades2 lexer: sub interfaces>+≡
  elemental module subroutine dag_token_assign_from_char_string &
    (dag_token, char_string)
    type(dag_token_t), intent(out) :: dag_token
    character(len=*), intent(in) :: char_string
  end subroutine dag_token_assign_from_char_string

```

```

<Cascades2 lexer: procedures>+≡
  elemental module subroutine dag_token_assign_from_char_string &
    (dag_token, char_string)
    type(dag_token_t), intent(out) :: dag_token
    character(len=*), intent(in) :: char_string
    integer :: i, j
    logical :: set_bincode
    integer :: bit_pos
    character(len=10) :: index_char
    dag_token%char_len = len (char_string)
    if (dag_token%char_len == 1) then
      select case (char_string(1:1))
        case (BACKSLASH_CHAR)
          dag_token%type = NEW_LINE_TK
        case (" ")
          dag_token%type = BLANC_SPACE_TK
        case (":")
          dag_token%type = COLON_TK

```

```

case (",")
    dag_token%type = COMMA_TK
case ("|")
    dag_token%type = VERTICAL_BAR_TK
case "("
    dag_token%type = OPEN_PAR_TK
case (")"
    dag_token%type = CLOSED_PAR_TK
case "{"
    dag_token%type = OPEN_CURLY_TK
case "}"
    dag_token%type = CLOSED_CURLY_TK
end select
else if (char_string(1:1) == "<") then
    select case (char_string(2:2))
        case ("N")
            dag_token%type = DAG_NODE_TK
        case ("O")
            dag_token%type = DAG_OPTIONS_TK
        case ("C")
            dag_token%type = DAG_COMBINATION_TK
    end select
    read(char_string(3:dag_token%char_len-1), fmt="(I10)") dag_token%index
else
    dag_token%bincode = 0
    set_bincode = .false.
    do i=1, dag_token%char_len
        select case (char_string(i:i))
            case ("["
                dag_token%type = NODE_TK
                if (i > 1) then
                    do j = 1, i - 1
                        dag_token%particle_name(j:j) = char_string(j:j)
                    end do
                end if
                set_bincode = .true.
            case ("]")
                set_bincode = .false.
            case default
                dag_token%type = NODE_TK
                if (set_bincode) then
                    select case (char_string(i:i))
                        case ("1", "2", "3", "4", "5", "6", "7", "8", "9")
                            read(char_string(i:i), fmt="(I1)") bit_pos
                        case ("A")
                            bit_pos = 10
                        case ("B")
                            bit_pos = 11
                        case ("C")
                            bit_pos = 12
                    end select
                    dag_token%bincode = ibset(dag_token%bincode, bit_pos - 1)
                end if
            end select
        end select
    end do
end select

```



```

        if (dag_token%type /= NODE_TK) exit
    end do
end if
end subroutine dag_token_assign_from_char_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module subroutine dag_token_assign_from_dag_token &
        (token_out, token_in)
        type(dag_token_t), intent(out) :: token_out
        type(dag_token_t), intent(in) :: token_in
    end subroutine dag_token_assign_from_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module subroutine dag_token_assign_from_dag_token &
        (token_out, token_in)
        type(dag_token_t), intent(out) :: token_out
        type(dag_token_t), intent(in) :: token_in
        token_out%type = token_in%type
        token_out%char_len = token_in%char_len
        token_out%bincode = token_in%bincode
        token_out%particle_name = token_in%particle_name
        token_out%index = token_in%index
    end subroutine dag_token_assign_from_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module subroutine dag_string_assign_from_dag_token &
        (dag_string, dag_token)
        type(dag_string_t), intent(out) :: dag_string
        type(dag_token_t), intent(in) :: dag_token
    end subroutine dag_string_assign_from_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module subroutine dag_string_assign_from_dag_token &
        (dag_string, dag_token)
        type(dag_string_t), intent(out) :: dag_string
        type(dag_token_t), intent(in) :: dag_token
        allocate (dag_string%t(1))
        dag_string%t(1) = dag_token
        dag_string%char_len = dag_token%char_len
    end subroutine dag_string_assign_from_dag_token

<Cascades2 lexer: sub interfaces>+≡
    module subroutine dag_string_assign_from_dag_token_array &
        (dag_string, dag_token)
        type(dag_string_t), intent(out) :: dag_string
        type(dag_token_t), dimension(:), intent(in) :: dag_token
    end subroutine dag_string_assign_from_dag_token_array

<Cascades2 lexer: procedures>+≡
    module subroutine dag_string_assign_from_dag_token_array &
        (dag_string, dag_token)
        type(dag_string_t), intent(out) :: dag_string
        type(dag_token_t), dimension(:), intent(in) :: dag_token
        allocate (dag_string%t(size(dag_token)))
        dag_string%t = dag_token

```

```

dag_string%char_len = sum(dag_token%char_len)
end subroutine dag_string_assign_from_dag_token_array

```

<Cascades2 lexer: sub interfaces>+≡

```

elemental module subroutine dag_string_assign_from_char_string &
(dag_string, char_string)
type(dag_string_t), intent(out) :: dag_string
character(len=*), intent(in) :: char_string
end subroutine dag_string_assign_from_char_string

```

<Cascades2 lexer: procedures>+≡

```

elemental module subroutine dag_string_assign_from_char_string &
(dag_string, char_string)
type(dag_string_t), intent(out) :: dag_string
character(len=*), intent(in) :: char_string
type(dag_token_t), dimension(:), allocatable :: token
integer :: token_pos
integer :: i
character(len=len(char_string)) :: node_char
integer :: node_char_len
node_char = ""
dag_string%char_len = len (char_string)
if (dag_string%char_len > 0) then
allocate (token(dag_string%char_len))
token_pos = 0
node_char_len = 0
do i=1, dag_string%char_len
select case (char_string(i:i))
case (BACKSLASH_CHAR, " ", ":", ",", "|", "(", ")", "{", "}")
if (node_char_len > 0) then
token_pos = token_pos + 1
token(token_pos) = node_char(:node_char_len)
node_char_len = 0
end if
token_pos = token_pos + 1
token(token_pos) = char_string(i:i)
case default
node_char_len = node_char_len + 1
node_char(node_char_len:node_char_len) = char_string(i:i)
end select
end do
if (node_char_len > 0) then
token_pos = token_pos + 1
token(token_pos) = node_char(:node_char_len)
end if
if (token_pos > 0) then
allocate (dag_string%t(token_pos))
dag_string%t = token(:token_pos)
deallocate (token)
end if
end if
end subroutine dag_string_assign_from_char_string

```

<Cascades2 lexer: sub interfaces>+≡

```

        elemental module subroutine dag_string_assign_from_dag_string &
            (string_out, string_in)
            type(dag_string_t), intent(out) :: string_out
            type(dag_string_t), intent(in) :: string_in
        end subroutine dag_string_assign_from_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module subroutine dag_string_assign_from_dag_string &
        (string_out, string_in)
        type(dag_string_t), intent(out) :: string_out
        type(dag_string_t), intent(in) :: string_in
        if (allocated (string_in%t)) then
            allocate (string_out%t (size(string_in%t)))
            string_out%t = string_in%t
        end if
        string_out%char_len = string_in%char_len
    end subroutine dag_string_assign_from_dag_string

Concatenate strings/tokens. The result is always a dag_string.

<Cascades2 lexer: public>+≡
    public :: operator (//)

<Cascades2 lexer: interfaces>+≡
    interface operator (//)
        module procedure concat_dag_token_dag_token
        module procedure concat_dag_string_dag_token
        module procedure concat_dag_token_dag_string
        module procedure concat_dag_string_dag_string
    end interface operator (//)

<Cascades2 lexer: sub interfaces>+≡
    module function concat_dag_token_dag_token &
        (token1, token2) result (res_string)
        type(dag_token_t), intent(in) :: token1, token2
        type(dag_string_t) :: res_string
    end function concat_dag_token_dag_token

<Cascades2 lexer: procedures>+≡
    module function concat_dag_token_dag_token &
        (token1, token2) result (res_string)
        type(dag_token_t), intent(in) :: token1, token2
        type(dag_string_t) :: res_string
        if (token1%type == EMPTY_TK) then
            call dag_string_assign_from_dag_token (res_string, token2)
        else if (token2%type == EMPTY_TK) then
            call dag_string_assign_from_dag_token (res_string, token1)
        else
            allocate (res_string%t(2))
            res_string%t(1) = token1
            res_string%t(2) = token2
            res_string%char_len = token1%char_len + token2%char_len
        end if
    end function concat_dag_token_dag_token

```

```

<Cascades2 lexer: sub interfaces>+≡
    module function concat_dag_string_dag_token &
        (dag_string, dag_token) result (res_string)
        type(dag_string_t), intent(in) :: dag_string
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t) :: res_string
    end function concat_dag_string_dag_token

<Cascades2 lexer: procedures>+≡
    module function concat_dag_string_dag_token &
        (dag_string, dag_token) result (res_string)
        type(dag_string_t), intent(in) :: dag_string
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t) :: res_string
        integer :: t_size
        if (dag_string%char_len == 0) then
            call dag_string_assign_from_dag_token (res_string, dag_token)
        else if (dag_token%type == EMPTY_TK) then
            res_string = dag_string
        else
            t_size = size (dag_string%t)
            allocate (res_string%t(t_size+1))
            res_string%t(:t_size) = dag_string%t
            res_string%t(t_size+1) = dag_token
            res_string%char_len = dag_string%char_len + dag_token%char_len
        end if
    end function concat_dag_string_dag_token

<Cascades2 lexer: sub interfaces>+≡
    module function concat_dag_token_dag_string &
        (dag_token, dag_string) result (res_string)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        type(dag_string_t) :: res_string
        integer :: t_size
    end function concat_dag_token_dag_string

<Cascades2 lexer: procedures>+≡
    module function concat_dag_token_dag_string &
        (dag_token, dag_string) result (res_string)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        type(dag_string_t) :: res_string
        integer :: t_size
        if (dag_token%type == EMPTY_TK) then
            res_string = dag_string
        else if (dag_string%char_len == 0) then
            call dag_string_assign_from_dag_token (res_string, dag_token)
        else
            t_size = size (dag_string%t)
            allocate (res_string%t(t_size+1))
            res_string%t(2:t_size+1) = dag_string%t
            res_string%t(1) = dag_token
            res_string%char_len = dag_token%char_len + dag_string%char_len
        end if

```

```

end function concat_dag_token_dag_string

<Cascades2 lexer: sub interfaces>+=
  module function concat_dag_string_dag_string &
    (string1, string2) result (res_string)
    type(dag_string_t), intent(in) :: string1, string2
    type(dag_string_t) :: res_string
  end function concat_dag_string_dag_string

<Cascades2 lexer: procedures>+=
  module function concat_dag_string_dag_string &
    (string1, string2) result (res_string)
    type(dag_string_t), intent(in) :: string1, string2
    type(dag_string_t) :: res_string
    integer :: t1_size, t2_size, t_size
    if (string1%char_len == 0) then
      res_string = string2
    else if (string2%char_len == 0) then
      res_string = string1
    else
      t1_size = size (string1%t)
      t2_size = size (string2%t)
      t_size = t1_size + t2_size
      if (t_size > 0) then
        allocate (res_string%t(t_size))
        res_string%t(:t1_size) = string1%t
        res_string%t(t1_size+1:) = string2%t
        res_string%char_len = string1%char_len + string2%char_len
      end if
    end if
  end function concat_dag_string_dag_string

```

Compare strings/tokens/characters. Each character is relevant, including all blanc spaces. An exception is the `newline` character which is not treated by the types used in this module (not to confused with the type parameter `NEW_LINE_TK` which corresponds to the backslash character and simply tells us that the string continues on the next line in the file).

```

<Cascades2 lexer: public>+=
  public :: operator (==)

<Cascades2 lexer: interfaces>+=
  interface operator (==)
    module procedure dag_token_eq_dag_token
    module procedure dag_string_eq_dag_string
    module procedure dag_token_eq_dag_string
    module procedure dag_string_eq_dag_token
    module procedure dag_token_eq_char_string
    module procedure char_string_eq_dag_token
    module procedure dag_string_eq_char_string
    module procedure char_string_eq_dag_string
  end interface operator (==)

```

```

<Cascades2 lexer: sub interfaces>+=

```

```

        elemental module function dag_token_eq_dag_token &
            (token1, token2) result (flag)
            type(dag_token_t), intent(in) :: token1, token2
            logical :: flag
        end function dag_token_eq_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_eq_dag_token &
        (token1, token2) result (flag)
        type(dag_token_t), intent(in) :: token1, token2
        logical :: flag
        flag = (token1%type == token2%type) .and. &
            (token1%char_len == token2%char_len) .and. &
            (token1%bincode == token2%bincode) .and. &
            (token1%index == token2%index) .and. &
            (token1%particle_name == token2%particle_name)
    end function dag_token_eq_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_eq_dag_string &
        (string1, string2) result (flag)
        type(dag_string_t), intent(in) :: string1, string2
        logical :: flag
    end function dag_string_eq_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_eq_dag_string &
        (string1, string2) result (flag)
        type(dag_string_t), intent(in) :: string1, string2
        logical :: flag
        flag = (string1%char_len == string2%char_len) .and. &
            (allocated (string1%t) .eqv. allocated (string2%t))
        if (flag) then
            if (allocated (string1%t)) flag = all (string1%t == string2%t)
        end if
    end function dag_string_eq_dag_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_token_eq_dag_string &
        (dag_token, dag_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
    end function dag_token_eq_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_eq_dag_string &
        (dag_token, dag_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
        flag = size (dag_string%t) == 1 .and. &
            dag_string%char_len == dag_token%char_len
        if (flag) flag = (dag_string%t(1) == dag_token)
    end function dag_token_eq_dag_string

```

```

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_eq_dag_token &
        (dag_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
    end function dag_string_eq_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_eq_dag_token &
        (dag_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
        flag = (dag_token == dag_string)
    end function dag_string_eq_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_token_eq_char_string &
        (dag_token, char_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function dag_token_eq_char_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_eq_char_string &
        (dag_token, char_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = (char (dag_token) == char_string)
    end function dag_token_eq_char_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function char_string_eq_dag_token &
        (char_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function char_string_eq_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function char_string_eq_dag_token &
        (char_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = (char (dag_token) == char_string)
    end function char_string_eq_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_eq_char_string &
        (dag_string, char_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string

```

```

        character(len=*), intent(in) :: char_string
        logical :: flag
    end function dag_string_eq_char_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_eq_char_string &
        (dag_string, char_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = (char (dag_string) == char_string)
    end function dag_string_eq_char_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function char_string_eq_dag_string &
        (char_string, dag_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function char_string_eq_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function char_string_eq_dag_string &
        (char_string, dag_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = (char (dag_string) == char_string)
    end function char_string_eq_dag_string

<Cascades2 lexer: public>+≡
    public :: operator (/=)

<Cascades2 lexer: interfaces>+≡
    interface operator (/=)
        module procedure dag_token_ne_dag_token
        module procedure dag_string_ne_dag_string
        module procedure dag_token_ne_dag_string
        module procedure dag_string_ne_dag_token
        module procedure dag_token_ne_char_string
        module procedure char_string_ne_dag_token
        module procedure dag_string_ne_char_string
        module procedure char_string_ne_dag_string
    end interface operator (/=)

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_token_ne_dag_token &
        (token1, token2) result (flag)
        type(dag_token_t), intent(in) :: token1, token2
        logical :: flag
    end function dag_token_ne_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_ne_dag_token &
        (token1, token2) result (flag)

```



```

    type(dag_token_t), intent(in) :: token1, token2
    logical :: flag
    flag = .not. (token1 == token2)
end function dag_token_ne_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_ne_dag_string &
        (string1, string2) result (flag)
        type(dag_string_t), intent(in) :: string1, string2
        logical :: flag
    end function dag_string_ne_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_ne_dag_string &
        (string1, string2) result (flag)
        type(dag_string_t), intent(in) :: string1, string2
        logical :: flag
        flag = .not. (string1 == string2)
    end function dag_string_ne_dag_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_token_ne_dag_string &
        (dag_token, dag_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
    end function dag_token_ne_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_ne_dag_string &
        (dag_token, dag_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
        flag = .not. (dag_token == dag_string)
    end function dag_token_ne_dag_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_ne_dag_token &
        (dag_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
    end function dag_string_ne_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_ne_dag_token &
        (dag_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        type(dag_string_t), intent(in) :: dag_string
        logical :: flag
        flag = .not. (dag_string == dag_token)
    end function dag_string_ne_dag_token

```

```

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_token_ne_char_string &
        (dag_token, char_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function dag_token_ne_char_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_token_ne_char_string &
        (dag_token, char_string) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = .not. (dag_token == char_string)
    end function dag_token_ne_char_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function char_string_ne_dag_token &
        (char_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function char_string_ne_dag_token

<Cascades2 lexer: procedures>+≡
    elemental module function char_string_ne_dag_token &
        (char_string, dag_token) result (flag)
        type(dag_token_t), intent(in) :: dag_token
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = .not. (char_string == dag_token)
    end function char_string_ne_dag_token

<Cascades2 lexer: sub interfaces>+≡
    elemental module function dag_string_ne_char_string &
        (dag_string, char_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
    end function dag_string_ne_char_string

<Cascades2 lexer: procedures>+≡
    elemental module function dag_string_ne_char_string &
        (dag_string, char_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = .not. (dag_string == char_string)
    end function dag_string_ne_char_string

<Cascades2 lexer: sub interfaces>+≡
    elemental module function char_string_ne_dag_string &
        (char_string, dag_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string

```

```

        character(len=*), intent(in) :: char_string
        logical :: flag
    end function char_string_ne_dag_string

<Cascades2 lexer: procedures>+≡
    elemental module function char_string_ne_dag_string &
        (char_string, dag_string) result (flag)
        type(dag_string_t), intent(in) :: dag_string
        character(len=*), intent(in) :: char_string
        logical :: flag
        flag = .not. (char_string == dag_string)
    end function char_string_ne_dag_string

Convert a dag_token or dag_string to character.

<Cascades2 lexer: public>+≡
    public :: char

<Cascades2 lexer: interfaces>+≡
    interface char
        module procedure char_dag_token
        module procedure char_dag_string
    end interface char

<Cascades2 lexer: sub interfaces>+≡
    pure module function char_dag_token (dag_token) result (char_string)
        type(dag_token_t), intent(in) :: dag_token
        character (dag_token%char_len) :: char_string
    end function char_dag_token

<Cascades2 lexer: procedures>+≡
    pure module function char_dag_token (dag_token) result (char_string)
        type(dag_token_t), intent(in) :: dag_token
        character (dag_token%char_len) :: char_string
        integer :: i
        integer :: name_len
        integer :: bc_pos
        integer :: n_digits
        character(len=9) :: fmt_spec
        select case (dag_token%type)
        case (EMPTY_TK)
            char_string = ""
        case (NEW_LINE_TK)
            char_string = BACKSLASH_CHAR
        case (BLANC_SPACE_TK)
            char_string = " "
        case (COLON_TK)
            char_string = ":"
        case (COMMA_TK)
            char_string = ","
        case (VERTICAL_BAR_TK)
            char_string = "|"
        case (OPEN_PAR_TK)
            char_string = "("
        case (CLOSED_PAR_TK)
            char_string = ")"

```

```

case (OPEN_CURLY_TK)
    char_string = "{"
case (CLOSED_CURLY_TK)
    char_string = "}"
case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
    n_digits = dag_token%char_len - 3
    fmt_spec = ""
    if (n_digits > 9) then
        write (fmt_spec, fmt="(A,I2,A)") "(A,I", n_digits, ",A)"
    else
        write (fmt_spec, fmt="(A,I1,A)") "(A,I", n_digits, ",A)"
    end if
    select case (dag_token%type)
        case (DAG_NODE_TK)
            write (char_string, fmt=fmt_spec) "<N", dag_token%index, ">"
        case (DAG_OPTIONS_TK)
            write (char_string, fmt=fmt_spec) "<O", dag_token%index, ">"
        case (DAG_COMBINATION_TK)
            write (char_string, fmt=fmt_spec) "<C", dag_token%index, ">"
        end select
case (NODE_TK)
    name_len = len_trim (dag_token%particle_name)
    char_string = dag_token%particle_name
    bc_pos = name_len + 1
    char_string(bc_pos:bc_pos) = "["
    do i=0, bit_size (dag_token%bincode) - 1
        if (btest (dag_token%bincode, i)) then
            bc_pos = bc_pos + 1
            select case (i)
                case (0, 1, 2, 3, 4, 5, 6, 7, 8)
                    write (char_string(bc_pos:bc_pos), fmt="(I1)") i + 1
                case (9)
                    write (char_string(bc_pos:bc_pos), fmt="(A1)") "A"
                case (10)
                    write (char_string(bc_pos:bc_pos), fmt="(A1)") "B"
                case (11)
                    write (char_string(bc_pos:bc_pos), fmt="(A1)") "C"
            end select
            bc_pos = bc_pos + 1
        if (bc_pos == dag_token%char_len) then
            write (char_string(bc_pos:bc_pos), fmt="(A1)") "]"
            return
        else
            write (char_string(bc_pos:bc_pos), fmt="(A1)") "/"
        end if
    end if
    end do
end select
end function char_dag_token

```

<Cascades2 lexer: sub interfaces>+≡

```

pure module function char_dag_string (dag_string) result (char_string)
    type(dag_string_t), intent(in) :: dag_string
    character (dag_string%char_len) :: char_string

```

```

        end function char_dag_string
<Cascades2 lexer: procedures>+≡
pure module function char_dag_string (dag_string) result (char_string)
    type(dag_string_t), intent(in) :: dag_string
    character (dag_string%char_len) :: char_string
    integer :: pos
    integer :: i
    char_string = ""
    pos = 0
    do i=1, size(dag_string%t)
        char_string(pos+1:pos+dag_string%t(i)%char_len) = char (dag_string%t(i))
        pos = pos + dag_string%t(i)%char_len
    end do
end function char_dag_string

```

Remove all tokens which are irrelevant for parsing. These are of type NEW_LINE_TK, BLANC_SPACE_TK and EMTPTY_TK.

```

<Cascades2 lexer: dag string: TBP>≡
    procedure :: clean => dag_string_clean

<Cascades2 lexer: sub interfaces>+≡
    module subroutine dag_string_clean (dag_string)
        class(dag_string_t), intent(inout) :: dag_string
    end subroutine dag_string_clean

<Cascades2 lexer: procedures>+≡
module subroutine dag_string_clean (dag_string)
    class(dag_string_t), intent(inout) :: dag_string
    type(dag_token_t), dimension(:), allocatable :: tmp_token
    integer :: n_keep
    integer :: i
    n_keep = 0
    dag_string%char_len = 0
    allocate (tmp_token (size(dag_string%t)))
    do i=1, size (dag_string%t)
        select case (dag_string%t(i)%type)
            case(NEW_LINE_TK, BLANC_SPACE_TK, EMPTY_TK)
            case default
                n_keep = n_keep + 1
                tmp_token(n_keep) = dag_string%t(i)
                dag_string%char_len = dag_string%char_len + dag_string%t(i)%char_len
        end select
    end do
    deallocate (dag_string%t)
    allocate (dag_string%t(n_keep))
    dag_string%t = tmp_token(:n_keep)
end subroutine dag_string_clean

```

If we operate explicitly on the token array `t` of a `dag_string`, the variable `char_len` is not automatically modified. It can however be determined afterwards using the following subroutine.

```

<Cascades2 lexer: dag string: TBP>+≡
    procedure :: update_char_len => dag_string_update_char_len

```

```

<Cascades2 lexer: sub interfaces>+≡
    module subroutine dag_string_update_char_len (dag_string)
        class(dag_string_t), intent(inout) :: dag_string
        end subroutine dag_string_update_char_len
<Cascades2 lexer: procedures>+≡
    module subroutine dag_string_update_char_len (dag_string)
        class(dag_string_t), intent(inout) :: dag_string
        integer :: char_len
        integer :: i
        char_len = 0
        if (allocated (dag_string%t)) then
            do i=1, size (dag_string%t)
                char_len = char_len + dag_string%t(i)%char_len
            end do
        end if
        dag_string%char_len = char_len
    end subroutine dag_string_update_char_len

```

Append a `dag_string` to a `dag_chain`. The argument `char_string` is of type `character` because the subroutine is used for reading from the file produced by O'Mega which is first read line by line to a character variable.

```

<Cascades2 lexer: dag chain: TBP>≡
    procedure :: append => dag_chain_append_string
<Cascades2 lexer: sub interfaces>+≡
    module subroutine dag_chain_append_string (dag_chain, char_string)
        class(dag_chain_t), intent(inout) :: dag_chain
        character(len=*), intent(in) :: char_string
        end subroutine dag_chain_append_string
<Cascades2 lexer: procedures>+≡
    module subroutine dag_chain_append_string (dag_chain, char_string)
        class(dag_chain_t), intent(inout) :: dag_chain
        character(len=*), intent(in) :: char_string
        if (.not. associated (dag_chain%first)) then
            allocate (dag_chain%first)
            dag_chain%last => dag_chain%first
        else
            allocate (dag_chain%last%next)
            dag_chain%last => dag_chain%last%next
        end if
        dag_chain%last = char_string
        dag_chain%char_len = dag_chain%char_len + dag_chain%last%char_len
        dag_chain%t_size = dag_chain%t_size + size (dag_chain%last%t)
    end subroutine dag_chain_append_string

```

Reduce the linked list of `dag_string` objects which are attached to a given `dag_chain` object to a single `dag_string`.

```

<Cascades2 lexer: dag chain: TBP>+≡
    procedure :: compress => dag_chain_compress
<Cascades2 lexer: sub interfaces>+≡
    module subroutine dag_chain_compress (dag_chain)
        class(dag_chain_t), intent(inout) :: dag_chain
        end subroutine dag_chain_compress

```

```

<Cascades2 lexer: procedures>+≡
module subroutine dag_chain_compress (dag_chain)
  class(dag_chain_t), intent(inout) :: dag_chain
  type(dag_string_t), pointer :: current
  type(dag_string_t), pointer :: remove
  integer :: filled_t
  current => dag_chain%first
  dag_chain%first => null ()
  allocate (dag_chain%first)
  dag_chain%last => dag_chain%first
  dag_chain%first%char_len = dag_chain%char_len
  allocate (dag_chain%first%t (dag_chain%t_size))
  filled_t = 0
  do while (associated (current))
    dag_chain%first%t(filled_t+1:filled_t+size(current%t)) = current%t
    filled_t = filled_t + size (current%t)
    remove => current
    current => current%next
    deallocate (remove)
  end do
end subroutine dag_chain_compress

```

Finalizer for dag_string_t.

```

<Cascades2 lexer: dag string: TBP>+≡
  procedure :: final => dag_string_final

<Cascades2 lexer: sub interfaces>+≡
  module subroutine dag_string_final (dag_string)
    class(dag_string_t), intent(inout) :: dag_string
  end subroutine dag_string_final

<Cascades2 lexer: procedures>+≡
module subroutine dag_string_final (dag_string)
  class(dag_string_t), intent(inout) :: dag_string
  if (allocated (dag_string%t)) deallocate (dag_string%t)
  dag_string%next => null ()
end subroutine dag_string_final

```

Finalizer for dag_chain_t.

```

<Cascades2 lexer: dag chain: TBP>+≡
  procedure :: final => dag_chain_final

<Cascades2 lexer: sub interfaces>+≡
  module subroutine dag_chain_final (dag_chain)
    class(dag_chain_t), intent(inout) :: dag_chain
  end subroutine dag_chain_final

<Cascades2 lexer: procedures>+≡
module subroutine dag_chain_final (dag_chain)
  class(dag_chain_t), intent(inout) :: dag_chain
  type(dag_string_t), pointer :: current
  current => dag_chain%first
  do while (associated (current))
    dag_chain%first => dag_chain%first%next
    call current%final ()
  end do
end subroutine dag_chain_final

```

```

        deallocate (current)
        current => dag_chain%first
    end do
    dag_chain%last => null ()
end subroutine dag_chain_final

<cascades2_lexer_ut.f90>≡
<File header>

module cascades2_lexer_ut
    use unit_tests
    use cascades2_lexer_util

    <Standard module head>

    <Cascades2 lexer: public test>

contains

    <Cascades2 lexer: test driver>

end module cascades2_lexer_ut

<cascades2_lexer_util.f90>≡
<File header>

module cascades2_lexer_util

    <Use kinds>
    <Use strings>
    use numeric_utils

    use cascades2_lexer

    <Standard module head>

    <Cascades2 lexer: test declarations>

contains

    <Cascades2 lexer: tests>

end module cascades2_lexer_util
API: driver for the unit tests below.
<Cascades2 lexer: public test>≡
    public :: cascades2_lexer_test
<Cascades2 lexer: test driver>≡
    subroutine cascades2_lexer_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Cascades2 lexer: execute tests>
    end subroutine cascades2_lexer_test

```



```

<Cascades2 lexer: execute tests>≡
  call test (cascades2_lexer_1, "cascades2_lexer_1", &
    "make phase-space", u, results)

<Cascades2 lexer: test declarations>≡
  public :: cascades2_lexer_1

<Cascades2 lexer: tests>≡
  subroutine cascades2_lexer_1 (u)
    integer, intent(in) :: u
    integer :: u_in = 8
    character(len=300) :: line
    integer :: stat
    logical :: fail
    type(dag_string_t) :: dag_string

    write (u, "(A)")  "* Test output: cascades2_lexer_1"
    write (u, "(A)")  "* Purpose: read lines of 0'Mega's phase space output, translate"
    write (u, "(A)")  "*           to dag_string, retranslate to character string and"
    write (u, "(A)")  "*           compare"
    write (u, "(A)")

    open (unit=u_in, file="cascades2_lexer_1.fds", status='old', action='read')

    stat = 0
    fail = .false.
    read (unit=u_in, fmt="(A)", iostat=stat) line
    do while (stat == 0 .and. .not. fail)
      read (unit=u_in, fmt="(A)", iostat=stat) line
      if (stat /= 0) exit
      dag_string = line
      fail = (char(dag_string) /= line)
    end do
    if (fail) then
      write (u, "(A)")  "* Test result: Test failed!"
    else
      write (u, "(A)")  "* Test result: Test passed"
    end if

    close (u_in)
    write (u, *)
    write (u, "(A)")  "* Test output end: cascades2_lexer_1"
  end subroutine cascades2_lexer_1

```

@

19.11 An alternative cascades module

This module might replace the module `cascades`, which generates suitable phase space parametrizations and generates the phase space file. The mappings, as well as the criteria to determine these, do not change.

The advantage of this module is that it makes use of the 0'Mega matrix element generator which provides the relevant Feynman diagrams (the ones

which can be constructed only from 3-vertices). In principle, the construction of these diagrams is also one of the tasks of the existing `cascades` module, in which the diagrams would correspond to a set of cascades. It starts by creating cascades which correspond to the outgoing particles. These are combined to a new cascade using the vertices of the model. In this way, since each cascade knows the daughter cascades from which it is built, complete Feynman diagrams are represented by sets of cascades, as soon as the existing cascades can be recombined with the incoming particle(s).

In this module, the Feynman diagrams are represented by the type `feyngraph_t`, which represents the Feynman diagrams as a tree of nodes. The object which contains the necessary kinematical information to determine mappings, and hence sensible phase space parametrizations is of another type, called `kingraph_t`, which is built from a corresponding `feyngraph` object.

There are two types of output which can be produced by `O'Mega` and are potentially relevant here. The first type contains all tree diagrams for the process under consideration, where each line of the output corresponds to one Feynman diagram. This output is easy to read, but can be very large, depending on the number of particles involved in the process. Moreover, it repeats substructures of the diagrams which are part of more than one diagram. One could in principle work with this output and construct a `feyngraph` from each line, if allowed, i.e. if there are only 3-vertices.

The other output contains also all of these Feynman diagrams, but in a factorized form. This means that the substructures which appear in several Feynman diagrams, are written only once, if possible. This leads to a much shorter input file, which speeds up the parsing process. Furthermore it makes it possible to reconstruct the `feyngraphs` in such a way that the calculations concerning subdiagrams which reappear in other `feyngraphs` have to be performed only once. This is already the case in the existing `cascades` module but can be exploited more efficiently here because the possible graphs are well known from the input file, whereas the `cascades` module would create a large number of `cascades` which do not lead to a complete Feynman diagram of the given process.

```
<cascades2.f90>≡
  <File header>
```

```
module cascades2
```

```
  use, intrinsic :: iso_fortran_env, only : input_unit, output_unit, error_unit
  <Use kinds>
  use kinds, only: TC, i8
  <Use strings>
  <Use debug>
  use diagnostics
  use flavors
  use model_data
  use pbs_forests, only: pbs_parameters_t
  use resonances, only: resonance_info_t
  use resonances, only: resonance_history_t
  use resonances, only: resonance_history_set_t
  use cascades2_lexer
```

```

    <Standard module head>

    <Cascades2: public>

    <Cascades2: parameters>

    <Cascades2: types>

    <Cascades2: interfaces>

    interface
    <Cascades2: sub interfaces>
    end interface

contains

    <Cascades2: main procedures>

end module cascades2

<cascades2_sub.f90>≡
    <File header>

    submodule (cascades2) cascades2_s

        use sorting
        use io_units
        use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
        use hashes
        use cascades, only: phase_space_vanishes, MAX_WARN_RESONANCE

        implicit none

contains

    <Cascades2: procedures>

end submodule cascades2_s

```

19.11.1 Particle properties

We define a type holding the properties of the particles which are needed for parsing and finding the phase space parametrizations and mappings. The properties of all particles which appear in the parsed Feynman diagrams for the given process will be stored in a central place, and only pointers to these objects are used.

```

<Cascades2: types>≡
    type :: part_prop_t
        character(len=LABEL_LEN) :: particle_label
        integer :: pdg = 0
        real(default) :: mass = 0.
        real :: width = 0.

```

```

integer :: spin_type = 0
logical :: is_vector = .false.
logical :: empty = .true.
type(part_prop_t), pointer :: anti => null ()
type(string_t) :: tex_name
contains
  <Cascades2: part prop: TBP>
end type part_prop_t

```

The `particle_label` in `part_prop_t` is simply the particle name (e.g. 'W+'). The corresponding variable in the type `f_node_t` contains some additional information related to the external momenta, see below. The length of the `character` variable is fixed as:

```

<Cascades2: parameters>≡
  integer, parameter :: LABEL_LEN=30

<Cascades2: part prop: TBP>≡
  procedure :: final => part_prop_final

<Cascades2: sub interfaces>≡
  module subroutine part_prop_final (part)
    class(part_prop_t), intent(inout) :: part
  end subroutine part_prop_final

<Cascades2: procedures>≡
  module subroutine part_prop_final (part)
    class(part_prop_t), intent(inout) :: part
    part%anti => null ()
  end subroutine part_prop_final

```

19.11.2 The mapping modes

The possible mappings are essentially the same as in `cascades`, but we introduce in addition the mapping constant `NON_RESONANT`, which does not refer to a new mapping; it corresponds to the nonresonant version of a potentially resonant particle (or `k_node`). This becomes relevant when we compare `k_nodes` to eliminate equivalences.

```

<Cascades2: parameters>+≡
  integer, parameter :: &
    & NONRESONANT = -2, EXTERNAL_PRT = -1, &
    & NO_MAPPING = 0, S_CHANNEL = 1, T_CHANNEL = 2, U_CHANNEL = 3, &
    & RADIATION = 4, COLLINEAR = 5, INFRARED = 6, &
    & STEP_MAPPING_E = 11, STEP_MAPPING_H = 12, &
    & ON_SHELL = 99

```

19.11.3 Grove properties

The channels or `kingraphs` will be grouped in groves, i.e. sets of channels, which share some characteristic numbers. These numbers are stored in the following type:

```

<Cascades2: types>+≡
  type :: grove_prop_t

```

```

integer :: multiplicity = 0
integer :: n_resonances = 0
integer :: n_log_enhanced = 0
integer :: n_off_shell = 0
integer :: n_t_channel = 0
integer :: res_hash = 0
end type grove_prop_t

```

19.11.4 The tree type

This type contains all the information which is needed to reconstruct a **feyngraph** or **kingraph**. We store bincodes, pdg codes and mappings for all nodes of a valid **kingraph**. If we label the external particles as given in the process definition with integer numbers representing their position in the process definition, the bincode would be the number that one obtains by setting the bit at the position that is given by this number. If we combine two particles/nodes to a third one (using a three-vertex of the given model), the bincode is the number which one obtains by setting all the bits which are set for the two particles. The **pdg** and **mapping** are simply the pdg-code and mapping at the position (i.e. propagator or external particle) which is specified by the corresponding bincode. We use **tree_t** not only for completed **kingraphs**, but also for all **k_nodes**, which are a subtree of a **kingraph**.

```

<Cascades2: types>+≡
type :: tree_t
integer(TC), dimension(:), allocatable :: bc
integer, dimension(:), allocatable :: pdg
integer, dimension(:), allocatable :: mapping
integer :: n_entries = 0
logical :: keep = .true.
logical :: empty = .true.
contains
<Cascades2: tree: TBP>
end type tree_t

<Cascades2: tree: TBP>≡
procedure :: final => tree_final

<Cascades2: sub interfaces>+≡
module subroutine tree_final (tree)
class(tree_t), intent(inout) :: tree
end subroutine tree_final

<Cascades2: procedures>+≡
module subroutine tree_final (tree)
class(tree_t), intent(inout) :: tree
if (allocated (tree%bc)) deallocate (tree%bc)
if (allocated (tree%pdg)) deallocate (tree%pdg)
if (allocated (tree%mapping)) deallocate (tree%mapping)
end subroutine tree_final

```

```

<Cascades2: interfaces>≡
  interface assignment (=)
    module procedure tree_assign
    end interface assignment (=)

<Cascades2: sub interfaces>+≡
  module subroutine tree_assign (tree1, tree2)
    type(tree_t), intent(inout) :: tree1
    type(tree_t), intent(in) :: tree2
  end subroutine tree_assign

<Cascades2: procedures>+≡
  module subroutine tree_assign (tree1, tree2)
    type(tree_t), intent(inout) :: tree1
    type(tree_t), intent(in) :: tree2
    if (allocated (tree2%bc)) then
      allocate (tree1%bc(size(tree2%bc)))
      tree1%bc = tree2%bc
    end if
    if (allocated (tree2%pdg)) then
      allocate (tree1%pdg(size(tree2%pdg)))
      tree1%pdg = tree2%pdg
    end if
    if (allocated (tree2%mapping)) then
      allocate (tree1%mapping(size(tree2%mapping)))
      tree1%mapping = tree2%mapping
    end if
    tree1%n_entries = tree2%n_entries
    tree1%keep = tree2%keep
    tree1%empty = tree2%empty
  end subroutine tree_assign

```

19.11.5 Add entries to the tree

The following procedures fill the arrays in `tree_t` with entries resulting from the bincode and mapping assignment.

```

<Cascades2: tree: TBP>+≡
  procedure :: add_entry_from_numbers => tree_add_entry_from_numbers
  procedure :: add_entry_from_node => tree_add_entry_from_node
  generic :: add_entry => add_entry_from_numbers, add_entry_from_node

```

Here we add a single entry to each of the arrays. This will exclusively be used for external particles.

```

<Cascades2: sub interfaces>+≡
  module subroutine tree_add_entry_from_numbers (tree, bincode, pdg, mapping)
    class(tree_t), intent(inout) :: tree
    integer(TC), intent(in) :: bincode
    integer, intent(in) :: pdg
    integer, intent(in) :: mapping
  end subroutine tree_add_entry_from_numbers

```

```

<Cascades2: procedures>+≡
module subroutine tree_add_entry_from_numbers (tree, bincode, pdg, mapping)
  class(tree_t), intent(inout) :: tree
  integer(TC), intent(in) :: bincode
  integer, intent(in) :: pdg
  integer, intent(in) :: mapping
  integer :: pos
  if (tree%empty) then
    allocate (tree%bc(1))
    allocate (tree%pdg(1))
    allocate (tree%mapping(1))
    pos = tree%n_entries + 1
    tree%bc(pos) = bincode
    tree%pdg(pos) = pdg
    tree%mapping(pos) = mapping
    tree%n_entries = pos
    tree%empty = .false.
  end if
end subroutine tree_add_entry_from_numbers

```

Here we merge two existing subtrees and a single entry (bc, pdg and mapping).

```

<Cascades2: procedures>+≡
subroutine tree_merge (tree, tree1, tree2, bc, pdg, mapping)
  class(tree_t), intent(inout) :: tree
  type(tree_t), intent(in) :: tree1, tree2
  integer(TC), intent(in) :: bc
  integer, intent(in) :: pdg, mapping
  integer :: tree_size
  integer :: i1, i2
  if (tree%empty) then
    i1 = tree1%n_entries
    i2 = tree1%n_entries + tree2%n_entries
    !! Proof: tree_size > 0 (always)
    tree_size = tree1%n_entries + tree2%n_entries + 1
    allocate (tree%bc (tree_size))
    allocate (tree%pdg (tree_size))
    allocate (tree%mapping (tree_size))
    if (.not. tree1%empty) then
      tree%bc(:i1) = tree1%bc
      tree%pdg(:i1) = tree1%pdg
      tree%mapping(:i1) = tree1%mapping
    end if
    if (.not. tree2%empty) then
      tree%bc(i1+1:i2) = tree2%bc
      tree%pdg(i1+1:i2) = tree2%pdg
      tree%mapping(i1+1:i2) = tree2%mapping
    end if
    tree%bc(tree_size) = bc
    tree%pdg(tree_size) = pdg
    tree%mapping(tree_size) = mapping
    tree%n_entries = tree_size
    tree%empty = .false.
  end if
end subroutine tree_merge

```

```
end subroutine tree_merge
```

Here we add entries to a tree for a given `k_node`, which means that we first have to determine whether the node is external or internal. The arrays are sorted after the entries have been added (see below for details).

<Cascades2: sub interfaces>+≡

```
module subroutine tree_add_entry_from_node (tree, node)
  class(tree_t), intent(inout) :: tree
  type(k_node_t), intent(in) :: node
end subroutine tree_add_entry_from_node
```

<Cascades2: procedures>+≡

```
module subroutine tree_add_entry_from_node (tree, node)
  class(tree_t), intent(inout) :: tree
  type(k_node_t), intent(in) :: node
  integer :: pdg
  if (node%t_line) then
    pdg = abs (node%particle%pdg)
  else
    pdg = node%particle%pdg
  end if
  if (associated (node%daughter1) .and. &
      associated (node%daughter2)) then
    call tree_merge (tree, node%daughter1%subtree, &
                    node%daughter2%subtree, node%bincode, &
                    node%particle%pdg, node%mapping)
  else
    call tree_add_entry_from_numbers (tree, node%bincode, &
                                     node%particle%pdg, node%mapping)
  end if
  call tree%sort ()
end subroutine tree_add_entry_from_node
```

For a well-defined order of the elements of the arrays in `tree_t`, the elements can be sorted. The bincodes (entries of `bc`) are simply ordered by size, the `pdg` and `mapping` entries go to the positions of the corresponding `bc` values.

<Cascades2: tree: TBP>+≡

```
procedure :: sort => tree_sort
```

<Cascades2: sub interfaces>+≡

```
module subroutine tree_sort (tree)
  class(tree_t), intent(inout) :: tree
end subroutine tree_sort
```

<Cascades2: procedures>+≡

```
module subroutine tree_sort (tree)
  class(tree_t), intent(inout) :: tree
  integer(TC), dimension(size(tree%bc)) :: bc_tmp
  integer, dimension(size(tree%pdg)) :: pdg_tmp, mapping_tmp
  integer, dimension(1) :: pos
  integer :: i
  bc_tmp = tree%bc
  pdg_tmp = tree%pdg
  mapping_tmp = tree%mapping
```



```

do i = size(tree%bc),1,-1
  pos = maxloc (bc_tmp)
  tree%bc(i) = bc_tmp (pos(1))
  tree%pdg(i) = pdg_tmp (pos(1))
  tree%mapping(i) = mapping_tmp (pos(1))
  bc_tmp(pos(1)) = 0
end do
end subroutine tree_sort

```

19.11.6 Graph types

We define an abstract type which will give rise to two different types: The type `feyngraph_t` contains the pure information of the corresponding Feynman diagram, but also a list of objects of the `kingraph` type which contain the kinematically relevant data for the mapping calculation as well as the mappings themselves. Every graph should have an index which is unique. Graphs which are not needed any more can be disabled by setting the `keep` variable to `false`.

```

<Cascades2: types>+≡
type, abstract :: graph_t
  integer :: index = 0
  integer :: n_nodes = 0
  logical :: keep = .true.
end type graph_t

```

This is the type representing the Feynman diagrams which are read from an input file created by O'Mega. It is a tree of nodes, which we call `f_nodes`, so that `feyngraph_t` contains a pointer to the root of this tree, and each node can have two daughter nodes. The case of only one associated daughter should never appear, because in the method of phase space parametrization which is used here, we combine always two particle momenta to a third one. The `feyngraphs` will be arranged in a linked list. This is why we have a pointer to the next graph. The `kingraphs` on the other hand are arranged in linked lists which are attached to the corresponding `feyngraph`. In general, a `feyngraph` can give rise to more than one `kingraph` because we make a copy every time a particle can be resonant, so that in the copy we keep the particle nonresonant.

```

<Cascades2: types>+≡
type, extends (graph_t) :: feyngraph_t
  type(string_t) :: omega_feyngraph_output
  type(f_node_t), pointer :: root => null ()
  type(feyngraph_t), pointer :: next => null()
  type(kingraph_t), pointer :: kin_first => null ()
  type(kingraph_t), pointer :: kin_last => null ()
contains
  <Cascades2: feyngraph: TBP>
end type feyngraph_t

```

A container for a pointer of type `feyngraph_t`. This is used to realize arrays of these pointers.

```

<Cascades2: types>+≡
type :: feyngraph_ptr_t

```

```

    type(feyngraph_t), pointer :: graph => null ()
end type feyngraph_ptr_t

```

The length of a string describing a Feynman diagram which is produced by O'Mega is fixed by the parameter

```

<Cascades2: parameters>+≡
    integer, parameter :: FEYNGRAPH_LEN=300

<Cascades2: feyngraph: TBP>≡
    procedure :: final => feyngraph_final

<Cascades2: sub interfaces>+≡
    module subroutine feyngraph_final (graph)
        class(feyngraph_t), intent(inout) :: graph
    end subroutine feyngraph_final

<Cascades2: procedures>+≡
    module subroutine feyngraph_final (graph)
        class(feyngraph_t), intent(inout) :: graph
        type(kingraph_t), pointer :: current
        graph%root => null ()
        graph%kin_last => null ()
        do while (associated (graph%kin_first))
            current => graph%kin_first
            graph%kin_first => graph%kin_first%next
            call current%final ()
            deallocate (current)
        end do
    end subroutine feyngraph_final

```

This is the type of graph which is used to find the phase space channels, or in other words, each kingraph could correspond to a channel, if it is not eliminated for kinematical reasons or due to an equivalence. For the linked list which is attached to the corresponding `feyngraph`, we need the `next` pointer, whereas `grove_next` points to the next `kingraph` within a grove. The information which is relevant for the specification of a channel is stored in `tree`. We use `grove_prop` to sort the `kingraph` in a grove in which all `kingraphs` are characterized by the numbers contained in `grove_prop`. Later these groves are further subdivided using the resonance hash. A `kingraph` which is constructed directly from the output of O'Mega, is not `inverse`. In this case the first incoming particle is the root of the tree. In a scattering process, we can also construct a `kingraph` where the root of the tree is the second incoming particle. In this case the value of `inverse` is `.true.`.

```

<Cascades2: types>+≡
    type, extends (graph_t) :: kingraph_t
        type(k_node_t), pointer :: root => null ()
        type(kingraph_t), pointer :: next => null()
        type(kingraph_t), pointer :: grove_next => null ()
    type(tree_t) :: tree
    type(grove_prop_t) :: grove_prop
    logical :: inverse = .false.
    integer :: prc_component = 0
contains

```

```

    <Cascades2: kingraph: TBP>
end type kingraph_t

```

Another container for a pointer to emulate arrays of pointers:

```

<Cascades2: types>+≡
type :: kingraph_ptr_t
    type(kingraph_t), pointer :: graph => null ()
end type kingraph_ptr_t

<Cascades2: kingraph: TBP>≡
procedure :: final => kingraph_final

<Cascades2: sub interfaces>+≡
module subroutine kingraph_final (graph)
    class(kingraph_t), intent(inout) :: graph
end subroutine kingraph_final

<Cascades2: procedures>+≡
module subroutine kingraph_final (graph)
    class(kingraph_t), intent(inout) :: graph
    graph%root => null ()
    graph%next => null ()
    graph%grove_next => null ()
    call graph%tree%final ()
end subroutine kingraph_final

```

19.11.7 The node types

We define an abstract type containing variables which are needed for `f_node_t` as well as `k_node_t`. We say that a node is on the t-line if it lies between the two nodes which correspond to the two incoming particles. `incoming` and `tline` are used only for scattering processes and remain `.false.` in decay processes. The variable `n_subtree_nodes` holds the number of nodes (including the node itself) of the subtree of which the node is the root.

```

<Cascades2: types>+≡
type, abstract :: node_t
    type(part_prop_t), pointer :: particle => null ()
    logical :: incoming = .false.
    logical :: t_line = .false.
    integer :: index = 0
    logical :: keep = .true.
    integer :: n_subtree_nodes = 1
end type node_t

```

We use two different list types for the different kinds of nodes. We therefore start with an abstract type:

```

<Cascades2: types>+≡
type, abstract :: list_t
    integer :: n_entries = 0
end type list_t

```

Since the contents of the lists are different, we introduce two different entry types. Since the trees of nodes use pointers, the nodes should only be allocated by a type-bound procedure of the corresponding list type, such that we can keep track of all nodes, eventually reuse and in the end deallocate nodes correctly, without forgetting any nodes. Here is the type for the `k_nodes`. The list is a linked list. We want to reuse (recycle) the `k_nodes` which are neither incoming nor `t_line`.

```

<Cascades2: types>+≡
  type :: k_node_entry_t
    type(k_node_t), pointer :: node => null ()
    type(k_node_entry_t), pointer :: next => null ()
    logical :: recycle = .false.
  contains
    <Cascades2: k node entry: TBP>
  end type k_node_entry_t

<Cascades2: k node entry: TBP>≡
  procedure :: final => k_node_entry_final

<Cascades2: sub interfaces>+≡
  module subroutine k_node_entry_final (entry)
    class(k_node_entry_t), intent(inout) :: entry
  end subroutine k_node_entry_final

<Cascades2: procedures>+≡
  module subroutine k_node_entry_final (entry)
    class(k_node_entry_t), intent(inout) :: entry
    if (associated (entry%node)) then
      call entry%node%final
      deallocate (entry%node)
    end if
    entry%next => null ()
  end subroutine k_node_entry_final

<Cascades2: k node entry: TBP>+≡
  procedure :: write => k_node_entry_write

<Cascades2: sub interfaces>+≡
  module subroutine k_node_entry_write (k_node_entry, u)
    class(k_node_entry_t), intent(in) :: k_node_entry
    integer, intent(in) :: u
  end subroutine k_node_entry_write

<Cascades2: procedures>+≡
  module subroutine k_node_entry_write (k_node_entry, u)
    class(k_node_entry_t), intent(in) :: k_node_entry
    integer, intent(in) :: u
  end subroutine k_node_entry_write

```

Here is the list type for `k_nodes`. A `k_node_list` can be declared to be an observer. In this case it does not create any nodes by itself, but the entries set their pointers to existing nodes. In this way we can use the list structure and the type bound procedures for existing nodes.

```

<Cascades2: types>+≡

```

```

type, extends (list_t) :: k_node_list_t
  type(k_node_entry_t), pointer :: first => null ()
  type(k_node_entry_t), pointer :: last => null ()
  integer :: n_recycle
  logical :: observer = .false.
contains
  <Cascades2: k node list: TBP>
end type k_node_list_t

<Cascades2: k node list: TBP>≡
  procedure :: final => k_node_list_final

<Cascades2: sub interfaces>+≡
  module subroutine k_node_list_final (list)
    class(k_node_list_t), intent(inout) :: list
  end subroutine k_node_list_final

<Cascades2: procedures>+≡
  module subroutine k_node_list_final (list)
    class(k_node_list_t), intent(inout) :: list
    type(k_node_entry_t), pointer :: current
    do while (associated (list%first))
      current => list%first
      list%first => list%first%next
      if (list%observer) current%node => null ()
      call current%final ()
      deallocate (current)
    end do
  end subroutine k_node_list_final

```

The `f_node_t` type contains the `particle_label` variable which is extracted from the input file. It consists not only of the particle name, but also of some numbers in brackets. These numbers indicate which external particles are part of the subtree of this node. The `f_node` contains also a list of `k_nodes`. Therefore, if the nodes are not `incoming` or `t_line`, the mapping calculations for these `k_nodes` which can appear in several `kingraphs` have to be performed only once.

```

<Cascades2: types>+≡
  type, extends (node_t) :: f_node_t
    type(f_node_t), pointer :: daughter1 => null ()
    type(f_node_t), pointer :: daughter2 => null ()
    character(len=LABEL_LEN) :: particle_label
    type(k_node_list_t) :: k_node_list
  contains
    <Cascades2: f node: TBP>
  end type f_node_t

```

The finalizer nullifies the daughter pointers, since they are deallocated, like the `f_node` itself, with the finalizer of the `f_node_list`.

```

<Cascades2: f node: TBP>≡
  procedure :: final => f_node_final

```

```

<Cascades2: sub interfaces>+≡
    recursive module subroutine f_node_final (node)
        class(f_node_t), intent(inout) :: node
    end subroutine f_node_final

```

```

<Cascades2: procedures>+≡
    recursive module subroutine f_node_final (node)
        class(f_node_t), intent(inout) :: node
        call node%k_node_list%final ()
        node%daughter1 => null ()
        node%daughter2 => null ()
    end subroutine f_node_final

```

Finaliser for f_node_entry.

```

<Cascades2: f node entry: TBP>≡
    procedure :: final => f_node_entry_final

<Cascades2: sub interfaces>+≡
    module subroutine f_node_entry_final (entry)
        class(f_node_entry_t), intent(inout) :: entry
    end subroutine f_node_entry_final

<Cascades2: procedures>+≡
    module subroutine f_node_entry_final (entry)
        class(f_node_entry_t), intent(inout) :: entry
        if (associated (entry%node)) then
            call entry%node%final ()
            deallocate (entry%node)
        end if
        entry%next => null ()
    end subroutine f_node_entry_final

```

Set index if not yet done, i.e. if it is zero.

```

<Cascades2: f node: TBP>+≡
    procedure :: set_index => f_node_set_index

<Cascades2: sub interfaces>+≡
    module subroutine f_node_set_index (f_node)
        class(f_node_t), intent(inout) :: f_node
    end subroutine f_node_set_index

<Cascades2: procedures>+≡
    module subroutine f_node_set_index (f_node)
        class(f_node_t), intent(inout) :: f_node
        integer, save :: counter = 0
        if (f_node%index == 0) then
            counter = counter + 1
            f_node%index = counter
        end if
    end subroutine f_node_set_index

```

Type for the nodes of the tree (lines of the Feynman diagrams). We also need a type containing a pointer to a node, which is needed for creating arrays of pointers. This will be used for scattering processes where we can take either the first or the second particle to be the root of the tree. Since we need both

cases for the calculations and O'Mega only gives us one of these, we have to perform a transformation of the graph in which some nodes (on the line which we hereafter call t-line) need to know their mother and sister nodes, which become their daughters within this transformation.

```

<Cascades2: types>+≡
  type :: f_node_ptr_t
    type(f_node_t), pointer :: node => null ()
    contains
      <Cascades2: f node ptr: TBP>
    end type f_node_ptr_t

<Cascades2: f node ptr: TBP>≡
  procedure :: final => f_node_ptr_final

<Cascades2: sub interfaces>+≡
  module subroutine f_node_ptr_final (f_node_ptr)
    class(f_node_ptr_t), intent(inout) :: f_node_ptr
  end subroutine f_node_ptr_final

<Cascades2: procedures>+≡
  module subroutine f_node_ptr_final (f_node_ptr)
    class(f_node_ptr_t), intent(inout) :: f_node_ptr
    f_node_ptr%node => null ()
  end subroutine f_node_ptr_final

<Cascades2: interfaces>+≡
  interface assignment (=)
    module procedure f_node_ptr_assign
  end interface assignment (=)

<Cascades2: sub interfaces>+≡
  module subroutine f_node_ptr_assign (ptr1, ptr2)
    type(f_node_ptr_t), intent(out) :: ptr1
    type(f_node_ptr_t), intent(in) :: ptr2
  end subroutine f_node_ptr_assign

<Cascades2: procedures>+≡
  module subroutine f_node_ptr_assign (ptr1, ptr2)
    type(f_node_ptr_t), intent(out) :: ptr1
    type(f_node_ptr_t), intent(in) :: ptr2
    ptr1%node => ptr2%node
  end subroutine f_node_ptr_assign

<Cascades2: types>+≡
  type :: k_node_ptr_t
    type(k_node_t), pointer :: node => null ()
  end type k_node_ptr_t

<Cascades2: types>+≡
  type, extends (node_t) :: k_node_t
    type(k_node_t), pointer :: daughter1 => null ()
    type(k_node_t), pointer :: daughter2 => null ()
    type(k_node_t), pointer :: inverse_daughter1 => null ()
    type(k_node_t), pointer :: inverse_daughter2 => null ()

```

```

type(f_node_t), pointer :: f_node => null ()
type(tree_t) :: subtree
real (default) :: ext_mass_sum = 0.
real (default) :: effective_mass = 0.
logical :: resonant = .false.
logical :: on_shell = .false.
logical :: log_enhanced = .false.
integer :: mapping = NO_MAPPING
integer(TC) :: bincode = 0
logical :: mapping_assigned = .false.
logical :: is_nonresonant_copy = .false.
logical :: subtree_checked = .false.
integer :: n_off_shell = 0
integer :: n_log_enhanced = 0
integer :: n_resonances = 0
integer :: multiplicity = 0
integer :: n_t_channel = 0
integer :: f_node_index = 0
contains
  <Cascades2: k_node: TBP>
end type k_node_t

```

Subroutine for k_node assignment.

```

<Cascades2: interfaces>+≡
  interface assignment (=)
    module procedure k_node_assign
  end interface assignment (=)

<Cascades2: sub interfaces>+≡
  module subroutine k_node_assign (k_node1, k_node2)
    type(k_node_t), intent(inout) :: k_node1
    type(k_node_t), intent(in) :: k_node2
  end subroutine k_node_assign

<Cascades2: procedures>+≡
  module subroutine k_node_assign (k_node1, k_node2)
    type(k_node_t), intent(inout) :: k_node1
    type(k_node_t), intent(in) :: k_node2
    k_node1%f_node => k_node2%f_node
    k_node1%particle => k_node2%particle
    k_node1%incoming = k_node2%incoming
    k_node1%t_line = k_node2%t_line
    k_node1%keep = k_node2%keep
    k_node1%n_subtree_nodes = k_node2%n_subtree_nodes
    k_node1%ext_mass_sum = k_node2%ext_mass_sum
    k_node1%effective_mass = k_node2%effective_mass
    k_node1%resonant = k_node2%resonant
    k_node1%on_shell = k_node2%on_shell
    k_node1%log_enhanced = k_node2%log_enhanced
    k_node1%mapping = k_node2%mapping
    k_node1%bincode = k_node2%bincode
    k_node1%mapping_assigned = k_node2%mapping_assigned
    k_node1%is_nonresonant_copy = k_node2%is_nonresonant_copy
    k_node1%n_off_shell = k_node2%n_off_shell
    k_node1%n_log_enhanced = k_node2%n_log_enhanced

```



```

    k_node1%n_resonances = k_node2%n_resonances
    k_node1%multiplicity = k_node2%multiplicity
    k_node1%n_t_channel = k_node2%n_t_channel
    k_node1%f_node_index = k_node2%f_node_index
end subroutine k_node_assign

```

The finalizer of `k_node_t` nullifies all pointers to nodes, since the deallocation of these nodes takes place in the finalizer of the list by which they were created.

```

<Cascades2: k node: TBP>≡
    procedure :: final => k_node_final

<Cascades2: sub interfaces>+≡
    recursive module subroutine k_node_final (k_node)
        class(k_node_t), intent(inout) :: k_node
    end subroutine k_node_final

<Cascades2: procedures>+≡
    recursive module subroutine k_node_final (k_node)
        class(k_node_t), intent(inout) :: k_node
        k_node%daughter1 => null ()
        k_node%daughter2 => null ()
        k_node%inverse_daughter1 => null ()
        k_node%inverse_daughter2 => null ()
        k_node%f_node => null ()
    end subroutine k_node_final

```

Set an index to a `k_node`, if not yet done, i.e. if it is zero. The indices are simply positive integer numbers starting from 1.

```

<Cascades2: k node: TBP>+≡
    procedure :: set_index => k_node_set_index

<Cascades2: sub interfaces>+≡
    module subroutine k_node_set_index (k_node)
        class(k_node_t), intent(inout) :: k_node
    end subroutine k_node_set_index

<Cascades2: procedures>+≡
    module subroutine k_node_set_index (k_node)
        class(k_node_t), intent(inout) :: k_node
        integer, save :: counter = 0
        if (k_node%index == 0) then
            counter = counter + 1
            k_node%index = counter
        end if
    end subroutine k_node_set_index

```

The process type (decay or scattering) is given by an integer which is equal to the number of incoming particles.

```

<Cascades2: public>≡
    public :: DECAY, SCATTERING

<Cascades2: parameters>+≡
    integer, parameter :: DECAY=1, SCATTERING=2

```

The entries of the `f_node_list` contain the substring of the input file from which the node's subtree will be constructed (or a modified string containing placeholders for substrings). We use the length of this string for fast comparison to find the nodes in the `f_node_list` which we want to reuse.

```

<Cascades2: types>+=
  type :: f_node_entry_t
    character(len=FEYNGRAPH_LEN) :: subtree_string
    integer :: string_len = 0
    type(f_node_t), pointer :: node => null ()
    type(f_node_entry_t), pointer :: next => null ()
    integer :: subtree_size = 0
  contains
    <Cascades2: f node entry: TBP>
  end type f_node_entry_t

```

A write method for `f_node_entry`.

```

<Cascades2: f node entry: TBP>+=
  procedure :: write => f_node_entry_write

<Cascades2: sub interfaces>+=
  module subroutine f_node_entry_write (f_node_entry, u)
    class(f_node_entry_t), intent(in) :: f_node_entry
    integer, intent(in) :: u
  end subroutine f_node_entry_write

<Cascades2: procedures>+=
  module subroutine f_node_entry_write (f_node_entry, u)
    class(f_node_entry_t), intent(in) :: f_node_entry
    integer, intent(in) :: u
    write (unit=u, fmt='(A)') trim(f_node_entry%subtree_string)
  end subroutine f_node_entry_write

<Cascades2: interfaces>+=
  interface assignment (=)
    module procedure f_node_entry_assign
  end interface assignment (=)

<Cascades2: sub interfaces>+=
  module subroutine f_node_entry_assign (entry1, entry2)
    type(f_node_entry_t), intent(out) :: entry1
    type(f_node_entry_t), intent(in) :: entry2
  end subroutine f_node_entry_assign

<Cascades2: procedures>+=
  module subroutine f_node_entry_assign (entry1, entry2)
    type(f_node_entry_t), intent(out) :: entry1
    type(f_node_entry_t), intent(in) :: entry2
    entry1%node => entry2%node
    entry1%subtree_string = entry2%subtree_string
    entry1%string_len = entry2%string_len
    entry1%subtree_size = entry2%subtree_size
  end subroutine f_node_entry_assign

```

This is the list type for `f_nodes`. The variable `max_tree_size` is the number of nodes which appear in a complete graph.

```

<Cascades2: types>+≡
type, extends (list_t) :: f_node_list_t
  type(f_node_entry_t), pointer :: first => null ()
  type(f_node_entry_t), pointer :: last => null ()
  type(k_node_list_t), pointer :: k_node_list => null ()
  integer :: max_tree_size = 0
contains
  <Cascades2: f node list: TBP>
end type f_node_list_t

```

Add an entry to the `f_node_list`. If the node might be reused, we check first using the `subtree_string` if there is already a node in the list which is the root of exactly the same subtree. Otherwise we add an entry to the list and allocate the node. In both cases we return a pointer to the node which allows to access the node.

```

<Cascades2: f node list: TBP>≡
  procedure :: add_entry => f_node_list_add_entry

<Cascades2: sub interfaces>+≡
  module subroutine f_node_list_add_entry (list, subtree_string, &
    ptr_to_node, recycle, subtree_size)
    class(f_node_list_t), intent(inout) :: list
    character(len=*), intent(in) :: subtree_string
    type(f_node_t), pointer, intent(out) :: ptr_to_node
    logical, intent(in) :: recycle
    integer, intent(in), optional :: subtree_size
  end subroutine f_node_list_add_entry

<Cascades2: procedures>+≡
  module subroutine f_node_list_add_entry (list, subtree_string, &
    ptr_to_node, recycle, subtree_size)
    class(f_node_list_t), intent(inout) :: list
    character(len=*), intent(in) :: subtree_string
    type(f_node_t), pointer, intent(out) :: ptr_to_node
    logical, intent(in) :: recycle
    integer, intent(in), optional :: subtree_size
    type(f_node_entry_t), pointer :: current
    type(f_node_entry_t), pointer :: second
    integer :: subtree_len
    ptr_to_node => null ()
    if (recycle) then
      subtree_len = len_trim (subtree_string)
      current => list%first
      do while (associated (current))
        if (present (subtree_size)) then
          if (current%subtree_size /= subtree_size) exit
        end if
        if (current%string_len == subtree_len) then
          if (trim (current%subtree_string) == trim (subtree_string)) then
            ptr_to_node => current%node
            exit
          end if
        end if
      end do
    end if
  end subroutine f_node_list_add_entry

```

```

        end if
        current => current%next
    end do
end if
if (.not. associated (ptr_to_node)) then
    if (list%n_entries == 0) then
        allocate (list%first)
        list%last => list%first
    else
        second => list%first
        list%first => null ()
        allocate (list%first)
        list%first%next => second
    end if
    list%n_entries = list%n_entries + 1
    list%first%subtree_string = trim(subtree_string)
    list%first%string_len = subtree_len
    if (present (subtree_size)) list%first%subtree_size = subtree_size
    allocate (list%first%node)
    call list%first%node%set_index ()
    ptr_to_node => list%first%node
end if
end subroutine f_node_list_add_entry

```

A write method for debugging.

<Cascades2: f_node_list: TBP>+≡

```

    procedure :: write => f_node_list_write

```

<Cascades2: sub interfaces>+≡

```

    module subroutine f_node_list_write (f_node_list, u)
        class(f_node_list_t), intent(in) :: f_node_list
        integer, intent(in) :: u
    end subroutine f_node_list_write

```

<Cascades2: procedures>+≡

```

    module subroutine f_node_list_write (f_node_list, u)
        class(f_node_list_t), intent(in) :: f_node_list
        integer, intent(in) :: u
        type(f_node_entry_t), pointer :: current
        integer :: pos = 0
        current => f_node_list%first
        do while (associated (current))
            pos = pos + 1
            write (unit=u, fmt='(A,I10)') 'entry #: ', pos
            call current%write (u)
            write (unit=u, fmt=*)
            current => current%next
        end do
    end subroutine f_node_list_write

```

<Cascades2: interfaces>+≡

```

    interface assignment (=)
        module procedure k_node_entry_assign
    end interface assignment (=)

```

```

<Cascades2: sub interfaces>+≡
    module subroutine k_node_entry_assign (entry1, entry2)
        type(k_node_entry_t), intent(out) :: entry1
        type(k_node_entry_t), intent(in)  :: entry2
    end subroutine k_node_entry_assign

<Cascades2: procedures>+≡
    module subroutine k_node_entry_assign (entry1, entry2)
        type(k_node_entry_t), intent(out) :: entry1
        type(k_node_entry_t), intent(in)  :: entry2
        entry1%node => entry2%node
        entry1%recycle = entry2%recycle
    end subroutine k_node_entry_assign

```

Add an entry to the `k_node_list`. We have to specify if the node can be reused. The check for existing reusable nodes happens with `k_node_list_get_nodes` (see below).

```

<Cascades2: k node list: TBP>+≡
    procedure :: add_entry => k_node_list_add_entry

<Cascades2: sub interfaces>+≡
    recursive module subroutine k_node_list_add_entry &
        (list, ptr_to_node, recycle)
        class(k_node_list_t), intent(inout) :: list
        type(k_node_t), pointer, intent(out) :: ptr_to_node
        logical, intent(in) :: recycle
    end subroutine k_node_list_add_entry

<Cascades2: procedures>+≡
    recursive module subroutine k_node_list_add_entry &
        (list, ptr_to_node, recycle)
        class(k_node_list_t), intent(inout) :: list
        type(k_node_t), pointer, intent(out) :: ptr_to_node
        logical, intent(in) :: recycle
        if (list%n_entries == 0) then
            allocate (list%first)
            list%last => list%first
        else
            allocate (list%last%next)
            list%last => list%last%next
        end if
        list%n_entries = list%n_entries + 1
        list%last%recycle = recycle
        allocate (list%last%node)
        call list%last%node%set_index ()
        ptr_to_node => list%last%node
    end subroutine k_node_list_add_entry

```

We need a similar subroutine for adding only a pointer to a list. This is needed for a `k_node_list` which is only an observer, i.e. it does not create any nodes by itself.

```

<Cascades2: k node list: TBP>+≡
    procedure :: add_pointer => k_node_list_add_pointer

```

```

<Cascades2: sub interfaces>+≡
  module subroutine k_node_list_add_pointer (list, ptr_to_node, recycle)
    class(k_node_list_t), intent(inout) :: list
    type(k_node_t), pointer, intent(in) :: ptr_to_node
    logical, optional, intent(in) :: recycle
  end subroutine k_node_list_add_pointer

<Cascades2: procedures>+≡
  module subroutine k_node_list_add_pointer (list, ptr_to_node, recycle)
    class(k_node_list_t), intent(inout) :: list
    type(k_node_t), pointer, intent(in) :: ptr_to_node
    logical, optional, intent(in) :: recycle
    logical :: rec
    if (present (recycle)) then
      rec = recycle
    else
      rec = .false.
    end if
    if (list%n_entries == 0) then
      allocate (list%first)
      list%last => list%first
    else
      allocate (list%last%next)
      list%last => list%last%next
    end if
    list%n_entries = list%n_entries + 1
    list%last%recycle = rec
    list%last%node => ptr_to_node
  end subroutine k_node_list_add_pointer

```

The `k_node_list` can also be used to collect `k_nodes` which belong to different `f_nodes` in order to compare these. This is done only for nodes which have the same number of subtree nodes. We compare all nodes of the list with each other (as long as the node is not deactivated, i.e. if the `keep` variable is set to `.true.`) using the subroutine `subtree_select`. If it turns out that two nodes are equivalent, we keep only one of them. The term equivalent in this module refers to trees or subtrees which differ in the pdg codes at positions where the trivial mapping is used (`NO_MAPPING` or `NON_RESONANT`) so that the mass of the particle does not matter. Depending on the available couplings, two equivalent subtrees could eventually lead to the same phase space channels, which is why only one of them is kept.

```

<Cascades2: k node list: TBP>+≡
  procedure :: check_subtree_equivalences => &
    k_node_list_check_subtree_equivalences

<Cascades2: sub interfaces>+≡
  module subroutine k_node_list_check_subtree_equivalences (list, model)
    class(k_node_list_t), intent(inout) :: list
    type(model_data_t), intent(in) :: model
  end subroutine k_node_list_check_subtree_equivalences

<Cascades2: procedures>+≡
  module subroutine k_node_list_check_subtree_equivalences (list, model)
    class(k_node_list_t), intent(inout) :: list

```

```

type(model_data_t), intent(in) :: model
type(k_node_ptr_t), dimension (:), allocatable :: set
type(k_node_entry_t), pointer :: current
integer :: pos
integer :: i,j
if (list%n_entries == 0) return
allocate (set (list%n_entries))
current => list%first
pos = 0
do while (associated (current))
    pos = pos + 1
    set(pos)%node => current%node
    current => current%next
end do
do i=1, list%n_entries
    if (set(i)%node%keep) then
        do j=i+1, list%n_entries
            if (set(j)%node%keep) then
                if (set(i)%node%bincode == set(j)%node%bincode) then
                    call subtree_select (set(i)%node%subtree,set(j)%node%subtree, model)
                    if (.not. set(i)%node%subtree%keep) then
                        set(i)%node%keep = .false.
                        exit
                    else if (.not. set(j)%node%subtree%keep) then
                        set(j)%node%keep = .false.
                    end if
                end if
            end if
        end do
    end if
end do
deallocate (set)
end subroutine k_node_list_check_subtree_equivalences

```

This subroutine is used to obtain all `k_nodes` of a `k_node_list` which can be recycled and are not disabled for some reason. We pass an allocatable array of the type `k_node_ptr_t` which will be allocated if there are any such nodes in the list and the pointers will be associated with these nodes.

<Cascades2: k node list: TBP>+≡

```

procedure :: get_nodes => k_node_list_get_nodes

```

<Cascades2: sub interfaces>+≡

```

module subroutine k_node_list_get_nodes (list, nodes)
    class(k_node_list_t), intent(inout) :: list
    type(k_node_ptr_t), dimension(:), allocatable, intent(out) :: nodes
end subroutine k_node_list_get_nodes

```

<Cascades2: procedures>+≡

```

module subroutine k_node_list_get_nodes (list, nodes)
    class(k_node_list_t), intent(inout) :: list
    type(k_node_ptr_t), dimension(:), allocatable, intent(out) :: nodes
    integer :: n_nodes
    integer :: pos
    type(k_node_entry_t), pointer :: current, garbage

```

```

n_nodes = 0
current => list%first
do while (associated (current))
  if (current%recycle .and. current%node%keep) n_nodes = n_nodes + 1
  current => current%next
end do
if (n_nodes /= 0) then
  pos = 1
  allocate (nodes (n_nodes))
  do while (associated (list%first) .and. .not. list%first%node%keep)
    garbage => list%first
    list%first => list%first%next
    call garbage%final ()
    deallocate (garbage)
  end do
  current => list%first
  do while (associated (current))
    do while (associated (current%next))
      if (.not. current%next%node%keep) then
        garbage => current%next
        current%next => current%next%next
        call garbage%final
        deallocate (garbage)
      else
        exit
      end if
    end do
    if (current%recycle .and. current%node%keep) then
      nodes(pos)%node => current%node
      pos = pos + 1
    end if
    current => current%next
  end do
end if
end subroutine k_node_list_get_nodes

```

Gfortran 7/8/9 bug, has to remain in the main module:

```

<Cascades2: f node list: TBP>+≡
  procedure :: final => f_node_list_final

<Cascades2: main procedures>≡
  subroutine f_node_list_final (list)
    class(f_node_list_t) :: list
    type(f_node_entry_t), pointer :: current
    list%k_node_list => null ()
    do while (associated (list%first))
      current => list%first
      list%first => list%first%next
      call current%final ()
      deallocate (current)
    end do
  end subroutine f_node_list_final

```


19.11.8 The grove list

First a type is introduced in order to speed up the comparison of kingraphs with the purpose to quickly find the graphs that might be equivalent. This is done solely on the basis of a number (which is given by the value of `depth` in `compare_tree_t`) of bincodes, which are the highest ones that do not belong to external particles. The highest such value determines the index of the element in the `entry` array of the `compare_tree`. The next lower such value determines the index of the element in the `entry` array of this `entry`, and so on and so forth. This results in a tree structure where the number of levels is given by `depth` and should not be too large for reasons of memory. This is the entry type.

```

<Cascades2: types>+≡
  type :: compare_tree_entry_t
    type(compare_tree_entry_t), dimension(:), pointer :: entry => null ()
    type(kingraph_ptr_t), dimension(:), allocatable :: graph_entry
  contains
    <Cascades2: compare tree entry: TBP>
  end type compare_tree_entry_t

```

This is the tree type.

```

<Cascades2: types>+≡
  type :: compare_tree_t
    integer :: depth = 3
    type(compare_tree_entry_t), dimension(:), pointer :: entry => null ()
  contains
    <Cascades2: compare tree: TBP>
  end type compare_tree_t

```

Finalizers for both types. The one for the entry type has to be recursive.

```

<Cascades2: compare tree: TBP>≡
  procedure :: final => compare_tree_final

<Cascades2: sub interfaces>+≡
  module subroutine compare_tree_final (ctree)
    class(compare_tree_t), intent(inout) :: ctree
  end subroutine compare_tree_final

<Cascades2: procedures>+≡
  module subroutine compare_tree_final (ctree)
    class(compare_tree_t), intent(inout) :: ctree
    integer :: i
    if (associated (ctree%entry)) then
      do i=1, size (ctree%entry)
        call ctree%entry(i)%final ()
        deallocate (ctree%entry)
      end do
    end if
  end subroutine compare_tree_final

<Cascades2: compare tree entry: TBP>≡
  procedure :: final => compare_tree_entry_final

```

```

<Cascades2: sub interfaces>+≡
    recursive module subroutine compare_tree_entry_final (ct_entry)
        class(compare_tree_entry_t), intent(inout) :: ct_entry
    end subroutine compare_tree_entry_final

<Cascades2: procedures>+≡
    recursive module subroutine compare_tree_entry_final (ct_entry)
        class(compare_tree_entry_t), intent(inout) :: ct_entry
        integer :: i
        if (associated (ct_entry%entry)) then
            do i=1, size (ct_entry%entry)
                call ct_entry%entry(i)%final ()
            end do
            deallocate (ct_entry%entry)
        else
            deallocate (ct_entry%graph_entry)
        end if
    end subroutine compare_tree_entry_final

```

Check the presence of a graph which is considered as equivalent and select between the two. If there is no such graph, the current one is added to the list. First the entry has to be found:

```

<Cascades2: compare tree: TBP>+≡
    procedure :: check_kingraph => compare_tree_check_kingraph

<Cascades2: sub interfaces>+≡
    module subroutine compare_tree_check_kingraph &
        (ctree, kingraph, model, preliminary)
        class(compare_tree_t), intent(inout) :: ctree
        type(kingraph_t), intent(inout), pointer :: kingraph
        type(model_data_t), intent(in) :: model
        logical, intent(in) :: preliminary
    end subroutine compare_tree_check_kingraph

<Cascades2: procedures>+≡
    module subroutine compare_tree_check_kingraph &
        (ctree, kingraph, model, preliminary)
        class(compare_tree_t), intent(inout) :: ctree
        type(kingraph_t), intent(inout), pointer :: kingraph
        type(model_data_t), intent(in) :: model
        logical, intent(in) :: preliminary
        integer :: i
        integer :: pos
        integer(TC) :: sz
        integer(TC), dimension(:), allocatable :: identifier
        if (.not. associated (ctree%entry)) then
            sz = 0_TC
            do i = size(kingraph%tree%bc), 1, -1
                sz = ior (sz, kingraph%tree%bc(i))
            end do
            if (sz > 0) then
                allocate (ctree%entry (sz))
            else
                call msg_bug ("Compare tree could not be created")
            end if
        end if
    end subroutine compare_tree_check_kingraph

```

```

end if
allocate (identifier (ctree%depth))
pos = 0
do i = size(kingraph%tree%bc), 1, -1
  if (popcnt (kingraph%tree%bc(i)) /= 1) then
    pos = pos + 1
    identifier(pos) = kingraph%tree%bc(i)
    if (pos == ctree%depth) exit
  end if
end do
if (size (identifier) > 1) then
  call ctree%entry(identifier(1))%check_kingraph (kingraph, model, &
    preliminary, identifier(1), identifier(2:))
else if (size (identifier) == 1) then
  call ctree%entry(identifier(1))%check_kingraph &
    (kingraph, model, preliminary)
end if
deallocate (identifier)
end subroutine compare_tree_check_kingraph

```

Then the graphs of the entry are checked.

```

<Cascades2: compare tree entry: TBP>+≡
  procedure :: check_kingraph => compare_tree_entry_check_kingraph

<Cascades2: sub interfaces>+≡
  recursive module subroutine compare_tree_entry_check_kingraph (ct_entry, &
    kingraph, model, preliminary, subtree_size, identifier)
    class(compare_tree_entry_t), intent(inout) :: ct_entry
    type(kingraph_t), pointer, intent(inout) :: kingraph
    type(model_data_t), intent(in) :: model
    logical, intent(in) :: preliminary
    integer, intent(in), optional :: subtree_size
    integer, dimension (:), intent(in), optional :: identifier
  end subroutine compare_tree_entry_check_kingraph

<Cascades2: procedures>+≡
  recursive module subroutine compare_tree_entry_check_kingraph (ct_entry, &
    kingraph, model, preliminary, subtree_size, identifier)
    class(compare_tree_entry_t), intent(inout) :: ct_entry
    type(kingraph_t), pointer, intent(inout) :: kingraph
    type(model_data_t), intent(in) :: model
    logical, intent(in) :: preliminary
    integer, intent(in), optional :: subtree_size
    integer, dimension (:), intent(in), optional :: identifier
    if (present (identifier)) then
      if (.not. associated (ct_entry%entry)) &
        allocate (ct_entry%entry(subtree_size))
      if (size (identifier) > 1) then
        call ct_entry%entry(identifier(1))%check_kingraph (kingraph, &
          model, preliminary, identifier(1), identifier(2:))
      else if (size (identifier) == 1) then
        call ct_entry%entry(identifier(1))%check_kingraph (kingraph, &
          model, preliminary)
      end if
    else

```

```

        if (allocated (ct_entry%graph_entry)) then
            call perform_check
        else
            allocate (ct_entry%graph_entry(1))
            ct_entry%graph_entry(1)%graph => kingraph
        end if
    end if

contains

    subroutine perform_check
        integer :: i
        logical :: rebuild
        rebuild = .true.
        do i=1, size(ct_entry%graph_entry)
            if (ct_entry%graph_entry(i)%graph%keep) then
                if (preliminary .or. &
                    ct_entry%graph_entry(i)%graph%prc_component /= &
                    kingraph%prc_component) then
                    call kingraph_select (ct_entry%graph_entry(i)%graph, &
                        kingraph, model, preliminary)
                    if (.not. kingraph%keep) then
                        return
                    else if (rebuild .and. .not. &
                        ct_entry%graph_entry(i)%graph%keep) then
                        ct_entry%graph_entry(i)%graph => kingraph
                        rebuild = .false.
                    end if
                end if
            end if
        end do
        if (rebuild) call rebuild_graph_entry
    end subroutine perform_check

    subroutine rebuild_graph_entry
        type(kingraph_ptr_t), dimension(:), allocatable :: tmp_ptr
        integer :: i
        integer :: pos
        allocate (tmp_ptr(size(ct_entry%graph_entry)+1))
        pos = 0
        do i=1, size(ct_entry%graph_entry)
            pos = pos + 1
            tmp_ptr(pos)%graph => ct_entry%graph_entry(i)%graph
        end do
        pos = pos + 1
        tmp_ptr(pos)%graph => kingraph
        deallocate (ct_entry%graph_entry)
        allocate (ct_entry%graph_entry (pos))
        do i=1, pos
            ct_entry%graph_entry(i)%graph => tmp_ptr(i)%graph
        end do
        deallocate (tmp_ptr)
    end subroutine rebuild_graph_entry
end subroutine compare_tree_entry_check_kingraph

```

The grove to which a completed `kingraph` will be added is determined by the entries of `grove_prop`. We use another list type (linked list) to arrange the groves. Each `grove` contains again a linked list of `kingraphs`.

```

<Cascades2: types>+≡
  type :: grove_t
    type(grove_prop_t) :: grove_prop
    type(grove_t), pointer :: next => null ()
    type(kingraph_t), pointer :: first => null ()
    type(kingraph_t), pointer :: last => null ()
    type(compare_tree_t) :: compare_tree
  contains
    <Cascades2: grove: TBP>
  end type grove_t

```

Container for a pointer of type `grove_t`:

```

<Cascades2: types>+≡
  type :: grove_ptr_t
    type(grove_t), pointer :: grove => null ()
  end type grove_ptr_t

```

```

<Cascades2: grove: TBP>≡
  procedure :: final => grove_final

<Cascades2: sub interfaces>+≡
  module subroutine grove_final (grove)
    class(grove_t), intent(inout) :: grove
  end subroutine grove_final

<Cascades2: procedures>+≡
  module subroutine grove_final (grove)
    class(grove_t), intent(inout) :: grove
    grove%first => null ()
    grove%last  => null ()
    grove%next => null ()
  end subroutine grove_final

```

This is the list type:

```

<Cascades2: types>+≡
  type :: grove_list_t
    type(grove_t), pointer :: first => null ()
  contains
    <Cascades2: grove list: TBP>
  end type grove_list_t

```

Gfortran 7/8/9 bug, has to remain in the main module:

```

<Cascades2: grove list: TBP>≡
  procedure :: final => grove_list_final

<Cascades2: main procedures>+≡
  subroutine grove_list_final (list)
    class(grove_list_t), intent(inout) :: list

```

```

class(grove_t), pointer :: current
do while (associated (list%first))
  current => list%first
  list%first => list%first%next
  call current%final ()
  deallocate (current)
end do
end subroutine grove_list_final

```

19.11.9 The feyngraph set

The fundament of the module is the public type `feyngraph_set_t`. It is not only a linked list of all `feyngraphs` but contains an array of all particle properties (`particle`), an `f_node_list` and a pointer of the type `grove_list_t`, since several `feyngraph_sets` can share a common `grove_list`. In addition it keeps the data which unambiguously specifies the process, as well as the model which provides information which allows us to choose between equivalent subtrees or complete `kingraphs`.

```

<Cascades2: public>+≡
  public :: feyngraph_set_t

<Cascades2: types>+≡
  type :: feyngraph_set_t
    type(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(:, :), allocatable :: flv
    integer :: n_in = 0
    integer :: n_out = 0
    integer :: process_type = DECAY
    type(pbs_parameters_t) :: pbs_par
    logical :: fatal_beam_decay = .true.
    type(part_prop_t), dimension (:), pointer :: particle => null ()
    type(f_node_list_t) :: f_node_list
    type(feyngraph_t), pointer :: first => null ()
    type(feyngraph_t), pointer :: last => null ()
    integer :: n_graphs = 0
    type(grove_list_t), pointer :: grove_list => null ()
    logical :: use_dag = .true.
    type(dag_t), pointer :: dag => null ()
    type(feyngraph_set_t), dimension (:), pointer :: fset => null ()
    contains
    <Cascades2: feyngraph set: TBP>
  end type feyngraph_set_t

```

This final procedure contains calls to all other necessary final procedures. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Cascades2: feyngraph set: TBP>≡
  procedure :: final => feyngraph_set_final

<Cascades2: main procedures>+≡
  recursive subroutine feyngraph_set_final (set)
    class(feyngraph_set_t), intent(inout) :: set
    class(feyngraph_t), pointer :: current

```

```

integer :: i
if (associated (set%fset)) then
  do i=1, size (set%fset)
    call set%fset(i)%final ()
  end do
  deallocate (set%fset)
else
  set%particle => null ()
  set%grove_list => null ()
end if
set%model => null ()
if (allocated (set%flv)) deallocate (set%flv)
set%last => null ()
do while (associated (set%first))
  current => set%first
  set%first => set%first%next
  call current%final ()
  deallocate (current)
end do
if (associated (set%particle)) then
  do i = 1, size (set%particle)
    call set%particle(i)%final ()
  end do
  deallocate (set%particle)
end if
if (associated (set%grove_list)) then
  if (debug_on) call msg_debug (D_PHASESPACE, "grove_list: final")
  call set%grove_list%final ()
  deallocate (set%grove_list)
end if
if (debug_on) call msg_debug (D_PHASESPACE, "f_node_list: final")
call set%f_node_list%final ()
if (associated (set%dag)) then
  if (debug_on) call msg_debug (D_PHASESPACE, "dag: final")
  if (associated (set%dag)) then
    call set%dag%final ()
    deallocate (set%dag)
  end if
end if
end if
end subroutine feyngraph_set_final

```

19.11.10 Construct the feyngraph set

We construct the `feyngraph_set` from an input file. Therefore we pass a unit to `feyngraph_set_build`. The parsing subroutines are chosen depending on the value of `use_dag`. In the DAG output, which is the one that is produced by default, we have to work on a string of one line, where the length of this string becomes larger the more particles are involved in the process. The other output (which is now only used in a unit test) contains one Feynman diagram per line and each line starts with an open parenthesis so that we read the file line per line and create a `feyngraph` for every line. Only after this, nodes are created. In both decay and scattering processes the diagrams are represented like in a

decay process, i.e. in a scattering process one of the incoming particles appears as an outgoing particle.

```

(Cascades2: feyngraph set: TBP)+≡
    procedure :: build => feyngraph_set_build

(Cascades2: sub interfaces)+≡
    module subroutine feyngraph_set_build (feyngraph_set, u_in)
        class(feyngraph_set_t), intent(inout) :: feyngraph_set
        integer, intent(in) :: u_in
    end subroutine feyngraph_set_build

(Cascades2: procedures)+≡
    module subroutine feyngraph_set_build (feyngraph_set, u_in)
        class(feyngraph_set_t), intent(inout) :: feyngraph_set
        integer, intent(in) :: u_in
        integer :: stat = 0
        character(len=FEYNGRAPH_LEN) :: omega_feyngraph_output
        type(feyngraph_t), pointer :: current_graph
        type(feyngraph_t), pointer :: compare_graph
        logical :: present
        if (feyngraph_set%use_dag) then
            allocate (feyngraph_set%dag)
            if (.not. associated (feyngraph_set%first)) then
                call feyngraph_set%dag%read_string (u_in, feyngraph_set%flv(:,1))
                call feyngraph_set%dag%construct (feyngraph_set)
                call feyngraph_set%dag%make_feyngraphs (feyngraph_set)
            end if
        else
            if (.not. associated (feyngraph_set%first)) then
                read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') &
                    omega_feyngraph_output
                if (omega_feyngraph_output(1:1) == '(') then
                    allocate (feyngraph_set%first)
                    feyngraph_set%first%omega_feyngraph_output = &
                        trim(omega_feyngraph_output)
                    feyngraph_set%last => feyngraph_set%first
                    feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
                else
                    call msg_fatal ("Invalid input file")
                end if
            end if
            read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') &
                omega_feyngraph_output
            do while (stat == 0)
                if (omega_feyngraph_output(1:1) == '(') then
                    compare_graph => feyngraph_set%first
                    present = .false.
                    do while (associated (compare_graph))
                        if (len_trim(compare_graph%omega_feyngraph_output) &
                            == len_trim(omega_feyngraph_output)) then
                            if (compare_graph%omega_feyngraph_output == &
                                omega_feyngraph_output) then
                                present = .true.
                                exit
                            end if
                        end if
                    end if
                end if
            end while
        end if
    end subroutine feyngraph_set_build

```



```

        compare_graph => compare_graph%next
    end do
    if (.not. present) then
        allocate (feyngraph_set%last%next)
        feyngraph_set%last => feyngraph_set%last%next
        feyngraph_set%last%omega_feyngraph_output = &
            trim(omega_feyngraph_output)
        feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
    end if
    read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') &
        omega_feyngraph_output
    else
        exit
    end if
end do
current_graph => feyngraph_set%first
do while (associated (current_graph))
    call feyngraph_construct (feyngraph_set, current_graph)
    current_graph => current_graph%next
end do
feyngraph_set%f_node_list%max_tree_size = feyngraph_set%first%n_nodes
end if
end if
end subroutine feyngraph_set_build

```

Read the string from the file. The output which is produced by O'Mega contains the DAG in a factorised form as a long string, distributed over several lines (in addition, in the case of a scattering process, it contains a similar string for the same process, but with the other incoming particle as the root of the tree structure). In general, such a file can contain many of these strings, belonging to different process components. Therefore we first have to find the correct position of the string for the process in question. Therefore we look for a line containing a pair of colons, in which case the line contains a process string. Then we check if the process string describes the correct process, which is done by checking for all the incoming and outgoing particle names. If the process is correct, the dag output should start in the following line. As long as we do not find the correct process string, we continue searching. If we reach the end of the file, we rewind the unit once, and repeat searching. If the process is still not found, there must be some sort of error.

```

<Cascades2: dag: TBP>≡
    procedure :: read_string => dag_read_string

<Cascades2: sub interfaces>+≡
    module subroutine dag_read_string (dag, u_in, flv)
        class(dag_t), intent(inout) :: dag
        integer, intent(in) :: u_in
        type(flavor_t), dimension(:), intent(in) :: flv
    end subroutine dag_read_string

<Cascades2: procedures>+≡
    module subroutine dag_read_string (dag, u_in, flv)
        class(dag_t), intent(inout) :: dag
        integer, intent(in) :: u_in

```

```

type(flavor_t), dimension(:), intent(in) :: flv
character(len=BUFFER_LEN) :: process_string
logical :: process_found
logical :: rewound
!!! Find process string in file
process_found = .false.
rewound = .false.
do while (.not. process_found)
  process_string = ""
  read (unit=u_in, fmt='(A)') process_string
  if (len_trim(process_string) /= 0) then
    if (index (process_string, "::") > 0) then
      process_found = process_string_match (trim (process_string), flv)
    end if
  else if (.not. rewound) then
    rewind (u_in)
    rewound = .true.
  else
    call msg_bug ("Process string not found in O'Mega input file.")
  end if
end do
call fds_file_get_line (u_in, dag%string)
call dag%string%clean ()
if (.not. allocated (dag%string%t) .or. dag%string%char_len == 0) &
  call msg_bug ("Process string not found in O'Mega input file.")
end subroutine dag_read_string

```

The output of factorized Feynman diagrams which is created by O'Mega for a given process could in principle be written to a single line in the file. This can however lead to different problems with different compilers as soon as such lines become too long. This is the reason why the line is cut into smaller pieces. This means that a new line starts after each vertical bar. For this long string the type `dag_string_t` has been introduced. In order to read the file quickly into such a `dag_string` we use another type, `dag_chain_t` which is a linked list of such `dag_strings`. This has the advantage that we do not have to recreate a new `dag_string` for every line which has been read from file. Only in the end of this operation we compress the list of strings to a single string, removing useless `dag_tokens`, such as blanc space tokens. This subroutine reads all lines starting from the position in the file the unit is connected to, until no backslash character is found at the end of a line (the backslash means that the next line also belongs to the current string).

```

<Cascades2: parameters>+≡
integer, parameter :: BUFFER_LEN = 1000
integer, parameter :: STACK_SIZE = 100

<Cascades2: procedures>+≡
subroutine fds_file_get_line (u, string)
  integer, intent(in) :: u
  type(dag_string_t), intent(out) :: string
  type(dag_chain_t) :: chain
  integer :: string_size, current_len
  character(len=BUFFER_LEN) :: buffer
  integer :: fragment_len

```

```

integer :: stat
current_len = 0
stat = 0
string_size = 0
do while (stat == 0)
  read (unit=u, fmt='(A)', iostat=stat) buffer
  if (stat /= 0) exit
  fragment_len = len_trim (buffer)
  if (fragment_len == 0) then
    exit
  else if (buffer (fragment_len:fragment_len) == BACKSLASH_CHAR) then
    fragment_len = fragment_len - 1
  end if
  call chain%append (buffer(:fragment_len))
  if (buffer(fragment_len+1:fragment_len+1) /= BACKSLASH_CHAR) exit
end do
if (associated (chain%first)) then
  call chain%compress ()
  string = chain%first
  call chain%final ()
end if
end subroutine fds_file_get_line

```

We check, if the process string which has been read from file corresponds to the process for which we want to extract the Feynman diagrams.

(Cascades2: procedures) +=

```

function process_string_match (string, flv) result (match)
  character(len=*), intent(in) :: string
  type(flavor_t), dimension(:), intent(in) :: flv
  logical :: match
  integer :: pos
  integer :: occurrence
  integer :: i
  pos = 1
  match = .false.
  do i=1, size (flv)
    occurrence = index (string(pos:), char(flv(i)%get_name()))
    if (occurrence > 0) then
      pos = pos + occurrence
      match = .true.
    else
      match = .false.
    end if
    exit
  end do
end function process_string_match

```

19.11.11 Particle properties

This subroutine initializes a model instance with the Standard Model data. It is only relevant for a unit test. We do not have to care about the model initializa-

tion in this module because the model is passed to feyngraph_set_generate when it is called.

```

<Cascades2: public>+=
    public :: init_sm_full_test

<Cascades2: sub interfaces>+=
    module subroutine init_sm_full_test (model)
        class(model_data_t), intent(out) :: model
    end subroutine init_sm_full_test

<Cascades2: procedures>+=
    module subroutine init_sm_full_test (model)
        class(model_data_t), intent(out) :: model
        type(field_data_t), pointer :: field
        integer, parameter :: n_real = 17
        integer, parameter :: n_field = 21
        integer, parameter :: n_vtx = 56
        integer :: i
        call model%init (var_str ("SM_vertex_test"), &
            n_real, 0, n_field, n_vtx)
        call model%init_par (1, var_str ("mZ"), 91.1882_default)
        call model%init_par (2, var_str ("mW"), 80.419_default)
        call model%init_par (3, var_str ("mH"), 125._default)
        call model%init_par (4, var_str ("me"), 0.000510997_default)
        call model%init_par (5, var_str ("mmu"), 0.105658389_default)
        call model%init_par (6, var_str ("mtau"), 1.77705_default)
        call model%init_par (7, var_str ("ms"), 0.095_default)
        call model%init_par (8, var_str ("mc"), 1.2_default)
        call model%init_par (9, var_str ("mb"), 4.2_default)
        call model%init_par (10, var_str ("mtop"), 173.1_default)
        call model%init_par (11, var_str ("wtop"), 1.523_default)
        call model%init_par (12, var_str ("wZ"), 2.443_default)
        call model%init_par (13, var_str ("wW"), 2.049_default)
        call model%init_par (14, var_str ("wH"), 0.004143_default)
        call model%init_par (15, var_str ("ee"), 0.3079561542961_default)
        call model%init_par (16, var_str ("cw"), 8.819013863636E-01_default)
        call model%init_par (17, var_str ("sw"), 4.714339240339E-01_default)
        i = 0
        i = i + 1
        field => model%get_field_ptr_by_index (i)
        call field%init (var_str ("D_QUARK"), 1)
        call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
        call field%set (name = [var_str ("d")], anti = [var_str ("dbar")])
        i = i + 1
        field => model%get_field_ptr_by_index (i)
        call field%init (var_str ("U_QUARK"), 2)
        call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
        call field%set (name = [var_str ("u")], anti = [var_str ("ubar")])
        i = i + 1
        field => model%get_field_ptr_by_index (i)
        call field%init (var_str ("S_QUARK"), 3)
        call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
        call field%set (mass_data=model%get_par_real_ptr (7))
        call field%set (name = [var_str ("s")], anti = [var_str ("sbar")])
        i = i + 1

```

```

field => model%get_field_ptr_by_index (i)
call field%init (var_str ("C_QUARK"), 4)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("c")], anti = [var_str ("cbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("B_QUARK"), 5)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (mass_data=model%get_par_real_ptr (9))
call field%set (name = [var_str ("b")], anti = [var_str ("bbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("T_QUARK"), 6)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (10))
call field%set (width_data=model%get_par_real_ptr (11))
call field%set (name = [var_str ("t")], anti = [var_str ("tbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_LEPTON"), 11)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (4))
call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_NEUTRINO"), 12)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nue")], anti = [var_str ("nuebar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_LEPTON"), 13)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (5))
call field%set (name = [var_str ("mu-")], anti = [var_str ("mu+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_NEUTRINO"), 14)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("numu")], anti = [var_str ("numubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("TAU_LEPTON"), 15)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (6))
call field%set (name = [var_str ("tau-")], anti = [var_str ("tau+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("TAU_NEUTRINO"), 16)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nutau")], anti = [var_str ("nutaubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("GLUON"), 21)

```

```

call field%set (spin_type=3, color_type=8)
call field%set (name = [var_str ("gl")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PHOTON"), 22)
call field%set (spin_type=3)
call field%set (name = [var_str ("A")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("Z_BOSON"), 23)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (1))
call field%set (width_data=model%get_par_real_ptr (12))
call field%set (name = [var_str ("Z")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("W_BOSON"), 24)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (2))
call field%set (width_data=model%get_par_real_ptr (13))
call field%set (name = [var_str ("W+")] , anti = [var_str ("W-")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HIGGS"), 25)
call field%set (spin_type=1)
call field%set (mass_data=model%get_par_real_ptr (3))
call field%set (width_data=model%get_par_real_ptr (14))
call field%set (name = [var_str ("H")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PROTON"), 2212)
call field%set (spin_type=2)
call field%set (name = [var_str ("p")] , anti = [var_str ("pbar")])
!   call field%set (mass_data=model%get_par_real_ptr (12))
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_SINGLET"), 91)
call field%set (color_type=1)
call field%set (name = [var_str ("hr1")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_TRIPLET"), 92)
call field%set (color_type=3)
call field%set (name = [var_str ("hr3")] , anti = [var_str ("hr3bar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_OCTET"), 93)
call field%set (color_type=8)
call field%set (name = [var_str ("hr8")])
call model%freeze_fields ()
i = 0
i = i + 1
!!! QED
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("A")])

```

```

i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("A")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("e+"), var_str ("e-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("mu-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("tau-"), var_str ("A")])
i = i + 1
!!! QCD
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), &
var_str ("gl"), var_str ("gl")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("gl")])
i = i + 1
!!! Neutral currents
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("Z")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("e+"), var_str ("e-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("mu-"), var_str ("Z")])

```

```

i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("tau-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("nuebar"), var_str ("nue"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("numubar"), var_str ("numu"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("nutaubar"), var_str ("nutau"), &
    var_str ("Z")])
i = i + 1
!!! Charged currents
call model%set_vertex (i, [var_str ("ubar"), var_str ("d"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("s"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("b"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("u"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("c"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("t"), var_str ("W-")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("nuebar"), var_str ("e-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("numubar"), var_str ("mu-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("nutaubar"), var_str ("tau-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("e+"), var_str ("nue"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("numu"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("nutau"), var_str ("W-")])
i = i + 1
!!! Yukawa
!!! keeping only 3rd generation for the moment
! call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("H")])
! i = i + 1
! call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("H")])
! i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("H")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("H")])
i = i + 1
! call model%set_vertex (i, [var_str ("mubar"), var_str ("mu"), var_str ("H")])
! i = i + 1
call model%set_vertex (i, [var_str ("taubar"), var_str ("tau"), var_str ("H")])
i = i + 1
!!! Vector-boson self-interactions
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("Z")])

```



```

i = i + 1
!!!
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("Z"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W+"), var_str ("W-"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("Z"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("A"), var_str ("A")])
i = i + 1
!!! Higgs - vector boson
! call model%set_vertex (i, [var_str ("H"), var_str ("Z"), var_str ("A")])
! i = i + 1
! call model%set_vertex (i, [var_str ("H"), var_str ("A"), var_str ("A")])
! i = i + 1
! call model%set_vertex (i, [var_str ("H"), var_str ("gl"), var_str ("gl")])
! i = i + 1
!!!
call model%set_vertex (i, [var_str ("H"), var_str ("W+"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("Z"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("W+"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("Z"), var_str ("Z")])
i = i + 1
!!! Higgs self-interactions
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("H")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("H"), var_str ("H")])
i = i + 1
call model%freeze_vertices ()
end subroutine init_sm_full_test

```

Initialize a `part_prop` object by passing a `particle_label`, which is simply the particle name. `part_prop` should be part of the `particle` array of `feyngraph_set`. We use the model of `feyngraph_set` to obtain the relevant data of the particle which is needed to find `phase_space` parametrizations. When a `part_prop` is initialized, we add and initialize also the corresponding anti- particle `part_prop` if it is not yet in the array.

```

<Cascades2: part prop: TBP>+≡
  procedure :: init => part_prop_init

<Cascades2: sub interfaces>+≡
  recursive module subroutine part_prop_init &
    (part_prop, feyngraph_set, particle_label)
    class(part_prop_t), intent(out), target :: part_prop
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    character(len=*), intent(in) :: particle_label
  end subroutine part_prop_init

<Cascades2: procedures>+≡
  recursive module subroutine part_prop_init &
    (part_prop, feyngraph_set, particle_label)

```

```

class(part_prop_t), intent(out), target :: part_prop
type(feyngraph_set_t), intent(inout) :: feyngraph_set
character(len=*), intent(in) :: particle_label
type(flavor_t) :: flv, anti
type(string_t) :: name
integer :: i
name = particle_label
call flv%init (name, feyngraph_set%model)
part_prop%particle_label = particle_label
part_prop%pdg = flv%get_pdg ()
part_prop%mass = flv%get_mass ()
part_prop%width = flv%get_width()
part_prop%spin_type = flv%get_spin_type ()
part_prop%is_vector = flv%get_spin_type () == VECTOR
part_prop%empty = .false.
part_prop%tex_name = flv%get_tex_name ()
anti = flv%anti ()
if (flv%get_pdg() == anti%get_pdg()) then
  select type (part_prop)
  type is (part_prop_t)
    part_prop%anti => part_prop
  end select
else
  do i=1, size (feyngraph_set%particle)
    if (feyngraph_set%particle(i)%pdg == (- part_prop%pdg)) then
      part_prop%anti => feyngraph_set%particle(i)
      exit
    else if (feyngraph_set%particle(i)%empty) then
      part_prop%anti => feyngraph_set%particle(i)
      call feyngraph_set%particle(i)%init &
        (feyngraph_set, char(anti%get_name()))
      exit
    end if
  end do
end if
end subroutine part_prop_init

```

This subroutine assigns to a node the particle properties. Since these properties do not change and are simply read from the model file, we use pointers to the elements of the `particle` array of the `feyngraph_set`. If there is no corresponding array element, we have to initialize the first empty element of the array.

```

<Cascades2: parameters>+≡
  integer, parameter :: PRT_ARRAY_SIZE = 200

<Cascades2: f node: TBP>+≡
  procedure :: assign_particle_properties => f_node_assign_particle_properties

<Cascades2: sub interfaces>+≡
  module subroutine f_node_assign_particle_properties (node, feyngraph_set)
    class(f_node_t), intent(inout) :: node
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
  end subroutine f_node_assign_particle_properties

```

```

<Cascades2: procedures>+=
module subroutine f_node_assign_particle_properties (node, feyngraph_set)
  class(f_node_t), intent(inout) :: node
  type(feyngraph_set_t), intent(inout) :: feyngraph_set
  character(len=LABEL_LEN) :: particle_label
  integer :: i
  particle_label = node%particle_label(1:index (node%particle_label, '[')-1)
  if (.not. associated (feyngraph_set%particle)) then
    allocate (feyngraph_set%particle (PRT_ARRAY_SIZE))
  end if
  do i = 1, size (feyngraph_set%particle)
    if (particle_label == feyngraph_set%particle(i)%particle_label) then
      node%particle => feyngraph_set%particle(i)
      exit
    else if (feyngraph_set%particle(i)%empty) then
      call feyngraph_set%particle(i)%init (feyngraph_set, particle_label)
      node%particle => feyngraph_set%particle(i)
      exit
    end if
  end do
  !!! Since the O'Mega output uses the anti-particles instead of the
  !!! particles specified in the process definition, we revert this
  !!! here. An exception is the first particle in the parsable DAG output
  node%particle => node%particle%anti
end subroutine f_node_assign_particle_properties

```

From the output of a Feynman diagram (in the non-factorized output) we need to find out how many daughter nodes would be required to reconstruct it correctly, to make sure that we keep only those **feyngraphs** which are constructed solely on the basis of the 3-vertices which are provided by the model. The number of daughter particles can easily be determined from the syntax of O'Mega's output: The particle which appears before the colon ':' is the mother particle. The particles or subtrees (i.e. whole parentheses) follow after the colon and are separated by commas.

```

<Cascades2: procedures>+=
function get_n_daughters (subtree_string, pos_first_colon) &
  result (n_daughters)
  character(len=*), intent(in) :: subtree_string
  integer, intent(in) :: pos_first_colon
  integer :: n_daughters
  integer :: n_open_par
  integer :: i
  n_open_par = 1
  n_daughters = 0
  if (len_trim(subtree_string) > 0) then
    if (pos_first_colon > 0) then
      do i=pos_first_colon, len_trim(subtree_string)
        if (subtree_string(i:i) == ',') then
          if (n_open_par == 1) n_daughters = n_daughters + 1
        else if (subtree_string(i:i) == '(') then
          n_open_par = n_open_par + 1
        else if (subtree_string(i:i) == ')') then
          n_open_par = n_open_par - 1
        end if
      end do
    end if
  end if
end function get_n_daughters

```

```

        end if
    end do
    if (n_open_par == 0) then
        n_daughters = n_daughters + 1
    end if
end if
end if
end if
end function get_n_daughters

```

19.11.12 Reconstruction of trees

The reconstruction of a tree or subtree with the non-factorized input can be done recursively, i.e. we first find the root of the tree in the string and create an `f_node`. Then we look for daughters, which in the string appear either as single particles or subtrees (which are of the same form as the tree which we want to reconstruct. Therefore the subroutine can simply be called again and again until there are no more daughter nodes to create. When we meet a vertex which requires more than two daughter particles, we stop the recursion and disable the node using its `keep` variable. Whenever a daughter node is not kept, we do not keep the mother node as well.

(Cascades2: procedures) +=

```

recursive subroutine node_construct_subtree_rec (feyngraph_set, &
    feyngraph, subtree_string, mother_node)
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(feyngraph_t), intent(inout) :: feyngraph
    character(len=*), intent(in) :: subtree_string
    type(f_node_t), pointer, intent(inout) :: mother_node
    integer :: n_daughters
    integer :: pos_first_colon
    integer :: current_daughter
    integer :: pos_subtree_begin, pos_subtree_end
    integer :: i
    integer :: n_open_par
    if (.not. associated (mother_node)) then
        call feyngraph_set%f_node_list%add_entry (subtree_string, mother_node, .true.)
        current_daughter = 1
        n_open_par = 1
        pos_first_colon = index (subtree_string, ':')
        n_daughters = get_n_daughters (subtree_string, pos_first_colon)
        if (pos_first_colon == 0) then
            mother_node%particle_label = subtree_string
        else
            mother_node%particle_label = subtree_string(2:pos_first_colon-1)
        end if
        if (.not. associated (mother_node%particle)) then
            call mother_node%assign_particle_properties (feyngraph_set)
        end if
        if (n_daughters /= 2 .and. n_daughters /= 0) then
            mother_node%keep = .false.
            feyngraph%keep = .false.
            return
        end if
    end if

```

```

pos_subtree_begin = pos_first_colon + 1
do i = pos_first_colon + 1, len(trim(subtree_string))
  if (current_daughter == 2) then
    pos_subtree_end = len(trim(subtree_string)) - 1
    call node_construct_subtree_rec (feyngraph_set, feyngraph, &
      subtree_string(pos_subtree_begin:pos_subtree_end), &
      mother_node%daughter2)
    exit
  else if (subtree_string(i:i) == ',') then
    if (n_open_par == 1) then
      pos_subtree_end = i - 1
      call node_construct_subtree_rec (feyngraph_set, feyngraph, &
        subtree_string(pos_subtree_begin:pos_subtree_end), &
        mother_node%daughter1)
      current_daughter = 2
      pos_subtree_begin = i + 1
    end if
  else if (subtree_string(i:i) == '(') then
    n_open_par = n_open_par + 1
  else if (subtree_string(i:i) == ')') then
    n_open_par = n_open_par - 1
  end if
end do
end if
if (associated (mother_node%daughter1)) then
  if (.not. mother_node%daughter1%keep) then
    mother_node%keep = .false.
  end if
end if
if (associated (mother_node%daughter2)) then
  if (.not. mother_node%daughter2%keep) then
    mother_node%keep = .false.
  end if
end if
if (associated (mother_node%daughter1) .and. &
  associated (mother_node%daughter2)) then
  mother_node%n_subtree_nodes = &
    mother_node%daughter1%n_subtree_nodes &
    + mother_node%daughter2%n_subtree_nodes + 1
end if
if (.not. mother_node%keep) then
  feyngraph%keep = .false.
end if
end subroutine node_construct_subtree_rec

```

When the non-factorized version of the O'Mega output is used, the feyngraph is reconstructed from the contents of its string_t variable omega_feyngraph_output. This can be used for the recursive reconstruction of the tree of k_nodes with node_construct_subtree_rec.

<Cascades2: procedures>+≡

```

subroutine feyngraph_construct (feyngraph_set, feyngraph)
  type(feyngraph_set_t), intent(inout) :: feyngraph_set
  type(feyngraph_t), pointer, intent(inout) :: feyngraph

```

```

call node_construct_subtree_rec (feyngraph_set, feyngraph, &
char(feyngraph%omega_feyngraph_output), feyngraph%root)
feyngraph%n_nodes = feyngraph%root%n_subtree_nodes
end subroutine feyngraph_construct

```

We introduce another node type, which is called `dag_node_t` and is used to reproduce the dag structure which is represented by the input. The `dag_nodes` can have several combinations of daughters 1 and 2. The `dag` type contains an array of `dag_nodes` and is only used for the reconstruction of `feyngraphs` which are factorized as well, but in the other direction as the original output. This means in particular that the outgoing particles in the output file (which there can appear many times) exist only once as `f_nodes`. To represent combinations of daughters and alternatives (options), we further use the types `dag_options_t` and `dag_combination_t`. The `dag_nodes`, `dag_options` and `dag_combinations` correspond to a substring of the string which has been read from file (and transformed into an object of type `dag_string_t`, which is simply another compact representation of this string), or a modified version of this substring. The aim is to create only one object for a given substring, even if it appears several times in the original string and then create trees of `f_nodes`, which build up the `feyngraph`, such that as many `f_nodes` as possible can be reused. An outgoing particle (always interpreting the input as a decay) is called a `leaf` in the context of a `dag`.

```

<Cascades2: types>+=
  type :: dag_node_t
    integer :: string_len
    type(dag_string_t) :: string
    logical :: leaf = .false.
    type(f_node_ptr_t), dimension (:), allocatable :: f_node
    integer :: subtree_size = 0
  contains
    <Cascades2: dag node: TBP>
  end type dag_node_t

<Cascades2: dag node: TBP>=
  procedure :: final => dag_node_final

<Cascades2: sub interfaces>+=
  module subroutine dag_node_final (dag_node)
    class(dag_node_t), intent(inout) :: dag_node
  end subroutine dag_node_final

<Cascades2: procedures>+=
  module subroutine dag_node_final (dag_node)
    class(dag_node_t), intent(inout) :: dag_node
    integer :: i
    call dag_node%string%final ()
    if (allocated (dag_node%f_node)) then
      do i=1, size (dag_node%f_node)
        if (associated (dag_node%f_node(i)%node)) then
          call dag_node%f_node(i)%node%final ()
          deallocate (dag_node%f_node(i)%node)
        end if
      end do
    end do
  end subroutine dag_node_final

```

```

        deallocate (dag_node%f_node)
    end if
end subroutine dag_node_final

```

Whenever there are more than one possible subtrees (represented by a `dag_node`) or combinations of subtrees to daughters (represented by `dag_combination_t`), we use the type `dag_options_t`. In the syntax of the factorized output, options are listed within curly braces, separated by horizontal bars.

```

<Cascades2: types>+≡
type :: dag_options_t
    integer :: string_len
    type(dag_string_t) :: string
    type(f_node_ptr_t), dimension (:), allocatable :: f_node_ptr1
    type(f_node_ptr_t), dimension (:), allocatable :: f_node_ptr2
contains
    <Cascades2: dag options: TBP>
end type dag_options_t

<Cascades2: dag options: TBP>≡
procedure :: final => dag_options_final

<Cascades2: sub interfaces>+≡
module subroutine dag_options_final (dag_options)
    class(dag_options_t), intent(inout) :: dag_options
end subroutine dag_options_final

<Cascades2: procedures>+≡
module subroutine dag_options_final (dag_options)
    class(dag_options_t), intent(inout) :: dag_options
    integer :: i
    call dag_options%string%final ()
    if (allocated (dag_options%f_node_ptr1)) then
        do i=1, size (dag_options%f_node_ptr1)
            dag_options%f_node_ptr1(i)%node => null ()
        end do
        deallocate (dag_options%f_node_ptr1)
    end if
    if (allocated (dag_options%f_node_ptr2)) then
        do i=1, size (dag_options%f_node_ptr2)
            dag_options%f_node_ptr2(i)%node => null ()
        end do
        deallocate (dag_options%f_node_ptr2)
    end if
end subroutine dag_options_final

```

A pair of two daughters (which can be `dag_nodes` or `dag_options`) is represented by the type `dag_combination_t`. In the original string, a `dag_combination` appears between parentheses, which contain a comma, but not a colon. If we find a colon between these parentheses, it is a `dag_node` instead.

```

<Cascades2: types>+≡
type :: dag_combination_t
    integer :: string_len
    type(dag_string_t) :: string

```

```

        integer, dimension (2) :: combination
        type(f_node_ptr_t), dimension (:), allocatable :: f_node_ptr1
        type(f_node_ptr_t), dimension (:), allocatable :: f_node_ptr2
    contains
        <Cascades2: dag combination: TBP>
    end type dag_combination_t

<Cascades2: dag combination: TBP>≡
    procedure :: final => dag_combination_final

<Cascades2: sub interfaces>+≡
    module subroutine dag_combination_final (dag_combination)
        class(dag_combination_t), intent(inout) :: dag_combination
    end subroutine dag_combination_final

<Cascades2: procedures>+≡
    module subroutine dag_combination_final (dag_combination)
        class(dag_combination_t), intent(inout) :: dag_combination
        integer :: i
        call dag_combination%string%final ()
        if (allocated (dag_combination%f_node_ptr1)) then
            do i=1, size (dag_combination%f_node_ptr1)
                dag_combination%f_node_ptr1(i)%node => null ()
            end do
            deallocate (dag_combination%f_node_ptr1)
        end if
        if (allocated (dag_combination%f_node_ptr2)) then
            do i=1, size (dag_combination%f_node_ptr2)
                dag_combination%f_node_ptr2(i)%node => null ()
            end do
            deallocate (dag_combination%f_node_ptr2)
        end if
    end subroutine dag_combination_final

```

Here is the type representing the DAG, i.e. it holds arrays of the `dag_nodes`, `dag_options` and `dag_combinations`. The root node of the `dag` is the last filled element of the `node` array.

```

<Cascades2: types>+≡
    type :: dag_t
        type(dag_string_t) :: string
        type(dag_node_t), dimension (:), allocatable :: node
        type(dag_options_t), dimension (:), allocatable :: options
        type(dag_combination_t), dimension (:), allocatable :: combination
        integer :: n_nodes = 0
        integer :: n_options = 0
        integer :: n_combinations = 0
    contains
        <Cascades2: dag: TBP>
    end type dag_t

<Cascades2: dag: TBP>+≡
    procedure :: final => dag_final

```



```

<Cascades2: sub interfaces>+≡
  module subroutine dag_final (dag)
    class(dag_t), intent(inout) :: dag
  end subroutine dag_final

<Cascades2: procedures>+≡
  module subroutine dag_final (dag)
    class(dag_t), intent(inout) :: dag
    integer :: i
    call dag%string%final ()
    if (allocated (dag%node)) then
      do i=1, size (dag%node)
        call dag%node(i)%final ()
      end do
      deallocate (dag%node)
    end if
    if (allocated (dag%options)) then
      do i=1, size (dag%options)
        call dag%options(i)%final ()
      end do
      deallocate (dag%options)
    end if
    if (allocated (dag%combination)) then
      do i=1, size (dag%combination)
        call dag%combination(i)%final ()
      end do
      deallocate (dag%combination)
    end if
  end subroutine dag_final

```

We construct the DAG from the given `dag_string` which is modified several times so that in the end the remaining string corresponds to a simple `dag_node`, the root of the factorized tree. This means that we first identify the leaves, i.e. outgoing particles. Then we identify `dag_nodes`, `dag_combinations` and `options` until the number of these objects does not change any more. Identifying means that we add a corresponding object to the array (if not yet present), which can be identified with the corresponding substring, and replace the substring in the original `dag_string` by a `dag_token` of the corresponding type (in the char output of this token, this corresponds to a place holder like e.g. '<O23>' which in this particular case corresponds to an option and can be found at the position 23 in the array). The character output of the substrings turns out to be very useful for debugging.

```

<Cascades2: dag: TBP>+≡
  procedure :: construct => dag_construct

<Cascades2: sub interfaces>+≡
  module subroutine dag_construct (dag, feyngraph_set)
    class(dag_t), intent(inout) :: dag
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
  end subroutine dag_construct

<Cascades2: procedures>+≡
  module subroutine dag_construct (dag, feyngraph_set)
    class(dag_t), intent(inout) :: dag

```

```

type(feyngraph_set_t), intent(inout) :: feyngraph_set
integer :: n_nodes
integer :: n_options
integer :: n_combinations
logical :: continue_loop
integer :: subtree_size
integer :: i,j
subtree_size = 1
call dag%get_nodes_and_combinations (leaves = .true.)
do i=1, dag%n_nodes
    call dag%node(i)%make_f_nodes (feyngraph_set, dag)
end do
continue_loop = .true.
subtree_size = subtree_size + 2
do while (continue_loop)
    n_nodes = dag%n_nodes
    n_options = dag%n_options
    n_combinations = dag%n_combinations
    call dag%get_nodes_and_combinations (leaves = .false.)
    if (n_nodes /= dag%n_nodes) then
        dag%node(n_nodes+1:dag%n_nodes)%subtree_size = subtree_size
        do i = n_nodes+1, dag%n_nodes
            call dag%node(i)%make_f_nodes (feyngraph_set, dag)
        end do
        subtree_size = subtree_size + 2
    end if
    if (n_combinations /= dag%n_combinations) then
        !$OMP PARALLEL DO
        do i = n_combinations+1, dag%n_combinations
            call dag%combination(i)%make_f_nodes (feyngraph_set, dag)
        end do
        !$OMP END PARALLEL DO
    end if
    call dag%get_options ()
    if (n_options /= dag%n_options) then
        !$OMP PARALLEL DO
        do i = n_options+1, dag%n_options
            call dag%options(i)%make_f_nodes (feyngraph_set, dag)
        end do
        !$OMP END PARALLEL DO
    end if
    if (n_nodes == dag%n_nodes .and. n_options == dag%n_options &
        .and. n_combinations == dag%n_combinations) then
        continue_loop = .false.
    end if
end do
!!! add root node to dag
call dag%add_node (dag%string%t, leaf = .false.)
dag%node(dag%n_nodes)%subtree_size = subtree_size
call dag%node(dag%n_nodes)%make_f_nodes (feyngraph_set, dag)
if (debug2_active (D_PHASESPACE)) then
    call dag%write (output_unit)
end if
!!! set indices for all f_nodes

```

```

do i=1, dag%n_nodes
  if (allocated (dag%node(i)%f_node)) then
    do j=1, size (dag%node(i)%f_node)
      if (associated (dag%node(i)%f_node(j)%node)) &
        call dag%node(i)%f_node(j)%node%set_index ( )
    end do
  end if
end do
end subroutine dag_construct

```

Identify `dag_nodes` and `dag_combinations`. Leaves are simply nodes (i.e. of type `NODE_TK`) where only one bit in the bincode is set. The `dag_nodes` and `dag_combinations` have in common that they are surrounded by parentheses. There is however a way to distinguish between them because the corresponding substring contains a colon (or `dag_token` with type `COLON_TK`) if it is a `dag_node`. Otherwise it is a `dag_combination`. The string of the `dag_node` or `dag_combination` should not contain curly braces, because these correspond to `dag_options` and should be identified before.

```

<Cascades2: dag: TBP>+=
  procedure :: get_nodes_and_combinations => dag_get_nodes_and_combinations

<Cascades2: sub interfaces>+=
  module subroutine dag_get_nodes_and_combinations (dag, leaves)
    class(dag_t), intent(inout) :: dag
    logical, intent(in) :: leaves
  end subroutine dag_get_nodes_and_combinations

<Cascades2: procedures>+=
  module subroutine dag_get_nodes_and_combinations (dag, leaves)
    class(dag_t), intent(inout) :: dag
    logical, intent(in) :: leaves
    type(dag_string_t) :: new_string
    integer :: i, j, k
    integer :: i_node
    integer :: new_size
    integer :: first_colon
    logical :: combination
    !!! Create nodes also for external particles, except for the incoming one
    !!! which appears as the root of the tree. These can easily be identified
    !!! by their bincodes, since they should contain only one bit which is set.
    if (leaves) then
      first_colon = &
        minloc (dag%string%t%type, 1, dag%string%t%type == COLON_TK)
      do i = first_colon + 1, size (dag%string%t)
        if (dag%string%t(i)%type == NODE_TK) then
          if (popcnt(dag%string%t(i)%bincode) == 1) then
            call dag%add_node (dag%string%t(i:i), .true., i_node)
            call dag%string%t(i)%init_dag_object_token (DAG_NODE_TK, i_node)
          end if
        end if
      end do
      call dag%string%update_char_len ( )
    else
      !!! Create a node or combination for every closed pair of parentheses
    end if
  end subroutine

```

```

!!! which do not contain any other parentheses or curly braces.
!!! A node (not outgoing) contains a colon. This is not the case
!!! for combinations, which we use as the criteria to distinguish
!!! between both.
    allocate (new_string%t (size (dag%string%t)))
    i = 1
    new_size = 0
    do while (i <= size(dag%string%t))
        if (dag%string%t(i)%type == OPEN_PAR_TK) then
            combination = .true.
            do j = i+1, size (dag%string%t)
                select case (dag%string%t(j)%type)
                    case (CLOSED_PAR_TK)
                        new_size = new_size + 1
                        if (combination) then
                            call dag%add_combination (dag%string%t(i:j), i_node)
                            call new_string%t(new_size)%init_dag_object_token &
                                (DAG_COMBINATION_TK, i_node)
                        else
                            call dag%add_node (dag%string%t(i:j), leaves, i_node)
                            call new_string%t(new_size)%init_dag_object_token &
                                (DAG_NODE_TK, i_node)
                        end if
                    i = j + 1
                    exit
                case (OPEN_PAR_TK, OPEN_CURLY_TK, CLOSED_CURLY_TK)
                    new_size = new_size + 1
                    new_string%t(new_size) = dag%string%t(i)
                    i = i + 1
                    exit
                case (COLON_TK)
                    combination = .false.
                end select
            end do
        else
            new_size = new_size + 1
            new_string%t(new_size) = dag%string%t(i)
            i = i + 1
        end if
    end do
    dag%string = new_string%t(:new_size)
    call dag%string%update_char_len ()
end if
end subroutine dag_get_nodes_and_combinations

```

Identify `dag_options`, i.e. lists of rival nodes or combinations of nodes. These are identified by the surrounding curly braces. They should not contain any parentheses any more, because these correspond either to nodes or to combinations and should be identified before.

```

<Cascades2: dag: TBP>+≡
    procedure :: get_options => dag_get_options

<Cascades2: sub interfaces>+≡
    module subroutine dag_get_options (dag)

```

```

        class(dag_t), intent(inout) :: dag
    end subroutine dag_get_options
<Cascades2: procedures>+≡
module subroutine dag_get_options (dag)
    class(dag_t), intent(inout) :: dag
    type(dag_string_t) :: new_string
    integer :: i, j, k
    integer :: new_size
    integer :: i_options
    character(len=10) :: index_char
    integer :: index_start, index_end
    !!! Create a node or combination for every closed pair of parentheses
    !!! which do not contain any other parentheses or curly braces.
    !!! A node (not outgoing) contains a colon. This is not the case
    !!! for combinations, which we use as the criteria to distinguish
    !!! between both.
    allocate (new_string%t (size (dag%string%t)))
    i = 1
    new_size = 0
    do while (i <= size(dag%string%t))
        if (dag%string%t(i)%type == OPEN_CURLY_TK) then
            do j = i+1, size (dag%string%t)
                select case (dag%string%t(j)%type)
                    case (CLOSED_CURLY_TK)
                        new_size = new_size + 1
                        call dag%add_options (dag%string%t(i:j), i_options)
                        call new_string%t(new_size)%init_dag_object_token (DAG_OPTIONS_TK, i_options)
                        i = j + 1
                        exit
                    case (OPEN_PAR_TK, CLOSED_PAR_TK, OPEN_CURLY_TK)
                        new_size = new_size + 1
                        new_string%t(new_size) = dag%string%t(i)
                        i = i + 1
                        exit
                end select
            end do
        else
            new_size = new_size + 1
            new_string%t(new_size) = dag%string%t(i)
            i = i + 1
        end if
    end do
    dag%string = new_string%t(:new_size)
    call dag%string%update_char_len ()
end subroutine dag_get_options

```

Add a `dag_node` to the list. The optional argument returns the index of the node. The node might already exist. In this case we only return the index.

```

<Cascades2: dag: TBP>+≡
    procedure :: add_node => dag_add_node
<Cascades2: parameters>+≡
    integer, parameter :: DAG_STACK_SIZE = 1000

```

```

<Cascades2: sub interfaces>+=
  module subroutine dag_add_node (dag, string, leaf, i_node)
    class(dag_t), intent(inout) :: dag
    type(dag_token_t), dimension (:), intent(in) :: string
    logical, intent(in) :: leaf
    integer, intent(out), optional :: i_node
  end subroutine dag_add_node

<Cascades2: procedures>+=
  module subroutine dag_add_node (dag, string, leaf, i_node)
    class(dag_t), intent(inout) :: dag
    type(dag_token_t), dimension (:), intent(in) :: string
    logical, intent(in) :: leaf
    integer, intent(out), optional :: i_node
    type(dag_node_t), dimension (:), allocatable :: tmp_node
    integer :: string_len
    integer :: i
    string_len = sum (string%char_len)
    if (.not. allocated (dag%node)) then
      allocate (dag%node (DAG_STACK_SIZE))
    else if (dag%n_nodes == size (dag%node)) then
      allocate (tmp_node (dag%n_nodes))
      tmp_node = dag%node
      deallocate (dag%node)
      allocate (dag%node (dag%n_nodes+DAG_STACK_SIZE))
      dag%node(:dag%n_nodes) = tmp_node
      deallocate (tmp_node)
    end if
    do i = 1, dag%n_nodes
      if (dag%node(i)%string_len == string_len) then
        if (size (dag%node(i)%string%t) == size (string)) then
          if (all(dag%node(i)%string%t == string)) then
            if (present (i_node)) i_node = i
            return
          end if
        end if
      end if
    end do
    dag%n_nodes = dag%n_nodes + 1
    dag%node(dag%n_nodes)%string = string
    dag%node(dag%n_nodes)%string_len = string_len
    if (present (i_node)) i_node = dag%n_nodes
    dag%node(dag%n_nodes)%leaf = leaf
  end subroutine dag_add_node

```

A similar subroutine for options.

```

<Cascades2: dag: TBP>+=
  procedure :: add_options => dag_add_options

<Cascades2: sub interfaces>+=
  module subroutine dag_add_options (dag, string, i_options)
    class(dag_t), intent(inout) :: dag
    type(dag_token_t), dimension (:), intent(in) :: string
    integer, intent(out), optional :: i_options
  end subroutine dag_add_options

```

```

<Cascades2: procedures>+≡
module subroutine dag_add_options (dag, string, i_options)
  class(dag_t), intent(inout) :: dag
  type(dag_token_t), dimension (:), intent(in) :: string
  integer, intent(out), optional :: i_options
  type(dag_options_t), dimension (:), allocatable :: tmp_options
  integer :: string_len
  integer :: i
  string_len = sum (string%char_len)
  if (.not. allocated (dag%options)) then
    allocate (dag%options (DAG_STACK_SIZE))
  else if (dag%n_options == size (dag%options)) then
    allocate (tmp_options (dag%n_options))
    tmp_options = dag%options
    deallocate (dag%options)
    allocate (dag%options (dag%n_options+DAG_STACK_SIZE))
    dag%options(:dag%n_options) = tmp_options
    deallocate (tmp_options)
  end if
  do i = 1, dag%n_options
    if (dag%options(i)%string_len == string_len) then
      if (size (dag%options(i)%string%t) == size (string)) then
        if (all(dag%options(i)%string%t == string)) then
          if (present (i_options)) i_options = i
          return
        end if
      end if
    end if
  end do
  dag%n_options = dag%n_options + 1
  dag%options(dag%n_options)%string = string
  dag%options(dag%n_options)%string_len = string_len
  if (present (i_options)) i_options = dag%n_options
end subroutine dag_add_options

```

A similar subroutine for combinations.

```

<Cascades2: dag: TBP>+≡
  procedure :: add_combination => dag_add_combination

<Cascades2: sub interfaces>+≡
  module subroutine dag_add_combination (dag, string, i_combination)
    class(dag_t), intent(inout) :: dag
    type(dag_token_t), dimension (:), intent(in) :: string
    integer, intent(out), optional :: i_combination
  end subroutine dag_add_combination

<Cascades2: procedures>+≡
module subroutine dag_add_combination (dag, string, i_combination)
  class(dag_t), intent(inout) :: dag
  type(dag_token_t), dimension (:), intent(in) :: string
  integer, intent(out), optional :: i_combination
  type(dag_combination_t), dimension (:), allocatable :: tmp_combination
  integer :: string_len
  integer :: i
  string_len = sum (string%char_len)

```

```

if (.not. allocated (dag%combination)) then
  allocate (dag%combination (DAG_STACK_SIZE))
else if (dag%n_combinations == size (dag%combination)) then
  allocate (tmp_combination (dag%n_combinations))
  tmp_combination = dag%combination
  deallocate (dag%combination)
  allocate (dag%combination (dag%n_combinations+DAG_STACK_SIZE))
  dag%combination(:dag%n_combinations) = tmp_combination
  deallocate (tmp_combination)
end if
do i = 1, dag%n_combinations
  if (dag%combination(i)%string_len == string_len) then
    if (size (dag%combination(i)%string%t) == size (string)) then
      if (all(dag%combination(i)%string%t == string)) then
        i_combination = i
        return
      end if
    end if
  end if
end do
dag%n_combinations = dag%n_combinations + 1
dag%combination(dag%n_combinations)%string = string
dag%combination(dag%n_combinations)%string_len = string_len
if (present (i_combination)) i_combination = dag%n_combinations
end subroutine dag_add_combination

```

For a given `dag_node` we want to create all `f_nodes`. If the node is not a leaf, it contains in its string placeholders for options or combinations. For these objects there are similar subroutines which are needed here to obtain the sets of daughter nodes. If the `dag_node` is a leaf, it corresponds to an external particle and the token contains the particle name.

<Cascades2: dag node: TBP>+≡

```

procedure :: make_f_nodes => dag_node_make_f_nodes

```

<Cascades2: sub interfaces>+≡

```

module subroutine dag_node_make_f_nodes (dag_node, feyngraph_set, dag)
  class(dag_node_t), intent(inout) :: dag_node
  type(feyngraph_set_t), intent(inout) :: feyngraph_set
  type(dag_t), intent(inout) :: dag
end subroutine dag_node_make_f_nodes

```

<Cascades2: procedures>+≡

```

module subroutine dag_node_make_f_nodes (dag_node, feyngraph_set, dag)
  class(dag_node_t), intent(inout) :: dag_node
  type(feyngraph_set_t), intent(inout) :: feyngraph_set
  type(dag_t), intent(inout) :: dag
  character(len=LABEL_LEN) :: particle_label
  integer :: i, j
  integer, dimension (2) :: obj
  integer, dimension (2) :: i_obj
  integer :: n_obj
  integer :: pos
  integer :: new_size, size1, size2
  integer, dimension(:), allocatable :: match

```



```

if (allocated (dag_node%f_node)) return
pos = minloc (dag_node%string%t%type, 1,dag_node%string%t%type == NODE_TK)
particle_label = char (dag_node%string%t(pos))
if (dag_node%leaf) then
!!! construct subtree with procedure similar to the one for the old output
    allocate (dag_node%f_node(1))
    allocate (dag_node%f_node(1)%node)
    dag_node%f_node(1)%node%particle_label = particle_label
    call dag_node%f_node(1)%node%assign_particle_properties (feyngraph_set)
    if (.not. dag_node%f_node(1)%node%keep) then
        deallocate (dag_node%f_node)
        return
    end if
else
    n_obj = 0
    do i = 1, size (dag_node%string%t)
        select case (dag_node%string%t(i)%type)
        case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
            n_obj = n_obj + 1
            if (n_obj > 2) return
            obj(n_obj) = dag_node%string%t(i)%type
            i_obj(n_obj) = dag_node%string%t(i)%index
        end select
    end do
    if (n_obj == 1) then
        if (obj(1) == DAG_OPTIONS_TK) then
            if (allocated (dag%options(i_obj(1))%f_node_ptr1)) then
                size1 = size(dag%options(i_obj(1))%f_node_ptr1)
                allocate (dag_node%f_node(size1))
                do i=1, size1
                    allocate (dag_node%f_node(i)%node)
                    dag_node%f_node(i)%node%particle_label = particle_label
                    call dag_node%f_node(i)%node%assign_particle_properties (feyngraph_set)
                    dag_node%f_node(i)%node%daughter1 => dag%options(i_obj(1))%f_node_ptr1(i)%node
                    dag_node%f_node(i)%node%daughter2 => dag%options(i_obj(1))%f_node_ptr2(i)%node
                    dag_node%f_node(i)%node%n_subtree_nodes = &
                        dag%options(i_obj(1))%f_node_ptr1(i)%node%n_subtree_nodes &
                        + dag%options(i_obj(1))%f_node_ptr2(i)%node%n_subtree_nodes + 1
                end do
            end if
        else if (obj(1) == DAG_COMBINATION_TK) then
            if (allocated (dag%combination(i_obj(1))%f_node_ptr1)) then
                size1 = size(dag%combination(i_obj(1))%f_node_ptr1)
                allocate (dag_node%f_node(size1))
                do i=1, size1
                    allocate (dag_node%f_node(i)%node)
                    dag_node%f_node(i)%node%particle_label = particle_label
                    call dag_node%f_node(i)%node%assign_particle_properties (feyngraph_set)
                    dag_node%f_node(i)%node%daughter1 => dag%combination(i_obj(1))%f_node_ptr1(i)%node
                    dag_node%f_node(i)%node%daughter2 => dag%combination(i_obj(1))%f_node_ptr2(i)%node
                    dag_node%f_node(i)%node%n_subtree_nodes = &
                        dag%combination(i_obj(1))%f_node_ptr1(i)%node%n_subtree_nodes &
                        + dag%combination(i_obj(1))%f_node_ptr2(i)%node%n_subtree_nodes + 1
                end do
            end if
        end if
    end if
end do

```

```

        end if
    end if
    !!! simply set daughter pointers, daughters are already combined correctly
    else if (n_obj == 2) then
        size1 = 0
        size2 = 0
        if (obj(1) == DAG_NODE_TK) then
            if (allocated (dag%node(i_obj(1))%f_node)) then
                do i=1, size (dag%node(i_obj(1))%f_node)
                    if (dag%node(i_obj(1))%f_node(i)%node%keep) size1 = size1 + 1
                end do
            end if
        else if (obj(1) == DAG_OPTIONS_TK) then
            if (allocated (dag%options(i_obj(1))%f_node_ptr1)) then
                do i=1, size (dag%options(i_obj(1))%f_node_ptr1)
                    if (dag%options(i_obj(1))%f_node_ptr1(i)%node%keep) size1 = size1 + 1
                end do
            end if
        end if
        if (obj(2) == DAG_NODE_TK) then
            if (allocated (dag%node(i_obj(2))%f_node)) then
                do i=1, size (dag%node(i_obj(2))%f_node)
                    if (dag%node(i_obj(2))%f_node(i)%node%keep) size2 = size2 + 1
                end do
            end if
        else if (obj(2) == DAG_OPTIONS_TK) then
            if (allocated (dag%options(i_obj(2))%f_node_ptr1)) then
                do i=1, size (dag%options(i_obj(2))%f_node_ptr1)
                    if (dag%options(i_obj(2))%f_node_ptr1(i)%node%keep) size2 = size2 + 1
                end do
            end if
        end if
    end if
    !!! make all combinations of daughters
    select case (obj(1))
    case (DAG_NODE_TK)
        select case (obj(2))
        case (DAG_NODE_TK)
            call combine_all_daughters(dag%node(i_obj(1))%f_node, &
                dag%node(i_obj(2))%f_node)
        case (DAG_OPTIONS_TK)
            call combine_all_daughters(dag%node(i_obj(1))%f_node, &
                dag%options(i_obj(2))%f_node_ptr1)
        end select
    case (DAG_OPTIONS_TK)
        select case (obj(2))
        case (DAG_NODE_TK)
            call combine_all_daughters(dag%options(i_obj(1))%f_node_ptr1, &
                dag%node(i_obj(2))%f_node)
        case (DAG_OPTIONS_TK)
            call combine_all_daughters(dag%options(i_obj(1))%f_node_ptr1, &
                dag%options(i_obj(2))%f_node_ptr1)
        end select
    end select
end if

```

```

end if

contains

subroutine combine_all_daughters (daughter1_ptr, daughter2_ptr)
  type(f_node_ptr_t), dimension (:), intent(in) :: daughter1_ptr
  type(f_node_ptr_t), dimension (:), intent(in) :: daughter2_ptr
  integer :: i, j
  integer :: pos
  new_size = size1*size2
  allocate (dag_node%f_node(new_size))
  pos = 0
  do i = 1, size (daughter1_ptr)
    if (daughter1_ptr(i)%node%keep) then
      do j = 1, size (daughter2_ptr)
        if (daughter2_ptr(j)%node%keep) then
          pos = pos + 1
          allocate (dag_node%f_node(pos)%node)
          dag_node%f_node(pos)%node%particle_label = particle_label
          call dag_node%f_node(pos)%node%assign_particle_properties (feyngraph_set)
          dag_node%f_node(pos)%node%daughter1 => daughter1_ptr(i)%node
          dag_node%f_node(pos)%node%daughter2 => daughter2_ptr(j)%node
          dag_node%f_node(pos)%node%n_subtree_nodes = daughter1_ptr(i)%node%n_subtree_nodes
            + daughter2_ptr(j)%node%n_subtree_nodes + 1
          call feyngraph_set%model%match_vertex (daughter1_ptr(i)%node%particle%pdg, &
            daughter2_ptr(j)%node%particle%pdg, match)
          if (allocated (match)) then
            if (any (abs(match) == abs(dag_node%f_node(pos)%node%particle%pdg))) then
              dag_node%f_node(pos)%node%keep = .true.
            else
              dag_node%f_node(pos)%node%keep = .false.
            end if
            deallocate (match)
          else
            dag_node%f_node(pos)%node%keep = .false.
          end if
        end if
      end do
    end if
  end do
end subroutine combine_all_daughters
end subroutine dag_node_make_f_nodes

```

In `dag_options_make_f_nodes_single` we obtain all `f_nodes` for `dag_nodes` which correspond to a set of rival subtrees or nodes, which is the first possibility for which `dag_options` can appear. In `dag_options_make_f_nodes_pair` the options are rival pairs (`daughter1`, `daughter2`). Therefore we have to pass two allocatable arrays of type `f_node_ptr_t` to the subroutine.

<Cascades2: dag options: TBP>+≡

```

  procedure :: make_f_nodes => dag_options_make_f_nodes

```

<Cascades2: sub interfaces>+≡

```

  module subroutine dag_options_make_f_nodes (dag_options, &
    feyngraph_set, dag)

```

```

        class(dag_options_t), intent(inout) :: dag_options
        type(feyngraph_set_t), intent(inout) :: feyngraph_set
        type(dag_t), intent(inout) :: dag
    end subroutine dag_options_make_f_nodes
<Cascades2: procedures>+≡
    module subroutine dag_options_make_f_nodes (dag_options, &
        feyngraph_set, dag)
        class(dag_options_t), intent(inout) :: dag_options
        type(feyngraph_set_t), intent(inout) :: feyngraph_set
        type(dag_t), intent(inout) :: dag
        integer, dimension (:), allocatable :: obj, i_obj
        integer :: n_obj
        integer :: i
        integer :: pos
    !!! read options
        if (allocated (dag_options%f_node_ptr1)) return
        n_obj = count ((dag_options%string%t%type == DAG_NODE_TK) .or. &
            (dag_options%string%t%type == DAG_OPTIONS_TK) .or. &
            (dag_options%string%t%type == DAG_COMBINATION_TK), 1)
        allocate (obj(n_obj)); allocate (i_obj(n_obj))
        pos = 0
        do i = 1, size (dag_options%string%t)
            select case (dag_options%string%t(i)%type)
            case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
                pos = pos + 1
                obj(pos) = dag_options%string%t(i)%type
                i_obj(pos) = dag_options%string%t(i)%index
            end select
        end do
        if (any (dag_options%string%t%type == DAG_NODE_TK)) then
            call dag_options_make_f_nodes_single
        else if (any (dag_options%string%t%type == DAG_COMBINATION_TK)) then
            call dag_options_make_f_nodes_pair
        end if
        deallocate (obj, i_obj)
contains
    subroutine dag_options_make_f_nodes_single
        integer :: i_start, i_end
        integer :: n_nodes
        n_nodes = 0
        do i=1, n_obj
            if (allocated (dag%node(i_obj(i))%f_node)) then
                n_nodes = n_nodes + size (dag%node(i_obj(i))%f_node)
            end if
        end do
        if (n_nodes /= 0) then
            allocate (dag_options%f_node_ptr1 (n_nodes))
            i_end = 0
            do i = 1, n_obj
                if (allocated (dag%node(i_obj(i))%f_node)) then
                    i_start = i_end + 1
                    i_end = i_end + size (dag%node(i_obj(i))%f_node)
                end if
            end do
        end if
    end subroutine
end module

```

```

        dag_options%f_node_ptr1(i_start:i_end) = dag%node(i_obj(i))%f_node
    end if
end do
end if
end subroutine dag_options_make_f_nodes_single

subroutine dag_options_make_f_nodes_pair
    integer :: i_start, i_end
    integer :: n_nodes
!!! get f_nodes from each combination
    n_nodes = 0
    do i=1, n_obj
        if (allocated (dag%combination(i_obj(i))%f_node_ptr1)) then
            n_nodes = n_nodes + size (dag%combination(i_obj(i))%f_node_ptr1)
        end if
    end do
    if (n_nodes /= 0) then
        allocate (dag_options%f_node_ptr1 (n_nodes))
        allocate (dag_options%f_node_ptr2 (n_nodes))
        i_end = 0
        do i=1, n_obj
            if (allocated (dag%combination(i_obj(i))%f_node_ptr1)) then
                i_start = i_end + 1
                i_end = i_end + size (dag%combination(i_obj(i))%f_node_ptr1)
                dag_options%f_node_ptr1(i_start:i_end) = dag%combination(i_obj(i))%f_node_ptr1
                dag_options%f_node_ptr2(i_start:i_end) = dag%combination(i_obj(i))%f_node_ptr2
            end if
        end do
    end if
end subroutine dag_options_make_f_nodes_pair
end subroutine dag_options_make_f_nodes

```

We create all combinations of daughter `f_nodes` for a combination. In the combination each daughter can be either a single `dag_node` or `dag_options` which are a set of single `dag_nodes`. Therefore, we first create all possible `f_nodes` for daughter1, then all possible `f_nodes` for daughter2. In the end we combine all daughter1 nodes with all daughter2 nodes.

<Cascades2: dag combination: TBP>+≡

```
procedure :: make_f_nodes => dag_combination_make_f_nodes
```

<Cascades2: sub interfaces>+≡

```

module subroutine dag_combination_make_f_nodes (dag_combination, &
    feyngraph_set, dag)
    class(dag_combination_t), intent(inout) :: dag_combination
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(dag_t), intent(inout) :: dag
end subroutine dag_combination_make_f_nodes

```

<Cascades2: procedures>+≡

```

module subroutine dag_combination_make_f_nodes (dag_combination, &
    feyngraph_set, dag)
    class(dag_combination_t), intent(inout) :: dag_combination
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(dag_t), intent(inout) :: dag

```

```

integer, dimension (2) :: obj, i_obj
integer :: n_obj
integer :: new_size, size1, size2
integer :: i, j, pos
if (allocated (dag_combination%f_node_ptr1)) return
n_obj = 0
do i = 1, size (dag_combination%string%t)
  select case (dag_combination%string%t(i)%type)
    case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
      n_obj = n_obj + 1
      if (n_obj > 2) return
      obj(n_obj) = dag_combination%string%t(i)%type
      i_obj(n_obj) = dag_combination%string%t(i)%index
  end select
end do
size1 = 0
size2 = 0
if (obj(1) == DAG_NODE_TK) then
  if (allocated (dag%node(i_obj(1))%f_node)) &
    size1 = size (dag%node(i_obj(1))%f_node)
else if (obj(1) == DAG_OPTIONS_TK) then
  if (allocated (dag%options(i_obj(1))%f_node_ptr1)) &
    size1 = size (dag%options(i_obj(1))%f_node_ptr1)
end if
if (obj(2) == DAG_NODE_TK) then
  if (allocated (dag%node(i_obj(2))%f_node)) &
    size2 = size (dag%node(i_obj(2))%f_node)
else if (obj(2) == DAG_OPTIONS_TK) then
  if (allocated (dag%options(i_obj(2))%f_node_ptr1)) &
    size2 = size (dag%options(i_obj(2))%f_node_ptr1)
end if
!!! combine the 2 arrays of f_nodes
new_size = size1*size2
if (new_size /= 0) then
  allocate (dag_combination%f_node_ptr1 (new_size))
  allocate (dag_combination%f_node_ptr2 (new_size))
  pos = 0
  select case (obj(1))
    case (DAG_NODE_TK)
      select case (obj(2))
        case (DAG_NODE_TK)
          do i = 1, size1
            do j = 1, size2
              pos = pos + 1
              dag_combination%f_node_ptr1(pos) = &
                dag%node(i_obj(1))%f_node(i)
              dag_combination%f_node_ptr2(pos) = &
                dag%node(i_obj(2))%f_node(j)
            end do
          end do
        case (DAG_OPTIONS_TK)
          do i = 1, size1
            do j = 1, size2
              pos = pos + 1

```

```

        dag_combination%f_node_ptr1(pos) = &
            dag%node(i_obj(1))%f_node(i)
        dag_combination%f_node_ptr2(pos) = &
            dag%options(i_obj(2))%f_node_ptr1(j)
    end do
end do
end select
case (DAG_OPTIONS_TK)
select case (obj(2))
case (DAG_NODE_TK)
do i = 1, size1
do j = 1, size2
pos = pos + 1
dag_combination%f_node_ptr1(pos) = &
    dag%options(i_obj(1))%f_node_ptr1(i)
dag_combination%f_node_ptr2(pos) = &
    dag%node(i_obj(2))%f_node(j)
end do
end do
case (DAG_OPTIONS_TK)
do i = 1, size1
do j = 1, size2
pos = pos + 1
dag_combination%f_node_ptr1(pos) = &
    dag%options(i_obj(1))%f_node_ptr1(i)
dag_combination%f_node_ptr2(pos) = &
    dag%options(i_obj(2))%f_node_ptr1(j)
end do
end do
end select
end select
end if
end subroutine dag_combination_make_f_nodes

```

Here we create the **feyngraphs**. After the construction of the **dag** the remaining **dag_string** should contain a token for a single **dag_node** which corresponds to the roots of the **feyngraphs**. Therefore we make all **f_nodes** for this **dag_node** and create a **feyngraph** for each **f_node**. Note that only 3-vertices are accepted. All other vertices are rejected. The starting point is the last dag node which has been added to the list, since this corresponds to the root of the tree. It is important to understand that the structure of feyngraphs is not the same as the structure of the dag which is read from file, because for the calculations which are performed in this module we want to reuse the nodes for the outgoing particles, which means that they appear only once. In O'Mega's output, it is the first incoming particle which appears only once and the outgoing particles appear many times. This transition is incorporated in the subroutines which create **f_nodes** from the different dag objects.

```

<Cascades2: dag: TBP>+=
    procedure :: make_feyngraphs => dag_make_feyngraphs

<Cascades2: sub interfaces>+=
    module subroutine dag_make_feyngraphs (dag, feyngraph_set)
        class(dag_t), intent(inout) :: dag

```

```

        type(feyngraph_set_t), intent(inout) :: feyngraph_set
    end subroutine dag_make_feyngraphs

<Cascades2: procedures>+≡
    module subroutine dag_make_feyngraphs (dag, feyngraph_set)
        class(dag_t), intent(inout) :: dag
        type(feyngraph_set_t), intent(inout) :: feyngraph_set
        integer :: i
        integer :: max_subtree_size
        max_subtree_size = dag%node(dag%n_nodes)%subtree_size
        if (allocated (dag%node(dag%n_nodes)%f_node)) then
            do i = 1, size (dag%node(dag%n_nodes)%f_node)
                if (.not. associated (feyngraph_set%first)) then
                    allocate (feyngraph_set%last)
                    feyngraph_set%first => feyngraph_set%last
                else
                    allocate (feyngraph_set%last%next)
                    feyngraph_set%last => feyngraph_set%last%next
                end if
                feyngraph_set%last%root => dag%node(dag%n_nodes)%f_node(i)%node
                !!! The first particle was correct in the O'Mega parsable DAG output.
                !!! It was however changed to its anti-particle in
                !!! f_node_assign_particle_properties, which we revert here.
                feyngraph_set%last%root%particle => &
                    feyngraph_set%last%root%particle%anti
                feyngraph_set%last%n_nodes = feyngraph_set%last%root%n_subtree_nodes
                feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
            end do
            feyngraph_set%f_node_list%max_tree_size = feyngraph_set%first%n_nodes
        end if
    end subroutine dag_make_feyngraphs

```

A write procedure of the dag for debugging.

```

<Cascades2: dag: TBP>+≡
    procedure :: write => dag_write

<Cascades2: sub interfaces>+≡
    module subroutine dag_write (dag, u)
        class(dag_t), intent(in) :: dag
        integer, intent(in) :: u
    end subroutine dag_write

<Cascades2: procedures>+≡
    module subroutine dag_write (dag, u)
        class(dag_t), intent(in) :: dag
        integer, intent(in) :: u
        integer :: i
        write (u,fmt='(A)') 'nodes'
        do i=1, dag%n_nodes
            write (u,fmt='(I5,3X,A)') i, char (dag%node(i)%string)
        end do
        write (u,fmt='(A)') 'options'
        do i=1, dag%n_options
            write (u,fmt='(I5,3X,A)') i, char (dag%options(i)%string)
        end do
    end subroutine dag_write

```



```

write (u,fmt='(A)') 'combination'
do i=1, dag%n_combinations
  write (u,fmt='(I5,3X,A)') i, char (dag%combination(i)%string)
end do
end subroutine dag_write

```

Make a copy of a resonant `k_node`, where the copy is kept nonresonant.

```

<Cascades2: procedures>+≡
subroutine k_node_make_nonresonant_copy (k_node)
  type(k_node_t), intent(in) :: k_node
  type(k_node_t), pointer :: copy
  call k_node%f_node_list%add_entry (copy, recycle=.true.)
  copy%daughter1 => k_node%daughter1
  copy%daughter2 => k_node%daughter2
  copy = k_node
  copy%mapping = NONRESONANT
  copy%resonant = .false.
  copy%on_shell = .false.
  copy%mapping_assigned = .true.
  copy%is_nonresonant_copy = .true.
end subroutine k_node_make_nonresonant_copy

```

For a given `feyngraph` we create all possible `kingraphs`. Here we use existing `k_nodes` which have already been created when the mapping calculations of the pure s-channel subgraphs are performed. The nodes for the incoming particles or the nodes on the t-line will have to be created in all cases because they are not used in several graphs. To obtain the existing `k_nodes`, we use the subroutine `k_node_init_from_f_node` which itself uses `f_node_list_get_nodes` to obtain all active `k_nodes` in the `k_node_list` of the `f_node`. The created `kingraphs` are attached to the linked list of the `feyngraph`. For scattering processes we have to split up the t-line, because since all graphs are represented as a decay, different nodes can share daughter nodes. This happens also for the t-line or the incoming particle which appears as an outgoing particle. For the `t_line` or `incoming` nodes we do not want to recycle nodes but rather create a copy of this line for each `kingraph`.

```

<Cascades2: feyngraph: TBP>+≡
procedure :: make_kingraphs => feyngraph_make_kingraphs

<Cascades2: sub interfaces>+≡
module subroutine feyngraph_make_kingraphs (feyngraph, feyngraph_set)
  class(feyngraph_t), intent(inout) :: feyngraph
  type(feyngraph_set_t), intent(in) :: feyngraph_set
end subroutine feyngraph_make_kingraphs

<Cascades2: procedures>+≡
module subroutine feyngraph_make_kingraphs (feyngraph, feyngraph_set)
  class(feyngraph_t), intent(inout) :: feyngraph
  type(feyngraph_set_t), intent(in) :: feyngraph_set
  type(k_node_ptr_t), dimension (:), allocatable :: kingraph_root
  integer :: i
  if (.not. associated (feyngraph%kin_first)) then
    call k_node_init_from_f_node (feyngraph%root, &
      kingraph_root, feyngraph_set)

```

```

if (.not. feyngraph%root%keep) return
if (feyngraph_set%process_type == SCATTERING) then
  call split_up_t_lines (kingraph_root)
end if
do i=1, size (kingraph_root)
  if (associated (feyngraph%kin_last)) then
    allocate (feyngraph%kin_last%next)
    feyngraph%kin_last => feyngraph%kin_last%next
  else
    allocate (feyngraph%kin_last)
    feyngraph%kin_first => feyngraph%kin_last
  end if
  feyngraph%kin_last%root => kingraph_root(i)%node
  feyngraph%kin_last%n_nodes = feyngraph%n_nodes
  feyngraph%kin_last%keep = feyngraph%keep
  if (feyngraph_set%process_type == SCATTERING) then
    feyngraph%kin_last%root%bincode = &
      f_node_get_external_bincode (feyngraph_set, feyngraph%root)
  end if
end do
deallocate (kingraph_root)
end if
end subroutine feyngraph_make_kingraphs

```

Create all **k_nodes** for a given **f_node**. We return these nodes using **k_node_ptr**. If the node is external, we assign also the bincode to the **k_nodes** because this is determined from substrings of the input file which belong to the **feyngraphs** and **f_nodes**.

(Cascades2: procedures)+≡

```

recursive subroutine k_node_init_from_f_node (f_node, k_node_ptr, feyngraph_set)
  type(f_node_t), target, intent(inout) :: f_node
  type(k_node_ptr_t), allocatable, dimension (:), intent(out) :: k_node_ptr
  type(feyngraph_set_t), intent(in) :: feyngraph_set
  type(k_node_ptr_t), allocatable, dimension(:) :: daughter_ptr1, daughter_ptr2
  integer :: n_nodes
  integer :: i, j
  integer :: pos
  integer, save :: counter = 0
  if (.not. (f_node%incoming .or. f_node%t_line)) then
    call f_node%k_node_list%get_nodes (k_node_ptr)
    if (.not. allocated (k_node_ptr) .and. f_node%k_node_list%n_entries > 0) then
      f_node%keep = .false.
      return
    end if
  end if
  if (.not. allocated (k_node_ptr)) then
    if (associated (f_node%daughter1) .and. associated (f_node%daughter2)) then
      call k_node_init_from_f_node (f_node%daughter1, daughter_ptr1, &
        feyngraph_set)
      call k_node_init_from_f_node (f_node%daughter2, daughter_ptr2, &
        feyngraph_set)
    if (.not. (f_node%daughter1%keep .and. f_node%daughter2%keep)) then
      f_node%keep = .false.
    end if
  end if
end subroutine k_node_init_from_f_node

```

```

        return
    end if
    n_nodes = size (daughter_ptr1) * size (daughter_ptr2)
    allocate (k_node_ptr (n_nodes))
    pos = 1
    do i=1, size (daughter_ptr1)
        do j=1, size (daughter_ptr2)
            if (f_node%incoming .or. f_node%t_line) then
                call f_node%k_node_list%add_entry (k_node_ptr(pos)%node, recycle = .false.)
            else
                call f_node%k_node_list%add_entry (k_node_ptr(pos)%node, recycle = .true.)
            end if
            k_node_ptr(pos)%node%f_node => f_node
            k_node_ptr(pos)%node%daughter1 => daughter_ptr1(i)%node
            k_node_ptr(pos)%node%daughter2 => daughter_ptr2(j)%node
            k_node_ptr(pos)%node%f_node_index = f_node%index
            k_node_ptr(pos)%node%incoming = f_node%incoming
            k_node_ptr(pos)%node%t_line = f_node%t_line
            k_node_ptr(pos)%node%particle => f_node%particle
            pos = pos + 1
        end do
    end do
    deallocate (daughter_ptr1, daughter_ptr2)
else
    allocate (k_node_ptr(1))
    if (f_node%incoming .or. f_node%t_line) then
        call f_node%k_node_list%add_entry (k_node_ptr(1)%node, recycle=.false.)
    else
        call f_node%k_node_list%add_entry (k_node_ptr(1)%node, recycle=.true.)
    end if
    k_node_ptr(1)%node%f_node => f_node
    k_node_ptr(1)%node%f_node_index = f_node%index
    k_node_ptr(1)%node%incoming = f_node%incoming
    k_node_ptr(1)%node%t_line = f_node%t_line
    k_node_ptr(1)%node%particle => f_node%particle
    k_node_ptr(1)%node%bincode = f_node_get_external_bincode (feyngraph_set, &
        f_node)
    end if
end if
end subroutine k_node_init_from_f_node

```

The graphs resulting from `k_node_init_from_f_node` are fine if they are used only in one direction. This is however not the case when one wants to invert the graphs, i.e. take the other incoming particle of a scattering process as the decaying particle, because the outgoing `f_nodes` (and hence also the `k_nodes`) exist only once. This problem is solved here by creating a distinct t-line for each of the graphs. The following subroutine disentangles the data structure by creating new nodes such that the different t-lines are not connected any more.

(*Cascades2: procedures*) +=

```

recursive subroutine split_up_t_lines (t_node)
    type(k_node_ptr_t), dimension(:), intent(inout) :: t_node
    type(k_node_t), pointer :: ref_node => null ()
    type(k_node_t), pointer :: ref_daughter => null ()

```

```

type(k_node_t), pointer :: new_daughter => null ()
type(k_node_ptr_t), dimension(:), allocatable :: t_daughter
integer :: ref_daughter_index
integer :: i, j
allocate (t_daughter (size (t_node)))
do i=1, size (t_node)
  ref_node => t_node(i)%node
  if (associated (ref_node%daughter1) .and. associated (ref_node%daughter2)) then
    ref_daughter => null ()
    if (ref_node%daughter1%incoming .or. ref_node%daughter1%t_line) then
      ref_daughter => ref_node%daughter1
      ref_daughter_index = 1
    else if (ref_node%daughter2%incoming .or. ref_node%daughter2%t_line) then
      ref_daughter => ref_node%daughter2
      ref_daughter_index = 2
    end if
    do j=1, size (t_daughter)
      if (.not. associated (t_daughter(j)%node)) then
        t_daughter(j)%node => ref_daughter
        exit
      else if (t_daughter(j)%node%index == ref_daughter%index) then
        new_daughter => null ()
        call ref_daughter%f_node%k_node_list%add_entry (new_daughter, recycle=.false.)
        new_daughter = ref_daughter
        new_daughter%daughter1 => ref_daughter%daughter1
        new_daughter%daughter2 => ref_daughter%daughter2
        if (ref_daughter_index == 1) then
          ref_node%daughter1 => new_daughter
        else if (ref_daughter_index == 2) then
          ref_node%daughter2 => new_daughter
        end if
        ref_daughter => new_daughter
      end if
    end do
  else
    return
  end if
end do
call split_up_t_lines (t_daughter)
deallocate (t_daughter)
end subroutine split_up_t_lines

```

This subroutine sets the `inverse_daughters` of a `k_node`. If we invert a `kingraph` such that not the first but the second incoming particle appears as the root of the tree, the `incoming` and `t_line` particles obtain other daughters. These are the former mother node and the sister node `s_daughter`. Here we set only the pointers for the `inverse_daughters`. The inversion happens in `kingraph_make_inverse_copy` and `node_inverse_deep_copy`.

(*Cascades2: procedures*) +=

```

subroutine kingraph_set_inverse_daughters (kingraph)
  type(kingraph_t), intent(inout) :: kingraph
  type(k_node_t), pointer :: mother
  type(k_node_t), pointer :: t_daughter

```

```

type(k_node_t), pointer :: s_daughter
mother => kingraph%root
do while (associated (mother))
  if (associated (mother%daughter1) .and. &
      associated (mother%daughter2)) then
    if (mother%daughter1%t_line .or. mother%daughter1%incoming) then
      t_daughter => mother%daughter1; s_daughter => mother%daughter2
    else if (mother%daughter2%t_line .or. mother%daughter2%incoming) then
      t_daughter => mother%daughter2; s_daughter => mother%daughter1
    else
      exit
    end if
    t_daughter%inverse_daughter1 => mother
    t_daughter%inverse_daughter2 => s_daughter
    mother => t_daughter
  else
    exit
  end if
end do
end subroutine kingraph_set_inverse_daughters

```

Set the bincode of an `f_node` which corresponds to an external particle. This is done on the basis of the `particle_label` which is a substring of the input file. Here it is not the particle name which is important, but the number(s) in brackets which in general indicate the external particles which are connected to the current node. This function is however only used for external particles, so there can either be one or `n_out + 1` particles in the brackets (in the DAG input file always one, because also for the root there is only a single number). In all cases we check the number of particles (in the DAG input the numbers are separated by a slash).

(*Cascades2: procedures*) \equiv

```

function f_node_get_external_bincode (feyngraph_set, f_node) result (bincode)
  type(feyngraph_set_t), intent(in) :: feyngraph_set
  type(f_node_t), intent(in) :: f_node
  integer (TC) :: bincode
  character(len=LABEL_LEN) :: particle_label
  integer :: start_pos, end_pos, n_out_decay
  integer :: n_prt ! for DAG
  integer :: i
  bincode = 0
  if (feyngraph_set%process_type == DECAY) then
    n_out_decay = feyngraph_set%n_out
  else
    n_out_decay = feyngraph_set%n_out + 1
  end if
  particle_label = f_node%particle_label
  start_pos = index (particle_label, '[') + 1
  end_pos = index (particle_label, ']') - 1
  particle_label = particle_label(start_pos:end_pos)
  !!! n_out_decay is the number of outgoing particles in the
  !!! 0'Mega output, which is always represented as a decay
  if (feyngraph_set%use_dag) then
    n_prt = 1
  end if
end function

```

```

do i=1, len(particle_label)
  if (particle_label(i:i) == '/') n_prt = n_prt + 1
end do
else
  n_prt = end_pos - start_pos + 1
end if
if (n_prt == 1) then
  bincode = calculate_external_bincode (particle_label, &
    feyngraph_set%process_type, n_out_decay)
else if (n_prt == n_out_decay) then
  bincode = ibset (0, n_out_decay)
end if
end function f_node_get_external_bincode

```

Assign a bincode to an internal node, which is calculated from the bincodes of daughter1 and daughter2.

```

<Cascades2: procedures>+≡
subroutine node_assign_bincode (node)
  type(k_node_t), intent(inout) :: node
  if (associated (node%daughter1) .and. associated (node%daughter2) &
    .and. .not. node%incoming) then
    node%bincode = ior(node%daughter1%bincode, node%daughter2%bincode)
  end if
end subroutine node_assign_bincode

```

Calculate the bincode from the number in the brackets of the particle_label, if the node is external. For the root in the non-factorized output, this is calculated directly in f_node_get_external_bincode because in this case all the other external particle numbers appear between the brackets.

```

<Cascades2: procedures>+≡
function calculate_external_bincode (label_number_string, process_type, n_out_decay) result (bincode)
  character(len=*), intent(in) :: label_number_string
  integer, intent(in) :: process_type
  integer, intent(in) :: n_out_decay
  character :: number_char
  integer :: number_int
  integer (kind=TC) :: bincode
  bincode = 0
  read (label_number_string, fmt='(A)') number_char
  !!! check if the character is a letter (A,B,C,...) or a number (1...9)
  !!! numbers 1 and 2 are special cases
  select case (number_char)
  case ('1')
    if (process_type == SCATTERING) then
      number_int = n_out_decay + 3
    else
      number_int = n_out_decay + 2
    end if
  case ('2')
    if (process_type == SCATTERING) then
      number_int = n_out_decay + 2
    else
      number_int = 2
    end if
  end select
  bincode = ibset (number_int, n_out_decay)
end function calculate_external_bincode

```

```

        end if
    case ('A')
        number_int = 10
    case ('B')
        number_int = 11
    case ('C')
        number_int = 12
    case ('D')
        number_int = 13
    case default
        read (number_char, fmt='(I1)') number_int
    end select
    bincode = ibset (bincode, number_int - process_type - 1)
end function calculate_external_bincode

```

19.11.13 Mapping calculations

Once a `k_node` and its subtree nodes have been created, we can perform the kinematical calculations and assign mappings, depending on the particle properties and the results for the subtree nodes. This could in principle be done recursively, calling the procedure first for the daughter nodes and then perform the calculations for the actual node. But for parallization and comparing the nodes, this will be done simultaneously for all nodes with the same number of subtree nodes, and the number of subtree nodes increases, starting from one, in steps of two. The actual mapping calculations are done in complete analogy to cascades.

```

(Cascades2: procedures) +=
subroutine node_assign_mapping_s (feyngraph, node, feyngraph_set)
    type(feyngraph_t), intent(inout) :: feyngraph
    type(k_node_t), intent(inout) :: node
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    real(default) :: eff_mass_sum
    logical :: keep
    if (.not. node%mapping_assigned) then
        if (node%particle%mass > feyngraph_set%phs_par%m_threshold_s) then
            node%effective_mass = node%particle%mass
        end if
        if (associated (node%daughter1) .and. associated (node%daughter2)) then
            if (.not. (node%daughter1%keep .and. node%daughter2%keep)) then
                node%keep = .false.; return
            end if
            node%ext_mass_sum = node%daughter1%ext_mass_sum &
                + node%daughter2%ext_mass_sum
            keep = .false.
        !!! Potentially resonant cases [sqrts = m_rea for on-shell decay]
        if (node%particle%mass > node%ext_mass_sum &
            .and. node%particle%mass <= feyngraph_set%phs_par%sqrts) then
            if (node%particle%width /= 0) then
                if (node%daughter1%on_shell .or. node%daughter2%on_shell) then
                    keep = .true.
                    node%mapping = S_CHANNEL
                    node%resonant = .true.
                end if
            end if
        end if
    end if
end subroutine node_assign_mapping_s

```

```

        end if
    else
        call warn_decay (node%particle)
    end if
!!! Collinear and IR singular cases
    else if (node%particle%mass < feyngraph_set%phs_par%sqrts) then
!!! Massless splitting
        if (node%daughter1%effective_mass == 0 &
            .and. node%daughter2%effective_mass == 0 &
            .and. .not. associated (node%daughter1%daughter1) &
            .and. .not. associated (node%daughter1%daughter2) &
            .and. .not. associated (node%daughter2%daughter1) &
            .and. .not. associated (node%daughter2%daughter2)) then
            keep = .true.
            node%log_enhanced = .true.
            if (node%particle%is_vector) then
                if (node%daughter1%particle%is_vector &
                    .and. node%daughter2%particle%is_vector) then
                    node%mapping = COLLINEAR    !!! three-vector-splitting
                else
                    node%mapping = INFRARED      !!! vector splitting into matter
                end if
            else
                if (node%daughter1%particle%is_vector &
                    .or. node%daughter2%particle%is_vector) then
                    node%mapping = COLLINEAR    !!! vector radiation off matter
                else
                    node%mapping = INFRARED      !!! scalar radiation/splitting
                end if
            end if
        end if
!!! IR radiation off massive particle [cascades]
        else if (node%effective_mass > 0 .and. &
            node%daughter1%effective_mass > 0 .and. &
            node%daughter2%effective_mass == 0 .and. &
            (node%daughter1%on_shell .or. &
            node%daughter1%mapping == RADIATION) .and. &
            abs (node%effective_mass - &
            node%daughter1%effective_mass) < feyngraph_set%phs_par%m_threshold_s) &
            then
            keep = .true.
            node%log_enhanced = .true.
            node%mapping = RADIATION
        else if (node%effective_mass > 0 .and. &
            node%daughter2%effective_mass > 0 .and. &
            node%daughter1%effective_mass == 0 .and. &
            (node%daughter2%on_shell .or. &
            node%daughter2%mapping == RADIATION) .and. &
            abs (node%effective_mass - &
            node%daughter2%effective_mass) < feyngraph_set%phs_par%m_threshold_s) &
            then
            keep = .true.
            node%log_enhanced = .true.
            node%mapping = RADIATION
        end if
    end if

```



```

        end if
    !!! Non-singular cases, including failed resonances [from cascades]
        if (.not. keep) then
    !!! Two on-shell particles from a virtual mother [from cascades, here eventually more than 2]
            if (node%daughter1%on_shell .or. node%daughter2%on_shell) then
                keep = .true.
                eff_mass_sum = node%daughter1%effective_mass &
                    + node%daughter2%effective_mass
                node%effective_mass = max (node%ext_mass_sum, eff_mass_sum)
                if (node%effective_mass < feyngraph_set%phs_par%m_threshold_s) then
                    node%effective_mass = 0
                end if
            end if
        end if
    !!! Complete and register feyngraph (make copy in case of resonance)
        if (keep) then
            node%on_shell = node%resonant .or. node%log_enhanced
            if (node%resonant) then
                if (feyngraph_set%phs_par%keep_nonresonant) then
                    call k_node_make_nonresonant_copy (node)
                end if
                node%ext_mass_sum = node%particle%mass
            end if
            node%mapping_assigned = .true.
            call node_assign_bincode (node)
            call node%subtree%add_entry (node)
        else !!! external (outgoing) particle
            node%ext_mass_sum = node%particle%mass
            node%mapping = EXTERNAL_PRT
            node%multiplicity = 1
            node%mapping_assigned = .true.
            call node%subtree%add_entry (node)
            node%on_shell = .true.
            if (node%particle%mass >= feyngraph_set%phs_par%m_threshold_s) then
                node%effective_mass = node%particle%mass
            end if
        end if
    else if (node%is_nonresonant_copy) then
        call node_assign_bincode (node)
        call node%subtree%add_entry (node)
        node%is_nonresonant_copy = .false.
    end if
    call node_count_specific_properties (node)
    if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
        node%keep = .false.
    end if
contains
    subroutine warn_decay (particle)
        type(part_prop_t), intent(in) :: particle
        integer :: i
        integer, dimension(MAX_WARN_RESONANCE), save :: warned_code = 0
        LOOP_WARNED: do i = 1, MAX_WARN_RESONANCE
            if (warned_code(i) == 0) then

```

```

warned_code(i) = particle%pdg
write (msg_buffer, "(A)") &
    & " Intermediate decay of zero-width particle " &
    & // trim(particle%particle_label) &
    & // " may be possible."
call msg_warning
exit LOOP_WARNED
else if (warned_code(i) == particle%pdg) then
    exit LOOP_WARNED
end if
end do LOOP_WARNED
end subroutine warn_decay
end subroutine node_assign_mapping_s

```

We determine the numbers `n_resonances`, `multiplicity`, `n_off_shell` and `n_log_enhanced` for a given node.

```

<Cascades2: procedures>+=
subroutine node_count_specific_properties (node)
    type(k_node_t), intent(inout) :: node
    if (associated (node%daughter1) .and. associated(node%daughter2)) then
        if (node%resonant) then
            node%multiplicity = 1
            node%n_resonances &
                = node%daughter1%n_resonances &
                + node%daughter2%n_resonances + 1
        else
            node%multiplicity &
                = node%daughter1%multiplicity &
                + node%daughter2%multiplicity
            node%n_resonances &
                = node%daughter1%n_resonances &
                + node%daughter2%n_resonances
        end if
        if (node%log_enhanced) then
            node%n_log_enhanced &
                = node%daughter1%n_log_enhanced &
                + node%daughter2%n_log_enhanced + 1
        else
            node%n_log_enhanced &
                = node%daughter1%n_log_enhanced &
                + node%daughter2%n_log_enhanced
        end if
        if (node%resonant) then
            node%n_off_shell = 0
        else if (node%log_enhanced) then
            node%n_off_shell &
                = node%daughter1%n_off_shell &
                + node%daughter2%n_off_shell
        else
            node%n_off_shell &
                = node%daughter1%n_off_shell &
                + node%daughter2%n_off_shell + 1
        end if
    end if
end subroutine

```

```

    if (node%t_line) then
      if (node%daughter1%t_line .or. node%daughter1%incoming) then
        node%n_t_channel = node%daughter1%n_t_channel + 1
      else if (node%daughter2%t_line .or. node%daughter2%incoming) then
        node%n_t_channel = node%daughter2%n_t_channel + 1
      end if
    end if
  end if
end if
end subroutine node_count_specific_properties

```

The subroutine `kingraph_assign_mappings_s` completes kinematical calculations for a decay process, considering the root node.

(*Cascades2: procedures*) +=

```

subroutine kingraph_assign_mappings_s (feyngraph, kingraph, feyngraph_set)
  type(feyngraph_t), intent(inout) :: feyngraph
  type(kingraph_t), pointer, intent(inout) :: kingraph
  type(feyngraph_set_t), intent(inout) :: feyngraph_set
  if (.not. (kingraph%root%daughter1%keep .and. kingraph%root%daughter2%keep)) then
    kingraph%keep = .false.
    call kingraph%tree%final ()
  end if
  if (kingraph%keep) then
    kingraph%root%on_shell = .true.
    kingraph%root%mapping = EXTERNAL_PRT
    kingraph%root%mapping_assigned = .true.
    call node_assign_bincode (kingraph%root)
    kingraph%root%ext_mass_sum = &
      kingraph%root%daughter1%ext_mass_sum + &
      kingraph%root%daughter2%ext_mass_sum
    if (kingraph%root%ext_mass_sum >= feyngraph_set%phs_par%sqrts) then
      kingraph%root%keep = .false.
      kingraph%keep = .false.; call kingraph%tree%final (); return
    end if
    call kingraph%root%subtree%add_entry (kingraph%root)
    kingraph%root%multiplicity &
      = kingraph%root%daughter1%multiplicity &
      + kingraph%root%daughter2%multiplicity
    kingraph%root%n_resonances &
      = kingraph%root%daughter1%n_resonances &
      + kingraph%root%daughter2%n_resonances
    kingraph%root%n_off_shell &
      = kingraph%root%daughter1%n_off_shell &
      + kingraph%root%daughter2%n_off_shell
    kingraph%root%n_log_enhanced &
      = kingraph%root%daughter1%n_log_enhanced &
      + kingraph%root%daughter2%n_log_enhanced
    if (kingraph%root%n_off_shell > feyngraph_set%phs_par%off_shell) then
      kingraph%root%keep = .false.
      kingraph%keep = .false.; call kingraph%tree%final (); return
    else
      kingraph%grove_prop%multiplicity = &
        kingraph%root%multiplicity
      kingraph%grove_prop%n_resonances = &

```

```

        kinggraph%root%n_resonances
        kinggraph%grove_prop%n_off_shell = &
        kinggraph%root%n_off_shell
        kinggraph%grove_prop%n_log_enhanced = &
        kinggraph%root%n_log_enhanced
    end if
    kinggraph%tree = kinggraph%root%subtree
end if
end subroutine kinggraph_assign_mappings_s

```

Compute mappings for the `t_line` and incoming nodes. This is done recursively using `node_compute_t_line`.

(Cascades2: procedures) +=

```

subroutine kinggraph_compute_mappings_t_line (feyngraph, kinggraph, feyngraph_set)
    type(feyngraph_t), intent(inout) :: feyngraph
    type(kinggraph_t), pointer, intent(inout) :: kinggraph
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    call node_compute_t_line (feyngraph, kinggraph, kinggraph%root, feyngraph_set)
    if (.not. kinggraph%root%keep) then
        kinggraph%keep = .false.
        call kinggraph%tree%final ()
    end if
    if (kinggraph%keep) kinggraph%tree = kinggraph%root%subtree
end subroutine kinggraph_compute_mappings_t_line

```

Perform the kinematical calculations and mapping assignment for a node which is either `incoming` or `t_line`. This is done recursively, going first to the daughter node which has this property. Therefore we first set the pointer `t_node` to this daughter node and `s_node` to the other one. The mapping determination happens again in the same way as in `cascades`.

(Cascades2: procedures) +=

```

recursive subroutine node_compute_t_line (feyngraph, kinggraph, node, feyngraph_set)
    type(feyngraph_t), intent(inout) :: feyngraph
    type(kinggraph_t), intent(inout) :: kinggraph
    type(k_node_t), intent(inout) :: node
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(k_node_t), pointer :: s_node
    type(k_node_t), pointer :: t_node
    type(k_node_t), pointer :: new_s_node
    if (.not. (node%daughter1%keep .and. node%daughter2%keep)) then
        node%keep = .false.
        return
    end if
    s_node => null ()
    t_node => null ()
    new_s_node => null ()
    if (associated (node%daughter1) .and. associated (node%daughter2)) then
        if (node%daughter1%t_line .or. node%daughter1%incoming) then
            t_node => node%daughter1; s_node => node%daughter2
        else if (node%daughter2%t_line .or. node%daughter2%incoming) then
            t_node => node%daughter2; s_node => node%daughter1
        end if
        if (t_node%t_line) then

```

```

        call node_compute_t_line (feyngraph, kingraph, t_node, feyngraph_set)
        if (.not. t_node%keep) then
            node%keep = .false.
            return
        end if
    else if (t_node%incoming) then
        t_node%mapping = EXTERNAL_PRT
        t_node%on_shell = .true.
        t_node%ext_mass_sum = t_node%particle%mass
        if (t_node%particle%mass >= feyngraph_set%phs_par%m_threshold_t) then
            t_node%effective_mass = t_node%particle%mass
        end if
        call t_node%subtree%add_entry (t_node)
    end if
!!! root:
    if (.not. node%incoming) then
        if (t_node%incoming) then
            node%ext_mass_sum = s_node%ext_mass_sum
        else
            node%ext_mass_sum &
                = node%daughter1%ext_mass_sum &
                + node%daughter2%ext_mass_sum
        end if
        if (node%particle%mass > feyngraph_set%phs_par%m_threshold_t) then
            node%effective_mass = max (node%particle%mass, &
                s_node%effective_mass)
        else if (s_node%effective_mass > feyngraph_set%phs_par%m_threshold_t) then
            node%effective_mass = s_node%effective_mass
        else
            node%effective_mass = 0
        end if
!!! Allowed decay of beam particle
        if (t_node%incoming &
            .and. t_node%particle%mass > s_node%particle%mass &
            + node%particle%mass) then
            call beam_decay (feyngraph_set%fatal_beam_decay)
!!! Massless splitting
        else if (t_node%effective_mass == 0 &
            .and. s_node%effective_mass < feyngraph_set%phs_par%m_threshold_t &
            .and. node%effective_mass == 0) then
            node%mapping = U_CHANNEL
            node%log_enhanced = .true.
!!! IR radiation off massive particle
        else if (t_node%effective_mass /= 0 &
            .and. s_node%effective_mass == 0 &
            .and. node%effective_mass /= 0 &
            .and. (t_node%on_shell &
            .or. t_node%mapping == RADIATION) &
            .and. abs (t_node%effective_mass - node%effective_mass) &
            < feyngraph_set%phs_par%m_threshold_t) then
            node%log_enhanced = .true.
            node%mapping = RADIATION
        end if
        node%mapping_assigned = .true.

```

```

call node_assign_bincode (node)
call node%subtree%add_entry (node)
call node_count_specific_properties (node)
if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
  node%keep = .false.
  kingraph%keep = .false.; call kingraph%tree%final (); return
else if (node%n_t_channel > feyngraph_set%phs_par%t_channel) then
  node%keep = .false.;
  kingraph%keep = .false.; call kingraph%tree%final (); return
end if
else
  node%mapping = EXTERNAL_PRT
  node%on_shell = .true.
  node%ext_mass_sum &
    = t_node%ext_mass_sum &
    + s_node%ext_mass_sum
  node%effective_mass = node%particle%mass
  if (.not. (node%ext_mass_sum < feyngraph_set%phs_par%sqrts)) then
    node%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
  end if
  if (kingraph%keep) then
    if (t_node%incoming .and. s_node%log_enhanced) then
      call s_node%f_node%k_node_list%add_entry (new_s_node, recycle=.false.)
      new_s_node = s_node
      new_s_node%daughter1 => s_node%daughter1
      new_s_node%daughter2 => s_node%daughter2
      if (s_node%index == node%daughter1%index) then
        node%daughter1 => new_s_node
      else if (s_node%index == node%daughter2%index) then
        node%daughter2 => new_s_node
      end if
      new_s_node%subtree = s_node%subtree
      new_s_node%mapping = NO_MAPPING
      new_s_node%log_enhanced = .false.
      new_s_node%n_log_enhanced &
        = new_s_node%n_log_enhanced - 1
      new_s_node%log_enhanced = .false.
      where (new_s_node%subtree%bc == new_s_node%bincode)
        new_s_node%subtree%mapping = NO_MAPPING
      endwhere
    else if ((t_node%t_line .or. t_node%incoming) .and. &
      t_node%mapping == U_CHANNEL) then
      t_node%mapping = T_CHANNEL
      where (t_node%subtree%bc == t_node%bincode)
        t_node%subtree%mapping = T_CHANNEL
      endwhere
    else if (t_node%incoming .and. &
      .not. associated (s_node%daughter1) .and. &
      .not. associated (s_node%daughter2)) then
      call s_node%f_node%k_node_list%add_entry (new_s_node, recycle=.false.)
      new_s_node = s_node
      new_s_node%mapping = ON_SHELL
      new_s_node%daughter1 => s_node%daughter1

```

```

        new_s_node%daughter2 => s_node%daughter2
        new_s_node%subtree = s_node%subtree
        if (s_node%index == node%daughter1%index) then
            node%daughter1 => new_s_node
        else if (s_node%index == node%daughter2%index) then
            node%daughter2 => new_s_node
        end if
        where (new_s_node%subtree%bc == new_s_node%bincode)
            new_s_node%subtree%mapping = ON_SHELL
        endwhere
    end if
end if
call node%subtree%add_entry (node)
node%multiplicity &
    = node%daughter1%multiplicity &
    + node%daughter2%multiplicity
node%n_resonances &
    = node%daughter1%n_resonances &
    + node%daughter2%n_resonances
node%n_off_shell &
    = node%daughter1%n_off_shell &
    + node%daughter2%n_off_shell
node%n_log_enhanced &
    = node%daughter1%n_log_enhanced &
    + node%daughter2%n_log_enhanced
node%n_t_channel &
    = node%daughter1%n_t_channel &
    + node%daughter2%n_t_channel
if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
    node%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
else if (node%n_t_channel > feyngraph_set%phs_par%t_channel) then
    node%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
else
    kingraph%grove_prop%multiplicity = node%multiplicity
    kingraph%grove_prop%n_resonances = node%n_resonances
    kingraph%grove_prop%n_off_shell = node%n_off_shell
    kingraph%grove_prop%n_log_enhanced = node%n_log_enhanced
    kingraph%grove_prop%n_t_channel = node%n_t_channel
end if
end if
end if
contains
subroutine beam_decay (fatal_beam_decay)
    logical, intent(in) :: fatal_beam_decay
    write (msg_buffer, "(1x,A,1x,'->',1x,A,1x,A)") &
        t_node%particle%particle_label, &
        node%particle%particle_label, &
        s_node%particle%particle_label
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,') =' ,1x,E17.10)") &
        t_node%particle%particle_label, t_node%particle%mass
    call msg_message

```

```

write (msg_buffer, "(1x,'mass(',A,') =' ,1x,E17.10)") &
node%particle%particle_label, node%particle%mass
call msg_message
write (msg_buffer, "(1x,'mass(',A,') =' ,1x,E17.10)") &
s_node%particle%particle_label, s_node%particle%mass
call msg_message
if (fatal_beam_decay) then
call msg_fatal (" Phase space: Initial beam particle can decay")
else
call msg_warning (" Phase space: Initial beam particle can decay")
end if
end subroutine beam_decay
end subroutine node_compute_t_line

```

After all pure s-channel subdiagrams have already been created from the corresponding `f_nodes` and mappings have been determined for their nodes, we complete the calculations here. In a first step, the `kingraphs` have to be created on the basis of the existing `k_nodes`, which means in particular that a `feyngraph` can give rise to several `kingraphs` which will all be attached to the linked list of the `feyngraph`. The calculations which remain are of different kinds for decay and scattering processes. In a decay process the kinematical calculations have to be done for the `root` node. In a scattering process, after the creation of `kingraphs` in the first step, there will be only `kingraphs` with the first incoming particle as the `root` of the tree. For these graphs the `inverse` variable has the value `.false..` Before performing any calculations on these graphs we make a so-called inverse copy of the graph (see below), which will also be attached to the linked list. Since the s-channel subgraph calculations have already been completed, only the t-line computations remain.

```

<Cascades2: feyngraph: TBP>+≡
  procedure :: make_inverse_kingraphs => feyngraph_make_inverse_kingraphs

<Cascades2: sub interfaces>+≡
  module subroutine feyngraph_make_inverse_kingraphs (feyngraph)
    class(feyngraph_t), intent(inout) :: feyngraph
  end subroutine feyngraph_make_inverse_kingraphs

<Cascades2: procedures>+≡
  module subroutine feyngraph_make_inverse_kingraphs (feyngraph)
    class(feyngraph_t), intent(inout) :: feyngraph
    type(kingraph_t), pointer :: current
    current => feyngraph%kin_first
    do while (associated (current))
      if (current%inverse) exit
      call current%make_inverse_copy (feyngraph)
      current => current%next
    end do
  end subroutine feyngraph_make_inverse_kingraphs

<Cascades2: feyngraph: TBP>+≡
  procedure :: compute_mappings => feyngraph_compute_mappings

<Cascades2: sub interfaces>+≡
  module subroutine feyngraph_compute_mappings (feyngraph, feyngraph_set)
    class(feyngraph_t), intent(inout) :: feyngraph

```



```

        type(feyngraph_set_t), intent(inout) :: feyngraph_set
    end subroutine feyngraph_compute_mappings

<Cascades2: procedures>+=
module subroutine feyngraph_compute_mappings (feyngraph, feyngraph_set)
    class(feyngraph_t), intent(inout) :: feyngraph
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(kingraph_t), pointer :: current
    current => feyngraph%kin_first
    do while (associated (current))
        if (feyngraph_set%process_type == DECAY) then
            call kingraph_assign_mappings_s (feyngraph, current, feyngraph_set)
        else if (feyngraph_set%process_type == SCATTERING) then
            call kingraph_compute_mappings_t_line &
                (feyngraph, current, feyngraph_set)
        end if
        current => current%next
    end do
end subroutine feyngraph_compute_mappings

```

Here we control the mapping calculations for the nodes of s-channel subgraphs. We start with the nodes with the smallest number of subtree nodes and always increase this number by two because nodes have exactly zero or two daughter nodes. We create the `k_nodes` using the `k_node_list` of each `f_node`. The number of nodes which have to be created depends of the number of existing daughter nodes, which means that we have to create a node for each combination of existing and valid (the ones which we keep) daughter nodes. If the node corresponds to an external particle, we create only one node, since there are no daughter nodes. If the particle is not external and the daughter `f_nodes` do not contain any valid `k_nodes`, we do not create a new `k_nodes` either. When the calculations for all nodes with the same number of subtree nodes have been completed, we compare the valid nodes to eliminate equivalences (see below).

```

<Cascades2: procedures>+=
subroutine f_node_list_compute_mappings_s (feyngraph_set)
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(f_node_ptr_t), dimension(:), allocatable :: set
    type(k_node_ptr_t), dimension(:), allocatable :: k_set
    type(k_node_entry_t), pointer :: k_entry
    type(f_node_entry_t), pointer :: current
    type(k_node_list_t), allocatable :: compare_list
    integer :: n_entries
    integer :: pos
    integer :: i, j, k
    do i = 1, feyngraph_set%f_node_list%max_tree_size - 2, 2
        !!! Counter number of f_nodes with subtree size i for s channel calculations
        n_entries = 0
        if (feyngraph_set%use_dag) then
            do j=1, feyngraph_set%dag%n_nodes
                if (allocated (feyngraph_set%dag%node(j)%f_node)) then
                    do k=1, size(feyngraph_set%dag%node(j)%f_node)
                        if (associated (feyngraph_set%dag%node(j)%f_node(k)%node)) then
                            if (.not. (feyngraph_set%dag%node(j)%f_node(k)%node%incoming &
                                .or. feyngraph_set%dag%node(j)%f_node(k)%node%t_line) &

```

```

        .and. feyngraph_set%dag%node(j)%f_node(k)%node%n_subtree_nodes == i) th
        n_entries = n_entries + 1
    end if
    end if
    end do
    end if
    end do
else
    current => feyngraph_set%f_node_list%first
    do while (associated (current))
        if (.not. (current%node%incoming .or. current%node%t_line) &
            .and. current%node%n_subtree_nodes == i) then
            n_entries = n_entries + 1
        end if
        current => current%next
    end do
    end if
    if (n_entries == 0) exit
!!! Create a temporary k node list for comparison
    allocate (set(n_entries))
    pos = 0
    if (feyngraph_set%use_dag) then
        do j=1, feyngraph_set%dag%n_nodes
            if (allocated (feyngraph_set%dag%node(j)%f_node)) then
                do k=1, size(feyngraph_set%dag%node(j)%f_node)
                    if (associated (feyngraph_set%dag%node(j)%f_node(k)%node)) then
                        if (.not. (feyngraph_set%dag%node(j)%f_node(k)%node%incoming &
                            .or. feyngraph_set%dag%node(j)%f_node(k)%node%t_line) &
                            .and. feyngraph_set%dag%node(j)%f_node(k)%node%n_subtree_nodes == i) th
                            pos = pos + 1
                            set(pos)%node => feyngraph_set%dag%node(j)%f_node(k)%node
                        end if
                    end if
                end do
            end do
        end if
    else
        current => feyngraph_set%f_node_list%first
        do while (associated (current))
            if (.not. (current%node%incoming .or. current%node%t_line) &
                .and. current%node%n_subtree_nodes == i) then
                pos = pos + 1
                set(pos)%node => current%node
            end if
            current => current%next
        end do
    end if
    allocate (compare_list)
    compare_list%observer = .true.
    do j = 1, n_entries
        call k_node_init_from_f_node (set(j)%node, k_set, &
            feyngraph_set)
        if (allocated (k_set)) deallocate (k_set)
    end do

```

```

!$OMP PARALLEL DO PRIVATE (k_entry)
do j = 1, n_entries
  k_entry => set(j)%node%k_node_list%first
  do while (associated (k_entry))
    call node_assign_mapping_s(feyngraph_set%first, k_entry%node, feyngraph_set)
    k_entry => k_entry%next
  end do
end do
!$OMP END PARALLEL DO
do j = 1, size (set)
  k_entry => set(j)%node%k_node_list%first
  do while (associated (k_entry))
    if (k_entry%node%keep) then
      if (k_entry%node%mapping == NO_MAPPING .or. k_entry%node%mapping == NONRESONANT) t
        call compare_list%add_pointer (k_entry%node)
      end if
    end if
    k_entry => k_entry%next
  end do
end do
deallocate (set)
call compare_list%check_subtree_equivalences(feyngraph_set%model)
call compare_list%final
deallocate (compare_list)
end do
end subroutine f_node_list_compute_mappings_s

```

19.11.14 Fill the grove list

Find the **grove** within the **grove_list** for a **kingraph** for which the kinematical calculations and mapping assignments have been completed. The **groves** are defined by the **grove_prop** entries and the value of the resonance hash (**res_hash**). Whenever a matching grove does not exist, we create one. In a first step we consider only part of the grove properties (see **grove_prop_match**) and the resonance hash is ignored, which leads to a preliminary grove list. In the end all numbers in **grove_prop** as well as the resonance hash are compared, i.e. we create a new **grove_list**.

```

<Cascades2: grove list: TBP>+≡
  procedure :: get_grove => grove_list_get_grove

<Cascades2: sub interfaces>+≡
  module subroutine grove_list_get_grove (grove_list, kingraph, &
    return_grove, preliminary)
    class(grove_list_t), intent(inout) :: grove_list
    type(kingraph_t), intent(in), pointer :: kingraph
    type(grove_t), intent(inout), pointer :: return_grove
    logical, intent(in) :: preliminary
  end subroutine grove_list_get_grove

<Cascades2: procedures>+≡
  module subroutine grove_list_get_grove (grove_list, kingraph, &
    return_grove, preliminary)
    class(grove_list_t), intent(inout) :: grove_list

```

```

type(kingraph_t), intent(in), pointer :: kingraph
type(grove_t), intent(inout), pointer :: return_grove
logical, intent(in) :: preliminary
type(grove_t), pointer :: current_grove
return_grove => null ()
if (.not. associated(grove_list%first)) then
    allocate (grove_list%first)
    grove_list%first%grove_prop = kingraph%grove_prop
    return_grove => grove_list%first
    return
end if
current_grove => grove_list%first
do while (associated (current_grove))
    if ((preliminary .and. &
        (current_grove%grove_prop .match. kingraph%grove_prop)) .or. &
        (.not. preliminary .and. &
        current_grove%grove_prop == kingraph%grove_prop)) then
        return_grove => current_grove
        exit
    else if (.not. associated (current_grove%next)) then
        allocate (current_grove%next)
        current_grove%next%grove_prop = kingraph%grove_prop
        if (size (kingraph%tree%bc) < 9) &
            current_grove%compare_tree%depth = 1
        return_grove => current_grove%next
        exit
    end if
    if (associated (current_grove%next)) then
        current_grove => current_grove%next
    end if
end do
end subroutine grove_list_get_grove

```

Add a valid kingraph to a grove_list. We first look for the grove which has the grove properties of the kingraph. If no such grove exists so far, it is created.

<Cascades2: grove list: TBP>+≡

```

procedure :: add_kingraph => grove_list_add_kingraph

```

<Cascades2: sub interfaces>+≡

```

module subroutine grove_list_add_kingraph (grove_list, kingraph, &
    preliminary, check, model)
    class(grove_list_t), intent(inout) :: grove_list
    type(kingraph_t), pointer, intent(inout) :: kingraph
    logical, intent(in) :: preliminary
    logical, intent(in) :: check
    type(model_data_t), optional, intent(in) :: model
end subroutine grove_list_add_kingraph

```

<Cascades2: procedures>+≡

```

module subroutine grove_list_add_kingraph (grove_list, kingraph, &
    preliminary, check, model)
    class(grove_list_t), intent(inout) :: grove_list
    type(kingraph_t), pointer, intent(inout) :: kingraph

```

```

logical, intent(in) :: preliminary
logical, intent(in) :: check
type(model_data_t), optional, intent(in) :: model
type(grove_t), pointer :: grove
type(kingraph_t), pointer :: current
integer, save :: index = 0
grove => null ()
current => null ()
if (preliminary) then
  if (kingraph%index == 0) then
    index = index + 1
    kingraph%index = index
  end if
end if
call grove_list%get_grove (kingraph, grove, preliminary)
if (check) then
  call grove%compare_tree%check_kingraph (kingraph, model, preliminary)
end if
if (kingraph%keep) then
  if (associated (grove%first)) then
    grove%last%grove_next => kingraph
    grove%last => kingraph
  else
    grove%first => kingraph
    grove%last => kingraph
  end if
end if
end subroutine grove_list_add_kingraph

```

For a given feyngraph we store all valid kingraphs in the grove_list.

```

<Cascades2: grove list: TBP>+=
  procedure :: add_feyngraph => grove_list_add_feyngraph

<Cascades2: sub interfaces>+=
  module subroutine grove_list_add_feyngraph (grove_list, feyngraph, model)
    class(grove_list_t), intent(inout) :: grove_list
    type(feyngraph_t), intent(inout) :: feyngraph
    type(model_data_t), intent(in) :: model
  end subroutine grove_list_add_feyngraph

<Cascades2: procedures>+=
  module subroutine grove_list_add_feyngraph (grove_list, feyngraph, model)
    class(grove_list_t), intent(inout) :: grove_list
    type(feyngraph_t), intent(inout) :: feyngraph
    type(model_data_t), intent(in) :: model
    type(kingraph_t), pointer :: current_kingraph, add_kingraph
    do while (associated (feyngraph%kin_first))
      if (feyngraph%kin_first%keep) then
        add_kingraph => feyngraph%kin_first
        feyngraph%kin_first => feyngraph%kin_first%next
        add_kingraph%next => null ()
        call grove_list%add_kingraph (kingraph=add_kingraph, &
          preliminary=.true., check=.true., model=model)
      else
        exit
      end if
    end do
  end subroutine grove_list_add_feyngraph

```

```

        end if
    end do
    if (associated (feyngraph%kin_first)) then
        current_kingraph => feyngraph%kin_first
        do while (associated (current_kingraph%next))
            if (current_kingraph%next%keep) then
                add_kingraph => current_kingraph%next
                current_kingraph%next => current_kingraph%next%next
                add_kingraph%next => null ()
                call grove_list%add_kingraph (kingraph=add_kingraph, &
                    preliminary=.true., check=.true., model=model)
            else
                current_kingraph => current_kingraph%next
            end if
        end do
    end if
end subroutine grove_list_add_feyngraph

```

Compare two `grove_prop` objects. The `.match.` operator is used for preliminary groves in which the `kingraphs` share only the 3 numbers `n_resonances`, `n_log_enhanced` and `n_t_channel`. These groves are only used for comparing the kingraphs, because only graphs within these preliminary groves can be equivalent (the numbers which are compared here are unambiguously fixed by the combination of mappings in these channels).

```

<Cascades2: interfaces>+=
    interface operator (.match.)
        module procedure grove_prop_match
    end interface operator (.match.)

<Cascades2: sub interfaces>+=
    module function grove_prop_match (grove_prop1, grove_prop2) &
        result (gp_match)
        type(grove_prop_t), intent(in) :: grove_prop1
        type(grove_prop_t), intent(in) :: grove_prop2
        logical :: gp_match
    end function grove_prop_match

<Cascades2: procedures>+=
    module function grove_prop_match (grove_prop1, grove_prop2) result (gp_match)
        type(grove_prop_t), intent(in) :: grove_prop1
        type(grove_prop_t), intent(in) :: grove_prop2
        logical :: gp_match
        gp_match = (grove_prop1%n_resonances == grove_prop2%n_resonances) &
            .and. (grove_prop1%n_log_enhanced == grove_prop2%n_log_enhanced) &
            .and. (grove_prop1%n_t_channel == grove_prop2%n_t_channel)
    end function grove_prop_match

```

The equal operator on the other hand will be used when all valid `kingraphs` have been created and mappings have been determined, to split up the existing (preliminary) grove list, i.e. to create new groves which are determined by all entries in `grove_prop_t`.

```

<Cascades2: interfaces>+=
    interface operator (==)

```

```

        module procedure grove_prop_equal
    end interface operator (==)

<Cascades2: sub interfaces>+≡
    module function grove_prop_equal (grove_prop1, grove_prop2) &
        result (gp_equal)
        type(grove_prop_t), intent(in) :: grove_prop1
        type(grove_prop_t), intent(in) :: grove_prop2
        logical :: gp_equal
    end function grove_prop_equal

<Cascades2: procedures>+≡
    module function grove_prop_equal (grove_prop1, grove_prop2) result (gp_equal)
        type(grove_prop_t), intent(in) :: grove_prop1
        type(grove_prop_t), intent(in) :: grove_prop2
        logical :: gp_equal
        gp_equal = (grove_prop1%res_hash == grove_prop2%res_hash) &
            .and. (grove_prop1%n_resonances == grove_prop2%n_resonances) &
            .and. (grove_prop1%n_log_enhanced == grove_prop2%n_log_enhanced) &
            .and. (grove_prop1%n_off_shell == grove_prop2%n_off_shell) &
            .and. (grove_prop1%multiplicity == grove_prop2%multiplicity) &
            .and. (grove_prop1%n_t_channel == grove_prop2%n_t_channel)
    end function grove_prop_equal

```

19.11.15 Remove equivalent channels

Here we define the equivalence condition for completed **kingraphs**. The aim is to keep those **kingraphs** which describe the strongest peaks of the amplitude. The **bincodes** and **mappings** have to be the same for an equivalence, but the **pdgs** can be different. At the same time we check if the trees are exactly the same (up to the sign of **pdg** codes) in which case we do not keep both of them. This can be the case when the incoming particles are the same or their mutual anti-particles and there are no t-channel lines in the Feynman diagram to which the kingraph belongs.

```

<Cascades2: parameters>+≡
    integer, parameter :: EMPTY = -999

<Cascades2: procedures>+≡
    function kingraph_eqv (kingraph1, kingraph2) result (eqv)
        type(kingraph_t), intent(in) :: kingraph1
        type(kingraph_t), intent(inout) :: kingraph2
        logical :: eqv
        integer :: i
        logical :: equal
        eqv = .false.
        do i = kingraph1%tree%n_entries, 1, -1
            if (kingraph1%tree%bc(i) /= kingraph2%tree%bc(i)) return
        end do
        do i = kingraph1%tree%n_entries, 1, -1
            if ( .not. (kingraph1%tree%mapping(i) == kingraph2%tree%mapping(i) &
                .or. ((kingraph1%tree%mapping(i) == NO_MAPPING .or. &
                    kingraph1%tree%mapping(i) == NONRESONANT) .and. &
                    (kingraph2%tree%mapping(i) == NO_MAPPING .or. &

```

```

        kinggraph2%tree%mapping(i) == NONRESONANT)))) return
end do
equal = .true.
do i = kinggraph1%tree%n_entries, 1, -1
    if (abs(kinggraph1%tree%pdg(i)) /= abs(kinggraph2%tree%pdg(i))) then
        equal = .false.;
        select case (kinggraph1%tree%mapping(i))
        case (S_CHANNEL, RADIATION)
            select case (kinggraph2%tree%mapping(i))
            case (S_CHANNEL, RADIATION)
                return
            end select
        end select
    end if
end do
if (equal) then
    kinggraph2%keep = .false.
    call kinggraph2%tree%final ()
else
    eqv = .true.
end if
end function kinggraph_eqv

```

Select between two **kingraphs** which fulfill the equivalence condition above. This is done by comparing the **pdg** values of the **tree** for increasing bincode. If the particles are different at some place, we usually choose the one which would be returned first by the subroutine **match_vertex** of the model for the daughter **pdg** codes. Since we work here only on the basis of the **trees** of the completed **kingraphs**, we have to use the **bc** array to determine the positions of the daughter nodes' entries in the array. The graph which has to be kept should correspond to the stronger peak at the place which is compared.

(*Cascades2: procedures*) $\vdash\equiv$

```

subroutine kinggraph_select (kinggraph1, kinggraph2, model, preliminary)
    type(kinggraph_t), intent(inout) :: kinggraph1
    type(kinggraph_t), intent(inout) :: kinggraph2
    type(model_data_t), intent(in) :: model
    logical, intent(in) :: preliminary
    integer(TC), dimension(:), allocatable :: tmp_bc, daughter_bc
    integer, dimension(:), allocatable :: tmp_pdg, daughter_pdg
    integer, dimension(:), allocatable :: pdg_match
    integer :: i, j
    integer :: n_ext1, n_ext2
    if (kinggraph_eqv (kinggraph1, kinggraph2)) then
        if (.not. preliminary) then
            kinggraph2%keep = .false.; call kinggraph2%tree%final ()
            return
        end if
        do i=1, size (kinggraph1%tree%bc)
            if (abs(kinggraph1%tree%pdg(i)) /= abs(kinggraph2%tree%pdg(i))) then
                if (kinggraph1%tree%mapping(i) /= EXTERNAL_PRT) then
                    n_ext1 = popcnt (kinggraph1%tree%bc(i))
                    n_ext2 = n_ext1
                    do j=i+1, size (kinggraph1%tree%bc)

```



```

        if (abs(kingraph1%tree%pdg(j)) /= abs(kingraph2%tree%pdg(j))) then
            n_ext2 = popcnt (kingraph1%tree%bc(j))
            if (n_ext2 < n_ext1) exit
        end if
    end do
    if (n_ext2 < n_ext1) cycle
    allocate (tmp_bc(i-1))
    tmp_bc = kingraph1%tree%bc(:i-1)
    allocate (tmp_pdg(i-1))
    tmp_pdg = kingraph1%tree%pdg(:i-1)
    do j=i-1, 1, - 1
        where (iand (tmp_bc(:j-1),tmp_bc(j)) /= 0 &
            .or. iand(tmp_bc(:j-1),kingraph1%tree%bc(i)) == 0)
            tmp_bc(:j-1) = 0
            tmp_pdg(:j-1) = 0
        endwhere
    end do
    allocate (daughter_bc(size(pack(tmp_bc, tmp_bc /= 0))))
    daughter_bc = pack (tmp_bc, tmp_bc /= 0)
    allocate (daughter_pdg(size(pack(tmp_pdg, tmp_pdg /= 0))))
    daughter_pdg = pack (tmp_pdg, tmp_pdg /= 0)
    if (size (daughter_pdg) == 2) then
        call model%match_vertex(daughter_pdg(1), daughter_pdg(2), pdg_match)
    end if
    do j=1, size (pdg_match)
        if (abs(pdg_match(j)) == abs(kingraph1%tree%pdg(i))) then
            kingraph2%keep = .false.; call kingraph2%tree%final ()
            exit
        else if (abs(pdg_match(j)) == abs(kingraph2%tree%pdg(i))) then
            kingraph1%keep = .false.; call kingraph1%tree%final ()
            exit
        end if
    end do
    deallocate (tmp_bc, tmp_pdg, daughter_bc, daughter_pdg, pdg_match)
    if (.not. (kingraph1%keep .and. kingraph2%keep)) exit
end if
end if
end do
end if
end if
end subroutine kingraph_select

```

At the beginning we do not care about the resonance hash, but only about part of the grove properties, which is defined in `grove_prop_match`. In these resulting preliminary groves the kingraphs can be equivalent, i.e. we do not have to compare all graphs with each other but only all graphs within each of these preliminary groves. In the end we create a new grove list where the grove properties of the `kingraphs` within a `grove` have to be exactly the same and in addition the groves are distinguished by the resonance hash values. Here the kingraphs are not compared any more, which means that the number of channels is not reduced any more.

<Cascades2: grove list: TBP>+≡
 procedure :: merge => grove_list_merge
<Cascades2: sub interfaces>+≡

```

module subroutine grove_list_merge (target_list, grove_list, model, &
    prc_component)
    class(grove_list_t), intent(inout) :: target_list
    type(grove_list_t), intent(inout) :: grove_list
    type(model_data_t), intent(in) :: model
    integer, intent(in) :: prc_component
end subroutine grove_list_merge

<Cascades2: procedures>+=
module subroutine grove_list_merge (target_list, grove_list, model, &
    prc_component)
    class(grove_list_t), intent(inout) :: target_list
    type(grove_list_t), intent(inout) :: grove_list
    type(model_data_t), intent(in) :: model
    integer, intent(in) :: prc_component
    type(grove_t), pointer :: current_grove
    type(kingraph_t), pointer :: current_graph
    current_grove => grove_list%first
    do while (associated (current_grove))
        do while (associated (current_grove%first))
            current_graph => current_grove%first
            current_grove%first => current_grove%first%grove_next
            current_graph%grove_next => null ()
            if (current_graph%keep) then
                current_graph%prc_component = prc_component
                call target_list%add_kingraph(kingraph=current_graph, &
                    preliminary=.false., check=.true., model=model)
            else
                call current_graph%final ()
                deallocate (current_graph)
            end if
        end do
        current_grove => current_grove%next
    end do
end subroutine grove_list_merge

```

Recreate a grove list where we have different groves for different resonance hashes.

```

<Cascades2: grove list: TBP>+=
procedure :: rebuild => grove_list_rebuild

<Cascades2: sub interfaces>+=
module subroutine grove_list_rebuild (grove_list)
    class(grove_list_t), intent(inout) :: grove_list
end subroutine grove_list_rebuild

<Cascades2: procedures>+=
module subroutine grove_list_rebuild (grove_list)
    class(grove_list_t), intent(inout) :: grove_list
    type(grove_list_t) :: tmp_list
    type(grove_t), pointer :: current_grove
    type(grove_t), pointer :: remove_grove
    type(kingraph_t), pointer :: current_graph
    type(kingraph_t), pointer :: next_graph
    tmp_list%first => grove_list%first

```

```

grove_list%first => null ()
current_grove => tmp_list%first
do while (associated (current_grove))
  current_graph => current_grove%first
  do while (associated (current_graph))
    call current_graph%assign_resonance_hash ()
    next_graph => current_graph%grove_next
    current_graph%grove_next => null ()
    if (current_graph%keep) then
      call grove_list%add_kingraph (kingraph=current_graph, &
        preliminary=.false., check=.false.)
    end if
    current_graph => next_graph
  end do
  current_grove => current_grove%next
end do
call tmp_list%final
end subroutine grove_list_rebuild

```

19.11.16 Write the phase-space file

The phase-space file is written from the graphs which survive the calculations and equivalence checks and are in the grove list. It is written grove by grove. The output should be the same as in the corresponding procedure `cascade_set_write_file_format` of `cascades`, up to the order of groves and channels.

```

<Cascades2: public>+≡
  public :: feyngraph_set_write_file_format

<Cascades2: sub interfaces>+≡
  module subroutine feyngraph_set_write_file_format (feyngraph_set, u)
    type(feyngraph_set_t), intent(in) :: feyngraph_set
    integer, intent(in) :: u
  end subroutine feyngraph_set_write_file_format

<Cascades2: procedures>+≡
  module subroutine feyngraph_set_write_file_format (feyngraph_set, u)
    type(feyngraph_set_t), intent(in) :: feyngraph_set
    integer, intent(in) :: u
    type(grove_t), pointer :: grove
    integer :: channel_number
    integer :: grove_number
    channel_number = 0
    grove_number = 0
    grove => feyngraph_set%grove_list%first
    do while (associated (grove))
      grove_number = grove_number + 1
      call grove%write_file_format &
        (feyngraph_set, grove_number, channel_number, u)
      grove => grove%next
    end do
  end subroutine feyngraph_set_write_file_format

```

Write the relevant information of the kingraphs of a grove and the grove properties in the file format.

```

<Cascades2: grove: TBP>+≡
    procedure :: write_file_format => grove_write_file_format

<Cascades2: sub interfaces>+≡
    recursive module subroutine grove_write_file_format &
        (grove, feyngraph_set, gr_number, ch_number, u)
        class(grove_t), intent(in) :: grove
        type(feyngraph_set_t), intent(in) :: feyngraph_set
        integer, intent(in) :: u
        integer, intent(inout) :: gr_number
        integer, intent(inout) :: ch_number
    end subroutine grove_write_file_format

<Cascades2: procedures>+≡
    recursive module subroutine grove_write_file_format &
        (grove, feyngraph_set, gr_number, ch_number, u)
        class(grove_t), intent(in) :: grove
        type(feyngraph_set_t), intent(in) :: feyngraph_set
        integer, intent(in) :: u
        integer, intent(inout) :: gr_number
        integer, intent(inout) :: ch_number
        type(kingraph_t), pointer :: current
1   format(3x,A,1x,40(1x,I4))
    write (u, "(A)")
    write (u, "(1x,'!',1x,A,1x,I0,A)", advance='no') &
        'Multiplicity =', grove%grove_prop%multiplicity, ", "
    select case (grove%grove_prop%n_resonances)
    case (0)
        write (u, '(1x,A)', advance='no') 'no resonances, '
    case (1)
        write (u, '(1x,A)', advance='no') '1 resonance, '
    case default
        write (u, '(1x,I0,1x,A)', advance='no') &
            grove%grove_prop%n_resonances, 'resonances, '
    end select
    write (u, '(1x,I0,1x,A)', advance='no') &
        grove%grove_prop%n_log_enhanced, 'logs, '
    write (u, '(1x,I0,1x,A)', advance='no') &
        grove%grove_prop%n_off_shell, 'off-shell, '
    select case (grove%grove_prop%n_t_channel)
    case (0); write (u, '(1x,A)') 's-channel graph'
    case (1); write (u, '(1x,A)') '1 t-channel line'
    case default
        write(u, '(1x,I0,1x,A)') &
            grove%grove_prop%n_t_channel, 't-channel lines'
    end select
    write (u, '(1x,A,I0)') 'grove #', gr_number
    current => grove%first
    do while (associated (current))
        if (current%keep) then
            ch_number = ch_number + 1
            call current%write_file_format (feyngraph_set, ch_number, u)
        end if
    end do

```

```

        current => current%grove_next
    end do
end subroutine grove_write_file_format

```

Write the relevant information of a valid kingraph in the file format. The information is extracted from the tree.

```

<Cascades2: kingraph: TBP>+≡
    procedure :: write_file_format => kingraph_write_file_format

<Cascades2: sub interfaces>+≡
    module subroutine kingraph_write_file_format &
        (kingraph, feyngraph_set, ch_number, u)
    class(kingraph_t), intent(in) :: kingraph
    type(feyngraph_set_t), intent(in) :: feyngraph_set
    integer, intent(in) :: ch_number
    integer, intent(in) :: u
    end subroutine kingraph_write_file_format

<Cascades2: procedures>+≡
    module subroutine kingraph_write_file_format &
        (kingraph, feyngraph_set, ch_number, u)
    class(kingraph_t), intent(in) :: kingraph
    type(feyngraph_set_t), intent(in) :: feyngraph_set
    integer, intent(in) :: ch_number
    integer, intent(in) :: u
    integer :: i
    integer(TC) :: brcode_incoming
2   format(3X,'map',1X,I3,1X,A,1X,I9,1X,'!',1X,A)
    !!! determine brcode of incoming particle from tree
    brcode_incoming = maxval (kingraph%tree%bc)
    write (unit=u, fmt='(1X,A,I0)') '! Channel #', ch_number
    write (unit=u, fmt='(3X,A,1X)', advance='no') 'tree'
    do i=1, size (kingraph%tree%bc)
        if (kingraph%tree%mapping(i) >=0 &
            .or. kingraph%tree%mapping(i) == NONRESONANT &
            .or. (kingraph%tree%bc(i) == brcode_incoming &
                .and. feyngraph_set%process_type == DECAY)) then
            write (unit=u, fmt='(1X,I0)', advance='no') kingraph%tree%bc(i)
        end if
    end do
    write (unit=u, fmt='(A)', advance='yes')
    do i=1, size(kingraph%tree%bc)
        select case (kingraph%tree%mapping(i))
        case (NO_MAPPING, NONRESONANT, EXTERNAL_PRT)
        case (S_CHANNEL)
            write (unit=u, fmt=2) kingraph%tree%bc(i), 's_channel', &
                kingraph%tree%pdg(i), &
                trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
        case (T_CHANNEL)
            write (unit=u, fmt=2) kingraph%tree%bc(i), 't_channel', &
                abs (kingraph%tree%pdg(i)), &
                trim(get_particle_name (feyngraph_set, abs(kingraph%tree%pdg(i))))
        case (U_CHANNEL)
            write (unit=u, fmt=2) kingraph%tree%bc(i), 'u_channel', &
                abs (kingraph%tree%pdg(i)), &

```

```

        trim(get_particle_name (feyngraph_set, abs(kingraph%tree%pdg(i))))
case (RADIATION)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'radiation', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (COLLINEAR)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'collinear', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (INFRARED)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'infrared ', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (ON_SHELL)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'on_shell ', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case default
    call msg_bug (" Impossible mapping mode encountered")
end select
end do
end subroutine kingraph_write_file_format

```

Get the particle name from the particle array of the `feyngraph_set`. This is needed for the phs file creation.

(*Cascades2: procedures*) +=

```

function get_particle_name (feyngraph_set, pdg) result (particle_name)
    type(feyngraph_set_t), intent(in) :: feyngraph_set
    integer, intent(in) :: pdg
    character(len=LABEL_LEN) :: particle_name
    integer :: i
    do i=1, size (feyngraph_set%particle)
        if (feyngraph_set%particle(i)%pdg == pdg) then
            particle_name = feyngraph_set%particle(i)%particle_label
            exit
        end if
    end do
end function get_particle_name

```

19.11.17 Invert a graph

All Feynman diagrams given by O'Mega look like a decay. The `feyngraph` which is constructed from this output also looks like a decay, where one of the incoming particles is the decaying particle (or the root of the tree). The calculations can in principle be done on this data structure. However, it is also performed with the other incoming particle as the root. The first part of the calculation is the same for both cases. For the second part we need to transform/turn the graphs such that the other incoming particle becomes the root. This is done by identifying the incoming particles from the O'Mega output (the first one is simply the root of the existing tree, the second contains [2] in the `particle_label`) and the nodes/particles which connect both incoming particles (here we set `t_line`

= .true.). At the same time we set the pointers `inverse_daughter1` and `inverse_daughter2` for the corresponding node, which point to the mother node and the other daughter of the mother node; these will be the daughters of the node in the inverted `feyngraph`.

```

<Cascades2: feyngraph: TBP>+=
  procedure :: make_invertible => feyngraph_make_invertible

<Cascades2: sub interfaces>+=
  module subroutine feyngraph_make_invertible (feyngraph)
    class(feyngraph_t), intent(inout) :: feyngraph
  end subroutine feyngraph_make_invertible

<Cascades2: procedures>+=
  module subroutine feyngraph_make_invertible (feyngraph)
    class(feyngraph_t), intent(inout) :: feyngraph
    logical :: t_line_found
    feyngraph%root%incoming = .true.
    t_line_found = .false.
    if (associated (feyngraph%root%daughter1)) then
      call f_node_t_line_check (feyngraph%root%daughter1, t_line_found)
      if (.not. t_line_found) then
        if (associated (feyngraph%root%daughter2)) then
          call f_node_t_line_check (feyngraph%root%daughter2, t_line_found)
        end if
      end if
    end if

    contains

    <k node t line check>
    end subroutine feyngraph_make_invertible

```

Check if a node has to be `t_line` or `incoming` and assign inverse daughter pointers.

```

<k node t line check>≡
  recursive subroutine f_node_t_line_check (node, t_line_found)
    type(f_node_t), target, intent(inout) :: node
    integer :: pos
    logical, intent(inout) :: t_line_found
    if (associated (node%daughter1)) then
      call f_node_t_line_check (node%daughter1, t_line_found)
      if (node%daughter1%incoming .or. node%daughter1%t_line) then
        node%t_line = .true.
      else if (associated (node%daughter2)) then
        call f_node_t_line_check (node%daughter2, t_line_found)
        if (node%daughter2%incoming .or. node%daughter2%t_line) then
          node%t_line = .true.
        end if
      end if
    else
      pos = index (node%particle_label, '[') + 1
      if (node%particle_label(pos:pos) == '2') then
        node%incoming = .true.
        t_line_found = .true.
      end if
    end if
  end subroutine f_node_t_line_check

```

```

        end if
    end if
end subroutine f_node_t_line_check

```

Make an inverted copy of a `kingraph` using the inverse daughter pointers.

```

<Cascades2: kingraph: TBP>+≡
    procedure :: make_inverse_copy => kingraph_make_inverse_copy

<Cascades2: sub interfaces>+≡
    module subroutine kingraph_make_inverse_copy (original_kingraph, feyngraph)
        class(kingraph_t), intent(inout) :: original_kingraph
        type(feyngraph_t), intent(inout) :: feyngraph
    end subroutine kingraph_make_inverse_copy

<Cascades2: procedures>+≡
    module subroutine kingraph_make_inverse_copy (original_kingraph, feyngraph)
        class(kingraph_t), intent(inout) :: original_kingraph
        type(feyngraph_t), intent(inout) :: feyngraph
        type(kingraph_t), pointer :: kingraph_copy
        type(k_node_t), pointer :: potential_root
        allocate (kingraph_copy)
        if (associated (feyngraph%kin_last)) then
            allocate (feyngraph%kin_last%next)
            feyngraph%kin_last => feyngraph%kin_last%next
        else
            allocate(feyngraph%kin_first)
            feyngraph%kin_last => feyngraph%kin_first
        end if
        kingraph_copy => feyngraph%kin_last
        call kingraph_set_inverse_daughters (original_kingraph)
        kingraph_copy%inverse = .true.
        kingraph_copy%n_nodes = original_kingraph%n_nodes
        kingraph_copy%keep = original_kingraph%keep
        potential_root => original_kingraph%root
        do while (.not. potential_root%incoming .or. &
            (associated (potential_root%daughter1) .and. &
            associated (potential_root%daughter2)))
            if (potential_root%daughter1%incoming .or. &
                potential_root%daughter1%t_line) then
                potential_root => potential_root%daughter1
            else if (potential_root%daughter2%incoming .or. &
                potential_root%daughter2%t_line) then
                potential_root => potential_root%daughter2
            end if
        end do
        call node_inverse_deep_copy (potential_root, kingraph_copy%root)
    end subroutine kingraph_make_inverse_copy

```

Recursively deep-copy nodes, but along the t-line the inverse daughters become the new daughters. We need a deep copy only for the `incoming` or `t_line` nodes. For the other nodes (of s-channel subgraphs) we set only pointers to the existing nodes of the non-inverted graph.

```

<Cascades2: procedures>+≡
    recursive subroutine node_inverse_deep_copy (original_node, node_copy)

```



```

type(k_node_t), intent(in) :: original_node
type(k_node_t), pointer, intent(out) :: node_copy
call original_node%f_node%k_node_list%add_entry(node_copy, recycle=.false.)
node_copy = original_node
if (node_copy%t_line .or. node_copy%incoming) then
  node_copy%particle => original_node%particle%anti
else
  node_copy%particle => original_node%particle
end if
if (associated (original_node%inverse_daughter1) .and. associated (original_node%inverse_daughter2)) then
  if (original_node%inverse_daughter1%incoming .or. original_node%inverse_daughter1%t_line) then
    node_copy%daughter2 => original_node%inverse_daughter2
    call node_inverse_deep_copy (original_node%inverse_daughter1, &
      node_copy%daughter1)
  else if (original_node%inverse_daughter2%incoming .or. original_node%inverse_daughter2%t_line) then
    node_copy%daughter1 => original_node%inverse_daughter1
    call node_inverse_deep_copy (original_node%inverse_daughter2, &
      node_copy%daughter2)
  end if
end if
end subroutine node_inverse_deep_copy

```

19.11.18 Find phase-space parametrizations

Perform all mapping calculations for a single process and store valid kingraphs (channels) into the grove list, without caring for instance about the resonance hash values.

```

<Cascades2: public>+≡
  public :: feyngraph_set_generate_single

<Cascades2: sub interfaces>+≡
  module subroutine feyngraph_set_generate_single (feyngraph_set, model, &
    n_in, n_out, phs_par, fatal_beam_decay, u_in)
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(model_data_t), target, intent(in) :: model
    integer, intent(in) :: n_in, n_out
    type(phs_parameters_t), intent(in) :: phs_par
    logical, intent(in) :: fatal_beam_decay
    integer, intent(in) :: u_in
  end subroutine feyngraph_set_generate_single

<Cascades2: procedures>+≡
  module subroutine feyngraph_set_generate_single (feyngraph_set, model, &
    n_in, n_out, phs_par, fatal_beam_decay, u_in)
    type(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(model_data_t), target, intent(in) :: model
    integer, intent(in) :: n_in, n_out
    type(phs_parameters_t), intent(in) :: phs_par
    logical, intent(in) :: fatal_beam_decay
    integer, intent(in) :: u_in
    feyngraph_set%n_in = n_in
    feyngraph_set%n_out = n_out
    feyngraph_set%process_type = n_in
  end subroutine feyngraph_set_generate_single

```

```

feyngraph_set%phs_par = phs_par
feyngraph_set%model => model
if (debug_on) call msg_debug &
    (D_PHASESPACE, "Construct relevant Feynman diagrams from Omega output")
call feyngraph_set%build (u_in)
if (debug_on) call msg_debug &
    (D_PHASESPACE, "Find phase-space parametrizations")
call feyngraph_set_find_phs_parametrizations(feyngraph_set)
end subroutine feyngraph_set_generate_single

```

Find the phase space parametrizations. We start with the computation of pure s-channel subtrees, i.e. we determine mappings and compare subtrees in order to reduce the number of channels. This can be parallelized easily. When all s-channel `k_nodes` exist, the possible `kingraphs` are created using these nodes and we determine mappings for t-channel nodes.

(*Cascades2: procedures*) +=

```

subroutine feyngraph_set_find_phs_parametrizations (feyngraph_set)
    class(feyngraph_set_t), intent(inout) :: feyngraph_set
    type(feyngraph_t), pointer :: current => null ()
    type(feyngraph_ptr_t), dimension (:), allocatable :: set
    integer :: pos
    integer :: i
    allocate (set (feyngraph_set%n_graphs))
    pos = 0
    current => feyngraph_set%first
    do while (associated (current))
        pos = pos + 1
        set(pos)%graph => current
        current => current%next
    end do
    if (feyngraph_set%process_type == SCATTERING) then
        !$OMP PARALLEL DO
        do i=1, feyngraph_set%n_graphs
            if (set(i)%graph%keep) then
                call set(i)%graph%make_invertible ()
            end if
        end do
        !$OMP END PARALLEL DO
    end if
    call f_node_list_compute_mappings_s (feyngraph_set)
    do i=1, feyngraph_set%n_graphs
        if (set(i)%graph%keep) then
            call set(i)%graph%make_kingraphs (feyngraph_set)
        end if
    end do
    if (feyngraph_set%process_type == SCATTERING) then
        do i=1, feyngraph_set%n_graphs
            if (set(i)%graph%keep) then
                call set(i)%graph%make_inverse_kingraphs ()
            end if
        end do
    end if
    do i=1, feyngraph_set%n_graphs

```

```

        if (set(i)%graph%keep) then
            call set(i)%graph%compute_mappings (feyngraph_set)
        end if
    end do
do i=1, feyngraph_set%n_graphs
    if (set(i)%graph%keep) then
        call feyngraph_set%grove_list%add_feyngraph (set(i)%graph, &
            feyngraph_set%model)
    end if
end do
end subroutine feyngraph_set_find_phs_parametrizations

```

Compare objects of type `tree_t`.

```

<Cascades2: interfaces>+≡
    interface operator (==)
        module procedure tree_equal
    end interface operator (==)

<Cascades2: sub interfaces>+≡
    elemental module function tree_equal (tree1, tree2) result (flag)
        type(tree_t), intent(in) :: tree1, tree2
        logical :: flag
    end function tree_equal

<Cascades2: procedures>+≡
    elemental module function tree_equal (tree1, tree2) result (flag)
        type(tree_t), intent(in) :: tree1, tree2
        logical :: flag
        if (tree1%n_entries == tree2%n_entries) then
            if (tree1%bc(size(tree1%bc)) == tree2%bc(size(tree2%bc))) then
                flag = all (tree1%mapping == tree2%mapping) .and. &
                    all (tree1%bc == tree2%bc) .and. &
                    all (abs(tree1%pdg) == abs(tree2%pdg))
            else
                flag = .false.
            end if
        else
            flag = .false.
        end if
    end function tree_equal

```

Select between equivalent subtrees (type `tree_t`). This is similar to `kingraph_select`, but we compare only positions with mappings `NONRESONANT` and `NO_MAPPING`.

```

<Cascades2: interfaces>+≡
    interface operator (.eqv.)
        module procedure subtree_eqv
    end interface operator (.eqv.)

<Cascades2: sub interfaces>+≡
    pure module function subtree_eqv (subtree1, subtree2) result (eqv)
        type(tree_t), intent(in) :: subtree1, subtree2
        logical :: eqv
    end function subtree_eqv

```

```

<Cascades2: procedures>+≡
pure module function subtree_eqv (subtree1, subtree2) result (eqv)
  type(tree_t), intent(in) :: subtree1, subtree2
  logical :: eqv
  integer :: root_pos
  integer :: i
  logical :: equal
  eqv = .false.
  if (subtree1%n_entries /= subtree2%n_entries) return
  root_pos = subtree1%n_entries
  if (subtree1%mapping(root_pos) == NONRESONANT .or. &
      subtree2%mapping(root_pos) == NONRESONANT .or. &
      (subtree1%mapping(root_pos) == NO_MAPPING .and. &
       subtree2%mapping(root_pos) == NO_MAPPING .and. &
       abs(subtree1%pdg(root_pos)) == abs(subtree2%pdg(root_pos)))) then
    do i = subtree1%n_entries, 1, -1
      if (subtree1%bc(i) /= subtree2%bc(i)) return
    end do
    equal = .true.
    do i = subtree1%n_entries, 1, -1
      if (abs(subtree1%pdg(i)) /= abs(subtree2%pdg(i))) then
        select case (subtree1%mapping(i))
          case (NO_MAPPING, NONRESONANT)
            select case (subtree2%mapping(i))
              case (NO_MAPPING, NONRESONANT)
                equal = .false.
              case default
                return
            end select
          case default
            return
          end select
        end if
      end do
    do i = subtree1%n_entries, 1, -1
      if (subtree1%mapping(i) /= subtree2%mapping(i)) then
        select case (subtree1%mapping(i))
          case (NO_MAPPING, NONRESONANT)
            select case (subtree2%mapping(i))
              case (NO_MAPPING, NONRESONANT)
                case default
                  return
                end select
              case default
                return
              end select
            end if
          end do
        if (.not. equal) eqv = .true.
        end if
      end function subtree_eqv

```

```

<Cascades2: procedures>+≡
subroutine subtree_select (subtree1, subtree2, model)

```

```

type(tree_t), intent(inout) :: subtree1, subtree2
type(model_data_t), intent(in) :: model
integer :: j, k
integer(TC), dimension(:), allocatable :: tmp_bc, daughter_bc
integer, dimension(:), allocatable :: tmp_pdg, daughter_pdg
integer, dimension(:), allocatable :: pdg_match
if (subtree1 .eqv. subtree2) then
  do j=1, subtree1%n_entries
    if (abs(subtree1%pdg(j)) /= abs(subtree2%pdg(j))) then
      tmp_bc = subtree1%bc(:j-1); tmp_pdg = subtree1%pdg(:j-1)
      do k=j-1, 1, - 1
        where (iand (tmp_bc(:k-1),tmp_bc(k)) /= 0 &
               .or. iand(tmp_bc(:k-1),subtree1%bc(j)) == 0)
          tmp_bc(:k-1) = 0
          tmp_pdg(:k-1) = 0
        endwhile
      end do
      daughter_bc = pack (tmp_bc, tmp_bc /= 0)
      daughter_pdg = pack (tmp_pdg, tmp_pdg /= 0)
      if (size (daughter_pdg) == 2) then
        call model%match_vertex(daughter_pdg(1), daughter_pdg(2), pdg_match)
        if (.not. allocated (pdg_match)) then
          !!! Relevant if tree contains only abs (pdg). In this case, changing the
          !!! sign of one of the pdg codes should give a result.
          call model%match_vertex(-daughter_pdg(1), daughter_pdg(2), pdg_match)
        end if
      end if
    end if
    do k=1, size (pdg_match)
      if (abs(pdg_match(k)) == abs(subtree1%pdg(j))) then
        if (subtree1%keep) subtree2%keep = .false.
        exit
      else if (abs(pdg_match(k)) == abs(subtree2%pdg(j))) then
        if (subtree2%keep) subtree1%keep = .false.
        exit
      end if
    end do
    deallocate (tmp_bc, tmp_pdg, daughter_bc, daughter_pdg, pdg_match)
    if (.not. (subtree1%keep .and. subtree2%keep)) exit
  end if
end do
end if
end subroutine subtree_select

```

Assign a resonance hash value to a kingraph, like in cascades, but here without the array `tree_resonant`.

```

<Cascades2: kingraph: TBP>+=
  procedure :: assign_resonance_hash => kingraph_assign_resonance_hash

<Cascades2: sub interfaces>+=
  module subroutine kingraph_assign_resonance_hash (kingraph)
    class(kingraph_t), intent(inout) :: kingraph
  end subroutine kingraph_assign_resonance_hash

<Cascades2: procedures>+=
  module subroutine kingraph_assign_resonance_hash (kingraph)

```

```

class(kingraph_t), intent(inout) :: kingraph
logical, dimension (:), allocatable :: tree_resonant
integer(i8), dimension(1) :: mold
allocate (tree_resonant (kingraph%tree%n_entries))
tree_resonant = (kingraph%tree%mapping == S_CHANNEL)
kingraph%grove_prop%res_hash = hash (transfer &
    ([sort (pack (kingraph%tree%pdg, tree_resonant)), &
    sort (pack (abs (kingraph%tree%pdg), &
    kingraph%tree%mapping == T_CHANNEL .or. &
    kingraph%tree%mapping == U_CHANNEL))], mold))
deallocate (tree_resonant)
end subroutine kingraph_assign_resonance_hash

```

Write the process in the bincode format. This is again a copy of the corresponding procedure in `cascades`, using `feyngraph_set` instead of `cascade_set` as an argument.

```

<Cascades2: public>+≡
    public :: feyngraph_set_write_process_bincode_format

<Cascades2: sub interfaces>+≡
    module subroutine feyngraph_set_write_process_bincode_format &
        (feyngraph_set, unit)
        type(feyngraph_set_t), intent(in), target :: feyngraph_set
        integer, intent(in), optional :: unit
    end subroutine feyngraph_set_write_process_bincode_format

<Cascades2: procedures>+≡
    module subroutine feyngraph_set_write_process_bincode_format &
        (feyngraph_set, unit)
        type(feyngraph_set_t), intent(in), target :: feyngraph_set
        integer, intent(in), optional :: unit
        integer, dimension (:), allocatable :: bincode, field_width
        integer :: n_in, n_out, n_tot, n_flv
        integer :: u, f, i, bc
        character(20) :: str
        type(string_t) :: fmt_head
        type(string_t), dimension (:), allocatable :: fmt_proc
        u = given_output_unit (unit); if (u < 0) return
        if (.not. allocated (feyngraph_set%flv)) return
        write (u, "('!',1x,A)") "List of subprocesses with particle bincodes:"
        n_in = feyngraph_set%n_in
        n_out = feyngraph_set%n_out
        n_tot = n_in + n_out
        n_flv = size (feyngraph_set%flv, 2)
        allocate (bincode (n_tot), field_width (n_tot), fmt_proc (n_tot))
        bc = 1
        do i = 1, n_out
            bincode(n_in + i) = bc
            bc = 2 * bc
        end do
        do i = n_in, 1, -1
            bincode(i) = bc
            bc = 2 * bc
        end do
    end subroutine

```

```

do i = 1, n_tot
  write (str, "(I0)")  bincode(i)
  field_width(i) = len_trim (str)
  do f = 1, n_flv
    field_width(i) = max (field_width(i), &
      len (feyngraph_set%flv(i,f)%get_name ()))
  end do
end do
fmt_head = "('!'")
do i = 1, n_tot
  fmt_head = fmt_head // ",1x,"
  fmt_proc(i) = "(1x,"
  write (str, "(I0)")  field_width(i)
  fmt_head = fmt_head // "I" // trim(str)
  fmt_proc(i) = fmt_proc(i) // "A" // trim(str)
  if (i == n_in) then
    fmt_head = fmt_head // ",1x,'  '"
  end if
end do
do i = 1, n_tot
  fmt_proc(i) = fmt_proc(i) // ")"
end do
fmt_head = fmt_head // ")"
write (u, char (fmt_head))  bincode
do f = 1, n_flv
  write (u, "('!')", advance="no")
  do i = 1, n_tot
    write (u, char (fmt_proc(i)), advance="no") &
      char (feyngraph_set%flv(i,f)%get_name ())
    if (i == n_in) write (u, "(1x,'=>')", advance="no")
  end do
  write (u, *)
end do
write (u, char (fmt_head))  bincode
end subroutine feyngraph_set_write_process_bincode_format

```

Write tex file for graphical display of channels.

```

<Cascades2: public>+≡
  public :: feyngraph_set_write_graph_format

<Cascades2: sub interfaces>+≡
  module subroutine feyngraph_set_write_graph_format &
    (feyngraph_set, filename, process_id, unit)
    type(feyngraph_set_t), intent(in), target :: feyngraph_set
    type(string_t), intent(in) :: filename, process_id
    integer, intent(in), optional :: unit
  end subroutine feyngraph_set_write_graph_format

<Cascades2: procedures>+≡
  module subroutine feyngraph_set_write_graph_format &
    (feyngraph_set, filename, process_id, unit)
    type(feyngraph_set_t), intent(in), target :: feyngraph_set
    type(string_t), intent(in) :: filename, process_id
    integer, intent(in), optional :: unit
    type(kingraph_t), pointer :: kingraph

```

```

type(grove_t), pointer :: grove
integer :: u, n_grove, count, pgcount
logical :: first_in_grove
u = given_output_unit (unit); if (u < 0) return
write (u, '(A)') "\documentclass[10pt]{article}"
write (u, '(A)') "\usepackage{amsmath}"
write (u, '(A)') "\usepackage{feynmp}"
write (u, '(A)') "\usepackage{url}"
write (u, '(A)') "\usepackage{color}"
write (u, *)
write (u, '(A)') "\textwidth 18.5cm"
write (u, '(A)') "\evensidemargin -1.5cm"
write (u, '(A)') "\oddsidemargin -1.5cm"
write (u, *)
write (u, '(A)') "\newcommand{\blue}{\color{blue}}"
write (u, '(A)') "\newcommand{\green}{\color{green}}"
write (u, '(A)') "\newcommand{\red}{\color{red}}"
write (u, '(A)') "\newcommand{\magenta}{\color{magenta}}"
write (u, '(A)') "\newcommand{\cyan}{\color{cyan}}"
write (u, '(A)') "\newcommand{\sm}{\footnotesize}"
write (u, '(A)') "\setlength{\parindent}{0pt}"
write (u, '(A)') "\setlength{\parsep}{20pt}"
write (u, *)
write (u, '(A)') "\begin{document}"
write (u, '(A)') "\begin{fmffile}{ " // char (filename) // "}"
write (u, '(A)') "\fmfcmd{color magenta; magenta = red + blue;}"
write (u, '(A)') "\fmfcmd{color cyan; cyan = green + blue;}"
write (u, '(A)') "\begin{fmfshrink}{0.5}"
write (u, '(A)') "\begin{flushleft}"
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{\large\texttt{WHIZARD}} phase space channels}" // &
& "\hfill\today"
write (u, *)
write (u, '(A)') "\vspace{10pt}"
write (u, '(A)') "\noindent" // &
& "\textbf{Process:} \url{ " // char (process_id) // "}"
call feyngraph_set_write_process_tex_format (feyngraph_set, u)
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Note:} These are pseudo Feynman graphs that "
write (u, '(A)') "visualize phase-space parameterizations " // &
& "(‘integration channels’). "
write (u, '(A)') "They do \emph{not} indicate Feynman graphs used for the " // &
& "matrix element."
write (u, *)
write (u, '(A)') "\textbf{Color code:} " // &
& "{\blue resonance,} " // &
& "{\cyan t-channel,} " // &
& "{\green radiation,} "
write (u, '(A)') "{\red infrared,} " // &
& "{\magenta collinear,} " // &
& "external/off-shell"
write (u, *)

```



```

write (u, '(A)') "\noindent" // &
      & "\textbf{Black square:} Keystone, indicates ordering of " // &
      & "phase space parameters."
write (u, *)
write (u, '(A)') "\vspace{-20pt}"
count = 0
pgcount = 0
n_grove = 0
grove => feyngraph_set%grove_list%first
do while (associated (grove))
  n_grove = n_grove + 1
  write (u, *)
  write (u, '(A)') "\vspace{20pt}"
  write (u, '(A)') "\begin{tabular}{l}"
  write (u, '(A,I5,A)') &
    & "\fbox{\bf Grove \boldmath$, n_grove, "$} \\\[10pt]"
  write (u, '(A,I1,A)') "Multiplicity: ", &
    grove%grove_prop%multiplicity, "\\"
  write (u, '(A,I1,A)') "Resonances: ", &
    grove%grove_prop%n_resonances, "\\"
  write (u, '(A,I1,A)') "Log-enhanced: ", &
    grove%grove_prop%n_log_enhanced, "\\"
  write (u, '(A,I1,A)') "Off-shell: ", &
    grove%grove_prop%n_off_shell, "\\"
  write (u, '(A,I1,A)') "t-channel: ", &
    grove%grove_prop%n_t_channel, ""
  write (u, '(A)') "\end{tabular}"
  kingraph => grove%first
  do while (associated (kingraph))
    count = count + 1
    call kingraph_write_graph_format (kingraph, count, unit)
    kingraph => kingraph%grove_next
  end do
  grove => grove%next
end do
write (u, '(A)') "\end{flushleft}"
write (u, '(A)') "\end{fmfshrink}"
write (u, '(A)') "\end{fmffile}"
write (u, '(A)') "\end{document}"
end subroutine feyngraph_set_write_graph_format

```

Write the process as a L^AT_EX expression. This is a slightly modified copy of `cascade_set_write_process_tex_format` which has only been adapted to the types which are used here.

```

<Cascades2: procedures>+≡
subroutine feyngraph_set_write_process_tex_format (feyngraph_set, unit)
  type(feyngraph_set_t), intent(in), target :: feyngraph_set
  integer, intent(in), optional :: unit
  integer :: n_tot
  integer :: u, f, i
  n_tot = feyngraph_set%n_in + feyngraph_set%n_out
  u = given_output_unit (unit); if (u < 0) return
  if (.not. allocated (feyngraph_set%flv)) return

```

```

write (u, "(A)") "\begin{align*}"
do f = 1, size (feyngraph_set%flv, 2)
  do i = 1, feyngraph_set%n_in
    if (i > 1) write (u, "(A)", advance="no") "\quad "
    write (u, "(A)", advance="no") &
      char (feyngraph_set%flv(i,f)%get_tex_name ())
  end do
  write (u, "(A)", advance="no") "\quad &\to\quad "
  do i = feyngraph_set%n_in + 1, n_tot
    if (i > feyngraph_set%n_in + 1) write (u, "(A)", advance="no") "\quad "
    write (u, "(A)", advance="no") &
      char (feyngraph_set%flv(i,f)%get_tex_name ())
  end do
  if (f < size (feyngraph_set%flv, 2)) then
    write (u, "(A)") "\\ "
  else
    write (u, "(A)") ""
  end if
end do
write (u, "(A)") "\end{align*}"
end subroutine feyngraph_set_write_process_tex_format

```

This creates metapost source for graphical display for a given `kingraph`. It is the analogon to `cascade_write_graph_format` (a modified copy).

(*Cascades2: procedures*) \equiv

```

subroutine kingraph_write_graph_format (kingraph, count, unit)
  type(kingraph_t), intent(in) :: kingraph
  integer, intent(in) :: count
  integer, intent(in), optional :: unit
  integer :: u
  type(string_t) :: left_str, right_str
  u = given_output_unit (unit); if (u < 0) return
  left_str = ""
  right_str = ""
  write (u, '(A)') "\begin{minipage}{105pt}"
  write (u, '(A)') "\vspace{30pt}"
  write (u, '(A)') "\begin{center}"
  write (u, '(A)') "\begin{fmfgraph*}(55,55)"
  call graph_write_node (kingraph%root)
  write (u, '(A)') "\fmfleft{" // char (extract (left_str, 2)) // "}"
  write (u, '(A)') "\fmfright{" // char (extract (right_str, 2)) // "}"
  write (u, '(A)') "\end{fmfgraph*}\\ "
  write (u, '(A,I5,A)') "\fbox{$", count, "$}"
  write (u, '(A)') "\end{center}"
  write (u, '(A)') "\end{minipage}"
  write (u, '(A)') "%"
contains
  recursive subroutine graph_write_node (node)
    type(k_node_t), intent(in) :: node
    if (associated (node%daughter1) .or. associated (node%daughter2)) then
      if (node%daughter2%t_line .or. node%daughter2%incoming) then
        call vertex_write (node, node%daughter2)
      call vertex_write (node, node%daughter1)

```

```

        else
            call vertex_write (node, node%daughter1)
            call vertex_write (node, node%daughter2)
        end if
        if (node%mapping == EXTERNAL_PRT) then
            call line_write (node%bincode, 0, node%particle)
            call external_write (node%bincode, node%particle%tex_name, &
                left_str)
            write (u, '(A,I0,A)') "\fmfv{d.shape=square}{v0}"
        end if
    else
        if (node%incoming) then
            call external_write (node%bincode, node%particle%anti%tex_name, &
                left_str)
        else
            call external_write (node%bincode, node%particle%tex_name, &
                right_str)
        end if
    end if
end subroutine graph_write_node
recursive subroutine vertex_write (node, daughter)
    type(k_node_t), intent(in) :: node, daughter
    integer :: bincode
    if (associated (node%daughter1) .and. associated (node%daughter2) &
        .and. node%mapping == EXTERNAL_PRT) then
        bincode = 0
    else
        bincode = node%bincode
    end if
    call graph_write_node (daughter)
    if (associated (node%daughter1) .or. associated (node%daughter2)) then
        call line_write (bincode, daughter%bincode, daughter%particle, &
            mapping=daughter%mapping)
    else
        call line_write (bincode, daughter%bincode, daughter%particle)
    end if
end subroutine vertex_write
subroutine line_write (i1, i2, particle, mapping)
    integer(TC), intent(in) :: i1, i2
    type(part_prop_t), intent(in) :: particle
    integer, intent(in), optional :: mapping
    integer :: k1, k2
    type(string_t) :: prt_type
    select case (particle%spin_type)
    case (SCALAR);      prt_type = "plain"
    case (SPINOR);      prt_type = "fermion"
    case (VECTOR);      prt_type = "boson"
    case (VECTORSPINOR); prt_type = "fermion"
    case (TENSOR);      prt_type = "dbl_wiggly"
    case default;       prt_type = "dashes"
    end select
    if (particle%pdg < 0) then
!!! anti-particle
        k1 = i2; k2 = i1
    end if
end subroutine line_write

```

```

else
    k1 = i1; k2 = i2
end if
if (present (mapping)) then
    select case (mapping)
    case (S_CHANNEL)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=blue,lab=\sm\blue$" // &
            & char (particle%tex_name) // "$}" // &
            & "{v", k1, ",v", k2, "}"
    case (T_CHANNEL, U_CHANNEL)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=cyan,lab=\sm\cyan$" // &
            & char (particle%tex_name) // "$}" // &
            & "{v", k1, ",v", k2, "}"
    case (RADIATION)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=green,lab=\sm\green$" // &
            & char (particle%tex_name) // "$}" // &
            & "{v", k1, ",v", k2, "}"
    case (COLLINEAR)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=magenta,lab=\sm\magenta$" // &
            & char (particle%tex_name) // "$}" // &
            & "{v", k1, ",v", k2, "}"
    case (INFRARED)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=red,lab=\sm\red$" // &
            & char (particle%tex_name) // "$}" // &
            & "{v", k1, ",v", k2, "}"
    case default
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
            & ",f=black}" // &
            & "{v", k1, ",v", k2, "}"
    end select
else
    write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & "}" // &
        & "{v", k1, ",v", k2, "}"
end if
end subroutine line_write
subroutine external_write (bincode, name, ext_str)
    integer(TC), intent(in) :: bincode
    type(string_t), intent(in) :: name
    type(string_t), intent(inout) :: ext_str
    character(len=20) :: str
    write (str, '(A2,I0)') ",v", bincode
    ext_str = ext_str // trim (str)
    write (u, '(A,I0,A,I0,A)') "\fmflabel{\sm$" &
        // char (name) &
        // "\",(" , bincode, ")" &
        // "$}{v", bincode, "}"
end subroutine external_write
end subroutine kingraph_write_graph_format

```

Generate a `feyngraph_set` for several subprocesses. Mapping calculations are performed separately, but the final grove list is shared between the subsets `fset` of the `feyngraph_set`.

<Cascades2: public>+≡

`public :: feyngraph_set_generate`

<Cascades2: sub interfaces>+≡

```
module subroutine feyngraph_set_generate &
  (feyngraph_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay, &
   u_in, vis_channels, use_dag)
  type(feyngraph_set_t), intent(out) :: feyngraph_set
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_in, n_out
  type(flavor_t), dimension(:, :), intent(in) :: flv
  type(phs_parameters_t), intent(in) :: phs_par
  logical, intent(in) :: fatal_beam_decay
  integer, intent(in) :: u_in
  logical, intent(in) :: vis_channels
  logical, optional, intent(in) :: use_dag
end subroutine feyngraph_set_generate
```

<Cascades2: procedures>+≡

```
module subroutine feyngraph_set_generate &
  (feyngraph_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay, &
   u_in, vis_channels, use_dag)
  type(feyngraph_set_t), intent(out) :: feyngraph_set
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_in, n_out
  type(flavor_t), dimension(:, :), intent(in) :: flv
  type(phs_parameters_t), intent(in) :: phs_par
  logical, intent(in) :: fatal_beam_decay
  integer, intent(in) :: u_in
  logical, intent(in) :: vis_channels
  logical, optional, intent(in) :: use_dag
  type(grove_t), pointer :: grove
  integer :: i, j
  type(kingraph_t), pointer :: kingraph
  if (phase_space_vanishes (phs_par%sqrts, n_in, flv)) return
  if (present (use_dag)) feyngraph_set%use_dag = use_dag
  feyngraph_set%process_type = n_in
  feyngraph_set%n_in = n_in
  feyngraph_set%n_out = n_out
  allocate (feyngraph_set%flv (size (flv, 1), size (flv, 2)))
  do i = 1, size (flv, 2)
    do j = 1, size (flv, 1)
      call feyngraph_set%flv(j,i)%init (flv(j,i)%get_pdg (), model)
    end do
  end do
  allocate (feyngraph_set%particle (PRT_ARRAY_SIZE))
  allocate (feyngraph_set%grove_list)
  allocate (feyngraph_set%fset (size (flv, 2)))
  do i = 1, size (feyngraph_set%fset)
    feyngraph_set%fset(i)%use_dag = feyngraph_set%use_dag
    allocate (feyngraph_set%fset(i)%flv(size (flv,1),1))
```

```

    feyngraph_set%fset(i)%flv(:,1) = flv(:,i)
    feyngraph_set%fset(i)%particle => feyngraph_set%particle
    allocate (feyngraph_set%fset(i)%grove_list)
    call feyngraph_set%generate_single (feyngraph_set%fset(i), &
        model, n_in, n_out, phs_par, fatal_beam_decay, u_in)
    call feyngraph_set%grove_list%merge &
        (feyngraph_set%fset(i)%grove_list, model, i)
    if (.not. vis_channels) call feyngraph_set%fset(i)%final()
end do
call feyngraph_set%grove_list%rebuild ()
end subroutine feyngraph_set%generate

```

Check whether the `grove_list` of the `feyngraph_set` contains any `kingraphs` which are valid, i.e. where the `keep` variable has the value `.true.`. This is necessary to write a non-empty phase-space file. The function is the pendant to `cascade_set_is_valid`.

```

<Cascades2: public>+≡
    public :: feyngraph_set_is_valid

<Cascades2: sub interfaces>+≡
    module function feyngraph_set_is_valid (feyngraph_set) result (flag)
        class(feyngraph_set_t), intent(in) :: feyngraph_set
        logical :: flag
    end function feyngraph_set_is_valid

<Cascades2: procedures>+≡
    module function feyngraph_set_is_valid (feyngraph_set) result (flag)
        class(feyngraph_set_t), intent(in) :: feyngraph_set
        type(kingraph_t), pointer :: kingraph
        type(grove_t), pointer :: grove
        logical :: flag
        flag = .false.
        if (associated (feyngraph_set%grove_list)) then
            grove => feyngraph_set%grove_list%first
            do while (associated (grove))
                kingraph => grove%first
                do while (associated (kingraph))
                    if (kingraph%keep) then
                        flag = .true.
                        return
                    end if
                    kingraph => kingraph%next
                end do
                grove => grove%next
            end do
        end if
    end function feyngraph_set_is_valid

```

19.11.19 Return the resonance histories for subtraction

The following procedures are copies of corresponding procedures in `cascades`, which only have been adapted to the new types used in this module.

Extract the resonance set from a valid kingraph which is kept in the final grove list.

```

<Cascades2: kingraph: TBP>+≡
    procedure :: extract_resonance_history => kingraph_extract_resonance_history

<Cascades2: sub interfaces>+≡
    module subroutine kingraph_extract_resonance_history &
        (kingraph, res_hist, model, n_out)
        class(kingraph_t), intent(in), target :: kingraph
        type(resonance_history_t), intent(out) :: res_hist
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_out
    end subroutine kingraph_extract_resonance_history

<Cascades2: procedures>+≡
    module subroutine kingraph_extract_resonance_history &
        (kingraph, res_hist, model, n_out)
        class(kingraph_t), intent(in), target :: kingraph
        type(resonance_history_t), intent(out) :: res_hist
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_out
        type(resonance_info_t) :: resonance
        integer :: i, mom_id, pdg
        if (debug_on) call msg_debug2 &
            (D_PHASESPACE, "kingraph_extract_resonance_history")
        if (kingraph%grove_prop%n_resonances > 0) then
            if (associated (kingraph%root%daughter1) .or. &
                associated (kingraph%root%daughter2)) then
                if (debug_on) call msg_debug2 &
                    (D_PHASESPACE, "kingraph has resonances, root has children")
                do i = 1, kingraph%tree%n_entries
                    if (kingraph%tree%mapping(i) == S_CHANNEL) then
                        mom_id = kingraph%tree%bc (i)
                        pdg = kingraph%tree%pdg (i)
                        call resonance%init (mom_id, pdg, model, n_out)
                        if (debug2_active (D_PHASESPACE)) then
                            print *, 'D: Adding resonance'
                            call resonance%write ()
                        end if
                        call res_hist%add_resonance (resonance)
                    end if
                end do
            end if
        end if
    end subroutine kingraph_extract_resonance_history

```

Determine the number of valid kingraphs in grove_list.

```

<Cascades2: public>+≡
    public :: grove_list_get_n_trees

<Cascades2: sub interfaces>+≡
    module function grove_list_get_n_trees (grove_list) result (n)
        class(grove_list_t), intent(in) :: grove_list
        integer :: n
    end function grove_list_get_n_trees

```

```

<Cascades2: procedures>+≡
module function grove_list_get_n_trees (grove_list) result (n)
  class(grove_list_t), intent(in) :: grove_list
  integer :: n
  type(kingraph_t), pointer :: kingraph
  type(grove_t), pointer :: grove
  if (debug_on) call msg_debug (D_PHASESPACE, "grove_list_get_n_trees")
  n = 0
  grove => grove_list%first
  do while (associated (grove))
    kingraph => grove%first
    do while (associated (kingraph))
      if (kingraph%keep) n = n + 1
      kingraph => kingraph%grove_next
    end do
    grove => grove%next
  end do
  if (debug_on) call msg_debug (D_PHASESPACE, "n", n)
end function grove_list_get_n_trees

```

Extract the resonance histories from the feyngraph_set, in complete analogy to cascade_set_get_resonance_histories

```

<Cascades2: public>+≡
public :: feyngraph_set_get_resonance_histories

<Cascades2: sub interfaces>+≡
module subroutine feyngraph_set_get_resonance_histories &
  (feyngraph_set, n_filter, res_hists)
  type(feyngraph_set_t), intent(in), target :: feyngraph_set
  integer, intent(in), optional :: n_filter
  type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
    res_hists
end subroutine feyngraph_set_get_resonance_histories

<Cascades2: procedures>+≡
module subroutine feyngraph_set_get_resonance_histories &
  (feyngraph_set, n_filter, res_hists)
  type(feyngraph_set_t), intent(in), target :: feyngraph_set
  integer, intent(in), optional :: n_filter
  type(resonance_history_t), dimension(:), allocatable, intent(out) :: &
    res_hists
  type(kingraph_t), pointer :: kingraph
  type(grove_t), pointer :: grove
  type(resonance_history_t) :: res_hist
  type(resonance_history_set_t) :: res_hist_set
  integer :: i_grove
  if (debug_on) call msg_debug &
    (D_PHASESPACE, "grove_list_get_resonance_histories")
  call res_hist_set%init (n_filter = n_filter)
  grove => feyngraph_set%grove_list%first
  i_grove = 0
  do while (associated (grove))
    i_grove = i_grove + 1
    kingraph => grove%first
    do while (associated (kingraph))

```



```

        if (kingraph%keep) then
            if (debug_on) call msg_debug2 (D_PHASESPACE, "grove", i_grove)
            call kingraph%extract_resonance_history &
                (res_hist, feyngraph_set%model, feyngraph_set%n_out)
            call res_hist_set%enter (res_hist)
        end if
        kingraph => kingraph%grove_next
    end do
end do
call res_hist_set%freeze ()
call res_hist_set%to_array (res_hists)
end subroutine feyngraph_set_get_resonance_histories

<cascades2_ut.f90>≡
<File header>

module cascades2_ut
    use unit_tests
    use cascades2_uti

<Standard module head>

<Cascades2: public test>

contains

<Cascades2: test driver>

end module cascades2_ut

<cascades2_uti.f90>≡
<File header>

module cascades2_uti

<Use kinds>
<Use strings>
    use numeric_utils

    use cascades2
    use flavors
    use phs_forests, only: phs_parameters_t
    use model_data

<Standard module head>

<Cascades2: test declarations>

contains

<Cascades2: tests>

end module cascades2_uti

```

API: driver for the unit tests below.

```

<Cascades2: public test>≡
  public :: cascades2_test

<Cascades2: test driver>≡
  subroutine cascades2_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Cascades2: execute tests>
  end subroutine cascades2_test

<Cascades2: execute tests>≡
  call test (cascades2_1, "cascades2_1", &
    "make phase-space", u, results)
  call test (cascades2_2, "cascades2_2", &
    "make phase-space (scattering)", u, results)

<Cascades2: test declarations>≡
  public :: cascades2_1

<Cascades2: tests>≡
  subroutine cascades2_1 (u)
    integer, intent(in) :: u
    type(feyngraph_set_t) :: feyngraph_set
    type(model_data_t) :: model
    integer :: n_in = 1
    integer :: n_out = 6
    type(flavor_t), dimension(7,1) :: flv
    type(phs_parameters_t) :: phs_par
    logical :: fatal_beam_decay = .true.
    integer :: u_in = 8

    write (u, "(A)")  "* Test output: cascades2_1"
    write (u, "(A)")  "* Purpose: create a test phs file (decay) with the forest"
    write (u, "(A)")  "* output of 0'Mega"
    write (u, "(A)")

    write (u, "(A)")  "* Initializing"
    write (u, "(A)")

    call init_sm_full_test (model)

    call flv(1,1)%init (6, model)
    call flv(2,1)%init (5, model)
    call flv(3,1)%init (-11, model)
    call flv(4,1)%init (12, model)
    call flv(5,1)%init (21, model)
    call flv(6,1)%init (22, model)
    call flv(7,1)%init (21, model)

    phs_par%sqrts = 173.1_default
    phs_par%m_threshold_s = 50._default
    phs_par%m_threshold_t = 100._default
    phs_par%keep_nonresonant = .true.
    phs_par%off_shell = 2

```

```

open (unit=u_in, file="cascades2_1.fds", status='old', action='read')

write (u, "(A)")
write (u, "(A)")  "* Generating phase-space parametrizations"
write (u, "(A)")

call feyngraph_set_generate (feyngraph_set, model, n_in, n_out, &
    flv, phs_par, fatal_beam_decay, u_in, use_dag = .false., &
    vis_channels = .false.)
call feyngraph_set_write_process_bincode_format (feyngraph_set, u)
call feyngraph_set_write_file_format (feyngraph_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

close (u_in)
call feyngraph_set%final ()
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades2_1"
end subroutine cascades2_1

```

<Cascades2: test declarations>+≡

```
public :: cascades2_2
```

<Cascades2: tests>+≡

```

subroutine cascades2_2 (u)
    integer, intent(in) :: u
    type(feyngraph_set_t) :: feyngraph_set
    type(model_data_t) :: model
    integer :: n_in = 2
    integer :: n_out = 5
    type(flavor_t), dimension(7,1) :: flv
    type(phs_parameters_t) :: phs_par
    logical :: fatal_beam_decay = .true.
    integer :: u_in = 8

    write (u, "(A)")  "* Test output: cascades2_2"
    write (u, "(A)")  "* Purpose: create a test phs file (scattering) with the"
    write (u, "(A)")  "* parsable DAG output of 0'Mega"
    write (u, "(A)")

    write (u, "(A)")  "* Initializing"
    write (u, "(A)")

    call init_sm_full_test (model)

    call flv(1,1)%init (-11, model)
    call flv(2,1)%init (11, model)
    call flv(3,1)%init (-11, model)
    call flv(4,1)%init (12, model)
    call flv(5,1)%init (1, model)

```

```

call flv(6,1)%init (-2, model)
call flv(7,1)%init (22, model)

phs_par%sqrts = 500._default
phs_par%m_threshold_s = 50._default
phs_par%m_threshold_t = 100._default
phs_par%keep_nonresonant = .true.
phs_par%off_shell = 2
phs_par%t_channel = 6

open (unit=u_in, file="cascades2_2.fds", &
      status='old', action='read')

write (u, "(A)")
write (u, "(A)")  "* Generating phase-space parametrizations"
write (u, "(A)")

call feyngraph_set_generate (feyngraph_set, model, n_in, n_out, &
                             flv, phs_par, fatal_beam_decay, u_in, use_dag = .true., &
                             vis_channels = .false.)
call feyngraph_set_write_process_bincode_format (feyngraph_set, u)
call feyngraph_set_write_file_format (feyngraph_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

close (u_in)
call feyngraph_set%final ()
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades2_2"
end subroutine cascades2_2

```

19.12 WOOD phase space

This is the module that interfaces the `phs_forests` phase-space treatment and the `cascades` module for generating phase-space channels. As an extension of the `phs_base` abstract type, the phase-space configuration and instance implement the standard API.

(Currently, this is the only generic phase-space implementation of WHIZARD. For trivial two-particle phase space, there is `phs_wood` as an alternative.)

`<phs_wood.f90>` \equiv
<File header>

```
module phs_wood
```

```
<Use kinds>
```

```
<Use strings>
```

```
use os_interface
```

```
use lorentz
```

```

        use model_data
        use flavors
        use phs_base
        use mappings
        use resonances, only: resonance_history_set_t
        use phs_forests
        use cascades
        use cascades2

        <Standard module head>

        <PHS wood: public>

        <PHS wood: types>

        interface
        <PHS wood: sub interfaces>
        end interface

contains

        <PHS wood: main procedures>

    end module phs_wood
<phs_wood_sub.f90>≡
<File header>

    submodule (phs_wood) phs_wood_s

        use io_units
        use constants
        use numeric_utils
        use diagnostics
        use physics_defs
        use md5
        use process_constants
        use sf_mappings
        use sf_base

        implicit none

contains

        <PHS wood: procedures>

    end submodule phs_wood_s

```

19.12.1 Configuration

```

<PHS wood: public>≡
    public :: phs_wood_config_t

```

```

<PHS wood: types>≡
  type, extends (phs_config_t) :: phs_wood_config_t
    character(32) :: md5sum_forest = ""
    type(string_t) :: phs_path
    integer :: io_unit = 0
    logical :: io_unit_keep_open = .false.
    logical :: use_equivalences = .false.
    logical :: fatal_beam_decay = .true.
    type(mapping_defaults_t) :: mapping_defaults
    type(phs_parameters_t) :: par
    type(string_t) :: run_id
    type(cascade_set_t), allocatable :: cascade_set
    logical :: use_cascades2 = .false.
    type(feyngraph_set_t), allocatable :: feyngraph_set
    type(phs_forest_t) :: forest
    type(os_data_t) :: os_data
    logical :: is_combined_integration = .false.
  contains
    <PHS wood: phs wood config: TBP>
  end type phs_wood_config_t

```

Finalizer. We should delete the cascade set and the forest subobject.

Also close the I/O unit, just in case. (We assume that `io_unit` is not standard input/output.)

```

<PHS wood: phs wood config: TBP>≡
  procedure :: final => phs_wood_config_final

<PHS wood: sub interfaces>≡
  module subroutine phs_wood_config_final (object)
    class(phs_wood_config_t), intent(inout) :: object
  end subroutine phs_wood_config_final

<PHS wood: procedures>≡
  module subroutine phs_wood_config_final (object)
    class(phs_wood_config_t), intent(inout) :: object
    logical :: opened
    if (object%io_unit /= 0) then
      inquire (unit = object%io_unit, opened = opened)
      if (opened) close (object%io_unit)
    end if
    call object%clear_phase_space ()
    call object%forest%final ()
  end subroutine phs_wood_config_final

<PHS wood: phs wood config: TBP>+≡
  procedure :: increase_n_par => phs_wood_config_increase_n_par

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_increase_n_par (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
  end subroutine phs_wood_config_increase_n_par

<PHS wood: procedures>+≡
  module subroutine phs_wood_config_increase_n_par (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config

```

```

        if (phs_config%is_combined_integration) then
            phs_config%n_par = phs_config%n_par + 3
        end if
    end subroutine phs_wood_config_increase_n_par

```

Output. The contents of the PHS forest are not printed explicitly.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: write => phs_wood_config_write

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_write (object, unit, include_id)
        class(phs_wood_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
    end subroutine phs_wood_config_write

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_write (object, unit, include_id)
        class(phs_wood_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") &
            "Partonic phase-space configuration (phase-space forest):"
        call object%base_write (unit)
        write (u, "(1x,A)") "Phase-space configuration parameters:"
        call object%par%write (u)
        call object%mapping_defaults%write (u)
        write (u, "(3x,A,A,A)") "Run ID: ", char (object%run_id), ""
    end subroutine phs_wood_config_write

```

Print the PHS forest contents.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: write_forest => phs_wood_config_write_forest

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_write_forest (object, unit)
        class(phs_wood_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine phs_wood_config_write_forest

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_write_forest (object, unit)
        class(phs_wood_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call object%forest%write (u)
    end subroutine phs_wood_config_write_forest

```

Set the phase-space parameters that the configuration generator requests.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: set_parameters => phs_wood_config_set_parameters

```

```

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_set_parameters (phs_config, par)
    class(phs_wood_config_t), intent(inout) :: phs_config
    type(phs_parameters_t), intent(in) :: par
  end subroutine phs_wood_config_set_parameters

```

```

<PHS wood: procedures>+≡
  module subroutine phs_wood_config_set_parameters (phs_config, par)
    class(phs_wood_config_t), intent(inout) :: phs_config
    type(phs_parameters_t), intent(in) :: par
    phs_config%par = par
  end subroutine phs_wood_config_set_parameters

```

Enable the generation of channel equivalences (when calling configure).

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: enable_equivalences => phs_wood_config_enable_equivalences

```

```

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_enable_equivalences (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
  end subroutine phs_wood_config_enable_equivalences

```

```

<PHS wood: procedures>+≡
  module subroutine phs_wood_config_enable_equivalences (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    phs_config%use_equivalences = .true.
  end subroutine phs_wood_config_enable_equivalences

```

Set the phase-space mapping parameters that the configuration generator requests.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: set_mapping_defaults => phs_wood_config_set_mapping_defaults

```

```

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_set_mapping_defaults &
    (phs_config, mapping_defaults)
    class(phs_wood_config_t), intent(inout) :: phs_config
    type(mapping_defaults_t), intent(in) :: mapping_defaults
  end subroutine phs_wood_config_set_mapping_defaults

```

```

<PHS wood: procedures>+≡
  module subroutine phs_wood_config_set_mapping_defaults &
    (phs_config, mapping_defaults)
    class(phs_wood_config_t), intent(inout) :: phs_config
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    phs_config%mapping_defaults = mapping_defaults
  end subroutine phs_wood_config_set_mapping_defaults

```

Define the input stream for the phase-space file as an open logical unit. The unit must be connected.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: set_input => phs_wood_config_set_input

```



```

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_set_input (phs_config, unit)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer, intent(in) :: unit
    end subroutine phs_wood_config_set_input

```

```

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_set_input (phs_config, unit)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer, intent(in) :: unit
        phs_config%io_unit = unit
        rewind (unit)
    end subroutine phs_wood_config_set_input

```

19.12.2 Phase-space generation

This subroutine generates a phase space configuration using the `cascades` module. Note that this may take time, and the `cascade_set` subobject may consume a large amount of memory.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: generate_phase_space => phs_wood_config_generate_phase_space

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_generate_phase_space (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
    end subroutine phs_wood_config_generate_phase_space

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_generate_phase_space (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer :: off_shell, extra_off_shell
        logical :: valid
        integer :: unit_fds
        type(string_t) :: file_name
        logical :: file_exists
        call msg_message ("Phase space: generating configuration ...")
        off_shell = phs_config%par%off_shell
        if (phs_config%use_cascades2) then
            file_name = char (phs_config%id) // ".fds"
            inquire (file=char (file_name), exist=file_exists)
            if (.not. file_exists) call msg_fatal &
                ("The 0'Mega input file " // char (file_name) // &
                 " does not exist. " // "Please make sure that the " // &
                 "variable ?omega_write_phs_output has been set correctly.")
            unit_fds = free_unit ()
            open (unit=unit_fds, file=char(file_name), status='old', action='read')
            do extra_off_shell = 0, max (phs_config%n_tot - 3, 0)
                phs_config%par%off_shell = off_shell + extra_off_shell
                allocate (phs_config%feyngraph_set)
                call feyngraph_set_generate (phs_config%feyngraph_set, &
                    phs_config%model, phs_config%n_in, phs_config%n_out, &
                    phs_config%flv, &
                    phs_config%par, phs_config%fatal_beam_decay, unit_fds, &
                    phs_config%vis_channels)
            end do
        end if
    end subroutine phs_wood_config_generate_phase_space

```

```

        if (feyngraph_set_is_valid (phs_config%feyngraph_set)) then
            exit
        else
            call msg_message ("Phase space: ... failed. &
                &Increasing phs_off_shell ...")
            call phs_config%feyngraph_set%final ()
            deallocate (phs_config%feyngraph_set)
        end if
    end do
    close (unit_fds)
else
    allocate (phs_config%cascade_set)
    do extra_off_shell = 0, max (phs_config%n_tot - 3, 0)
        phs_config%par%off_shell = off_shell + extra_off_shell
        call cascade_set_generate (phs_config%cascade_set, &
            phs_config%model, phs_config%n_in, phs_config%n_out, &
            phs_config%flv, &
            phs_config%par, phs_config%fatal_beam_decay)
        if (cascade_set_is_valid (phs_config%cascade_set)) then
            exit
        else
            call msg_message ("Phase space: ... failed. &
                &Increasing phs_off_shell ...")
        end if
    end do
end if
if (phs_config%use_cascades2) then
    valid = feyngraph_set_is_valid (phs_config%feyngraph_set)
else
    valid = cascade_set_is_valid (phs_config%cascade_set)
end if
if (valid) then
    call msg_message ("Phase space: ... success.")
else
    call msg_fatal ("Phase-space: generation failed")
end if
end subroutine phs_wood_config_generate_phase_space

```

Using the generated phase-space configuration, write an appropriate phase-space file to the stored (or explicitly specified) I/O unit.

(PHS wood: phs wood config: TBP)+≡

```

    procedure :: write_phase_space => phs_wood_config_write_phase_space

```

(PHS wood: sub interfaces)+≡

```

    module subroutine phs_wood_config_write_phase_space (phs_config, &
        filename_vis, unit)
        class(phs_wood_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        type(string_t), intent(in), optional :: filename_vis
    end subroutine phs_wood_config_write_phase_space

```

(PHS wood: procedures)+≡

```

    module subroutine phs_wood_config_write_phase_space (phs_config, &
        filename_vis, unit)
        class(phs_wood_config_t), intent(in) :: phs_config

```

```

integer, intent(in), optional :: unit
type(string_t), intent(in), optional :: filename_vis
type(string_t) :: setenv_tex, setenv_mp, pipe, pipe_dvi
integer :: u, unit_tex, unit_dev, status
if (allocated (phs_config%cascade_set) .or. &
    allocated (phs_config%feyngraph_set)) then
    if (present (unit)) then
        u = unit
    else
        u = phs_config%io_unit
    end if
    write (u, "(1x,A,A)") "process ", char (phs_config%id)
    write (u, "(A)")
    if (phs_config%use_cascades2) then
        call feyngraph_set_write_process_bincode_format (phs_config%feyngraph_set, u)
    else
        call cascade_set_write_process_bincode_format (phs_config%cascade_set, u)
    end if
    write (u, "(A)")
    write (u, "(3x,A,A,A32,A)") "md5sum_process = ", &
        '', phs_config%md5sum_process, ''
    write (u, "(3x,A,A,A32,A)") "md5sum_model_par = ", &
        '', phs_config%md5sum_model_par, ''
    write (u, "(3x,A,A,A32,A)") "md5sum_phs_config = ", &
        '', phs_config%md5sum_phs_config, ''
    call phs_config%par%write (u)
    if (phs_config%use_cascades2) then
        call feyngraph_set_write_file_format (phs_config%feyngraph_set, u)
    else
        call cascade_set_write_file_format (phs_config%cascade_set, u)
    end if
    if (phs_config%vis_channels) then
        unit_tex = free_unit ()
        open (unit=unit_tex, file=char(filename_vis // ".tex"), &
            action="write", status="replace")
        if (phs_config%use_cascades2) then
            call feyngraph_set_write_graph_format (phs_config%feyngraph_set, &
                filename_vis // "-graphs", phs_config%id, unit_tex)
        else
            call cascade_set_write_graph_format (phs_config%cascade_set, &
                filename_vis // "-graphs", phs_config%id, unit_tex)
        end if
        close (unit_tex)
        call msg_message ("Phase space: visualizing channels in file " &
            // char(trim(filename_vis)) // "...")
        if (phs_config%os_data%event_analysis_ps) then
            BLOCK: do
                unit_dev = free_unit ()
                open (file = "/dev/null", unit = unit_dev, &
                    action = "write", iostat = status)
                if (status /= 0) then
                    pipe = ""
                    pipe_dvi = ""
                else

```

```

        pipe = " > /dev/null"
        pipe_dvi = " 2>/dev/null 1>/dev/null"
    end if
    close (unit_dev)
    if (phs_config%os_data%whizard_texpath /= "") then
        setenv_tex = "TEXINPUTS=" // &
            phs_config%os_data%whizard_texpath // " :$TEXINPUTS "
        setenv_mp = "MPINPUTS=" // &
            phs_config%os_data%whizard_texpath // " :$MPINPUTS "
    else
        setenv_tex = ""
        setenv_mp = ""
    end if
    call os_system_call (setenv_tex // &
        phs_config%os_data%latex // " " // &
        filename_vis // ".tex " // pipe, status)
    if (status /= 0) exit BLOCK
    if (phs_config%os_data%mpost /= "") then
        call os_system_call (setenv_mp // &
            phs_config%os_data%mpost // " " // &
            filename_vis // "-graphs.mp" // pipe, status)
    else
        call msg_fatal ("Could not use MetaPOST.")
    end if
    if (status /= 0) exit BLOCK
    call os_system_call (setenv_tex // &
        phs_config%os_data%latex // " " // &
        filename_vis // ".tex" // pipe, status)
    if (status /= 0) exit BLOCK
    call os_system_call &
        (phs_config%os_data%dvips // " -o " // filename_vis &
        // ".ps " // filename_vis // ".dvi" // pipe_dvi, status)
    if (status /= 0) exit BLOCK
    if (phs_config%os_data%event_analysis_pdf) then
        call os_system_call (phs_config%os_data%ps2pdf // " " // &
            filename_vis // ".ps", status)
        if (status /= 0) exit BLOCK
    end if
    exit BLOCK
end do BLOCK
if (status /= 0) then
    call msg_error ("Unable to compile analysis output file")
end if
end if
end if
else
    call msg_fatal ("Phase-space configuration: &
        &no phase space object generated")
end if
end subroutine phs_wood_config_write_phase_space

```

Clear the phase-space configuration. This is useful since the object may become *really* large.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: clear_phase_space => phs_wood_config_clear_phase_space
<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_clear_phase_space (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    end subroutine phs_wood_config_clear_phase_space
<PHS wood: procedures>+≡
  module subroutine phs_wood_config_clear_phase_space (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    if (allocated (phs_config%cascade_set)) then
      call cascade_set_final (phs_config%cascade_set)
      deallocate (phs_config%cascade_set)
    end if
    if (allocated (phs_config%feyngraph_set)) then
      call phs_config%feyngraph_set%final ()
      deallocate (phs_config%feyngraph_set)
    end if
  end subroutine phs_wood_config_clear_phase_space

```

Extract the set of resonance histories

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: extract_resonance_history_set &
    => phs_wood_config_extract_resonance_history_set
<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_config_extract_resonance_history_set &
    (phs_config, res_set, include_trivial)
    class(phs_wood_config_t), intent(in) :: phs_config
    type(resonance_history_set_t), intent(out) :: res_set
    logical, intent(in), optional :: include_trivial
    end subroutine phs_wood_config_extract_resonance_history_set
<PHS wood: procedures>+≡
  module subroutine phs_wood_config_extract_resonance_history_set &
    (phs_config, res_set, include_trivial)
    class(phs_wood_config_t), intent(in) :: phs_config
    type(resonance_history_set_t), intent(out) :: res_set
    logical, intent(in), optional :: include_trivial
    call phs_config%forest%extract_resonance_history_set &
      (res_set, include_trivial)
  end subroutine phs_wood_config_extract_resonance_history_set

```

19.12.3 Phase-space configuration

We read the phase-space configuration from the stored I/O unit. If this is not set, we assume that we have to generate a phase space configuration. When done, we open a scratch file and write the configuration.

If `rebuild` is set, we should trash any existing phase space file and build a new one. Otherwise, we try to use an old one, which we check for existence and integrity. If `ignore_mismatch` is set, we reuse an existing file even if it does not match the current setup.

```

<PHS wood: phs wood config: TBP>+≡

```

```

procedure :: configure => phs_wood_config_configure
<PHS wood: sub interfaces>+=
  module subroutine phs_wood_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
  end subroutine phs_wood_config_configure
<PHS wood: procedures>+=
  module subroutine phs_wood_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
    type(string_t) :: filename, filename_vis
    logical :: variable_limits
    logical :: ok, exist, found, check, match, rebuild_phs
    integer :: g, c0, c1, n
    if (present (nlo_type)) then
      phs_config%nlo_type = nlo_type
    else
      phs_config%nlo_type = BORN
    end if
    phs_config%sqrts = sqrts
    phs_config%par%sqrts = sqrts
    if (present (sqrts_fixed)) &
      phs_config%sqrts_fixed = sqrts_fixed
    if (present (lab_is_cm)) &
      phs_config%lab_is_cm = lab_is_cm
    if (present (azimuthal_dependence)) &
      phs_config%azimuthal_dependence = azimuthal_dependence
    if (present (rebuild)) then
      rebuild_phs = rebuild
    else
      rebuild_phs = .true.
    end if
    if (present (ignore_mismatch)) then
      check = .not. ignore_mismatch
      if (ignore_mismatch) &

```

```

        call msg_warning ("Reading phs file: MD5 sum check disabled")
else
    check = .true.
end if
phs_config%md5sum_forest = ""
call phs_config%compute_md5sum (include_id = .false.)
if (phs_config%io_unit == 0) then
    filename = phs_config%make_phs_filename (subdir)
    filename_vis = phs_config%make_phs_filename (subdir) // "-vis"
    if (.not. rebuild_phs) then
        if (check) then
            call phs_config%read_phs_file (exist, found, match, subdir=subdir)
            rebuild_phs = .not. (exist .and. found .and. match)
        else
            call phs_config%read_phs_file (exist, found, subdir=subdir)
            rebuild_phs = .not. (exist .and. found)
        end if
    end if
    if (.not. mpi_is_comm_master ()) then
        rebuild_phs = .false.
        call msg_message ("MPI: Workers do not build phase space configuration.")
    end if
    if (rebuild_phs) then
        call phs_config%generate_phase_space ()
        phs_config%io_unit = free_unit ()
        if (phs_config%id /= "") then
            call msg_message ("Phase space: writing configuration file '" &
                // char (filename) // "'")
            open (phs_config%io_unit, file = char (filename), &
                status = "replace", action = "readwrite")
        else
            open (phs_config%io_unit, status = "scratch", action = "readwrite")
        end if
        call phs_config%write_phase_space (filename_vis)
        rewind (phs_config%io_unit)
    else
        call msg_message ("Phase space: keeping configuration file '" &
            // char (filename) // "'")
    end if
end if
if (phs_config%io_unit == 0) then
    ok = .true.
else
    call phs_config%forest%read (phs_config%io_unit, phs_config%id, &
        phs_config%n_in, phs_config%n_out, phs_config%model, ok)
    if (.not. phs_config%io_unit_keep_open) then
        close (phs_config%io_unit)
        phs_config%io_unit = 0
    end if
end if
if (ok) then
    call phs_config%forest%set_flavors (phs_config%flv(:,1))
    variable_limits = .not. phs_config%lab_is_cm
    call phs_config%forest%set_parameters (phs_config%mapping_defaults, &

```

```

        variable_limits)
    call phs_config%forest%setup_prt_combinations ()
    phs_config%n_channel = phs_config%forest%get_n_channels ()
    phs_config%n_par = phs_config%forest%get_n_parameters ()
    allocate (phs_config%channel (phs_config%n_channel))
    if (phs_config%use_equivalences) then
        call phs_config%forest%set_equivalences ()
        call phs_config%forest%get_equivalences (phs_config%channel, &
            phs_config%azimuthal_dependence)
        phs_config%provides_equivalences = .true.
    end if
    call phs_config%forest%set_s_mappings ()
    call phs_config%record_on_shell ()
    if (phs_config%mapping_defaults%enable_s_mapping) then
        call phs_config%record_s_mappings ()
    end if
    allocate (phs_config%chain (phs_config%n_channel), source = 0)
    do g = 1, phs_config%forest%get_n_groves ()
        call phs_config%forest%get_grove_bounds (g, c0, c1, n)
        phs_config%chain (c0:c1) = g
    end do
    phs_config%provides_chains = .true.
    call phs_config%compute_md5sum_forest ()
else
    write (msg_buffer, "(A,A,A)") &
        "Phase space: process '", &
        char (phs_config%id), "' not found in configuration file"
    call msg_fatal ()
end if
end subroutine phs_wood_config_configure

```

The MD5 sum of the forest is computed in addition to the MD5 sum of the configuration. The reason is that the forest may depend on a user-provided external file. On the other hand, this MD5 sum encodes all information that is relevant for further processing. Therefore, the `get_md5sum` method returns this result, once it is available.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: compute_md5sum_forest => phs_wood_config_compute_md5sum_forest

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_compute_md5sum_forest (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
    end subroutine phs_wood_config_compute_md5sum_forest

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_compute_md5sum_forest (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer :: u
        u = free_unit ()
        open (u, status = "scratch", action = "readwrite")
        call phs_config%write_forest (u)
        rewind (u)
        phs_config%md5sum_forest = md5sum (u)
        close (u)
    end subroutine

```



```
end subroutine phs_wood_config_compute_md5sum_forest
```

Create filenames according to standard conventions. The `id` is the process name including the suffix `_iX` where `X` stands for the component identifier (an integer). The `run_id` may be set or unset.

The convention for file names that include the run ID is to separate prefix, run ID, and any extensions by dots. We construct the file name by concatenating the individual elements accordingly. If there is no run ID, we nevertheless replace `_iX` by `.iX`.

```
<PHS wood: phs wood config: TBP>+≡
```

```
procedure :: make_phs_filename => phs_wood_make_phs_filename
```

```
<PHS wood: sub interfaces>+≡
```

```
module function phs_wood_make_phs_filename &
  (phs_config, subdir) result (filename)
  class(phs_wood_config_t), intent(in) :: phs_config
  type(string_t), intent(in), optional :: subdir
  type(string_t) :: filename
end function phs_wood_make_phs_filename
```

```
<PHS wood: procedures>+≡
```

```
module function phs_wood_make_phs_filename &
  (phs_config, subdir) result (filename)
  class(phs_wood_config_t), intent(in) :: phs_config
  type(string_t), intent(in), optional :: subdir
  type(string_t) :: filename
  type(string_t) :: basename, suffix, comp_code, comp_index
  basename = phs_config%id
  call split (basename, suffix, "_", back=.true.)
  comp_code = extract (suffix, 1, 1)
  comp_index = extract (suffix, 2)
  if (comp_code == "i" .and. verify (comp_index, "1234567890") == 0) then
    suffix = "." // comp_code // comp_index
  else
    basename = phs_config%id
    suffix = ""
  end if
  if (phs_config%run_id /= "") then
    filename = basename // "." // phs_config%run_id // suffix // ".phs"
  else
    filename = basename // suffix // ".phs"
  end if
  if (present (subdir)) then
    filename = subdir // "/" // filename
  end if
end function phs_wood_make_phs_filename
```

```
<PHS wood: phs wood config: TBP>+≡
```

```
procedure :: reshuffle_flavors => phs_wood_config_reshuffle_flavors
```

```
<PHS wood: sub interfaces>+≡
```

```
module subroutine phs_wood_config_reshuffle_flavors &
  (phs_config, reshuffle, flv_extra)
  class(phs_wood_config_t), intent(inout) :: phs_config
```

```

        integer, intent(in), dimension(:), allocatable :: reshuffle
        type(flavor_t), intent(in) :: flv_extra
    end subroutine phs_wood_config_reshuffle_flavors

<PHS wood: procedures>+≡
module subroutine phs_wood_config_reshuffle_flavors &
    (phs_config, reshuffle, flv_extra)
    class(phs_wood_config_t), intent(inout) :: phs_config
    integer, intent(in), dimension(:), allocatable :: reshuffle
    type(flavor_t), intent(in) :: flv_extra
    call phs_config%forest%set_flavors (phs_config%flv(:,1), reshuffle, &
        flv_extra)
end subroutine phs_wood_config_reshuffle_flavors

<PHS wood: phs wood config: TBP>+≡
procedure :: set_momentum_links => phs_wood_config_set_momentum_links

<PHS wood: sub interfaces>+≡
module subroutine phs_wood_config_set_momentum_links (phs_config, reshuffle)
    class(phs_wood_config_t), intent(inout) :: phs_config
    integer, intent(in), dimension(:), allocatable :: reshuffle
end subroutine phs_wood_config_set_momentum_links

<PHS wood: procedures>+≡
module subroutine phs_wood_config_set_momentum_links (phs_config, reshuffle)
    class(phs_wood_config_t), intent(inout) :: phs_config
    integer, intent(in), dimension(:), allocatable :: reshuffle
    call phs_config%forest%set_momentum_links (reshuffle)
end subroutine phs_wood_config_set_momentum_links

```

Identify resonances which are marked by s-channel mappings for the whole phase space and report them to the channel array.

```

<PHS wood: phs wood config: TBP>+≡
procedure :: record_s_mappings => phs_wood_config_record_s_mappings

<PHS wood: sub interfaces>+≡
module subroutine phs_wood_config_record_s_mappings (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
end subroutine phs_wood_config_record_s_mappings

<PHS wood: procedures>+≡
module subroutine phs_wood_config_record_s_mappings (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    logical :: flag
    real(default) :: mass, width
    integer :: c
    do c = 1, phs_config%n_channel
        call phs_config%forest%get_s_mapping (c, flag, mass, width)
        if (flag) then
            if (mass == 0) then
                call msg_fatal ("Phase space: s-channel resonance " &
                    // " has zero mass")
            end if
            if (width == 0) then
                call msg_fatal ("Phase space: s-channel resonance " &

```

```

        // " has zero width")
    end if
    call phs_config%channel(c)%set_resonant (mass, width)
end if
end do
end subroutine phs_wood_config_record_s_mappings

```

Identify on-shell mappings for the whole phase space and report them to the channel array.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: record_on_shell => phs_wood_config_record_on_shell

<PHS wood: sub interfaces>+≡
    module subroutine phs_wood_config_record_on_shell (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
    end subroutine phs_wood_config_record_on_shell

<PHS wood: procedures>+≡
    module subroutine phs_wood_config_record_on_shell (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        logical :: flag
        real(default) :: mass
        integer :: c
        do c = 1, phs_config%n_channel
            call phs_config%forest%get_on_shell (c, flag, mass)
            if (flag) then
                call phs_config%channel(c)%set_on_shell (mass)
            end if
        end do
    end subroutine phs_wood_config_record_on_shell

```

Return the most relevant MD5 sum. This overrides the method of the base type.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: get_md5sum => phs_wood_config_get_md5sum

<PHS wood: sub interfaces>+≡
    module function phs_wood_config_get_md5sum (phs_config) result (md5sum)
        class(phs_wood_config_t), intent(in) :: phs_config
        character(32) :: md5sum
    end function phs_wood_config_get_md5sum

<PHS wood: procedures>+≡
    module function phs_wood_config_get_md5sum (phs_config) result (md5sum)
        class(phs_wood_config_t), intent(in) :: phs_config
        character(32) :: md5sum
        if (phs_config%md5sum_forest /= "") then
            md5sum = phs_config%md5sum_forest
        else
            md5sum = phs_config%md5sum_phs_config
        end if
    end function phs_wood_config_get_md5sum

```

Check whether a phase-space configuration for the current process exists. We look for the phase-space file that should correspond to the current process. If we find it, we check the MD5 sums stored in the file against the MD5 sums in the current configuration (if required).

If successful, read the PHS file.

```

(PHS wood: phs wood config: TBP)+≡
  procedure :: read_phs_file => phs_wood_read_phs_file

(PHS wood: sub interfaces)+≡
  module subroutine phs_wood_read_phs_file &
    (phs_config, exist, found, match, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    logical, intent(out) :: exist
    logical, intent(out) :: found
    logical, intent(out), optional :: match
    type(string_t), intent(in), optional :: subdir
  end subroutine phs_wood_read_phs_file

(PHS wood: procedures)+≡
  module subroutine phs_wood_read_phs_file &
    (phs_config, exist, found, match, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    logical, intent(out) :: exist
    logical, intent(out) :: found
    logical, intent(out), optional :: match
    type(string_t), intent(in), optional :: subdir
    type(string_t) :: filename
    integer :: u
    filename = phs_config%make_phs_filename (subdir)
    inquire (file = char (filename), exist = exist)
    if (exist) then
      u = free_unit ()
      open (u, file = char (filename), action = "read", status = "old")
      call phs_config%forest%read (u, phs_config%id, phs_config%n_in, &
        phs_config%n_out, phs_config%model, found, &
        phs_config%md5sum_process, phs_config%md5sum_model_par, &
        phs_config%md5sum_phs_config, match = match)
      close (u)
    else
      found = .false.
      if (present (match)) match = .false.
    end if
  end subroutine phs_wood_read_phs_file

```

Startup message, after configuration is complete.

```

(PHS wood: phs wood config: TBP)+≡
  procedure :: startup_message => phs_wood_config_startup_message

(PHS wood: sub interfaces)+≡
  module subroutine phs_wood_config_startup_message (phs_config, unit)
    class(phs_wood_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
  end subroutine phs_wood_config_startup_message

```

<PHS wood: procedures>+≡

```

module subroutine phs_wood_config_startup_message (phs_config, unit)
  class(phs_wood_config_t), intent(in) :: phs_config
  integer, intent(in), optional :: unit
  integer :: n_groves, n_eq
  n_groves = phs_config%forest%get_n_groves ()
  n_eq = phs_config%forest%get_n_equivalences ()
  call phs_config%base_startup_message (unit)
  if (phs_config%n_channel == 1) then
    write (msg_buffer, "(A,2(I0,A))") &
      "Phase space: found ", phs_config%n_channel, &
      " channel, collected in ", n_groves, &
      " grove."
  else if (n_groves == 1) then
    write (msg_buffer, "(A,2(I0,A))") &
      "Phase space: found ", phs_config%n_channel, &
      " channels, collected in ", n_groves, &
      " grove."
  else
    write (msg_buffer, "(A,2(I0,A))") &
      "Phase space: found ", phs_config%n_channel, &
      " channels, collected in ", n_groves, &
      " groves."
  end if
  call msg_message (unit = unit)
  if (phs_config%use_equivalences) then
    if (n_eq == 1) then
      write (msg_buffer, "(A,I0,A)") &
        "Phase space: Using ", n_eq, &
        " equivalence between channels."
    else
      write (msg_buffer, "(A,I0,A)") &
        "Phase space: Using ", n_eq, &
        " equivalences between channels."
    end if
  else
    write (msg_buffer, "(A)") &
      "Phase space: no equivalences between channels used."
  end if
  call msg_message (unit = unit)
  write (msg_buffer, "(A,2(1x,I0,1x,A))") &
    "Phase space: wood"
  call msg_message (unit = unit)
end subroutine phs_wood_config_startup_message

```

Allocate an instance: the actual phase-space object. Gfortran 7/8/9 bug, has to remain in the main module.

<PHS wood: phs wood config: TBP>+≡

```

procedure, nopass :: allocate_instance => phs_wood_config_allocate_instance

```

<PHS wood: main procedures>≡

```

subroutine phs_wood_config_allocate_instance (phs)
  class(phs_t), intent(inout), pointer :: phs
  allocate (phs_wood_t :: phs)

```

```
end subroutine phs_wood_config_allocate_instance
```

19.12.4 Kinematics implementation

We generate $\cos\theta$ and ϕ uniformly, covering the solid angle.

```
<PHS wood: public>+≡
  public :: phs_wood_t

<PHS wood: types>+≡
  type, extends (phs_t) :: phs_wood_t
    real(default) :: sqrts = 0
    type(phs_forest_t) :: forest
    real(default), dimension(3) :: r_real
    integer :: n_r_born = 0
  contains
    <PHS wood: phs wood: TBP>
  end type phs_wood_t
```

Output. The `verbose` setting is irrelevant, we just display the contents of the base object.

```
<PHS wood: phs wood: TBP>≡
  procedure :: write => phs_wood_write

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_write (object, unit, verbose)
    class(phs_wood_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine phs_wood_write

<PHS wood: procedures>+≡
  module subroutine phs_wood_write (object, unit, verbose)
    class(phs_wood_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    call object%base_write (u)
  end subroutine phs_wood_write
```

Write the forest separately.

```
<PHS wood: phs wood: TBP>+≡
  procedure :: write_forest => phs_wood_write_forest

<PHS wood: sub interfaces>+≡
  module subroutine phs_wood_write_forest (object, unit)
    class(phs_wood_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine phs_wood_write_forest
```

```

(PHS wood: procedures)+≡
module subroutine phs_wood_write_forest (object, unit)
  class(phs_wood_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  call object%forest%write (u)
end subroutine phs_wood_write_forest

```

Finalizer.

```

(PHS wood: phs wood: TBP)+≡
  procedure :: final => phs_wood_final

(PHS wood: sub interfaces)+≡
  module subroutine phs_wood_final (object)
    class(phs_wood_t), intent(inout) :: object
  end subroutine phs_wood_final

(PHS wood: procedures)+≡
module subroutine phs_wood_final (object)
  class(phs_wood_t), intent(inout) :: object
  call object%forest%final ()
end subroutine phs_wood_final

```

Initialization. We allocate arrays (`base_init`) and adjust the phase-space volume. The two-particle phase space volume is

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.55294034614 \times 10^{-5} \quad (19.64)$$

independent of the particle masses.

```

(PHS wood: phs wood: TBP)+≡
  procedure :: init => phs_wood_init

(PHS wood: sub interfaces)+≡
  module subroutine phs_wood_init (phs, phs_config)
    class(phs_wood_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
  end subroutine phs_wood_init

(PHS wood: procedures)+≡
module subroutine phs_wood_init (phs, phs_config)
  class(phs_wood_t), intent(out) :: phs
  class(phs_config_t), intent(in), target :: phs_config
  call phs%base_init (phs_config)
  select type(phs_config)
  type is (phs_wood_config_t)
    phs%forest = phs_config%forest
    if (phs_config%is_combined_integration) then
      phs%n_r_born = phs_config%n_par - 3
    end if
  end select
end subroutine phs_wood_init

```

19.12.5 Evaluation

We compute the outgoing momenta from the incoming momenta and the input parameter set `r_in` in channel `r_in`. We also compute the `r` parameters and Jacobians `f` for all other channels.

We do *not* need to apply a transformation from/to the c.m. frame, because in `phs_base` the momenta are already boosted to the c.m. frame before assigning them in the `phs` object, and inversely boosted when extracting them.

```

(PHS wood: phs wood: TBP)+≡
  procedure :: evaluate_selected_channel => phs_wood_evaluate_selected_channel
  procedure :: evaluate_other_channels => phs_wood_evaluate_other_channels

(PHS wood: sub interfaces)+≡
  module subroutine phs_wood_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_wood_t), intent(inout) :: phs
    real(default), intent(in), dimension(:) :: r_in
    integer, intent(in) :: c_in
  end subroutine phs_wood_evaluate_selected_channel
  module subroutine phs_wood_evaluate_other_channels (phs, c_in)
    class(phs_wood_t), intent(inout) :: phs
    integer, intent(in) :: c_in
  end subroutine phs_wood_evaluate_other_channels

(PHS wood: procedures)+≡
  module subroutine phs_wood_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_wood_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    logical :: ok
    phs%q_defined = .false.
    if (phs%p_defined) then
      call phs%forest%set_prt_in (phs%p)
      phs%r(:,c_in) = r_in
      call phs%forest%evaluate_selected_channel (c_in, phs%active_channel, &
        phs%sqrts_hat, phs%r, phs%f, phs%volume, ok)
      select type (config => phs%config)
      type is (phs_wood_config_t)
        if (config%is_combined_integration) then
          if (phs%n_r_born >= 0) then
            phs%r_real = r_in (phs%n_r_born + 1 : phs%n_r_born + 3)
          else
            call msg_fatal ("n_r_born should be larger than 0!")
          end if
        end if
      end select
      if (ok) then
        phs%q = phs%forest%get_momenta_out ()
        phs%q_defined = .true.
      end if
    end if
  end subroutine phs_wood_evaluate_selected_channel

  module subroutine phs_wood_evaluate_other_channels (phs, c_in)
    class(phs_wood_t), intent(inout) :: phs
    integer, intent(in) :: c_in

```



```

integer :: c
if (phs%q_defined) then
  call phs%forest%evaluate_other_channels (c_in, phs%active_channel, &
    phs%sqrts_hat, phs%r, phs%f, combine=.true.)
  select type (config => phs%config)
  type is (phs_wood_config_t)
    if (config%is_combined_integration) then
      if (phs%n_r_born >= 0) then
        do c = 1, size (phs%r, 2)
          phs%r(phs%n_r_born + 1 : phs%n_r_born + 3, c) = phs%r_real
        end do
      else
        phs%r_defined = .false.
      end if
    end if
  end select
  phs%r_defined = .true.
end if
end subroutine phs_wood_evaluate_other_channels

```

Inverse evaluation.

(PHS wood: phs wood: TBP)+≡

```

  procedure :: inverse => phs_wood_inverse

```

(PHS wood: sub interfaces)+≡

```

  module subroutine phs_wood_inverse (phs)
    class(phs_wood_t), intent(inout) :: phs
  end subroutine phs_wood_inverse

```

(PHS wood: procedures)+≡

```

  module subroutine phs_wood_inverse (phs)
    class(phs_wood_t), intent(inout) :: phs
    if (phs%p_defined .and. phs%q_defined) then
      call phs%forest%set_prt_in (phs%p)
      call phs%forest%set_prt_out (phs%q)
      call phs%forest%recover_channel (1, phs%sqrts_hat, phs%r, &
        phs%f, phs%volume)
      call phs%forest%evaluate_other_channels (1, phs%active_channel, &
        phs%sqrts_hat, phs%r, phs%f, combine=.false.)
      phs%r_defined = .true.
    end if
  end subroutine phs_wood_inverse

```

19.12.6 Unit tests

Test module, followed by the corresponding implementation module.

(phs_wood_ut.f90)≡

(File header)

```

module phs_wood_ut
  use unit_tests
  use phs_wood_uti

```

```

    <Standard module head>

    <PHS wood: public test>

    <PHS wood: public test auxiliary>

contains

    <PHS wood: test driver>

end module phs_wood_ut

<phs_wood_uti.f90>≡
    <File header>

module phs_wood_uti

    <Use kinds>
    <Use strings>
    use io_units
    use os_interface
    use lorentz
    use flavors
    use model_data
    use process_constants
    use mappings
    use phs_base
    use phs_forests

    use phs_wood

    use phs_base_ut, only: init_test_process_data, init_test_decay_data

    <Standard module head>

    <PHS wood: public test auxiliary>

    <PHS wood: test declarations>

contains

    <PHS wood: tests>

    <PHS wood: test auxiliary>

end module phs_wood_uti
API: driver for the unit tests below.
<PHS wood: public test>≡
    public :: phs_wood_test
<PHS wood: test driver>≡
    subroutine phs_wood_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS wood: execute tests>

```

```

end subroutine phs_wood_test

<PHS wood: public test>+≡
public :: phs_wood_vis_test

<PHS wood: test driver>+≡
subroutine phs_wood_vis_test (u, results)
  integer, intent(in) :: u
  type(test_results_t), intent(inout) :: results
  <PHS wood: execute vis tests>
end subroutine phs_wood_vis_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal_dependence flag.

This auxiliary routine writes a phase-space configuration file to unit `u_phs`.

```

<PHS wood: public test auxiliary>≡
public :: write_test_phs_file

<PHS wood: test auxiliary>≡
subroutine write_test_phs_file (u_phs, procname)
  integer, intent(in) :: u_phs
  type(string_t), intent(in), optional :: procname
  if (present (procname)) then
    write (u_phs, "(A,A)") "process ", char (procname)
  else
    write (u_phs, "(A)") "process testproc"
  end if
  write (u_phs, "(A,A)") " md5sum_process = ", ""
  write (u_phs, "(A,A)") " md5sum_model_par = ", ""
  write (u_phs, "(A,A)") " md5sum_phs_config = ", ""
  write (u_phs, "(A)") " sqrts = 1000"
  write (u_phs, "(A)") " m_threshold_s = 50"
  write (u_phs, "(A)") " m_threshold_t = 100"
  write (u_phs, "(A)") " off_shell = 2"
  write (u_phs, "(A)") " t_channel = 6"
  write (u_phs, "(A)") " keep_nonresonant = T"
  write (u_phs, "(A)") " grove #1"
  write (u_phs, "(A)") " tree 3"
end subroutine write_test_phs_file

<PHS wood: execute tests>≡
call test (phs_wood_1, "phs_wood_1", &
  "phase-space configuration", &
  u, results)

<PHS wood: test declarations>≡
public :: phs_wood_1

<PHS wood: tests>≡
subroutine phs_wood_1 (u)
  integer, intent(in) :: u

```

```

type(model_data_t), target :: model
type(process_constants_t) :: process_data
class(phs_config_t), allocatable :: phs_data
type(mapping_defaults_t) :: mapping_defaults
real(default) :: sqrts
integer :: u_phs, iostat
character(32) :: buffer

write (u, "(A)")  "* Test output: phs_wood_1"
write (u, "(A)")  "* Purpose: initialize and display &
    &phase-space configuration data"
write (u, "(A)")

call model%init_test ()

call syntax_phs_forest_init ()

write (u, "(A)")  "* Initialize a process"
write (u, "(A)")

call init_test_process_data (var_str ("phs_wood_1"), process_data)

write (u, "(A)")  "* Create a scratch phase-space file"
write (u, "(A)")

u_phs = free_unit ()
open (u_phs, status = "scratch", action = "readwrite")
call write_test_phs_file (u_phs, var_str ("phs_wood_1"))
rewind (u_phs)
do
    read (u_phs, "(A)", iostat = iostat) buffer
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do

write (u, "(A)")
write (u, "(A)")  "* Setup phase-space configuration object"
write (u, "(A)")

mapping_defaults%step_mapping = .false.

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_input (u_phs)
    call phs_data%set_mapping_defaults (mapping_defaults)
end select

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)
write (u, "(A)")

```

```

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%write_forest (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

close (u_phs)
call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_1"

end subroutine phs_wood_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS wood: execute tests>+≡
    call test (phs_wood_2, "phs_wood_2", &
        "phase-space evaluation", &
        u, results)

<PHS wood: test declarations>+≡
    public :: phs_wood_2

<PHS wood: tests>+≡
    subroutine phs_wood_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        real(default) :: sqrts, E
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(2) :: p, q
        integer :: u_phs

        write (u, "(A)")  "* Test output: phs_wood_2"
        write (u, "(A)")  "* Purpose: test simple single-channel phase space"
        write (u, "(A)")

        call model%init_test ()
        call flv%init (25, model)

        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_wood_2"), process_data)
        u_phs = free_unit ()

```

```

open (u_phs, status = "scratch", action = "readwrite")
call write_test_phs_file (u_phs, var_str ("phs_wood_2"))
rewind (u_phs)

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_input (u_phs)
end select

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrts / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.125, 0.5"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.125_default, 0.5_default])
call phs%evaluate_other_channels (1)
call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_t)
    call phs%write_forest (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

```

```

call phs%get_outgoing_momenta (q)
call phs%final ()
deallocate (phs)

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_t)
    call phs%write_forest (u)
end select

call phs%final ()
deallocate (phs)

close (u_phs)
call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_2"

end subroutine phs_wood_2

```

Phase-space generation

Generate phase space for a simple process.

```

<PHS wood: execute tests>+≡
    call test (phs_wood_3, "phs_wood_3", &
        "phase-space generation", &
        u, results)

<PHS wood: test declarations>+≡
    public :: phs_wood_3

<PHS wood: tests>+≡
    subroutine phs_wood_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        type(phs_parameters_t) :: phs_par
        class(phs_config_t), allocatable :: phs_data
        integer :: iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: phs_wood_3"
    end subroutine

```

```

write (u, "(A)")  "*"   Purpose: generate a phase-space configuration"
write (u, "(A)")

call model%init_test ()

call syntax_phs_forest_init ()

write (u, "(A)")  "*" Initialize a process and phase-space parameters"
write (u, "(A)")

call init_test_process_data (var_str ("phs_wood_3"), process_data)
allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)

phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%io_unit_keep_open = .true.
end select

write (u, "(A)")
write (u, "(A)")  "*" Generate a scratch phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)

select type (phs_data)
type is (phs_wood_config_t)
    rewind (phs_data%io_unit)
    do
        read (phs_data%io_unit, "(A)", iostat = iostat)  buffer
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
end select

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: phs_wood_3"

end subroutine phs_wood_3

```

Nontrivial process

Generate phase space for a $2 \rightarrow 3$ process.

(PHS wood: execute tests) \equiv


```

call test (phs_wood_4, "phs_wood_4", &
          "nontrivial process", &
          u, results)
<PHS wood: test declarations>+≡
public :: phs_wood_4
<PHS wood: tests>+≡
subroutine phs_wood_4 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(process_constants_t) :: process_data
  type(phs_parameters_t) :: phs_par
  class(phs_config_t), allocatable, target :: phs_data
  integer :: iostat
  character(80) :: buffer
  class(phs_t), pointer :: phs => null ()
  real(default) :: E, pL
  type(vector4_t), dimension(2) :: p
  type(vector4_t), dimension(3) :: q

  write (u, "(A)")  "* Test output: phs_wood_4"
  write (u, "(A)")  "* Purpose: generate a phase-space configuration"
  write (u, "(A)")

  call model%init_test ()

  call syntax_phs_forest_init ()

  write (u, "(A)")  "* Initialize a process and phase-space parameters"
  write (u, "(A)")

  process_data%id = "phs_wood_4"
  process_data%model_name = "Test"
  process_data%n_in = 2
  process_data%n_out = 3
  process_data%n_flv = 1
  allocate (process_data%flv_state (process_data%n_in + process_data%n_out, &
    process_data%n_flv))
  process_data%flv_state(:,1) = [25, 25, 25, 6, -6]

  allocate (phs_wood_config_t :: phs_data)
  call phs_data%init (process_data, model)

  phs_par%sqrts = 1000
  select type (phs_data)
  type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%io_unit_keep_open = .true.
  end select

  write (u, "(A)")
  write (u, "(A)")  "* Generate a scratch phase-space file"
  write (u, "(A)")

```

```

call phs_data%configure (phs_par%sqrts)

select type (phs_data)
type is (phs_wood_config_t)
  rewind (phs_data%io_unit)
  do
    read (phs_data%io_unit, "(A)", iostat = iostat) buffer
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
  end do
end select

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
  E = phs_data%sqrts / 2
  pL = sqrt (E**2 - phs_data%flv(1,1)%get_mass ()**2)
end select
p(1) = vector4_moving (E, pL, 3)
p(2) = vector4_moving (E, -pL, 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

write (u, "(A)")  "* Compute phase-space point &
  &for x = 0.1, 0.2, 0.3, 0.4, 0.5"
write (u, "(A)")

call phs%evaluate_selected_channel (1, &
  [0.1_default, 0.2_default, 0.3_default, 0.4_default, 0.5_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call phs%final ()
deallocate (phs)

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%set_incoming_momenta (p)

```

```

call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_4"

end subroutine phs_wood_4

```

Equivalences

Generate phase space for a simple process, including channel equivalences.

```

<PHS wood: execute tests>+≡
  call test (phs_wood_5, "phs_wood_5", &
    "equivalences", &
    u, results)

<PHS wood: test declarations>+≡
  public :: phs_wood_5

<PHS wood: tests>+≡
  subroutine phs_wood_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    type(phs_parameters_t) :: phs_par
    class(phs_config_t), allocatable :: phs_data

    write (u, "(A)")  "* Test output: phs_wood_5"
    write (u, "(A)")  "* Purpose: generate a phase-space configuration"
    write (u, "(A)")

    call model%init_test ()

    call syntax_phs_forest_init ()

    write (u, "(A)")  "* Initialize a process and phase-space parameters"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_wood_5"), process_data)
    allocate (phs_wood_config_t :: phs_data)
    call phs_data%init (process_data, model)

```

```

phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    call phs_data%enable_equivalences ()
end select

write (u, "(A)")
write (u, "(A)")  "* Generate a scratch phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)
call phs_data%write (u)
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%write_forest (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_5"

end subroutine phs_wood_5

```

MD5 sum checks

Generate phase space for a simple process. Repeat this with and without parameter change.

```

<PHS wood: execute tests>+≡
    call test (phs_wood_6, "phs_wood_6", &
        "phase-space generation", &
        u, results)

<PHS wood: test declarations>+≡
    public :: phs_wood_6

<PHS wood: tests>+≡
    subroutine phs_wood_6 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        type(phs_parameters_t) :: phs_par
        class(phs_config_t), allocatable :: phs_data
        logical :: exist, found, match
        integer :: u_phs
        character(*), parameter :: filename = "phs_wood_6.p.phs"

```

```

write (u, "(A)")  "* Test output: phs_wood_6"
write (u, "(A)")  "* Purpose: generate and check phase-space file"
write (u, "(A)")

call model%init_test ()

call syntax_phs_forest_init ()

write (u, "(A)")  "* Initialize a process and phase-space parameters"
write (u, "(A)")

call init_test_process_data (var_str ("phs_wood_6"), process_data)
process_data%id = "phs_wood_6_p"
process_data%md5sum = "1234567890abcdef1234567890abcdef"
allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)

phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
end select

write (u, "(A)")  "* Remove previous phs file, if any"
write (u, "(A)")

inquire (file = filename, exist = exist)
if (exist) then
    u_phs = free_unit ()
    open (u_phs, file = filename, action = "write")
    close (u_phs, status = "delete")
end if

write (u, "(A)")  "* Check phase-space file (should fail)"
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%read_phs_file (exist, found, match)
    write (u, "(1x,A,L1)") "exist = ", exist
    write (u, "(1x,A,L1)") "found = ", found
    write (u, "(1x,A,L1)") "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Generate a phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)

write (u, "(1x,A,A,A)") "MD5 sum (process)      = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)") "MD5 sum (model par) = '", &

```

```

        phs_data%md5sum_model_par, ""
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = ", &
        phs_data%md5sum_phs_config, ""

write (u, "(A)")
write (u, "(A)")  "* Check MD5 sum"
write (u, "(A)")

call phs_data%final ()
deallocate (phs_data)
allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = ", &
        phs_data%md5sum_process, ""
write (u, "(1x,A,A,A)") "MD5 sum (model par)   = ", &
        phs_data%md5sum_model_par, ""
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = ", &
        phs_data%md5sum_phs_config, ""

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%read_phs_file (exist, found, match)
    write (u, "(1x,A,L1)") "exist = ", exist
    write (u, "(1x,A,L1)") "found = ", found
    write (u, "(1x,A,L1)") "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Modify sqrts and check MD5 sum"
write (u, "(A)")

call phs_data%final ()
deallocate (phs_data)
allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
phs_par%sqrts = 500
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = ", &

```



```

process_data%md5sum = "1234567890abcdef1234567890abcdef"
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
phs_par%off_shell = 17
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)") "MD5 sum (model par) = '", &
    phs_data%md5sum_model_par, "'"
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = '", &
    phs_data%md5sum_phs_config, "'"

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%read_phs_file (exist, found, match)
    write (u, "(1x,A,L1)") "exist = ", exist
    write (u, "(1x,A,L1)") "found = ", found
    write (u, "(1x,A,L1)") "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Modify model parameter and check MD5 sum"
write (u, "(A)")

call phs_data%final ()
deallocate (phs_data)
allocate (phs_wood_config_t :: phs_data)
call model%set_par (var_str ("ms"), 100._default)
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
phs_par%off_shell = 1
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)") "MD5 sum (model par) = '", &
    phs_data%md5sum_model_par, "'"
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = '", &
    phs_data%md5sum_phs_config, "'"

select type (phs_data)

```



```

type is (phs_wood_config_t)
  call phs_data%read_phs_file (exist, found, match)
  write (u, "(1x,A,L1)") "exist = ", exist
  write (u, "(1x,A,L1)") "found = ", found
  write (u, "(1x,A,L1)") "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_6"

end subroutine phs_wood_6

<PHS wood: execute vis tests>≡
  call test (phs_wood_vis_1, "phs_wood_vis_1", &
    "visualizing phase space channels", &
    u, results)

<PHS wood: test declarations>+≡
  public :: phs_wood_vis_1

<PHS wood: tests>+≡
  subroutine phs_wood_vis_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable :: phs_data
    type(mapping_defaults_t) :: mapping_defaults
    type(string_t) :: vis_file, pdf_file, ps_file
    real(default) :: sqrts
    logical :: exist, exist_pdf, exist_ps
    integer :: u_phs, iostat, u_vis
    character(95) :: buffer

    write (u, "(A)")  "* Test output: phs_wood_vis_1"
    write (u, "(A)")  "* Purpose: visualizing the &
      &phase-space configuration"
    write (u, "(A)")

    call os_data%init ()
    call model%init_test ()

    call syntax_phs_forest_init ()

    write (u, "(A)")  "* Initialize a process"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_wood_vis_1"), process_data)

```

```

write (u, "(A)")  "* Create a scratch phase-space file"
write (u, "(A)")

u_phs = free_unit ()
open (u_phs, status = "scratch", action = "readwrite")
call write_test_phs_file (u_phs, var_str ("phs_wood_vis_1"))
rewind (u_phs)
do
  read (u_phs, "(A)", iostat = iostat)  buffer
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do

write (u, "(A)")
write (u, "(A)")  "* Setup phase-space configuration object"
write (u, "(A)")

mapping_defaults%step_mapping = .false.

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_wood_config_t)
  call phs_data%set_input (u_phs)
  call phs_data%set_mapping_defaults (mapping_defaults)
  phs_data%os_data = os_data
  phs_data%io_unit = 0
  phs_data%io_unit_keep_open = .true.
  phs_data%vis_channels = .true.
end select

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
  call phs_data%write_forest (u)
end select

vis_file = "phs_wood_vis_1.phs-vis.tex"
ps_file  = "phs_wood_vis_1.phs-vis.ps"
pdf_file = "phs_wood_vis_1.phs-vis.pdf"
inquire (file = char (vis_file), exist = exist)
if (exist) then
  u_vis = free_unit ()
  open (u_vis, file = char (vis_file), action = "read", status = "old")
  iostat = 0
  do while (iostat == 0)
    read (u_vis, "(A)", iostat = iostat)  buffer
    if (iostat == 0)  write (u, "(A)")  trim (buffer)
  end do

```

```

        close (u_vis)
    else
        write (u, "(A)") "[Visualize LaTeX file is missing]"
    end if
    inquire (file = char (ps_file), exist = exist_ps)
    if (exist_ps) then
        write (u, "(A)") "[Visualize Postscript file exists and is nonempty]"
    else
        write (u, "(A)") "[Visualize Postscript file is missing/non-regular]"
    end if
    inquire (file = char (pdf_file), exist = exist_pdf)
    if (exist_pdf) then
        write (u, "(A)") "[Visualize PDF file exists and is nonempty]"
    else
        write (u, "(A)") "[Visualize PDF file is missing/non-regular]"
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    close (u_phs)
    call phs_data%final ()
    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: phs_wood_vis_1"

end subroutine phs_wood_vis_1

```

19.13 The FKS phase space

```

⟨phs_fks.f90⟩≡
⟨File header⟩

module phs_fks

  ⟨Use kinds⟩
  ⟨Use strings⟩
  use constants
  use lorentz
  use phs_points
  use models, only: model_t
  use phs_base
  use resonances, only: resonance_contributors_t, resonance_history_t
  use phs_wood

  ⟨Standard module head⟩

  ⟨PHS fks: public⟩

  ⟨PHS fks: parameters⟩

```

```

    <PHS fks: types>

    interface
    <PHS fks: sub interfaces>
    end interface

    contains

    <PHS fks: main procedures>

    end module phs_fks

<phs_fks_sub.f90>≡
<File header>

submodule (phs_fks) phs_fks_s

<Use debug>
    use diagnostics
    use io_units, only: given_output_unit, free_unit
    use format_defs, only: FMT_17
    use format_utils, only: write_separator
    use physics_defs
    use flavors
    use pdg_arrays, only: is_colored
    use cascades
    use cascades2
    use ttv_formfactors, only: generate_on_shell_decay_threshold, mis_to_mpole

    implicit none

    <PHS fks: interfaces>

    contains

    <PHS fks: procedures>

    end submodule phs_fks_s

```

A container for the x_{\oplus} - and x_{\ominus} -values for initial-state phase spaces.

```

<PHS fks: public>≡
    public :: isr_kinematics_t

<PHS fks: types>≡
    type :: isr_kinematics_t
        integer :: n_in
        real(default), dimension(2) :: x = one
        real(default), dimension(2) :: z = zero
        real(default) :: sqrts_born = zero
        real(default), dimension(:), allocatable :: beam_energy
        real(default) :: fac_scale = zero
        real(default), dimension(2) :: jacobian = one
        integer :: isr_mode = SQRTS_FIXED

```

```

contains
  <PHS fks: isr kinematics: TBP>
end type isr_kinematics_t

<PHS fks: isr kinematics: TBP>≡
  procedure :: write => isr_kinematics_write

<PHS fks: sub interfaces>≡
  module subroutine isr_kinematics_write (isr, unit)
    class(isr_kinematics_t), intent(in) :: isr
    integer, intent(in), optional :: unit
  end subroutine isr_kinematics_write

<PHS fks: procedures>≡
  module subroutine isr_kinematics_write (isr, unit)
    class(isr_kinematics_t), intent(in) :: isr
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u,"(A)") "ISR kinematics: "
    write (u,"(A," // FMT_17 // ",1X)" "x(+):          ", isr%x(1)
    write (u,"(A," // FMT_17 // ",1X)" "x(-):          ", isr%x(2)
    write (u,"(A," // FMT_17 // ",1X)" "z(+):          ", isr%z(1)
    write (u,"(A," // FMT_17 // ",1X)" "z(-):          ", isr%z(2)
    write (u,"(A," // FMT_17 // ",1X)" "sqrts (Born): ", isr%sqrts_born
    if (allocated (isr%beam_energy)) then
      do i = 1, size (isr%beam_energy)
        write (u,"(A," // FMT_17 // ",1X)" "Beam energy:  ", &
          isr%beam_energy(i)
      end do
    end if
    write (u,"(A," // FMT_17 // ",1X)" "Fac. scale:    ", isr%fac_scale
    do i = 1, 2
      write (u,"(A," // FMT_17 // ",1X)" "Jacobian:      ", isr%jacobian(i)
    end do
    write (u,"(A,I0,1X)" "ISR mode:        ", isr%isr_mode
  end subroutine isr_kinematics_write

<PHS fks: public>+≡
  public :: phs_point_set_t

<PHS fks: types>+≡
  type :: phs_point_set_t
    type(phs_point_t), dimension(:), allocatable :: phs_point
    logical :: initialized = .false.
  contains
    <PHS fks: phs point set: TBP>
  end type phs_point_set_t

<PHS fks: phs point set: TBP>≡
  procedure :: init => phs_point_set_init

```

```

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_init (phs_point_set, n_particles, n_phs)
        class(phs_point_set_t), intent(out) :: phs_point_set
        integer, intent(in) :: n_particles, n_phs
    end subroutine phs_point_set_init

<PHS fks: procedures>+≡
    module subroutine phs_point_set_init (phs_point_set, n_particles, n_phs)
        class(phs_point_set_t), intent(out) :: phs_point_set
        integer, intent(in) :: n_particles, n_phs
        integer :: i_phs
        allocate (phs_point_set%phs_point (n_phs))
        do i_phs = 1, n_phs
            phs_point_set%phs_point(i_phs) = n_particles
        end do
        phs_point_set%initialized = .true.
    end subroutine phs_point_set_init

<PHS fks: phs point set: TBP>+≡
    procedure :: write => phs_point_set_write

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_write (phs_point_set, i_phs, contributors, &
        unit, show_mass, testflag, check_conservation, ultra, n_in)
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in), optional :: i_phs
        integer, intent(in), dimension(:), optional :: contributors
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
    end subroutine phs_point_set_write

<PHS fks: procedures>+≡
    module subroutine phs_point_set_write (phs_point_set, i_phs, contributors, &
        unit, show_mass, testflag, check_conservation, ultra, n_in)
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in), optional :: i_phs
        integer, intent(in), dimension(:), optional :: contributors
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
        integer :: i, u
        type(vector4_t) :: p_sum
        u = given_output_unit (unit); if (u < 0) return
        if (present (i_phs)) then
            call phs_point_set%phs_point(i_phs)%write &
                (unit = u, show_mass = show_mass, testflag = testflag, &
                check_conservation = check_conservation, ultra = ultra, n_in = n_in)
        else
            do i = 1, size(phs_point_set%phs_point)
                call phs_point_set%phs_point(i)%write &

```

```

        (unit = u, show_mass = show_mass, testflag = testflag, &
        check_conservation = check_conservation, ultra = ultra, &
        n_in = n_in)
    end do
end if
if (present (contributors)) then
    if (debug_on) call msg_debug &
        (D_SUBTRACTION, "Invariant masses for real emission: ")
    associate (pp => phs_point_set%phs_point(i_phs))
        p_sum = sum (pp, [contributors, size (pp)])
    end associate
    if (debug_active (D_SUBTRACTION)) &
        call vector4_write (p_sum, unit = unit, show_mass = show_mass, &
        testflag = testflag, ultra = ultra)
    end if
end if
end subroutine phs_point_set_write

```

<PHS fks: phs point set: TBP>+≡

```

    procedure :: get_n_momenta => phs_point_set_get_n_momenta

```

<PHS fks: sub interfaces>+≡

```

    elemental module function phs_point_set_get_n_momenta &
        (phs_point_set, i_res) result (n)
        integer :: n
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_res
    end function phs_point_set_get_n_momenta

```

<PHS fks: procedures>+≡

```

    elemental module function phs_point_set_get_n_momenta &
        (phs_point_set, i_res) result (n)
        integer :: n
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_res
        n = size (phs_point_set%phs_point(i_res))
    end function phs_point_set_get_n_momenta

```

<PHS fks: phs point set: TBP>+≡

```

    procedure :: get_momenta => phs_point_set_get_momenta

```

<PHS fks: sub interfaces>+≡

```

    pure module function phs_point_set_get_momenta &
        (phs_point_set, i_phs, n_in) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        integer, intent(in), optional :: n_in
    end function phs_point_set_get_momenta

```

<PHS fks: procedures>+≡

```

    pure module function phs_point_set_get_momenta &
        (phs_point_set, i_phs, n_in) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs

```

```

integer, intent(in), optional :: n_in
integer :: i
if (present (n_in)) then
    p = phs_point_set%phs_point(i_phs)%select ([(i, i=1, n_in)])
else
    p = phs_point_set%phs_point(i_phs)
end if
end function phs_point_set_get_momenta

<PHS fks: phs point set: TBP>+≡
procedure :: get_momentum => phs_point_set_get_momentum

<PHS fks: sub interfaces>+≡
pure module function phs_point_set_get_momentum &
    (phs_point_set, i_phs, i_mom) result (p)
    type(vector4_t) :: p
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs, i_mom
end function phs_point_set_get_momentum

<PHS fks: procedures>+≡
pure module function phs_point_set_get_momentum &
    (phs_point_set, i_phs, i_mom) result (p)
    type(vector4_t) :: p
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs, i_mom
    p = phs_point_set%phs_point(i_phs)%select (i_mom)
end function phs_point_set_get_momentum

<PHS fks: phs point set: TBP>+≡
procedure :: get_energy => phs_point_set_get_energy

<PHS fks: sub interfaces>+≡
pure module function phs_point_set_get_energy &
    (phs_point_set, i_phs, i_mom) result (E)
    real(default) :: E
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs, i_mom
end function phs_point_set_get_energy

<PHS fks: procedures>+≡
pure module function phs_point_set_get_energy &
    (phs_point_set, i_phs, i_mom) result (E)
    real(default) :: E
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs, i_mom
    E = energy (phs_point_set%phs_point(i_phs)%select (i_mom))
end function phs_point_set_get_energy

<PHS fks: phs point set: TBP>+≡
procedure :: get_sqrts => phs_point_set_get_sqrts

```



```

<PHS fks: sub interfaces>+≡
    module function phs_point_set_get_sqrts &
        (phs_point_set, i_phs) result (sqrts)
        real(default) :: sqrts
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
    end function phs_point_set_get_sqrts

<PHS fks: procedures>+≡
    module function phs_point_set_get_sqrts &
        (phs_point_set, i_phs) result (sqrts)
        real(default) :: sqrts
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        sqrts = sqrt (phs_point_set%phs_point(i_phs)%get_msq ([1,2]))
    end function phs_point_set_get_sqrts

<PHS fks: phs point set: TBP>+≡
    generic :: set_momenta => set_momenta_p, set_momenta_phs_point
    procedure :: set_momenta_p => phs_point_set_set_momenta_p

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_set_momenta_p (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(vector4_t), intent(in), dimension(:) :: p
    end subroutine phs_point_set_set_momenta_p

<PHS fks: procedures>+≡
    module subroutine phs_point_set_set_momenta_p (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(vector4_t), intent(in), dimension(:) :: p
        phs_point_set%phs_point(i_phs) = p
    end subroutine phs_point_set_set_momenta_p

<PHS fks: phs point set: TBP>+≡
    procedure :: set_momenta_phs_point => phs_point_set_set_momenta_phs_point

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_set_momenta_phs_point &
        (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(phs_point_t), intent(in) :: p
    end subroutine phs_point_set_set_momenta_phs_point

<PHS fks: procedures>+≡
    module subroutine phs_point_set_set_momenta_phs_point &
        (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(phs_point_t), intent(in) :: p
        phs_point_set%phs_point(i_phs) = p
    end subroutine phs_point_set_set_momenta_phs_point

```

```

<PHS fks: phs point set: TBP>+≡
  procedure :: get_n_particles => phs_point_set_get_n_particles

<PHS fks: sub interfaces>+≡
  module function phs_point_set_get_n_particles &
    (phs_point_set, i) result (n_particles)
    integer :: n_particles
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in), optional :: i
  end function phs_point_set_get_n_particles

<PHS fks: procedures>+≡
  module function phs_point_set_get_n_particles &
    (phs_point_set, i) result (n_particles)
    integer :: n_particles
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in), optional :: i
    integer :: j
    j = 1; if (present (i)) j = i
    n_particles = size (phs_point_set%phs_point(j))
  end function phs_point_set_get_n_particles

<PHS fks: phs point set: TBP>+≡
  procedure :: get_n_phs => phs_point_set_get_n_phs

<PHS fks: sub interfaces>+≡
  module function phs_point_set_get_n_phs (phs_point_set) result (n_phs)
    integer :: n_phs
    class(phs_point_set_t), intent(in) :: phs_point_set
  end function phs_point_set_get_n_phs

<PHS fks: procedures>+≡
  module function phs_point_set_get_n_phs (phs_point_set) result (n_phs)
    integer :: n_phs
    class(phs_point_set_t), intent(in) :: phs_point_set
    n_phs = size (phs_point_set%phs_point)
  end function phs_point_set_get_n_phs

<PHS fks: phs point set: TBP>+≡
  procedure :: get_invariant_mass => phs_point_set_get_invariant_mass

<PHS fks: sub interfaces>+≡
  module function phs_point_set_get_invariant_mass &
    (phs_point_set, i_phs, i_part) result (m2)
    real(default) :: m2
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs
    integer, intent(in), dimension(:) :: i_part
  end function phs_point_set_get_invariant_mass

<PHS fks: procedures>+≡
  module function phs_point_set_get_invariant_mass &
    (phs_point_set, i_phs, i_part) result (m2)
    real(default) :: m2
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in) :: i_phs

```

```

        integer, intent(in), dimension(:) :: i_part
        m2 = phs_point_set%phs_point(i_phs)%get_msq (i_part)
    end function phs_point_set_get_invariant_mass

<PHS fks: phs point set: TBP>+≡
    procedure :: write_phs_point => phs_point_set_write_phs_point

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_write_phs_point (phs_point_set, i_phs, &
        unit, show_mass, testflag, check_conservation, ultra, n_in)
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
    end subroutine phs_point_set_write_phs_point

<PHS fks: procedures>+≡
    module subroutine phs_point_set_write_phs_point (phs_point_set, i_phs, &
        unit, show_mass, testflag, check_conservation, ultra, n_in)
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_mass
        logical, intent(in), optional :: testflag, ultra
        logical, intent(in), optional :: check_conservation
        integer, intent(in), optional :: n_in
        call phs_point_set%phs_point(i_phs)%write (unit, show_mass, testflag, &
            check_conservation, ultra, n_in)
    end subroutine phs_point_set_write_phs_point

<PHS fks: phs point set: TBP>+≡
    procedure :: final => phs_point_set_final

<PHS fks: sub interfaces>+≡
    module subroutine phs_point_set_final (phs_point_set)
        class(phs_point_set_t), intent(inout) :: phs_point_set
    end subroutine phs_point_set_final

<PHS fks: procedures>+≡
    module subroutine phs_point_set_final (phs_point_set)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer :: i
        deallocate (phs_point_set%phs_point)
        phs_point_set%initialized = .false.
    end subroutine phs_point_set_final

<PHS fks: public>+≡
    public :: real_jacobian_t

```

```

<PHS fks: types>+≡
  type :: real_jacobian_t
    real(default), dimension(4) :: jac = 1._default
  end type real_jacobian_t

<PHS fks: public>+≡
  public :: real_kinematics_t

<PHS fks: types>+≡
  type :: real_kinematics_t
    logical :: supply_xi_max = .true.
    real(default) :: xi_tilde
    real(default) :: phi
    real(default), dimension(:), allocatable :: xi_max, y
    real(default) :: xi_mismatch, y_mismatch
    type(real_jacobian_t), dimension(:), allocatable :: jac
    real(default) :: jac_mismatch
    type(phs_point_set_t) :: p_born_cms
    type(phs_point_set_t) :: p_born_lab
    type(phs_point_set_t) :: p_real_cms
    type(phs_point_set_t) :: p_real_lab
    type(phs_point_set_t) :: p_born_onshell
    type(phs_point_set_t), dimension(2) :: p_real_onshell
    integer, dimension(:), allocatable :: alr_to_i_phs
    real(default), dimension(3) :: x_rad
    real(default), dimension(:), allocatable :: jac_rand
    real(default), dimension(:), allocatable :: y_soft
    real(default) :: cms_energy2
    type(vector4_t), dimension(:), allocatable :: xi_ref_momenta
  contains
    <PHS fks: real kinematics: TBP>
  end type real_kinematics_t

<PHS fks: real kinematics: TBP>≡
  procedure :: init => real_kinematics_init

<PHS fks: sub interfaces>+≡
  module subroutine real_kinematics_init (r, n_tot, n_phs, n_alr, n_contr)
    class(real_kinematics_t), intent(inout) :: r
    integer, intent(in) :: n_tot, n_phs, n_alr, n_contr
  end subroutine real_kinematics_init

<PHS fks: procedures>+≡
  module subroutine real_kinematics_init (r, n_tot, n_phs, n_alr, n_contr)
    class(real_kinematics_t), intent(inout) :: r
    integer, intent(in) :: n_tot, n_phs, n_alr, n_contr
    allocate (r%xi_max (n_phs))
    allocate (r%y (n_phs))
    allocate (r%y_soft (n_phs))
    call r%p_born_cms%init (n_tot - 1, 1)
    call r%p_born_lab%init (n_tot - 1, 1)
    call r%p_real_cms%init (n_tot, n_phs)
    call r%p_real_lab%init (n_tot, n_phs)
    allocate (r%jac (n_phs), r%jac_rand (n_phs))
    allocate (r%alr_to_i_phs (n_alr))

```

```

allocate (r%xi_ref_momenta (n_contr))
r%alr_to_i_phs = 0
r%xi_tilde = zero; r%xi_mismatch = zero
r%xi_max = zero
r%y = zero; r%y_mismatch = zero
r%y_soft = zero
r%phi = zero
r%cms_energy2 = zero
r%xi_ref_momenta = vector4_null
r%jac_mismatch = one
r%jac_rand = one
end subroutine real_kinematics_init

```

<PHS fks: real kinematics: TBP>+≡

```

procedure :: init_onshell => real_kinematics_init_onshell

```

<PHS fks: sub interfaces>+≡

```

module subroutine real_kinematics_init_onshell (r, n_tot, n_phs)
  class(real_kinematics_t), intent(inout) :: r
  integer, intent(in) :: n_tot, n_phs
end subroutine real_kinematics_init_onshell

```

<PHS fks: procedures>+≡

```

module subroutine real_kinematics_init_onshell (r, n_tot, n_phs)
  class(real_kinematics_t), intent(inout) :: r
  integer, intent(in) :: n_tot, n_phs
  call r%p_born_onshell%init (n_tot - 1, 1)
  call r%p_real_onshell(1)%init (n_tot, n_phs)
  call r%p_real_onshell(2)%init (n_tot, n_phs)
end subroutine real_kinematics_init_onshell

```

<PHS fks: real kinematics: TBP>+≡

```

procedure :: write => real_kinematics_write

```

<PHS fks: sub interfaces>+≡

```

module subroutine real_kinematics_write (r, unit)
  class(real_kinematics_t), intent(in) :: r
  integer, intent(in), optional :: unit
end subroutine real_kinematics_write

```

<PHS fks: procedures>+≡

```

module subroutine real_kinematics_write (r, unit)
  class(real_kinematics_t), intent(in) :: r
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u,"(A)") "Real kinematics: "
  write (u,"(A," // FMT_17 // ",1X)") "xi_tilde: ", r%xi_tilde
  write (u,"(A," // FMT_17 // ",1X)") "phi: ", r%phi
  do i = 1, size (r%xi_max)
    write (u,"(A,I1,1X)") "i_phs: ", i
    write (u,"(A," // FMT_17 // ",1X)") "xi_max: ", r%xi_max(i)
    write (u,"(A," // FMT_17 // ",1X)") "y: ", r%y(i)
    write (u,"(A," // FMT_17 // ",1X)") "jac_rand: ", r%jac_rand(i)
    write (u,"(A," // FMT_17 // ",1X)") "y_soft: ", r%y_soft(i)
  end do
end subroutine real_kinematics_write

```

```

end do
write (u, "(A)") "Born Momenta: "
write (u, "(A)") "CMS: "
call r%p_born_cms%write (unit = u)
write (u, "(A)") "Lab: "
call r%p_born_lab%write (unit = u)
write (u, "(A)") "Real Momenta: "
write (u, "(A)") "CMS: "
call r%p_real_cms%write (unit = u)
write (u, "(A)") "Lab: "
call r%p_real_lab%write (unit = u)
end subroutine real_kinematics_write

```

The boost to the center-of-mass system only has a reasonable meaning above the threshold. Below the threshold, we do not apply boost at all, so that the top quarks stay in the rest frame. However, with top quarks exactly at rest, problems arise in the matrix elements (e.g. in the computation of angles). Therefore, we apply a boost which is not exactly 1, but has a tiny value differing from that.

```

<PHS fks: public>+≡
public :: get_boost_for_threshold_projection

<PHS fks: sub interfaces>+≡
module function get_boost_for_threshold_projection &
  (p, sqrts, mtop) result (L)
  type(lorentz_transformation_t) :: L
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: sqrts, mtop
end function get_boost_for_threshold_projection

<PHS fks: procedures>+≡
module function get_boost_for_threshold_projection &
  (p, sqrts, mtop) result (L)
  type(lorentz_transformation_t) :: L
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: sqrts, mtop
  type(vector4_t) :: p_tmp
  type(vector3_t) :: dir
  real(default) :: scale_factor, arg
  p_tmp = p(THR_POS_WP) + p(THR_POS_B)
  arg = sqrts**2 - four * mtop**2
  if (arg > zero) then
    scale_factor = sqrt (arg) / two
  else
    scale_factor = tiny_07*1000
  end if
  dir = scale_factor * create_unit_vector (p_tmp)
  p_tmp = [sqrts / two, dir%p]
  L = boost (p_tmp, mtop)
end function get_boost_for_threshold_projection

```

This routine recomputes the value of ϕ used to generate the real phase space.

```

<PHS fks: procedures>+≡
function get_generation_phi (p_born, p_real, emitter, i_gluon) result (phi)

```

```

real(default) :: phi
type(vector4_t), intent(in), dimension(:) :: p_born, p_real
integer, intent(in) :: emitter, i_gluon
type(vector4_t) :: p1, p2, pp
type(lorentz_transformation_t) :: rot_to_gluon, rot_to_z
type(vector3_t) :: dir, z
real(default) :: cpsi
pp = p_real(emitter) + p_real(i_gluon)
cpsi = (space_part_norm (pp)**2 - space_part_norm (p_real(emitter))**2 &
        + space_part_norm (p_real(i_gluon))**2) / &
        (two * space_part_norm (pp) * space_part_norm (p_real(i_gluon)))
dir = create_orthogonal (space_part (p_born(emitter)))
rot_to_gluon = rotation (cpsi, sqrt (one - cpsi**2), dir)
pp = rot_to_gluon * p_born(emitter)
z%p = [0._default, 0._default, 1._default]
rot_to_z = rotation_to_2nd &
        (space_part (p_born(emitter)) / space_part_norm (p_born(emitter)), z)
p1 = rot_to_z * pp / space_part_norm (pp)
p2 = rot_to_z * p_real(i_gluon)
phi = azimuthal_distance (p1, p2)
if (phi < zero) phi = twopi - abs(phi)
end function get_generation_phi

```

<PHS fks: real kinematics: TBP>+≡

```

procedure :: apply_threshold_projection_real => &
        real_kinematics_apply_threshold_projection_real

```

<PHS fks: sub interfaces>+≡

```

module subroutine real_kinematics_apply_threshold_projection_real &
        (r, i_phs, mtop, L_to_cms, invert)
class(real_kinematics_t), intent(inout) :: r
integer, intent(in) :: i_phs
real(default), intent(in) :: mtop
type(lorentz_transformation_t), intent(in), dimension(:) :: L_to_cms
logical, intent(in) :: invert
end subroutine real_kinematics_apply_threshold_projection_real

```

<PHS fks: procedures>+≡

```

module subroutine real_kinematics_apply_threshold_projection_real &
        (r, i_phs, mtop, L_to_cms, invert)
class(real_kinematics_t), intent(inout) :: r
integer, intent(in) :: i_phs
real(default), intent(in) :: mtop
type(lorentz_transformation_t), intent(in), dimension(:) :: L_to_cms
logical, intent(in) :: invert
integer :: leg, other_leg
type(vector4_t), dimension(:), allocatable :: p_real
type(vector4_t), dimension(:), allocatable :: p_real_onshell
type(vector4_t), dimension(4) :: k_tmp
type(vector4_t), dimension(4) :: k_decay_onshell_real
type(vector4_t), dimension(3) :: k_decay_onshell_born
do leg = 1, 2
        other_leg = 3 - leg
        p_real = r%p_real_cms%phs_point(i_phs)
        allocate (p_real_onshell (size (p_real)))

```

```

p_real_onshell(1:2) = p_real(1:2)
k_tmp(1) = p_real(7)
k_tmp(2) = p_real(ass_quark(leg))
k_tmp(3) = p_real(ass_boson(leg))
k_tmp(4) = [mtop, zero, zero, zero]
call generate_on_shell_decay_threshold (k_tmp(1:3), &
    k_tmp(4), k_decay_onshell_real (2:4))
k_decay_onshell_real (1) = k_tmp(4)
k_tmp(1) = p_real(ass_quark(other_leg))
k_tmp(2) = p_real(ass_boson(other_leg))
k_decay_onshell_born = create_two_particle_decay (mtop**2, k_tmp(1), k_tmp(2))
p_real_onshell(THR_POS_GLUON) = L_to_cms(leg) * k_decay_onshell_real (2)
p_real_onshell(ass_quark(leg)) = L_to_cms(leg) * k_decay_onshell_real(3)
p_real_onshell(ass_boson(leg)) = L_to_cms(leg) * k_decay_onshell_real(4)
p_real_onshell(ass_quark(other_leg)) = L_to_cms(leg) * k_decay_onshell_born (2)
p_real_onshell(ass_boson(other_leg)) = L_to_cms(leg) * k_decay_onshell_born (3)
if (invert) then
    call vector4_invert_direction (p_real_onshell (ass_quark(other_leg)))
    call vector4_invert_direction (p_real_onshell (ass_boson(other_leg)))
end if
r%p_real_onshell(leg)%phs_point(i_phs) = p_real_onshell
deallocate (p_real_onshell)
end do
end subroutine real_kinematics_apply_threshold_projection_real

```

(PHS fks: public)+≡

```
public :: threshold_projection_born
```

(PHS fks: sub interfaces)+≡

```

module subroutine threshold_projection_born &
    (mtop, L_to_cms, p_in, p_onshell)
    real(default), intent(in) :: mtop
    type(lorentz_transformation_t), intent(in) :: L_to_cms
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:) :: p_onshell
end subroutine threshold_projection_born

```

(PHS fks: procedures)+≡

```

module subroutine threshold_projection_born &
    (mtop, L_to_cms, p_in, p_onshell)
    real(default), intent(in) :: mtop
    type(lorentz_transformation_t), intent(in) :: L_to_cms
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:) :: p_onshell
    type(vector4_t), dimension(3) :: k_decay_onshell
    type(vector4_t) :: p_tmp_1, p_tmp_2
    type(lorentz_transformation_t) :: L_to_cms_inv
    p_onshell(1:2) = p_in(1:2)
    L_to_cms_inv = inverse (L_to_cms)
    p_tmp_1 = L_to_cms_inv * p_in(THR_POS_B)
    p_tmp_2 = L_to_cms_inv * p_in(THR_POS_WP)
    k_decay_onshell = create_two_particle_decay (mtop**2, &
        p_tmp_1, p_tmp_2)
    p_onshell([THR_POS_B, THR_POS_WP]) = k_decay_onshell([2, 3])
    p_tmp_1 = L_to_cms * p_in(THR_POS_BBAR)

```



```

p_tmp_2 = L_to_cms * p_in(THR_POS_WM)
k_decay_onshell = create_two_particle_decay (mtop**2, &
    p_tmp_1, p_tmp_2)
p_onshell([THR_POS_BBAR, THR_POS_WM]) = k_decay_onshell([2, 3])
p_onshell([THR_POS_WP, THR_POS_B]) = L_to_cms * p_onshell([THR_POS_WP, THR_POS_B])
p_onshell([THR_POS_WM, THR_POS_BBAR]) = L_to_cms_inv * p_onshell([THR_POS_WM, THR_POS_BBAR])
end subroutine threshold_projection_born

```

This routine computes the bounds of the Dalitz region for massive emitters. The corresponding derivation can be found in 1202.0465, App. A. It is also used for the POWHEG matching so the routine is public. The input parameter `m2` corresponds to the squared mass of the emitter.

```

<PHS fks: public>+≡
    public :: compute_dalitz_bounds

<PHS fks: sub interfaces>+≡
    pure module subroutine compute_dalitz_bounds &
        (q0, m2, mrec2, z1, z2, k0_rec_max)
        real(default), intent(in) :: q0, m2, mrec2
        real(default), intent(out) :: z1, z2, k0_rec_max
    end subroutine compute_dalitz_bounds

<PHS fks: procedures>+≡
    pure module subroutine compute_dalitz_bounds &
        (q0, m2, mrec2, z1, z2, k0_rec_max)
        real(default), intent(in) :: q0, m2, mrec2
        real(default), intent(out) :: z1, z2, k0_rec_max
        k0_rec_max = (q0**2 - m2 + mrec2) / (two * q0)
        z1 = (k0_rec_max + sqrt(k0_rec_max**2 - mrec2)) / q0
        z2 = (k0_rec_max - sqrt(k0_rec_max**2 - mrec2)) / q0
    end subroutine compute_dalitz_bounds

```

Compute the `kt2` of a given emitter

```

<PHS fks: real kinematics: TBP>+≡
    procedure :: kt2 => real_kinematics_kt2

<PHS fks: sub interfaces>+≡
    module function real_kinematics_kt2 &
        (real_kinematics, i_phs, emitter, kt2_type, xi, y) result (kt2)
        real(default) :: kt2
        class(real_kinematics_t), intent(in) :: real_kinematics
        integer, intent(in) :: emitter, i_phs, kt2_type
        real(default), intent(in), optional :: xi, y
    end function real_kinematics_kt2

<PHS fks: procedures>+≡
    module function real_kinematics_kt2 &
        (real_kinematics, i_phs, emitter, kt2_type, xi, y) result (kt2)
        real(default) :: kt2
        class(real_kinematics_t), intent(in) :: real_kinematics
        integer, intent(in) :: emitter, i_phs, kt2_type
        real(default), intent(in), optional :: xi, y
        real(default) :: xii, yy
        real(default) :: q, E_em, z, z1, z2, m2, mrec2, k0_rec_max
        type(vector4_t) :: p_emitter

```

```

if (present (y)) then
  yy = y
else
  yy = real_kinematics%y (i_phs)
end if
if (present (xi)) then
  xii = xi
else
  xii = real_kinematics%xi_tilde * real_kinematics%xi_max (i_phs)
end if
select case (kt2_type)
case (UBF_FSR_SIMPLE)
  kt2 = real_kinematics%cms_energy2 / two * xii**2 * (1 - yy)
case (UBF_FSR_MASSIVE)
  q = sqrt (real_kinematics%cms_energy2)
  p_emitter = real_kinematics%p_born_cms%phs_point(1)%select (emitter)
  mrec2 = (q - p_emitter%p(0))**2 - sum (p_emitter%p(1:3)**2)
  m2 = p_emitter**2
  E_em = energy (p_emitter)
  call compute_dalitz_bounds (q, m2, mrec2, z1, z2, k0_rec_max)
  z = z2 - (z2 - z1) * (one + yy) / two
  kt2 = xii**2 * q**3 * (one - z) / &
    (two * E_em - z * xii * q)
case (UBF_FSR_MASSLESS_RECOIL)
  kt2 = real_kinematics%cms_energy2 / two * xii**2 * (1 - yy**2) / two
case (UBF_ISR)
  kt2 = real_kinematics%cms_energy2 / four * xii**2 * (1 - yy**2) / (1 - xii)
case default
  kt2 = zero
  call msg_bug ("kt2_type must be set to a known value")
end select
end function real_kinematics_kt2

```

These are the possible values for `upper_bound_func_type` and will be used to decide which UBF object is allocated and which K_T scale for the matching is computed.

(PHS fks: parameters)≡

```

integer, parameter, public :: UBF_FSR_SIMPLE = 1
integer, parameter, public :: UBF_FSR_MASSIVE = 2
integer, parameter, public :: UBF_FSR_MASSLESS_RECOIL = 3
integer, parameter, public :: UBF_ISR = 4

```

(PHS fks: real kinematics: TBP)+≡

```

procedure :: final => real_kinematics_final

```

(PHS fks: sub interfaces)+≡

```

module subroutine real_kinematics_final (real_kin)
  class(real_kinematics_t), intent(inout) :: real_kin
end subroutine real_kinematics_final

```

(PHS fks: procedures)+≡

```

module subroutine real_kinematics_final (real_kin)
  class(real_kinematics_t), intent(inout) :: real_kin
  if (allocated (real_kin%xi_max)) deallocate (real_kin%xi_max)
  if (allocated (real_kin%y)) deallocate (real_kin%y)

```

```

        if (allocated (real_kin%alr_to_i_phs)) deallocate (real_kin%alr_to_i_phs)
        if (allocated (real_kin%jac_rand)) deallocate (real_kin%jac_rand)
        if (allocated (real_kin%y_soft)) deallocate (real_kin%y_soft)
        if (allocated (real_kin%xi_ref_momenta)) &
            deallocate (real_kin%xi_ref_momenta)
        call real_kin%p_born_cms%final (); call real_kin%p_born_lab%final ()
        call real_kin%p_real_cms%final (); call real_kin%p_real_lab%final ()
    end subroutine real_kinematics_final

<PHS fks: parameters>+=
    integer, parameter, public :: I_XI = 1
    integer, parameter, public :: I_Y = 2
    integer, parameter, public :: I_PHI = 3

    integer, parameter, public :: PHS_MODE_UNDEFINED = 0
    integer, parameter, public :: PHS_MODE_ADDITIONAL_PARTICLE = 1
    integer, parameter, public :: PHS_MODE_COLLINEAR_REMNANT = 2

<PHS fks: public>+=
    public :: phs_fks_config_t

<PHS fks: types>+=
    type, extends (phs_wood_config_t) :: phs_fks_config_t
        integer :: mode = PHS_MODE_UNDEFINED
        character(32) :: md5sum_born_config
        logical :: born_2_to_1 = .false.
        logical :: make_dalitz_plot = .false.
    contains
        <PHS fks: fks config: TBP>
    end type phs_fks_config_t

<PHS fks: fks config: TBP>=
    procedure :: clear_phase_space => fks_config_clear_phase_space

<PHS fks: sub interfaces>+=
    module subroutine fks_config_clear_phase_space (phs_config)
        class(phs_fks_config_t), intent(inout) :: phs_config
    end subroutine fks_config_clear_phase_space

<PHS fks: procedures>+=
    module subroutine fks_config_clear_phase_space (phs_config)
        class(phs_fks_config_t), intent(inout) :: phs_config
    end subroutine fks_config_clear_phase_space

<PHS fks: fks config: TBP>+=
    procedure :: write => phs_fks_config_write

<PHS fks: sub interfaces>+=
    module subroutine phs_fks_config_write (object, unit, include_id)
        class(phs_fks_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
    end subroutine phs_fks_config_write

```

```

<PHS fks: procedures>+≡
module subroutine phs_fks_config_write (object, unit, include_id)
  class(phs_fks_config_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: include_id
  integer :: u
  u = given_output_unit (unit)
  call object%phs_wood_config_t%write (u)
  write (u, "(3x,A,I0)") "NLO mode = ", object%mode
  write (u, "(3x,A,L1)") "2->1 proc = ", object%born_2_to_1
  write (u, "(3x,A,L1)") "Dalitz = ", object%make_dalitz_plot
  write (u, "(A,A)") "Extra Born md5sum: ", object%md5sum_born_config
end subroutine phs_fks_config_write

<PHS fks: fks config: TBP>+≡
procedure :: set_mode => phs_fks_config_set_mode

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_config_set_mode (phs_config, mode)
  class(phs_fks_config_t), intent(inout) :: phs_config
  integer, intent(in) :: mode
end subroutine phs_fks_config_set_mode

<PHS fks: procedures>+≡
module subroutine phs_fks_config_set_mode (phs_config, mode)
  class(phs_fks_config_t), intent(inout) :: phs_config
  integer, intent(in) :: mode
  select case (mode)
  case (NLO_REAL, NLO_MISMATCH)
    phs_config%mode = PHS_MODE_ADDITIONAL_PARTICLE
  case (NLO_DGLAP)
    phs_config%mode = PHS_MODE_COLLINEAR_REMNANT
  end select
end subroutine phs_fks_config_set_mode

<PHS fks: fks config: TBP>+≡
procedure :: configure => phs_fks_config_configure

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_config_configure (phs_config, sqrts, &
  sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
  ignore_mismatch, nlo_type, subdir)
  class(phs_fks_config_t), intent(inout) :: phs_config
  real(default), intent(in) :: sqrts
  logical, intent(in), optional :: sqrts_fixed
  logical, intent(in), optional :: lab_is_cm
  logical, intent(in), optional :: azimuthal_dependence
  logical, intent(in), optional :: rebuild
  logical, intent(in), optional :: ignore_mismatch
  integer, intent(in), optional :: nlo_type
  type(string_t), intent(in), optional :: subdir
end subroutine phs_fks_config_configure

<PHS fks: procedures>+≡
module subroutine phs_fks_config_configure (phs_config, sqrts, &

```

```

        sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
        ignore_mismatch, nlo_type, subdir)
class(phs_fks_config_t), intent(inout) :: phs_config
real(default), intent(in) :: sqrts
logical, intent(in), optional :: sqrts_fixed
logical, intent(in), optional :: lab_is_cm
logical, intent(in), optional :: azimuthal_dependence
logical, intent(in), optional :: rebuild
logical, intent(in), optional :: ignore_mismatch
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: subdir
if (present (nlo_type)) phs_config%nlo_type = nlo_type
if (.not. phs_config%is_combined_integration) then
    select case (phs_config%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
        phs_config%n_par = phs_config%n_par + 3
        if (phs_config%nlo_type == NLO_REAL .and. phs_config%n_out == 2) then
            phs_config%born_2_to_1 = .true.
        end if
    case (PHS_MODE_COLLINEAR_REMNANT)
        phs_config%n_par = phs_config%n_par + 1
    end select
end if
call phs_config%compute_md5sum ()
end subroutine phs_fks_config_configure

```

<PHS fks: fks config: TBP>+≡

```

    procedure :: startup_message => phs_fks_config_startup_message

```

<PHS fks: sub interfaces>+≡

```

    module subroutine phs_fks_config_startup_message (phs_config, unit)
        class(phs_fks_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
    end subroutine phs_fks_config_startup_message

```

<PHS fks: procedures>+≡

```

    module subroutine phs_fks_config_startup_message (phs_config, unit)
        class(phs_fks_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        call phs_config%phs_wood_config_t%startup_message (unit)
    end subroutine phs_fks_config_startup_message

```

Gfortran 7/8/9 bug, has to remain in the main module:

<PHS fks: fks config: TBP>+≡

```

    procedure, nopass :: allocate_instance => phs_fks_config_allocate_instance

```

<PHS fks: main procedures>≡

```

    subroutine phs_fks_config_allocate_instance (phs)
        class(phs_t), intent(inout), pointer :: phs
        allocate (phs_fks_t :: phs)
    end subroutine phs_fks_config_allocate_instance

```

If the phase space is generated from file, but we want to have resonance histories, we must force the cascade sets to be generated. However, it must be assured that Born flavors are used for this.

```

<PHS fks: fks config: TBP>+≡
  procedure :: generate_phase_space_extra => &
    phs_fks_config_generate_phase_space_extra

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_config_generate_phase_space_extra (phs_config)
    class(phs_fks_config_t), intent(inout) :: phs_config
    end subroutine phs_fks_config_generate_phase_space_extra

<PHS fks: procedures>+≡
  module subroutine phs_fks_config_generate_phase_space_extra (phs_config)
    class(phs_fks_config_t), intent(inout) :: phs_config
    integer :: off_shell, extra_off_shell
    type(flavor_t), dimension(:, :), allocatable :: flv_born
    integer :: i, j
    integer :: n_state, n_flv_born
    integer :: unit_fds
    logical :: valid
    type(string_t) :: file_name
    logical :: file_exists
    if (phs_config%use_cascades2) then
      allocate (phs_config%feyngraph_set)
    else
      allocate (phs_config%cascade_set)
    end if
    n_flv_born = size (phs_config%flv, 1) - 1
    n_state = size (phs_config%flv, 2)
    allocate (flv_born (n_flv_born, n_state))
    do i = 1, n_flv_born
      do j = 1, n_state
        flv_born(i, j) = phs_config%flv(i, j)
      end do
    end do
    if (phs_config%use_cascades2) then
      file_name = char (phs_config%id) // ".fds"
      inquire (file=char (file_name), exist=file_exists)
      if (.not. file_exists) call msg_fatal &
        ("The O'Mega input file " // char (file_name) // &
         " does not exist. " // "Please make sure that the " // &
         "variable ?omega_write_phs_output has been set correctly.")
      unit_fds = free_unit ()
      open (unit=unit_fds, file=char(file_name), status='old', action='read')
    end if
    off_shell = phs_config%par%off_shell
    do extra_off_shell = 0, max (n_flv_born - 2, 0)
      phs_config%par%off_shell = off_shell + extra_off_shell
      if (phs_config%use_cascades2) then
        call feyngraph_set_generate (phs_config%feyngraph_set, &
          phs_config%model, phs_config%n_in, phs_config%n_out - 1, &
          flv_born, phs_config%par, phs_config%fatal_beam_decay, unit_fds, &
          phs_config%vis_channels)
        if (feyngraph_set_is_valid (phs_config%feyngraph_set)) exit
      end if
    end do
  end subroutine

```

```

else
  call cascade_set_generate (phs_config%cascade_set, &
    phs_config%model, phs_config%n_in, phs_config%n_out - 1, &
    flv_born, phs_config%par, phs_config%fatal_beam_decay)
  if (cascade_set_is_valid (phs_config%cascade_set)) exit
end if
end do
if (phs_config%use_cascades2) then
  close (unit_fds)
  valid = feyngraph_set_is_valid (phs_config%feyngraph_set)
else
  valid = cascade_set_is_valid (phs_config%cascade_set)
end if
if (.not. valid) &
  call msg_fatal ("Resonance extraction: Phase space generation failed")
end subroutine phs_fks_config_generate_phase_space_extra

```

(PHS fks: fks config: TBP)+≡

```

procedure :: set_born_config => phs_fks_config_set_born_config

```

(PHS fks: sub interfaces)+≡

```

module subroutine phs_fks_config_set_born_config (phs_config, phs_cfg_born)
  class(phs_fks_config_t), intent(inout) :: phs_config
  type(phs_wood_config_t), intent(in), target :: phs_cfg_born
end subroutine phs_fks_config_set_born_config

```

(PHS fks: procedures)+≡

```

module subroutine phs_fks_config_set_born_config (phs_config, phs_cfg_born)
  class(phs_fks_config_t), intent(inout) :: phs_config
  type(phs_wood_config_t), intent(in), target :: phs_cfg_born
  if (debug_on) &
    call msg_debug (D_PHASESPACE, "phs_fks_config_set_born_config")
  phs_config%forest = phs_cfg_born%forest
  phs_config%n_channel = phs_cfg_born%n_channel
  allocate (phs_config%channel (phs_config%n_channel))
  phs_config%channel = phs_cfg_born%channel
  phs_config%n_par = phs_cfg_born%n_par
  phs_config%n_state = phs_cfg_born%n_state
  phs_config%sqrts = phs_cfg_born%sqrts
  phs_config%par = phs_cfg_born%par
  phs_config%sqrts_fixed = phs_cfg_born%sqrts_fixed
  phs_config%azimuthal_dependence = phs_cfg_born%azimuthal_dependence
  phs_config%provides_chains = phs_cfg_born%provides_chains
  phs_config%lab_is_cm = phs_cfg_born%lab_is_cm
  phs_config%vis_channels = phs_cfg_born%vis_channels
  phs_config%provides_equivalences = phs_cfg_born%provides_equivalences
  allocate (phs_config%chain (size (phs_cfg_born%chain)))
  phs_config%chain = phs_cfg_born%chain
  phs_config%model => phs_cfg_born%model
  phs_config%use_cascades2 = phs_cfg_born%use_cascades2
  if (allocated (phs_cfg_born%cascade_set)) then
    allocate (phs_config%cascade_set)
    phs_config%cascade_set = phs_cfg_born%cascade_set
  end if
  if (allocated (phs_cfg_born%feyngraph_set)) then

```

```

        allocate (phs_config%feyngraph_set)
        phs_config%feyngraph_set = phs_cfg_born%feyngraph_set
    end if
    phs_config%md5sum_born_config = phs_cfg_born%md5sum_phs_config
end subroutine phs_fks_config_set_born_config

<PHS fks: fks config: TBP>+≡
    procedure :: get_resonance_histories => &
        phs_fks_config_get_resonance_histories

<PHS fks: sub interfaces>+≡
    module function phs_fks_config_get_resonance_histories &
        (phs_config) result (resonance_histories)
        type(resonance_history_t), dimension(:), allocatable :: &
            resonance_histories
        class(phs_fks_config_t), intent(inout) :: phs_config
    end function phs_fks_config_get_resonance_histories

<PHS fks: procedures>+≡
    module function phs_fks_config_get_resonance_histories &
        (phs_config) result (resonance_histories)
        type(resonance_history_t), dimension(:), allocatable :: resonance_histories
        class(phs_fks_config_t), intent(inout) :: phs_config
        if (allocated (phs_config%cascade_set)) then
            call cascade_set_get_resonance_histories (phs_config%cascade_set, &
                n_filter = 2, res_hists = resonance_histories)
        else if (allocated (phs_config%feyngraph_set)) then
            call feyngraph_set_get_resonance_histories (phs_config%feyngraph_set, &
                n_filter = 2, res_hists = resonance_histories)
        else
            if (debug_on) call msg_debug (D_PHASESPACE, "Have to rebuild phase space for resonance hist
            call phs_config%generate_phase_space_extra ()
            if (phs_config%use_cascades2) then
                call feyngraph_set_get_resonance_histories &
                    (phs_config%feyngraph_set, n_filter = 2, res_hists = resonance_histories)
            else
                call cascade_set_get_resonance_histories &
                    (phs_config%cascade_set, n_filter = 2, res_hists = resonance_histories)
            end if
        end if
    end function phs_fks_config_get_resonance_histories

<PHS fks: public>+≡
    public :: dalitz_plot_t

<PHS fks: types>+≡
    type :: dalitz_plot_t
        integer :: unit = -1
        type(string_t) :: filename
        logical :: active = .false.
        logical :: inverse = .false.
    contains
        <PHS fks: dalitz plot: TBP>
    end type dalitz_plot_t

```



```

<PHS fks: dalitz plot: TBP>≡
  procedure :: init => dalitz_plot_init

<PHS fks: sub interfaces>+≡
  module subroutine dalitz_plot_init (plot, unit, filename, inverse)
    class(dalitz_plot_t), intent(inout) :: plot
    integer, intent(in) :: unit
    type(string_t), intent(in) :: filename
    logical, intent(in) :: inverse
  end subroutine dalitz_plot_init

<PHS fks: procedures>+≡
  module subroutine dalitz_plot_init (plot, unit, filename, inverse)
    class(dalitz_plot_t), intent(inout) :: plot
    integer, intent(in) :: unit
    type(string_t), intent(in) :: filename
    logical, intent(in) :: inverse
    plot%active = .true.
    plot%unit = unit
    plot%inverse = inverse
    open (plot%unit, file = char (filename), action = "write")
  end subroutine dalitz_plot_init

<PHS fks: dalitz plot: TBP>+≡
  procedure :: write_header => dalitz_plot_write_header

<PHS fks: sub interfaces>+≡
  module subroutine dalitz_plot_write_header (plot)
    class(dalitz_plot_t), intent(in) :: plot
  end subroutine dalitz_plot_write_header

<PHS fks: procedures>+≡
  module subroutine dalitz_plot_write_header (plot)
    class(dalitz_plot_t), intent(in) :: plot
    write (plot%unit, "(A36)") "### Dalitz plot generated by WHIZARD"
    if (plot%inverse) then
      write (plot%unit, "(A10,1x,A4)") "### k0_n+1", "k0_n"
    else
      write (plot%unit, "(A8,1x,A6)") "### k0_n", "k0_n+1"
    end if
  end subroutine dalitz_plot_write_header

<PHS fks: dalitz plot: TBP>+≡
  procedure :: register => dalitz_plot_register

<PHS fks: sub interfaces>+≡
  module subroutine dalitz_plot_register (plot, k0_n, k0_np1)
    class(dalitz_plot_t), intent(in) :: plot
    real(default), intent(in) :: k0_n, k0_np1
  end subroutine dalitz_plot_register

<PHS fks: procedures>+≡
  module subroutine dalitz_plot_register (plot, k0_n, k0_np1)
    class(dalitz_plot_t), intent(in) :: plot
    real(default), intent(in) :: k0_n, k0_np1
    if (plot%inverse) then

```

```

        write (plot%unit, "(F8.4,1X,F8.4)") k0_np1, k0_n
    else
        write (plot%unit, "(F8.4,1X,F8.4)") k0_np1, k0_n
    end if
end subroutine dalitz_plot_register

<PHS fks: dalitz plot: TBP>+≡
    procedure :: final => dalitz_plot_final
<PHS fks: sub interfaces>+≡
    module subroutine dalitz_plot_final (plot)
        class(dalitz_plot_t), intent(inout) :: plot
    end subroutine dalitz_plot_final
<PHS fks: procedures>+≡
    module subroutine dalitz_plot_final (plot)
        class(dalitz_plot_t), intent(inout) :: plot
        logical :: opened
        plot%active = .false.
        plot%inverse = .false.
        if (plot%unit >= 0) then
            inquire (unit = plot%unit, opened = opened)
            if (opened) close (plot%unit)
        end if
        plot%filename = var_str ('')
        plot%unit = -1
    end subroutine dalitz_plot_final

<PHS fks: parameters>+≡
    integer, parameter, public :: GEN_REAL_PHASE_SPACE = 1
    integer, parameter, public :: GEN_SOFT_MISMATCH = 2
    integer, parameter, public :: GEN_SOFT_LIMIT_TEST = 3
    integer, parameter, public :: GEN_COLL_LIMIT_TEST = 4
    integer, parameter, public :: GEN_ANTI_COLL_LIMIT_TEST = 5
    integer, parameter, public :: GEN_SOFT_COLL_LIMIT_TEST = 6
    integer, parameter, public :: GEN_SOFT_ANTI_COLL_LIMIT_TEST = 7

    integer, parameter, public :: SQRTS_FIXED = 1
    integer, parameter, public :: SQRTS_VAR = 2

    real(default), parameter :: xi_tilde_test_soft = 0.00001_default
    real(default), parameter :: xi_tilde_test_coll = 0.5_default
    real(default), parameter :: y_test_soft = 0.5_default
    real(default), parameter :: y_test_coll = 0.9999999_default
    !!! for testing EW singularities: y_test_coll = 0.99999999_default

```

Very soft or collinear phase-space points can become a problem for matrix elements providers, as some scalar products cannot be evaluated properly. Here, a nonsensical result can spoil the whole integration. We therefore check the scalar products appearing to be below a certain tolerance.

Naturally, this happens very rarely but for some processes, setting `?test_coll_limit = true` and/or `?test_soft_limit = true` leads to all phase space points being discarded by this routine.

```

<PHS fks: public>+≡

```

```

    public :: check_scalar_products

<PHS fks: sub interfaces>+≡
    module function check_scalar_products (p) result (valid)
        logical :: valid
        type(vector4_t), intent(in), dimension(:) :: p
    end function check_scalar_products

<PHS fks: procedures>+≡
    module function check_scalar_products (p) result (valid)
        logical :: valid
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), parameter :: tolerance = 1E-7_default
        !!! for testing EW singularities: tolerance = 5E-9_default
        integer :: i, j
        valid = .true.
        do i = 1, size (p)
            do j = i, size (p)
                if (i /= j) then
                    if (abs(p(i) * p(j)) < tolerance) then
                        valid = .false.
                        exit
                    end if
                end if
            end do
        end do
    end function check_scalar_products

```

xi_min should be set to a non-zero value in order to avoid phase-space points with p_real(emitter) = 0.

```

<PHS fks: public>+≡
    public :: phs_fks_generator_t

<PHS fks: types>+≡
    type :: phs_fks_generator_t
        integer, dimension(:), allocatable :: emitters
        type(real_kinematics_t), pointer :: real_kinematics => null()
        type(isr_kinematics_t), pointer :: isr_kinematics => null()
        integer :: n_in
        real(default) :: xi_min
        real(default) :: y_max
        real(default) :: sqrts
        real(default) :: E_gluon
        real(default) :: mrec2
        real(default), dimension(:), allocatable :: m2
        logical :: massive_phsp = .false.
        logical, dimension(:), allocatable :: is_massive
        logical :: singular_jacobian = .false.
        integer :: i_fsr_first = -1
        type(resonance_contributors_t), dimension(:), allocatable :: resonance_contributors !!! Put so
        integer :: mode = GEN_REAL_PHASE_SPACE
    contains
    <PHS fks: phs fks generator: TBP>
    end type phs_fks_generator_t

```

```

<PHS fks: phs fks generator: TBP>≡
  procedure :: connect_kinematics => phs_fks_generator_connect_kinematics

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_connect_kinematics &
    (generator, isr_kinematics, real_kinematics, massive_phsp)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(isr_kinematics_t), intent(in), pointer :: isr_kinematics
    type(real_kinematics_t), intent(in), pointer :: real_kinematics
    logical, intent(in) :: massive_phsp
  end subroutine phs_fks_generator_connect_kinematics

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_connect_kinematics &
    (generator, isr_kinematics, real_kinematics, massive_phsp)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(isr_kinematics_t), intent(in), pointer :: isr_kinematics
    type(real_kinematics_t), intent(in), pointer :: real_kinematics
    logical, intent(in) :: massive_phsp
    generator%real_kinematics => real_kinematics
    generator%isr_kinematics => isr_kinematics
    generator%massive_phsp = massive_phsp
  end subroutine phs_fks_generator_connect_kinematics

<PHS fks: phs fks generator: TBP>+≡
  procedure :: compute_isr_kinematics => &
    phs_fks_generator_compute_isr_kinematics

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_compute_isr_kinematics &
    (generator, r, p_in)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: r
    type(vector4_t), dimension(2), intent(in), optional :: p_in
  end subroutine phs_fks_generator_compute_isr_kinematics

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_compute_isr_kinematics &
    (generator, r, p_in)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: r
    type(vector4_t), dimension(2), intent(in), optional :: p_in
    integer :: em
    type(vector4_t), dimension(2) :: p

    if (present (p_in)) then
      p = p_in
    else
      p = generator%real_kinematics%p_born_lab%phs_point(1)%select ([1,2])
    end if

    associate (isr_kinematics => generator%isr_kinematics)
      do em = 1, 2
        isr_kinematics%x(em) = p(em)%p(0) / isr_kinematics%beam_energy(em)
        isr_kinematics%z(em) = one - (one - isr_kinematics%x(em)) * r
        isr_kinematics%jacobian(em) = one - isr_kinematics%x(em)
      end do
    end associate
  end subroutine

```

```

        end do
        isr_kinematics%sqrts_born = (p(1) + p(2))*1
    end associate
end subroutine phs_fks_generator_compute_isr_kinematics

<PHS fks: phs fks generator: TBP>+=
    procedure :: final => phs_fks_generator_final

<PHS fks: sub interfaces>+=
    module subroutine phs_fks_generator_final (generator)
        class(phs_fks_generator_t), intent(inout) :: generator
    end subroutine phs_fks_generator_final

<PHS fks: procedures>+=
    module subroutine phs_fks_generator_final (generator)
        class(phs_fks_generator_t), intent(inout) :: generator
        if (allocated (generator%emitters)) deallocate (generator%emitters)
        if (associated (generator%real_kinematics)) &
            nullify (generator%real_kinematics)
        if (associated (generator%isr_kinematics)) &
            nullify (generator%isr_kinematics)
        if (allocated (generator%m2)) deallocate (generator%m2)
        generator%massive_phsp = .false.
        if (allocated (generator%is_massive)) deallocate (generator%is_massive)
        generator%singular_jacobian = .false.
        generator%i_fsr_first = -1
        if (allocated (generator%resonance_contributors)) &
            deallocate (generator%resonance_contributors)
        generator%mode = GEN_REAL_PHASE_SPACE
    end subroutine phs_fks_generator_final

A resonance phase space is uniquely specified via the resonance contributors
and the corresponding emitters. The phs_identifier type also checks whether
the given contributor-emitter configuration has already been evaluated to avoid
duplicate computations.

<PHS fks: public>+=
    public :: phs_identifier_t

<PHS fks: types>+=
    type :: phs_identifier_t
        integer, dimension(:), allocatable :: contributors
        integer :: emitter = -1
        logical :: evaluated = .false.
    contains
        <PHS fks: phs identifier: TBP>
    end type phs_identifier_t

<PHS fks: phs identifier: TBP>=
    generic :: init => init_from_emitter, init_from_emitter_and_contributors
    procedure :: init_from_emitter => phs_identifier_init_from_emitter
    procedure :: init_from_emitter_and_contributors &
        => phs_identifier_init_from_emitter_and_contributors

```

```

<PHS fks: sub interfaces>+≡
    module subroutine phs_identifier_init_from_emitter (phs_id, emitter)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
    end subroutine phs_identifier_init_from_emitter
    module subroutine phs_identifier_init_from_emitter_and_contributors &
        (phs_id, emitter, contributors)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
        integer, intent(in), dimension(:) :: contributors
    end subroutine phs_identifier_init_from_emitter_and_contributors

<PHS fks: procedures>+≡
    module subroutine phs_identifier_init_from_emitter (phs_id, emitter)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
        phs_id%emitter = emitter
    end subroutine phs_identifier_init_from_emitter

    module subroutine phs_identifier_init_from_emitter_and_contributors &
        (phs_id, emitter, contributors)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
        integer, intent(in), dimension(:) :: contributors
        allocate (phs_id%contributors (size (contributors)))
        phs_id%contributors = contributors
        phs_id%emitter = emitter
    end subroutine phs_identifier_init_from_emitter_and_contributors

<PHS fks: phs identifier: TBP>+≡
    procedure :: check => phs_identifier_check

<PHS fks: sub interfaces>+≡
    module function phs_identifier_check &
        (phs_id, emitter, contributors) result (check)
        logical :: check
        class(phs_identifier_t), intent(in) :: phs_id
        integer, intent(in) :: emitter
        integer, intent(in), dimension(:), optional :: contributors
    end function phs_identifier_check

<PHS fks: procedures>+≡
    module function phs_identifier_check &
        (phs_id, emitter, contributors) result (check)
        logical :: check
        class(phs_identifier_t), intent(in) :: phs_id
        integer, intent(in) :: emitter
        integer, intent(in), dimension(:), optional :: contributors
        check = phs_id%emitter == emitter
        if (present (contributors)) then
            if (.not. allocated (phs_id%contributors)) &
                call msg_fatal ("Phs identifier: contributors not allocated!")
            check = check .and. all (phs_id%contributors == contributors)
        end if
    end function phs_identifier_check

```

```

<PHS fks: phs identifier: TBP>+≡
    procedure :: write => phs_identifier_write

<PHS fks: sub interfaces>+≡
    module subroutine phs_identifier_write (phs_id, unit)
        class(phs_identifier_t), intent(in) :: phs_id
        integer, intent(in), optional :: unit
    end subroutine phs_identifier_write

<PHS fks: procedures>+≡
    module subroutine phs_identifier_write (phs_id, unit)
        class(phs_identifier_t), intent(in) :: phs_id
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, '(A)') 'phs_identifier: '
        write (u, '(A,1X,I1)') 'Emitter: ', phs_id%emitter
        if (allocated (phs_id%contributors)) then
            write (u, '(A)', advance = 'no') 'Resonance contributors: '
            do i = 1, size (phs_id%contributors)
                write (u, '(I1,1X)', advance = 'no') phs_id%contributors(i)
            end do
        else
            write (u, '(A)') 'No Contributors allocated'
        end if
    end subroutine phs_identifier_write

<PHS fks: public>+≡
    public :: check_for_phs_identifier

<PHS fks: sub interfaces>+≡
    module subroutine check_for_phs_identifier &
        (phs_id, n_in, emitter, contributors, phs_exist, i_phs)
        type(phs_identifier_t), intent(in), dimension(:) :: phs_id
        integer, intent(in) :: n_in, emitter
        integer, intent(in), dimension(:), optional :: contributors
        logical, intent(out) :: phs_exist
        integer, intent(out) :: i_phs
    end subroutine check_for_phs_identifier

<PHS fks: procedures>+≡
    module subroutine check_for_phs_identifier &
        (phs_id, n_in, emitter, contributors, phs_exist, i_phs)
        type(phs_identifier_t), intent(in), dimension(:) :: phs_id
        integer, intent(in) :: n_in, emitter
        integer, intent(in), dimension(:), optional :: contributors
        logical, intent(out) :: phs_exist
        integer, intent(out) :: i_phs
        integer :: i
        phs_exist = .false.
        i_phs = -1
        do i = 1, size (phs_id)
            if (phs_id(i)%emitter < 0) then
                i_phs = i
                exit
            end if
        end do
    end subroutine

```

```

    phs_exist = phs_id(i)%emitter == emitter
    if (present (contributors)) &
        phs_exist = phs_exist .and. &
        all (phs_id(i)%contributors == contributors)
    if (phs_exist) then
        i_phs = i
        exit
    end if
end do
end subroutine check_for_phs_identifier

```

The fks phase space type contains the wood phase space and separately the in- and outgoing momenta for the real process and the corresponding Born momenta. Additionally, there are the variables ξ, ξ_{max}, y and ϕ which are used to create the real phase space, as well as the jacobian and its corresponding soft and collinear limit. Lastly, the array `ch_to_em` connects each channel with an emitter.

```

<PHS fks: public>+≡
    public :: phs_fks_t

<PHS fks: types>+≡
    type, extends (phs_wood_t) :: phs_fks_t
        integer :: mode = PHS_MODE_UNDEFINED
        type(vector4_t), dimension(:), allocatable :: p_born
        type(vector4_t), dimension(:), allocatable :: q_born
        type(vector4_t), dimension(:), allocatable :: p_real
        type(vector4_t), dimension(:), allocatable :: q_real
        type(vector4_t), dimension(:), allocatable :: p_born_tot
        type(phs_fks_generator_t) :: generator
        real(default) :: r_isr
        type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
    contains
        <PHS fks: phs fks: TBP>
    end type phs_fks_t

<PHS fks: interfaces>≡

    interface compute_beta
        module procedure compute_beta_massless
        module procedure compute_beta_massive
    end interface

    interface get_xi_max_fsr
        module procedure get_xi_max_fsr_massless
        module procedure get_xi_max_fsr_massive
    end interface

<PHS fks: phs fks: TBP>≡
    procedure :: write => phs_fks_write

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_write (object, unit, verbose)
        class(phs_fks_t), intent(in) :: object

```



```

        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine phs_fks_write
<PHS fks: procedures>+≡
module subroutine phs_fks_write (object, unit, verbose)
    class(phs_fks_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i, n_id
    u = given_output_unit (unit)
    call object%base_write ()
    n_id = size (object%phs_identifiers)
    if (n_id == 0) then
        write (u, "(A)") "No phs identifiers allocated! "
    else
        do i = 1, n_id
            call object%phs_identifiers(i)%write (u)
        end do
    end if
end subroutine phs_fks_write

```

Initializer for the phase space. Calls the initialization of the corresponding Born phase space, sets up the channel-emitter-association and allocates space for the momenta.

```

<PHS fks: phs fks: TBP>+≡
    procedure :: init => phs_fks_init
<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_init (phs, phs_config)
        class(phs_fks_t), intent(out) :: phs
        class(phs_config_t), intent(in), target :: phs_config
    end subroutine phs_fks_init
<PHS fks: procedures>+≡
module subroutine phs_fks_init (phs, phs_config)
    class(phs_fks_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config

    call phs%base_init (phs_config)
    select type (phs_config)
    type is (phs_fks_config_t)
        phs%config => phs_config
        phs%forest = phs_config%forest
    end select

    select type (phs)
    type is (phs_fks_t)
        select type (phs_config)
        type is (phs_fks_config_t)
            phs%mode = phs_config%mode
        end select

        select case (phs%mode)
        case (PHS_MODE_ADDITIONAL_PARTICLE)

```

```

        phs%n_r_born = phs%config%n_par - 3
    case (PHS_MODE_COLLINEAR_REMNANT)
        phs%n_r_born = phs%config%n_par - 1
    end select
end select
end subroutine phs_fks_init

```

For real components of $2 \rightarrow 1$ NLO processes we have to recompute the flux factor as this has to be the one of the underlying Born.

```

<PHS fks: phs fks: TBP>+≡
    procedure :: compute_flux => phs_fks_compute_flux

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_compute_flux (phs)
        class(phs_fks_t), intent(inout) :: phs
    end subroutine phs_fks_compute_flux

<PHS fks: procedures>+≡
    module subroutine phs_fks_compute_flux (phs)
        class(phs_fks_t), intent(inout) :: phs
        call phs%compute_base_flux ()
        select type (config => phs%config)
        type is (phs_fks_config_t)
            if (config%born_2_to_1) then
                phs%flux = conv * twopi &
                    / (2 * config%sqrts ** 2 * phs%m_out(1) ** 2)
            end if
        end select
    end subroutine phs_fks_compute_flux

<PHS fks: phs fks: TBP>+≡
    procedure :: allocate_momenta => phs_fks_allocate_momenta

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_allocate_momenta (phs, phs_config, data_is_born)
        class(phs_fks_t), intent(inout) :: phs
        class(phs_config_t), intent(in) :: phs_config
        logical, intent(in) :: data_is_born
    end subroutine phs_fks_allocate_momenta

<PHS fks: procedures>+≡
    module subroutine phs_fks_allocate_momenta (phs, phs_config, data_is_born)
        class(phs_fks_t), intent(inout) :: phs
        class(phs_config_t), intent(in) :: phs_config
        logical, intent(in) :: data_is_born
        integer :: n_out_born
        allocate (phs%p_born (phs_config%n_in))
        allocate (phs%p_real (phs_config%n_in))
        select case (phs%mode)
        case (PHS_MODE_ADDITIONAL_PARTICLE)
            if (data_is_born) then
                n_out_born = phs_config%n_out
            else
                n_out_born = phs_config%n_out - 1
            end if

```

```

        allocate (phs%q_born (n_out_born))
        allocate (phs%q_real (n_out_born + 1))
        allocate (phs%p_born_tot (phs_config%n_in + n_out_born))
    end select
end subroutine phs_fks_allocate_momenta

```

Evaluate selected channel. First, the subroutine calls the evaluation procedure of the underlying Born phase space, using $n_r - 3$ random numbers. Then, the remaining three random numbers are used to create ξ , y and ϕ , from which the real momenta are calculated from the Born momenta.

```

<PHS fks: phs fks: TBP>+≡
    procedure :: evaluate_selected_channel => phs_fks_evaluate_selected_channel

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_evaluate_selected_channel (phs, c_in, r_in)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: c_in
        real(default), intent(in), dimension(:) :: r_in
    end subroutine phs_fks_evaluate_selected_channel

<PHS fks: procedures>+≡
    module subroutine phs_fks_evaluate_selected_channel (phs, c_in, r_in)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: c_in
        real(default), intent(in), dimension(:) :: r_in
        integer :: n_in

        call phs%phs_wood_t%evaluate_selected_channel (c_in, r_in)
        phs%r(:,c_in) = r_in

        phs%q_defined = phs%phs_wood_t%q_defined
        if (.not. phs%q_defined) return

        select case (phs%mode)
        case (PHS_MODE_ADDITIONAL_PARTICLE)
            n_in = phs%config%n_in
            phs%p_born = phs%phs_wood_t%p
            phs%q_born = phs%phs_wood_t%q
            phs%p_born_tot (1: n_in) = phs%p_born
            phs%p_born_tot (n_in + 1 :) = phs%q_born
            call phs%set_reference_frames (.true.)
            call phs%set_isr_kinematics (.true.)
        case (PHS_MODE_COLLINEAR_REMNANT)
            call phs%compute_isr_kinematics (r_in(phs%n_r_born + 1))
            phs%r_isr = r_in(phs%n_r_born + 1)
        end select
    end subroutine phs_fks_evaluate_selected_channel

<PHS fks: phs fks: TBP>+≡
    procedure :: evaluate_other_channels => phs_fks_evaluate_other_channels

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_evaluate_other_channels (phs, c_in)
        class(phs_fks_t), intent(inout) :: phs

```

```

        integer, intent(in) :: c_in
    end subroutine phs_fks_evaluate_other_channels
<PHS fks: procedures>+≡
    module subroutine phs_fks_evaluate_other_channels (phs, c_in)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: c_in
        call phs%phs_wood_t%evaluate_other_channels (c_in)
        phs%r_defined = .true.
    end subroutine phs_fks_evaluate_other_channels

<PHS fks: phs fks: TBP>+≡
    procedure :: get_mcpair => phs_fks_get_mcpair
<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_get_mcpair (phs, c, r)
        class(phs_fks_t), intent(in) :: phs
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
    end subroutine phs_fks_get_mcpair
<PHS fks: procedures>+≡
    module subroutine phs_fks_get_mcpair (phs, c, r)
        class(phs_fks_t), intent(in) :: phs
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
        r(1 : phs%n_r_born) = phs%r(1 : phs%n_r_born,c)
        select case (phs%mode)
        case (PHS_MODE_ADDITIONAL_PARTICLE)
            r(phs%n_r_born + 1 :) = phs%r_real
        case (PHS_MODE_COLLINEAR_REMNANT)
            r(phs%n_r_born + 1 :) = phs%r_isr
        end select
    end subroutine phs_fks_get_mcpair

<PHS fks: phs fks: TBP>+≡
    procedure :: set_beam_energy => phs_fks_set_beam_energy
<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_set_beam_energy (phs)
        class(phs_fks_t), intent(inout) :: phs
    end subroutine phs_fks_set_beam_energy
<PHS fks: procedures>+≡
    module subroutine phs_fks_set_beam_energy (phs)
        class(phs_fks_t), intent(inout) :: phs
        call phs%generator%set_sqrts_hat (phs%config%sqrts)
    end subroutine phs_fks_set_beam_energy

<PHS fks: phs fks: TBP>+≡
    procedure :: set_emitters => phs_fks_set_emitters
<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_set_emitters (phs, emitters)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in), dimension(:), allocatable :: emitters
    end subroutine phs_fks_set_emitters

```

```

<PHS fks: procedures>+≡
  module subroutine phs_fks_set_emitters (phs, emitters)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in), dimension(:), allocatable :: emitters
    call phs%generator%set_emitters (emitters)
  end subroutine phs_fks_set_emitters

<PHS fks: phs fks: TBP>+≡
  procedure :: set_momenta => phs_fks_set_momenta

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_set_momenta (phs, p)
    class(phs_fks_t), intent(inout) :: phs
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine phs_fks_set_momenta

<PHS fks: procedures>+≡
  module subroutine phs_fks_set_momenta (phs, p)
    class(phs_fks_t), intent(inout) :: phs
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: n_in, n_tot_born
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      n_in = phs%config%n_in; n_tot_born = phs%config%n_tot - 1
      phs%p_born = p(1 : n_in)
      phs%q_born = p(n_in + 1 : n_tot_born)
      phs%p_born_tot = p
    end select
  end subroutine phs_fks_set_momenta

<PHS fks: phs fks: TBP>+≡
  procedure :: setup_masses => phs_fks_setup_masses

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_setup_masses (phs, n_tot)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: n_tot
  end subroutine phs_fks_setup_masses

<PHS fks: procedures>+≡
  module subroutine phs_fks_setup_masses (phs, n_tot)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: n_tot
    call phs%generator%setup_masses (n_tot)
  end subroutine phs_fks_setup_masses

<PHS fks: phs fks: TBP>+≡
  procedure :: get_born_momenta => phs_fks_get_born_momenta

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_get_born_momenta (phs, p)
    class(phs_fks_t), intent(inout) :: phs
    type(vector4_t), intent(out), dimension(:) :: p
  end subroutine phs_fks_get_born_momenta

```

```

<PHS fks: procedures>+≡
module subroutine phs_fks_get_born_momenta (phs, p)
  class(phs_fks_t), intent(inout) :: phs
  type(vector4_t), intent(out), dimension(:) :: p
  select case (phs%mode)
  case (PHS_MODE_ADDITIONAL_PARTICLE)
    p(1 : phs%config%n_in) = phs%p_born
    p(phs%config%n_in + 1 :) = phs%q_born
  case (PHS_MODE_COLLINEAR_REMNANT)
    p(1:phs%config%n_in) = phs%phs_wood_t%p
    p(phs%config%n_in + 1 :) = phs%phs_wood_t%q
  end select
  if (.not. phs%config%lab_is_cm) p = phs%lt_cm_to_lab * p
end subroutine phs_fks_get_born_momenta

<PHS fks: phs fks: TBP>+≡
procedure :: get_outgoing_momenta => phs_fks_get_outgoing_momenta

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_get_outgoing_momenta (phs, q)
  class(phs_fks_t), intent(in) :: phs
  type(vector4_t), intent(out), dimension(:) :: q
end subroutine phs_fks_get_outgoing_momenta

<PHS fks: procedures>+≡
module subroutine phs_fks_get_outgoing_momenta (phs, q)
  class(phs_fks_t), intent(in) :: phs
  type(vector4_t), intent(out), dimension(:) :: q
  select case (phs%mode)
  case (PHS_MODE_ADDITIONAL_PARTICLE)
    q = phs%q_real
  case (PHS_MODE_COLLINEAR_REMNANT)
    q = phs%phs_wood_t%q
  end select
end subroutine phs_fks_get_outgoing_momenta

<PHS fks: phs fks: TBP>+≡
procedure :: get_incoming_momenta => phs_fks_get_incoming_momenta

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_get_incoming_momenta (phs, p)
  class(phs_fks_t), intent(in) :: phs
  type(vector4_t), intent(inout), dimension(:), allocatable :: p
end subroutine phs_fks_get_incoming_momenta

<PHS fks: procedures>+≡
module subroutine phs_fks_get_incoming_momenta (phs, p)
  class(phs_fks_t), intent(in) :: phs
  type(vector4_t), intent(inout), dimension(:), allocatable :: p
  p = phs%p_real
end subroutine phs_fks_get_incoming_momenta

<PHS fks: phs fks: TBP>+≡
procedure :: set_isr_kinematics => phs_fks_set_isr_kinematics

```

```

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_set_isr_kinematics (phs, requires_boost)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: requires_boost
  end subroutine phs_fks_set_isr_kinematics

<PHS fks: procedures>+≡
  module subroutine phs_fks_set_isr_kinematics (phs, requires_boost)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: requires_boost
    type(vector4_t), dimension(2) :: p
    if (phs%generator%isr_kinematics%isr_mode == SQRTS_VAR) then
      if (requires_boost) then
        p = phs%lt_cm_to_lab &
          * phs%generator%real_kinematics%p_born_cms%phs_point(1)%select ([1,2])
      else
        p = phs%generator%real_kinematics%p_born_lab%phs_point(1)%select ([1,2])
      end if
      call phs%generator%set_isr_kinematics (p)
    end if
  end subroutine phs_fks_set_isr_kinematics

<PHS fks: phs fks: TBP>+≡
  procedure :: generate_radiation_variables => &
    phs_fks_generate_radiation_variables

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generate_radiation_variables &
    (phs, r_in, threshold)
    class(phs_fks_t), intent(inout) :: phs
    real(default), intent(in), dimension(:) :: r_in
    logical, intent(in) :: threshold
  end subroutine phs_fks_generate_radiation_variables

<PHS fks: procedures>+≡
  module subroutine phs_fks_generate_radiation_variables &
    (phs, r_in, threshold)
    class(phs_fks_t), intent(inout) :: phs
    real(default), intent(in), dimension(:) :: r_in
    logical, intent(in) :: threshold
    type(vector4_t), dimension(:), allocatable :: p_born
    if (size (r_in) /= 3) call msg_fatal &
      ("Real kinematics need to be generated using three random numbers!")
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      allocate (p_born (size (phs%p_born_tot)))
      if (threshold) then
        p_born = phs%get_onshell_projected_momenta ()
      else
        p_born = phs%p_born_tot
        if (.not. phs%lab_is_cm ()) &
          p_born = inverse (phs%lt_cm_to_lab) * p_born
        end if
      call phs%generator%generate_radiation_variables &
        (r_in, p_born, phs%phs_identifiers, threshold)
    end case
  end subroutine

```

```

        phs%r_real = r_in
    end select
end subroutine phs_fks_generate_radiation_variables

<PHS fks: phs fks: TBP>+≡
    procedure :: compute_xi_ref_momenta => phs_fks_compute_xi_ref_momenta

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_compute_xi_ref_momenta (phs, p_in, contributors)
        class(phs_fks_t), intent(inout) :: phs
        type(vector4_t), intent(in), dimension(:), optional :: p_in
        type(resonance_contributors_t), intent(in), dimension(:), optional :: &
            contributors
    end subroutine phs_fks_compute_xi_ref_momenta

<PHS fks: procedures>+≡
    module subroutine phs_fks_compute_xi_ref_momenta (phs, p_in, contributors)
        class(phs_fks_t), intent(inout) :: phs
        type(vector4_t), intent(in), dimension(:), optional :: p_in
        type(resonance_contributors_t), intent(in), dimension(:), optional :: &
            contributors
        if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) then
            if (present (p_in)) then
                call phs%generator%compute_xi_ref_momenta (p_in, contributors)
            else
                call phs%generator%compute_xi_ref_momenta &
                    (phs%p_born_tot, contributors)
            end if
        end if
    end subroutine phs_fks_compute_xi_ref_momenta

<PHS fks: phs fks: TBP>+≡
    procedure :: compute_xi_ref_momenta_threshold => &
        phs_fks_compute_xi_ref_momenta_threshold

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_compute_xi_ref_momenta_threshold (phs)
        class(phs_fks_t), intent(inout) :: phs
    end subroutine phs_fks_compute_xi_ref_momenta_threshold

<PHS fks: procedures>+≡
    module subroutine phs_fks_compute_xi_ref_momenta_threshold (phs)
        class(phs_fks_t), intent(inout) :: phs
        select case (phs%mode)
        case (PHS_MODE_ADDITIONAL_PARTICLE)
            call phs%generator%compute_xi_ref_momenta_threshold &
                (phs%get_onshell_projected_momenta ())
        end select
    end subroutine phs_fks_compute_xi_ref_momenta_threshold

<PHS fks: phs fks: TBP>+≡
    procedure :: compute_cms_energy => phs_fks_compute_cms_energy

```



```

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_compute_cms_energy (phs)
    class(phs_fks_t), intent(inout) :: phs
  end subroutine phs_fks_compute_cms_energy

<PHS fks: procedures>+≡
  module subroutine phs_fks_compute_cms_energy (phs)
    class(phs_fks_t), intent(inout) :: phs
    if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) &
      call phs%generator%compute_cms_energy (phs%p_born_tot)
  end subroutine phs_fks_compute_cms_energy

```

When initial-state radiation is involved, either due to beamstrahlung or QCD/QED corrections, it is important to have access to both the phase space points in the center-of-mass and lab frame.

```

<PHS fks: phs fks: TBP>+≡
  procedure :: set_reference_frames => phs_fks_set_reference_frames

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_set_reference_frames (phs, is_cms)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: is_cms
  end subroutine phs_fks_set_reference_frames

<PHS fks: procedures>+≡
  module subroutine phs_fks_set_reference_frames (phs, is_cms)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: is_cms
    associate (real_kinematics => phs%generator%real_kinematics)
      if (phs%config%lab_is_cm) then
        real_kinematics%p_born_cms%phs_point(1) = phs%p_born_tot
        real_kinematics%p_born_lab%phs_point(1) = phs%p_born_tot
      else
        if (is_cms) then
          real_kinematics%p_born_cms%phs_point(1) &
            = phs%p_born_tot
          real_kinematics%p_born_lab%phs_point(1) &
            = phs%lt_cm_to_lab * phs%p_born_tot
        else
          real_kinematics%p_born_cms%phs_point(1) &
            = inverse (phs%lt_cm_to_lab) * phs%p_born_tot
          real_kinematics%p_born_lab%phs_point(1) &
            = phs%p_born_tot
        end if
      end if
    end associate
  end subroutine phs_fks_set_reference_frames

```

```

<PHS fks: phs fks: TBP>+≡
  procedure :: i_phs_is_isr => phs_fks_i_phs_is_isr

<PHS fks: sub interfaces>+≡
  module function phs_fks_i_phs_is_isr (phs, i_phs) result (is_isr)
    logical :: is_isr
    class(phs_fks_t), intent(in) :: phs

```

```

integer, intent(in) :: i_phs
end function phs_fks_i_phs_is_isr

<PHS fks: procedures>+≡
module function phs_fks_i_phs_is_isr (phs, i_phs) result (is_isr)
logical :: is_isr
class(phs_fks_t), intent(in) :: phs
integer, intent(in) :: i_phs
is_isr = phs%phs_identifiers(i_phs)%emitter <= phs%generator%n_in
end function phs_fks_i_phs_is_isr

```

19.13.1 Creation of the real phase space - FSR

At this point, the Born phase space has been generated, as well as the three random variables ξ , y and ϕ . The question is how the real phase space is generated for a final-state emission configuration. We work with two different sets of momenta, the Born configuration $\{\bar{k}_\oplus, \bar{k}_\ominus, \bar{k}_1, \dots, \bar{k}_n\}$ and the real configuration $\{k_\oplus, k_\ominus, k_1, \dots, k_n, k_{n+1}\}$. We define the momentum of the emitter to be on the n -th position and the momentum of the radiated particle to be at position $n+1$. The magnitude of the spatial component of \mathbf{k} is denoted by \underline{k} .

For final-state emissions, it is $\bar{k}_\oplus = k_\oplus$ and $\bar{k}_\ominus = k_\ominus$. Thus, the center-of-mass systems coincide and it is

$$q = \sum_{i=1}^n \bar{k}_i = \sum_{i=1}^{n+1} k_i, \quad (19.65)$$

with $\vec{q} = 0$ and $q^2 = (q^0)^2$.

We want to construct the real phase space from the Born phase space using three random numbers. They are defined as follows:

- $\xi = \frac{2k_{n+1}^0}{\sqrt{s}} \in [0, \xi_{max}]$, where k_{n+1} denotes the four-momentum of the radiated particle.
- $y = \cos \theta = \frac{\vec{k}_n \cdot \vec{k}_{n+1}}{\underline{k}_n \underline{k}_{n+1}}$ is the splitting angle.
- The angle between the two splitting particles in the transversal plane, $\phi \in [0, 2\pi]$.

Further, $k_{rec} = \sum_{i=1}^{n-1} k_i$ denotes the sum of all recoiling momenta.

```

<PHS fks: phs fks generator: TBP>+≡
generic :: generate_fsr => generate_fsr_default, generate_fsr_resonances

<PHS fks: phs fks generator: TBP>+≡
procedure :: generate_fsr_default => phs_fks_generator_generate_fsr_default

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_generator_generate_fsr_default &
(generator, emitter, i_phs, &
p_born, p_real, xi_y_phi, no_jacobians)
class(phs_fks_generator_t), intent(inout) :: generator
integer, intent(in) :: emitter, i_phs

```

```

        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(out), dimension(:) :: p_real
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians
    end subroutine phs_fks_generator_generate_fsr_default

<PHS fks: procedures>+≡
    module subroutine phs_fks_generator_generate_fsr_default &
        (generator, emitter, i_phs, &
         p_born, p_real, xi_y_phi, no_jacobians)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: emitter, i_phs
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(out), dimension(:) :: p_real
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians
        real(default) :: q0

        call generator%generate_fsr_in (p_born, p_real)
        q0 = sum (p_born(1:generator%n_in))*1
        generator%i_fsr_first = generator%n_in + 1
        call generator%generate_fsr_out (emitter, i_phs, p_born, p_real, q0, &
            xi_y_phi = xi_y_phi, no_jacobians = no_jacobians)
        if (debug_active (D_PHASESPACE)) then
            call vector4_check_momentum_conservation (p_real, generator%n_in, &
                rel_smallness = 1000 * tiny_07, abs_smallness = tiny_07)
        end if
    end subroutine phs_fks_generator_generate_fsr_default

<PHS fks: phs fks generator: TBP>+≡
    procedure :: generate_fsr_resonances => &
        phs_fks_generator_generate_fsr_resonances

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_generator_generate_fsr_resonances (generator, &
        emitter, i_phs, i_con, p_born, p_real, xi_y_phi, no_jacobians)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: emitter, i_phs
        integer, intent(in) :: i_con
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(inout), dimension(:) :: p_real
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians
    end subroutine phs_fks_generator_generate_fsr_resonances

<PHS fks: procedures>+≡
    module subroutine phs_fks_generator_generate_fsr_resonances (generator, &
        emitter, i_phs, i_con, p_born, p_real, xi_y_phi, no_jacobians)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: emitter, i_phs
        integer, intent(in) :: i_con
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(inout), dimension(:) :: p_real
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians

```

```

integer, dimension(:), allocatable :: resonance_list
integer, dimension(size(p_born)) :: inv_resonance_list
type(vector4_t), dimension(:), allocatable :: p_tmp_born
type(vector4_t), dimension(:), allocatable :: p_tmp_real
type(vector4_t) :: p_resonance
real(default) :: q0
integer :: i, j, nlegborn, nlegreal
integer :: i_emitter
type(lorentz_transformation_t) :: boost_to_resonance
integer :: n_resonant_particles
if (debug_on) call msg_debug2 (D_PHASESPACE, "phs_fks_generator_generate_fsr_resonances")
nlegborn = size (p_born); nlegreal = nlegborn + 1
allocate (resonance_list (size (generator%resonance_contributors(i_con)%c)))
resonance_list = generator%resonance_contributors(i_con)%c
n_resonant_particles = size (resonance_list)

if (.not. any (resonance_list == emitter)) then
    call msg_fatal ("Emitter must be included in the resonance list!")
else
    do i = 1, n_resonant_particles
        if (resonance_list (i) == emitter) i_emitter = i
    end do
end if

inv_resonance_list = &
    create_inverse_resonance_list (nlegborn, resonance_list)

allocate (p_tmp_born (n_resonant_particles))
allocate (p_tmp_real (n_resonant_particles + 1))
p_tmp_born = vector4_null
p_tmp_real = vector4_null
j = 1
do i = 1, n_resonant_particles
    p_tmp_born(j) = p_born(resonance_list(i))
    j = j + 1
end do

call generator%generate_fsr_in (p_born, p_real)

p_resonance = generator%real_kinematics%xi_ref_momenta(i_con)
q0 = p_resonance**1

boost_to_resonance = inverse (boost (p_resonance, q0))
p_tmp_born = boost_to_resonance * p_tmp_born

generator%i_fsr_first = 1
call generator%generate_fsr_out (emitter, i_phs, p_tmp_born, p_tmp_real, &
    q0, i_emitter, xi_y_phi)
p_tmp_real = inverse (boost_to_resonance) * p_tmp_real

do i = generator%n_in + 1, nlegborn
    if (any (resonance_list == i)) then
        p_real(i) = p_tmp_real(inv_resonance_list (i))
    else

```

```

        p_real(i) = p_born (i)
    end if
end do
p_real(nlegreal) = p_tmp_real (n_resonant_particles + 1)

if (debug_active (D_PHASESPACE)) then
    call vector4_check_momentum_conservation (p_real, generator%n_in, &
        rel_smallness = 1000 * tiny_07, abs_smallness = tiny_07)
end if

```

contains

```

function create_inverse_resonance_list (nlegborn, resonance_list) &
    result (inv_resonance_list)
    integer, intent(in) :: nlegborn
    integer, intent(in), dimension(:) :: resonance_list
    integer, dimension(nlegborn) :: inv_resonance_list
    integer :: i, j
    inv_resonance_list = 0
    j = 1
    do i = 1, nlegborn
        if (any (i == resonance_list)) then
            inv_resonance_list (i) = j
            j = j + 1
        end if
    end do
end function create_inverse_resonance_list

function boosted_energy () result (E)
    real(default) :: E
    type(vector4_t) :: p_boost
    p_boost = boost_to_resonance * p_resonance
    E = p_boost%p(0)
end function boosted_energy
end subroutine phs_fks_generator_generate_fsr_resonances

```

<PHS fks: phs fks generator: TBP>+≡

```

procedure :: generate_fsr_threshold => &
    phs_fks_generator_generate_fsr_threshold

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_generate_fsr_threshold (generator, &
    emitter, i_phs, p_born, p_real, xi_y_phi)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default), intent(in), dimension(3), optional :: xi_y_phi
end subroutine phs_fks_generator_generate_fsr_threshold

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generator_generate_fsr_threshold (generator, &
    emitter, i_phs, p_born, p_real, xi_y_phi)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs

```

```

type(vector4_t), intent(in), dimension(:) :: p_born
type(vector4_t), intent(inout), dimension(:) :: p_real
real(default), intent(in), dimension(3), optional :: xi_y_phi
type(vector4_t), dimension(2) :: p_tmp_born
type(vector4_t), dimension(3) :: p_tmp_real
integer :: nlegborn, nlegreal
type(vector4_t) :: p_top
real(default) :: q0
type(lorentz_transformation_t) :: boost_to_top
integer :: leg, other_leg
real(default) :: sqrts, mtop
if (debug_on) call msg_debug2 &
    (D_PHASESPACE, "phs_fks_generator_generate_fsr_resonances")
nlegborn = size (p_born); nlegreal = nlegborn + 1

leg = thr_leg(emitter); other_leg = 3 - leg

p_tmp_born(1) = p_born (ass_boson(leg))
p_tmp_born(2) = p_born (ass_quark(leg))

call generator%generate_fsr_in (p_born, p_real)

p_top = generator%real_kinematics%xi_ref_momenta(leg)

q0 = p_top**1
sqrts = two * p_born(1)%p(0)
mtop = mls_to_mpole (sqrts)
if (sqrts**2 - four * mtop**2 > zero) then
    boost_to_top = inverse (boost (p_top, q0))
else
    boost_to_top = identity
end if
p_tmp_born = boost_to_top * p_tmp_born

generator%i_fsr_first = 1
call generator%generate_fsr_out (emitter, i_phs, p_tmp_born, &
    p_tmp_real, q0, 2, xi_y_phi)
p_tmp_real = inverse (boost_to_top) * p_tmp_real

p_real(ass_boson(leg)) = p_tmp_real(1)
p_real(ass_quark(leg)) = p_tmp_real(2)
p_real(ass_boson(other_leg)) = p_born(ass_boson(other_leg))
p_real(ass_quark(other_leg)) = p_born(ass_quark(other_leg))
p_real(THR_POS_GLUON) = p_tmp_real(3)

end subroutine phs_fks_generator_generate_fsr_threshold

<PHS fks: phs fks generator: TBP>+≡
    procedure :: generate_fsr_in => phs_fks_generator_generate_fsr_in
<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_generator_generate_fsr_in &
        (generator, p_born, p_real)
        class(phs_fks_generator_t), intent(inout) :: generator

```

```

        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(out), dimension(:) :: p_real
    end subroutine phs_fks_generator_generate_fsr_in

<PHS fks: procedures>+≡
module subroutine phs_fks_generator_generate_fsr_in &
    (generator, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
    integer :: i
    do i = 1, generator%n_in
        p_real(i) = p_born(i)
    end do
end subroutine phs_fks_generator_generate_fsr_in

<PHS fks: phs fks generator: TBP>+≡
procedure :: generate_fsr_out => phs_fks_generator_generate_fsr_out

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_generator_generate_fsr_out (generator, &
    emitter, i_phs, p_born, p_real, q0, p_emitter_index, &
    xi_y_phi, no_jacobians)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default), intent(in) :: q0
    integer, intent(in), optional :: p_emitter_index
    real(default), intent(in), dimension(3), optional :: xi_y_phi
    logical, intent(in), optional :: no_jacobians
end subroutine phs_fks_generator_generate_fsr_out

<PHS fks: procedures>+≡
module subroutine phs_fks_generator_generate_fsr_out (generator, &
    emitter, i_phs, p_born, p_real, q0, p_emitter_index, &
    xi_y_phi, no_jacobians)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default), intent(in) :: q0
    integer, intent(in), optional :: p_emitter_index
    real(default), intent(in), dimension(3), optional :: xi_y_phi
    logical, intent(in), optional :: no_jacobians
    real(default) :: xi, y, phi
    integer :: nlegborn, nlegreal
    real(default) :: uk_np1, uk_n
    real(default) :: uk_rec, k_rec0
    type(vector3_t) :: k_n_born, k
    real(default) :: uk_n_born, uk, k2, k0_n
    real(default) :: cpsi, beta
    type(vector3_t) :: vec, vec_orth
    type(lorentz_transformation_t) :: rot
    integer :: i, p_em

```

```

logical :: compute_jac
p_em = emitter; if (present (p_emitter_index)) p_em = p_emitter_index
compute_jac = .true.
if (present (no_jacobians)) compute_jac = .not. no_jacobians
if (generator%i_fsr_first < 0) &
    call msg_fatal ("FSR generator is called for outgoing particles but "&
        &"i_fsr_first is not set!")

if (present (xi_y_phi)) then
    xi = xi_y_phi(I_XI)
    y = xi_y_phi(I_Y)
    phi = xi_y_phi(I_PHI)
else
    associate (rad_var => generator%real_kinematics)
        xi = rad_var%xi_tilde
        if (rad_var%supply_xi_max) xi = xi * rad_var%xi_max(i_phs)
        y = rad_var%y(i_phs)
        phi = rad_var%phi
    end associate
end if

nlegborn = size (p_born)
nlegreal = nlegborn + 1
generator%E_gluon = q0 * xi / two
uk_np1 = generator%E_gluon
k_n_born = p_born(p_em)%p(1:3)
uk_n_born = k_n_born**1

generator%mrec2 = (q0 - p_born(p_em)%p(0))**2 &
    - space_part_norm(p_born(p_em))**2
if (generator%is_massive(emitter)) then
    call generator%compute_emitter_kinematics (y, emitter, &
        i_phs, q0, k0_n, uk_n, uk, compute_jac)
else
    call generator%compute_emitter_kinematics (y, q0, uk_n, uk)
    generator%real_kinematics%y_soft(i_phs) = y
    k0_n = uk_n
end if

if (debug_on) call msg_debug2 &
    (D_PHASESPACE, "phs_fks_generator_generate_fsr_out")
call debug_input_values ()

vec = uk_n / uk_n_born * k_n_born
vec_orth = create_orthogonal (vec)
p_real(p_em)%p(0) = k0_n
p_real(p_em)%p(1:3) = vec%p(1:3)
cpsi = (uk_n**2 + uk**2 - uk_np1**2) / (two * uk_n * uk)
!!! This is to catch the case where cpsi = 1, but numerically
!!! turns out to be slightly larger than 1.
call check_cpsi_bound (cpsi)
rot = rotation (cpsi, - sqrt (one - cpsi**2), vec_orth)
p_real(p_em) = rot * p_real(p_em)
vec = uk_np1 / uk_n_born * k_n_born

```



```

    vec_orth = create_orthogonal (vec)
    p_real(nlegreal)%p(0) = uk_np1
    p_real(nlegreal)%p(1:3) = vec%p(1:3)
    cpsi = (uk_np1**2 + uk**2 - uk_n**2) / (two * uk_np1 * uk)
    call check_cpsi_bound (cpsi)
    rot = rotation (cpsi, sqrt (one - cpsi**2), vec_orth)
    p_real(nlegreal) = rot * p_real(nlegreal)
    call construct_recoiling_momenta ()
    if (compute_jac) call compute_jacobians ()

contains

<PHS fks: generator generate fsr out procedures>

end subroutine phs_fks_generator_generate_fsr_out

<PHS fks: generator generate fsr out procedures>≡
subroutine debug_input_values ()
  if (debug2_active (D_PHASESPACE)) then
    call generator%write ()
    print *, 'emitter = ', emitter
    print *, 'p_born:'
    call vector4_write_set (p_born)
    print *, 'p_real:'
    call vector4_write_set (p_real)
    print *, 'q0 = ', q0
    if (present(p_emitter_index)) then
      print *, 'p_emitter_index = ', p_emitter_index
    else
      print *, 'p_emitter_index not given'
    end if
  end if
end if
end subroutine debug_input_values

<PHS fks: generator generate fsr out procedures>+≡
subroutine check_cpsi_bound (cpsi)
  real(default), intent(inout) :: cpsi
  if (cpsi > one) then
    cpsi = one
  else if (cpsi < -one) then
    cpsi = - one
  end if
end subroutine check_cpsi_bound

```

Construction of the recoiling momenta. The reshuffling of momenta must not change the invariant mass of the recoiling system, which means $k_{\text{rec}}^2 = k_{\text{rec}}^{-2}$. Therefore, the momenta are related by a boost, $\bar{k}_i = \Lambda k_i$. The boost parameter is

$$\beta = \frac{q^2 - (k_{\text{rec}}^0 + \underline{k}_{\text{rec}})^2}{q^2 + (k_{\text{rec}}^0 + \underline{k}_{\text{rec}})^2}$$

```

<PHS fks: generator generate fsr out procedures>+≡
subroutine construct_recoiling_momenta ()

```

```

type(lorentz_transformation_t) :: lambda
k_rec0 = q0 - p_real(p_em)%p(0) - p_real(nlegreal)%p(0)
if (k_rec0**2 > generator%mrec2) then
    uk_rec = sqrt (k_rec0**2 - generator%mrec2)
else
    uk_rec = 0
end if
if (generator%is_massive(emitter)) then
    beta = compute_beta (q0**2, k_rec0, uk_rec, &
        p_born(p_em)%p(0), uk_n_born)
else
    beta = compute_beta (q0**2, k_rec0, uk_rec)
end if
k = p_real(p_em)%p(1:3) + p_real(nlegreal)%p(1:3)
vec%p(1:3) = one / uk * k%p(1:3)
lambda = boost (beta / sqrt(one - beta**2), vec)
do i = generator%i_fsr_first, nlegborn
    if (i /= p_em) then
        p_real(i) = lambda * p_born(i)
    end if
end do
vec%p(1:3) = p_born(p_em)%p(1:3) / uk_n_born
rot = rotation (cos(phi), sin(phi), vec)
p_real(nlegreal) = rot * p_real(nlegreal)
p_real(p_em) = rot * p_real(p_em)
end subroutine construct_recoiling_momenta

```

The factor $\frac{q^2}{(4\pi)^3}$ is not included here since it is supplied during phase space generation. Also, we already divide by ξ .

(PHS fks: generator generate fsr out procedures)+≡

```

subroutine compute_jacobians ()
    associate (jac => generator%real_kinematics%jac(i_phs))
        if (generator%is_massive(emitter)) then
            jac%jac(1) = jac%jac(1) * four / q0 / uk_n_born / xi
        else
            k2 = two * uk_n * uk_np1* (one - y)
            jac%jac(1) = uk_n**2 / uk_n_born / (uk_n - k2 / (two * q0))
        end if
        jac%jac(2) = one
        jac%jac(3) = one - xi / two * q0 / uk_n_born
    end associate
end subroutine compute_jacobians

```

(PHS fks: phs fks: TBP)+≡

```

procedure :: generate_fsr_in => phs_fks_generate_fsr_in

```

(PHS fks: sub interfaces)+≡

```

module subroutine phs_fks_generate_fsr_in (phs)
    class(phs_fks_t), intent(inout) :: phs
end subroutine phs_fks_generate_fsr_in

```

(PHS fks: procedures)+≡

```

module subroutine phs_fks_generate_fsr_in (phs)
    class(phs_fks_t), intent(inout) :: phs

```

```

        type(vector4_t), dimension(:), allocatable :: p
        p = phs%generator%real_kinematics%p_born_lab%get_momenta &
            (1, phs%generator%n_in)
    end subroutine phs_fks_generate_fsr_in

<PHS fks: phs fks: TBP>+≡
    procedure :: generate_fsr => phs_fks_generate_fsr

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_generate_fsr (phs, emitter, i_phs, p_real, &
        i_con, xi_y_phi, no_jacobians)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: emitter, i_phs
        type(vector4_t), intent(out), dimension(:) :: p_real
        integer, intent(in), optional :: i_con
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians
    end subroutine phs_fks_generate_fsr

<PHS fks: procedures>+≡
    module subroutine phs_fks_generate_fsr (phs, emitter, i_phs, p_real, &
        i_con, xi_y_phi, no_jacobians)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: emitter, i_phs
        type(vector4_t), intent(out), dimension(:) :: p_real
        integer, intent(in), optional :: i_con
        real(default), intent(in), dimension(3), optional :: xi_y_phi
        logical, intent(in), optional :: no_jacobians
        type(vector4_t), dimension(:), allocatable :: p
        associate (generator => phs%generator)
            p = generator%real_kinematics%p_born_cms%phs_point(1)
            generator%real_kinematics%supply_xi_max = .true.
            if (present (i_con)) then
                call generator%generate_fsr (emitter, i_phs, i_con, p, p_real, &
                    xi_y_phi, no_jacobians)
            else
                call generator%generate_fsr (emitter, i_phs, p, p_real, &
                    xi_y_phi, no_jacobians)
            end if
            generator%real_kinematics%p_real_cms%phs_point(i_phs) = p_real
            if (.not. phs%config%lab_is_cm) p_real = phs%lt_cm_to_lab * p_real
            generator%real_kinematics%p_real_lab%phs_point(i_phs) = p_real
        end associate
    end subroutine phs_fks_generate_fsr

<PHS fks: phs fks: TBP>+≡
    procedure :: get_onshell_projected_momenta => &
        phs_fks_get_onshell_projected_momenta

<PHS fks: sub interfaces>+≡
    pure module function phs_fks_get_onshell_projected_momenta (phs) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(phs_fks_t), intent(in) :: phs
    end function phs_fks_get_onshell_projected_momenta

```

```

<PHS fks: procedures>+≡
pure module function phs_fks_get_onshell_projected_momenta (phs) result (p)
  type(vector4_t), dimension(:), allocatable :: p
  class(phs_fks_t), intent(in) :: phs
  p = phs%generator%real_kinematics%p_born_onshell%phs_point(1)
end function phs_fks_get_onshell_projected_momenta

<PHS fks: phs fks: TBP>+≡
procedure :: generate_fsr_threshold => phs_fks_generate_fsr_threshold

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_generate_fsr_threshold &
  (phs, emitter, i_phs, p_real)
  class(phs_fks_t), intent(inout) :: phs
  integer, intent(in) :: emitter, i_phs
  type(vector4_t), intent(inout), dimension(:), optional :: p_real
end subroutine phs_fks_generate_fsr_threshold

<PHS fks: procedures>+≡
module subroutine phs_fks_generate_fsr_threshold &
  (phs, emitter, i_phs, p_real)
  class(phs_fks_t), intent(inout) :: phs
  integer, intent(in) :: emitter, i_phs
  type(vector4_t), intent(inout), dimension(:), optional :: p_real
  type(vector4_t), dimension(:), allocatable :: p_born
  type(vector4_t), dimension(:), allocatable :: pp
  integer :: leg
  associate (generator => phs%generator)
    generator%real_kinematics%supply_xi_max = .true.
    allocate (p_born (1 : generator%real_kinematics%p_born_cms%get_n_particles()))
    p_born = generator%real_kinematics%p_born_onshell%get_momenta (1)
    allocate (pp (size (p_born) + 1))
    call generator%generate_fsr_threshold (emitter, i_phs, p_born, pp)
    leg = thr_leg (emitter)
    call generator%real_kinematics%p_real_onshell(leg)%set_momenta (i_phs, pp)
    if (present (p_real)) p_real = pp
  end associate
end subroutine phs_fks_generate_fsr_threshold

<PHS fks: phs fks: TBP>+≡
generic :: compute_xi_max => &
  compute_xi_max_internal, compute_xi_max_with_output
procedure :: compute_xi_max_internal => phs_fks_compute_xi_max_internal

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_compute_xi_max_internal (phs, p, threshold)
  class(phs_fks_t), intent(inout) :: phs
  type(vector4_t), intent(in), dimension(:) :: p
  logical, intent(in) :: threshold
end subroutine phs_fks_compute_xi_max_internal

<PHS fks: procedures>+≡
module subroutine phs_fks_compute_xi_max_internal (phs, p, threshold)
  class(phs_fks_t), intent(inout) :: phs
  type(vector4_t), intent(in), dimension(:) :: p

```

```

logical, intent(in) :: threshold
integer :: i_phs, i_con, emitter
do i_phs = 1, size (phs%phs_identifiers)
  associate (phs_id => phs%phs_identifiers(i_phs), generator => phs%generator)
    emitter = phs_id%emitter
    if (threshold) then
      call generator%compute_xi_max (emitter, i_phs, p, &
        generator%real_kinematics%xi_max(i_phs), i_con = thr_leg(emitter))
    else if (allocated (phs_id%contributors)) then
      do i_con = 1, size (phs_id%contributors)
        call generator%compute_xi_max (emitter, i_phs, p, &
          generator%real_kinematics%xi_max(i_phs), i_con = 1)
      end do
    else
      call generator%compute_xi_max (emitter, i_phs, p, &
        generator%real_kinematics%xi_max(i_phs))
    end if
  end associate
end do
end subroutine phs_fks_compute_xi_max_internal

```

(PHS fks: phs fks: TBP)+≡

```

procedure :: compute_xi_max_with_output => phs_fks_compute_xi_max_with_output

```

(PHS fks: sub interfaces)+≡

```

module subroutine phs_fks_compute_xi_max_with_output &
  (phs, emitter, i_phs, y, p, xi_max)
  class(phs_fks_t), intent(inout) :: phs
  integer, intent(in) :: i_phs, emitter
  real(default), intent(in) :: y
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(out) :: xi_max
end subroutine phs_fks_compute_xi_max_with_output

```

(PHS fks: procedures)+≡

```

module subroutine phs_fks_compute_xi_max_with_output &
  (phs, emitter, i_phs, y, p, xi_max)
  class(phs_fks_t), intent(inout) :: phs
  integer, intent(in) :: i_phs, emitter
  real(default), intent(in) :: y
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(out) :: xi_max
  call phs%generator%compute_xi_max (emitter, i_phs, p, xi_max, y_in = y)
end subroutine phs_fks_compute_xi_max_with_output

```

(PHS fks: phs fks generator: TBP)+≡

```

generic :: compute_emitter_kinematics => &
  compute_emitter_kinematics_massless, &
  compute_emitter_kinematics_massive
procedure :: compute_emitter_kinematics_massless => &
  phs_fks_generator_compute_emitter_kinematics_massless
procedure :: compute_emitter_kinematics_massive => &
  phs_fks_generator_compute_emitter_kinematics_massive

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_compute_emitter_kinematics_massless &
  (generator, y, q0, uk_em, uk)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in) :: y, q0
  real(default), intent(out) :: uk_em, uk
end subroutine phs_fks_generator_compute_emitter_kinematics_massless
module subroutine phs_fks_generator_compute_emitter_kinematics_massive &
  (generator, y, em, i_phs, q0, k0_em, uk_em, uk, compute_jac)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in) :: y
  integer, intent(in) :: em, i_phs
  real(default), intent(in) :: q0
  real(default), intent(inout) :: k0_em, uk_em, uk
  logical, intent(in) :: compute_jac
end subroutine phs_fks_generator_compute_emitter_kinematics_massive

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generator_compute_emitter_kinematics_massless &
  (generator, uk)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in) :: y, q0
  real(default), intent(out) :: uk_em, uk
  real(default) :: k0_np1, q2

  k0_np1 = generator%E_gluon
  q2 = q0**2

  uk_em = (q2 - generator%mrec2 - two * q0 * k0_np1) / &
    (two * (q0 - k0_np1 * (one - y)))
  uk = sqrt (uk_em**2 + k0_np1**2 + two * uk_em * k0_np1 * y)
end subroutine phs_fks_generator_compute_emitter_kinematics_massless

module subroutine phs_fks_generator_compute_emitter_kinematics_massive &
  (generator, y, em, i_phs, q0, k0_em, uk_em, uk, compute_jac)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in) :: y
  integer, intent(in) :: em, i_phs
  real(default), intent(in) :: q0
  real(default), intent(inout) :: k0_em, uk_em, uk
  logical, intent(in) :: compute_jac
  real(default) :: k0_np1, q2, mrec2, m2
  real(default) :: k0_rec_max, k0_em_max, k0_rec, uk_rec
  real(default) :: z, z1, z2

  k0_np1 = generator%E_gluon
  q2 = q0**2
  mrec2 = generator%mrec2
  m2 = generator%m2(em)

  k0_rec_max = (q2 - m2 + mrec2) / (two * q0)
  k0_em_max = (q2 + m2 - mrec2) / (two * q0)
  z1 = (k0_rec_max + sqrt (k0_rec_max**2 - mrec2)) / q0
  z2 = (k0_rec_max - sqrt (k0_rec_max**2 - mrec2)) / q0
  z = z2 - (z2 - z1) * (one + y) / two

```

```

k0_em = k0_em_max - k0_np1 * z
k0_rec = q0 - k0_np1 - k0_em
uk_em = sqrt(k0_em**2 - m2)
uk_rec = sqrt(k0_rec**2 - mrec2)
uk = uk_rec
if (compute_jac) &
    generator%real_kinematics%jac(i_phs)%jac = q0 * (z1 - z2) / four * k0_np1
generator%real_kinematics%y_soft(i_phs) = &
    (two * q2 * z - q2 - mrec2 + m2) / (sqrt(k0_em_max**2 - m2) * q0) / two
end subroutine phs_fks_generator_compute_emitter_kinematics_massive

```

(PHS fks: procedures)+≡

```

function recompute_xi_max (q0, mrec2, m2, y) result (xi_max)
    real(default) :: xi_max
    real(default), intent(in) :: q0, mrec2, m2, y
    real(default) :: q2, k0_np1_max, k0_rec_max
    real(default) :: z1, z2, z
    q2 = q0**2
    k0_rec_max = (q2 - m2 + mrec2) / (two * q0)
    z1 = (k0_rec_max + sqrt(k0_rec_max**2 - mrec2)) / q0
    z2 = (k0_rec_max - sqrt(k0_rec_max**2 - mrec2)) / q0
    z = z2 - (z2 - z1) * (one + y) / 2
    k0_np1_max = - (q2 * z**2 - two * q0 * k0_rec_max * z + mrec2) / (two * q0 * z * (one - z))
    xi_max = two * k0_np1_max / q0
end function recompute_xi_max

```

(PHS fks: procedures)+≡

```

function compute_beta_massless (q2, k0_rec, uk_rec) result (beta)
    real(default), intent(in) :: q2, k0_rec, uk_rec
    real(default) :: beta
    beta = (q2 - (k0_rec + uk_rec)**2) / (q2 + (k0_rec + uk_rec)**2)
end function compute_beta_massless

function compute_beta_massive (q2, k0_rec, uk_rec, &
    k0_em_born, uk_em_born) result (beta)
    real(default), intent(in) :: q2, k0_rec, uk_rec
    real(default), intent(in) :: k0_em_born, uk_em_born
    real(default) :: beta
    real(default) :: k0_rec_born, uk_rec_born, alpha
    k0_rec_born = sqrt(q2) - k0_em_born
    uk_rec_born = uk_em_born
    alpha = (k0_rec + uk_rec) / (k0_rec_born + uk_rec_born)
    beta = (one - alpha**2) / (one + alpha**2)
end function compute_beta_massive

```

The momentum of the radiated particle is computed according to

$$\underline{k}_n = \frac{q^2 - M_{\text{rec}}^2 - 2q^0 \underline{k}_{n+1}}{2(q^0 - \underline{k}_{n+1}(1 - y))}, \quad (19.66)$$

with $k = k_n + k_{n+1}$ and $M_{\text{rec}}^2 = k_{\text{rec}}^2 = (q - k)^2$. Because of $\bar{\mathbf{k}}_n \parallel \mathbf{k}_n + \mathbf{k}_{n+1}$ we find $M_{\text{rec}}^2 = (q - \bar{\mathbf{k}}_n)^2$. Equation 19.66 follows from the fact that $(\mathbf{k} - \mathbf{k}_n)^2 =$

\mathbf{k}_{n+1}^2 , which is equivalent to $\mathbf{k}_n \cdot \mathbf{k} = \frac{1}{2}(\underline{k}_n^2 + \underline{k}^2 - \underline{k}_{n+1}^2)$.
 \mathbf{k}_n and \mathbf{k}_{n+1} are obtained by first setting up vectors parallel to $\bar{\mathbf{k}}_n$,

$$\mathbf{k}'_n = \underline{k}_n \frac{\bar{\mathbf{k}}_n}{\underline{k}_n}, \quad \mathbf{k}'_{n+1} = \underline{k}_{n+1} \frac{\bar{\mathbf{k}}_n}{\underline{k}_n},$$

and then rotating these vectors by an amount of $\cos \psi_n = \frac{\mathbf{k}_n \cdot \mathbf{k}}{\underline{k}_n \underline{k}}$. The emitted particle cannot have more momentum than the emitter has in the Born phase space. Thus, there is an upper bound for ξ , determined by the condition $k_{n+1}^0 = \underline{k}_n$, which is equal to

$$\xi_{\max} = \frac{2}{\underline{k}_n} q^0.$$

(PHS fks: procedures)+≡

```
pure function get_xi_max_fsr_massless (p_born, q0, emitter) result (xi_max)
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: q0
  integer, intent(in) :: emitter
  real(default) :: xi_max
  real(default) :: uk_n_born
  uk_n_born = space_part_norm (p_born(emitter))
  xi_max = two * uk_n_born / q0
end function get_xi_max_fsr_massless
```

The computation of ξ_{\max} for massive emitters is described in arXiv:1202.0465. Let's recapitulate it here.

We consider the Dalitz-domain created by k_{n+1}^0 , k_n^0 and k_{rec}^0 and introduce the parameterization

$$k_n^0 = \bar{k}_n^0 - z k_{n+1}^0$$

Then, for each value of z , there exists a maximum value of \underline{k}_{n+1} from which ξ_{\max} can be extracted via $\xi_{\max} = 2k_{n+1}^0/q$. It is determined by the condition

$$\underline{k}_{n+1} \pm \underline{k}_n \pm \underline{k}_{\text{rec}} = 0.$$

This can be manipulated to yield

$$(\underline{k}_{n+1}^2 + \underline{k}_n^2 - \underline{k}_{\text{rec}}^2)^2 = 4\underline{k}_{n+1}^2 \underline{k}_n^2.$$

Here we can use $\underline{k}_n^2 = (k_n^0)^2 - m^2$ and $\underline{k}_{\text{rec}}^2 = (q - k_n^0 - k_{n+1}^0)^2 - M_{\text{rec}}^2$, as well as the above parameterization of k_n^0 , to obtain

$$4\underline{k}_{n+1}^2 (2\underline{k}_{n+1} q z (1 - z) + q^2 z^2 - 2q \bar{k}_{\text{rec}}^0 z + M_{\text{rec}}^2) = 0.$$

Solving for k_{n+1}^0 gives

$$k_{n+1}^0 = \frac{2q \bar{k}_{\text{rec}}^0 z - q^2 z^2 - M_{\text{rec}}^2}{2q z (1 - z)}. \quad (19.67)$$

It is still open how to compute z . For this, consider that the right-hand-side of equation (19.67) vanishes for

$$z_{1,2} = \left(\bar{k}_{\text{rec}}^0 \pm \sqrt{(\bar{k}_{\text{rec}}^0)^2 - M_{\text{rec}}^2} \right) / q,$$

which corresponds to the borders of the Dalitz-region where the gluon momentum vanishes. Thus we define

$$z = z_2 - \frac{1}{2}(z_2 - z_1)(1 + y).$$

(PHS fks: procedures)+≡

```
pure function get_xi_max_fsr_massive (p_born, q0, emitter, m2, y) result (xi_max)
  real(default) :: xi_max
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: q0
  integer, intent(in) :: emitter
  real(default), intent(in) :: m2, y
  real(default) :: mrec2
  real(default) :: k0_rec_max
  real(default) :: z, z1, z2
  real(default) :: k0_np1_max
  associate (p => p_born(emitter)%p)
    mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
  end associate
  call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
  z = z2 - (z2 - z1) * (one + y) / two
  k0_np1_max = - (q0**2 * z**2 - two * q0 * k0_rec_max * z + mrec2) &
    / (two * q0 * z * (one - z))
  xi_max = two * k0_np1_max / q0
end function get_xi_max_fsr_massive
```

(PHS fks: parameters)+≡

```
integer, parameter, public :: I_PLUS = 1
integer, parameter, public :: I_MINUS = 2
```

Computes ξ_{\max} in the case of ISR as documented in eq. 27.39. It is also used for the POWHEG matching.

(PHS fks: public)+≡

```
public :: get_xi_max_isr
```

(PHS fks: sub interfaces)+≡

```
module function get_xi_max_isr (xb, y) result (xi_max)
  real(default) :: xi_max
  real(default), dimension(2), intent(in) :: xb
  real(default), intent(in) :: y
end function get_xi_max_isr
```

(PHS fks: procedures)+≡

```
module function get_xi_max_isr (xb, y) result (xi_max)
  real(default) :: xi_max
  real(default), dimension(2), intent(in) :: xb
  real(default), intent(in) :: y
  xi_max = one - max (xi_max_isr_plus (xb(I_PLUS), y), xi_max_isr_minus (xb(I_MINUS), y))
contains
  function xi_max_isr_plus (x, y)
    real(default) :: xi_max_isr_plus
    real(default), intent(in) :: x, y
    real(default) :: deno
    deno = sqrt ((one + x**2)**2 * (one - y)**2 + 16 * y * x**2) + (one - y) * (1 - x**2)
```

```

        xi_max_isr_plus = two * (one + y) * x**2 / deno
end function xi_max_isr_plus

function xi_max_isr_minus (x, y)
    real(default) :: xi_max_isr_minus
    real(default), intent(in) :: x, y
    real(default) :: deno
    deno = sqrt ((one + x**2)**2 * (one + y)**2 - 16 * y * x**2) + (one + y) * (1 - x**2)
    xi_max_isr_minus = two * (one - y) * x**2 / deno
end function xi_max_isr_minus
end function get_xi_max_isr

```

<PHS fks: procedures>+≡

```

recursive function get_xi_max_isr_decay (p) result (xi_max)
    real(default) :: xi_max
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: n_tot
    type(vector4_t), dimension(:), allocatable :: p_dec_new
    n_tot = size (p)
    if (n_tot == 3) then
        xi_max = xi_max_one_to_two (p(1), p(2), p(3))
    else
        allocate (p_dec_new (n_tot - 1))
        p_dec_new(1) = sum (p (3 : ))
        p_dec_new(2 : n_tot - 1) = p (3 : n_tot)
        xi_max = min (xi_max_one_to_two (p(1), p(2), sum(p(3 : ))), &
            get_xi_max_isr_decay (p_dec_new))
    end if
contains
    function xi_max_one_to_two (p_in, p_out1, p_out2) result (xi_max)
        real(default) :: xi_max
        type(vector4_t), intent(in) :: p_in, p_out1, p_out2
        real(default) :: m_in, m_out1, m_out2
        m_in = p_in**1
        m_out1 = p_out1**1; m_out2 = p_out2**1
        xi_max = one - (m_out1 + m_out2)**2 / m_in**2
    end function xi_max_one_to_two
end function get_xi_max_isr_decay

```

19.13.2 Creation of the real phase space - ISR

<PHS fks: phs fks: TBP>+≡

```

procedure :: generate_isr => phs_fks_generate_isr

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generate_isr (phs, i_phs, p_real)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: i_phs
    type(vector4_t), intent(out), dimension(:) :: p_real
end subroutine phs_fks_generate_isr

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generate_isr (phs, i_phs, p_real)

```

```

class(phs_fks_t), intent(inout) :: phs
integer, intent(in) :: i_phs
type(vector4_t), intent(out), dimension(:) :: p_real
type(vector4_t) :: p0, p1
type(lorentz_transformation_t) :: lt
real(default) :: sqrts_hat
type(vector4_t), dimension(:), allocatable :: p_work

associate (generator => phs%generator)
  select case (generator%n_in)
  case (1)
    p_work = generator%real_kinematics%p_born_cms%phs_point(1)
    call generator%generate_isr_fixed_beam_energy (i_phs, p_work, p_real)
    phs%config%lab_is_cm = .true.
  case (2)
    select case (generator%isr_kinematics%isr_mode)
    case (SQRTS_FIXED)
      p_work = generator%real_kinematics%p_born_cms%phs_point(1)
      call generator%generate_isr_fixed_beam_energy (i_phs, p_work, p_real)
    case (SQRTS_VAR)
      p_work = generator%real_kinematics%p_born_lab%phs_point(1)
      call generator%generate_isr (i_phs, p_work, p_real)
    end select
  end select
  generator%real_kinematics%p_real_lab%phs_point(i_phs) = p_real
  if (.not. phs%config%lab_is_cm) then
    sqrts_hat = (p_real(1) + p_real(2))*1
    p0 = p_real(1) + p_real(2)
    lt = boost (p0, sqrts_hat)
    p1 = inverse(lt) * p_real(1)
    lt = lt * rotation_to_2nd (3, space_part (p1))
    phs%generator%real_kinematics%p_real_cms%phs_point(i_phs) &
      = inverse (lt) * p_real
  else
    phs%generator%real_kinematics%p_real_cms%phs_point(i_phs) &
      = p_real
  end if
end if
end associate
end subroutine phs_fks_generate_isr

```

The real phase space for an initial-state emission involved in a decay process is generated by first setting the gluon momentum like in the scattering case by using its angular coordinates y and ϕ and then adjusting the gluon energy with ξ . The emitter momentum is kept identical to the Born case, i.e. $p_{\text{in}} = \bar{p}_{\text{in}}$, so that after the emission it has momentum $p_{\text{virt}} = p_{\text{in}} - p_g$ and invariant mass $m^2 = p_{\text{virt}}^2$. Note that the final state momenta have to remain on-shell, so that $p_1^2 = \bar{p}_1^2 = m_1^2$ and $p_2^2 = \bar{p}_2^2 = m_2^2$. Let Λ be the boost from into the rest frame of the emitter after emission, i.e. $\Lambda p_{\text{virt}} = (m, 0, 0, 0)$. In this reference frame, the spatial components of the final-state momenta sum up to zero, and their magnitude is

$$p = \frac{\sqrt{\lambda(m^2, m_1^2, m_2^2)}}{2m},$$

a fact already used in the evaluation of the phase space trees of `phs_forest`. Obviously, from this, the final-state energies can be deferred via $E_i^2 = m_i^2 - p^2$. In the next step, the $p_{1,2}$ are set up as vectors $(E, 0, 0, \pm p)$ along the z-axis and then rotated about the same azimuthal and polar angles as in the Born system. Finally, the momenta are boosted out of the rest frame by multiplying with Λ .

```

(PHS fks: phs fks generator: TBP)+≡
  procedure :: generate_isr_fixed_beam_energy => &
    phs_fks_generator_generate_isr_fixed_beam_energy

(PHS fks: sub interfaces)+≡
  module subroutine phs_fks_generator_generate_isr_fixed_beam_energy &
    (generator, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
  end subroutine phs_fks_generator_generate_isr_fixed_beam_energy

(PHS fks: procedures)+≡
  module subroutine phs_fks_generator_generate_isr_fixed_beam_energy &
    (generator, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
    real(default) :: xi_max, xi, y, phi
    integer :: nlegborn, nlegreal, i
    real(default) :: k0_np1
    real(default) :: msq_in
    type(vector4_t) :: p_virt
    real(default) :: jac_real

    associate (rad_var => generator%real_kinematics)
      xi_max = rad_var%xi_max(i_phs)
      xi = rad_var%xi_tilde * xi_max
      y = rad_var%y(i_phs)
      phi = rad_var%phi
      rad_var%y_soft(i_phs) = y
    end associate

    nlegborn = size (p_born)
    nlegreal = nlegborn + 1

    msq_in = sum (p_born(1:generator%n_in))**2
    generator%real_kinematics%jac(i_phs)%jac = one

    p_real(1) = p_born(1)
    if (generator%n_in > 1) p_real(2) = p_born(2)
    k0_np1 = zero
    do i = 1, generator%n_in
      k0_np1 = k0_np1 + p_real(i)%p(0) * xi / two
    end do
    p_real(nlegreal)%p(0) = k0_np1
    p_real(nlegreal)%p(1) = k0_np1 * sqrt(one - y**2) * sin(phi)
    p_real(nlegreal)%p(2) = k0_np1 * sqrt(one - y**2) * cos(phi)

```

```

p_real(nlegreal)%p(3) = k0_np1 * y

p_virt = sum (p_real(1:generator%n_in)) - p_real(nlegreal)

jac_real = one
call generate_on_shell_decay (p_virt, &
    p_born(generator%n_in + 1 : nlegborn), &
    p_real(generator%n_in + 1 : nlegreal - 1), 1, msq_in, jac_real)

associate (jac => generator%real_kinematics%jac(i_phs))
    jac%jac(1) = jac_real
    jac%jac(2) = one
end associate

end subroutine phs_fks_generator_generate_isr_fixed_beam_energy

<PHS fks: phs fks generator: TBP>+≡
procedure :: generate_isr_factorized => &
    phs_fks_generator_generate_isr_factorized

<PHS fks: sub interfaces>+≡
module subroutine phs_fks_generator_generate_isr_factorized &
    (generator, i_phs, emitter, p_born, p_real)
class(phs_fks_generator_t), intent(inout) :: generator
integer, intent(in) :: i_phs, emitter
type(vector4_t), intent(in), dimension(:) :: p_born
type(vector4_t), intent(out), dimension(:) :: p_real
end subroutine phs_fks_generator_generate_isr_factorized

<PHS fks: procedures>+≡
module subroutine phs_fks_generator_generate_isr_factorized &
    (generator, i_phs, emitter, p_born, p_real)
class(phs_fks_generator_t), intent(inout) :: generator
integer, intent(in) :: i_phs, emitter
type(vector4_t), intent(in), dimension(:) :: p_born
type(vector4_t), intent(out), dimension(:) :: p_real
type(vector4_t), dimension(3) :: p_tmp_born
type(vector4_t), dimension(4) :: p_tmp_real
type(vector4_t) :: p_top
type(lorentz_transformation_t) :: boost_to_rest_frame
integer, parameter :: nlegreal = 7
!!! Factorized phase space so far only required for ee -> bwbw

p_tmp_born = vector4_null; p_tmp_real = vector4_null
p_real(1:2) = p_born(1:2)
if (emitter == THR_POS_B) then
    p_top = p_born (THR_POS_WP) + p_born (THR_POS_B)
    p_tmp_born(2) = p_born (THR_POS_WP)
    p_tmp_born(3) = p_born (THR_POS_B)
else if (emitter == THR_POS_BBAR) then
    p_top = p_born (THR_POS_WM) + p_born (THR_POS_BBAR)
    p_tmp_born(2) = p_born (THR_POS_WM)
    p_tmp_born(3) = p_born (THR_POS_BBAR)
else
    call msg_fatal ("Threshold computation requires emitters to be at position 5 and 6 " // &

```

```

        "Please check if your process specification fulfills this requirement.")
    end if
    p_tmp_born (1) = p_top
    boost_to_rest_frame = inverse (boost (p_top, p_top**1))
    p_tmp_born = boost_to_rest_frame * p_tmp_born
    call generator%compute_xi_max_isr_factorized (i_phs, p_tmp_born)
    call generator%generate_isr_fixed_beam_energy &
        (i_phs, p_tmp_born, p_tmp_real)
    p_tmp_real = inverse (boost_to_rest_frame) * p_tmp_real
    if (emitter == THR_POS_B) then
        p_real(THR_POS_WP) = p_tmp_real(2)
        p_real(THR_POS_B) = p_tmp_real(3)
        p_real(THR_POS_WM) = p_born(THR_POS_WM)
        p_real(THR_POS_BBAR) = p_born(THR_POS_BBAR)
        !!! Exception has been handled above
    else
        p_real(THR_POS_WM) = p_tmp_real(2)
        p_real(THR_POS_BBAR) = p_tmp_real(3)
        p_real(THR_POS_WP) = p_born(THR_POS_WP)
        p_real(THR_POS_B) = p_born(THR_POS_B)
    end if
    p_real(nlegreal) = p_tmp_real(4)
end subroutine phs_fks_generator_generate_isr_factorized

```

Construction of the real momenta `p_real` in case of ISR. Follows the discussion in [0709.2092] sec. 5.1. The sequence of Lorentz boosts required to construct `p_real` from `p_born` is as follows:

- We construct the IS momenta of `p_real` from the Born momenta via rescaling: $\mathbf{p_real}(1:2) = \frac{x}{\bar{x}} \cdot \mathbf{p_born}(1:2)$. If the Born momenta are imported in the lab frame, these will define the real lab frame.
- We construct the momentum of the radiated particle in the real CMS: $k_{n+1} = \frac{s\xi}{2} \cdot (1, \sin(\theta) \sin(\phi), \sin(\theta) \cos(\phi), \cos(\theta))$
- 0. We first boost the momentum of the radiated particle from the real CMS to the real lab frame determined from `p_real(1:2)`.
- 1. We initialize the non-radiated real FS momenta by a longitudinal boost of `p_born` to a system with zero rapidity, i.e. zero longitudinal momentum. This is \mathbb{B}_L .
- 2. We boost these momenta in a transverse direction to compensate the transverse momentum of the radiation. This is \mathbb{B}_T . Note: we switched \mathbb{B}_T and \mathbb{B}_T^{-1} in Eq. (5.16) and their definition w.r.t. [0709.2092].
- 3. We restore longitudinal momentum conservation by applying the inverse boost of \mathbb{B}_L to all non-radiated real FS momenta.

This way, all components of `p_real` are constructed in the real Lab frame.

```

⟨PHS fks: phs fks generator: TBP⟩ +=
  procedure :: generate_isr => phs_fks_generator_generate_isr

```

```

(PHS fks: sub interfaces)+≡
module subroutine phs_fks_generator_generate_isr &
  (generator, i_phs, p_born, p_real)
  class(phs_fks_generator_t), intent(inout) :: generator
  integer, intent(in) :: i_phs
  type(vector4_t), intent(in) , dimension(:) :: p_born
  type(vector4_t), intent(out), dimension(:) :: p_real
end subroutine phs_fks_generator_generate_isr

(PHS fks: procedures)+≡
module subroutine phs_fks_generator_generate_isr &
  (generator, i_phs, p_born, p_real)
  !!! Important: Import Born momenta in the lab frame
  class(phs_fks_generator_t), intent(inout) :: generator
  integer, intent(in) :: i_phs
  type(vector4_t), intent(in) , dimension(:) :: p_born
  type(vector4_t), intent(out), dimension(:) :: p_real
  real(default) :: xi_max, xi_tilde, xi, y, phi
  integer :: nlegborn, nlegreal
  real(default) :: sqrts_real
  real(default) :: k0_np1
  type(lorentz_transformation_t) :: &
    lambda_transv, lambda_longit, lambda_longit_inv
  real(default) :: x_plus, x_minus, xb_plus, xb_minus
  real(default) :: onemy, onepy
  integer :: i
  real(default) :: xi_plus, xi_minus
  real(default) :: beta_gamma
  type(vector3_t) :: beta_vec

  associate (rad_var => generator%real_kinematics)
    xi_max = rad_var%xi_max(i_phs)
    xi_tilde = rad_var%xi_tilde
    xi = xi_tilde * xi_max
    y = rad_var%y(i_phs)
    onemy = one - y; onepy = one + y
    phi = rad_var%phi
    rad_var%y_soft(i_phs) = y
  end associate

  nlegborn = size (p_born)
  nlegreal = nlegborn + 1
  generator%isr_kinematics%sqrts_born = (p_born(1) + p_born(2))*1

  !!! Initial state real momenta
  xb_plus = generator%isr_kinematics%x(I_PLUS)
  xb_minus = generator%isr_kinematics%x(I_MINUS)
  x_plus = xb_plus / sqrt(one - xi) * sqrt ((two - xi * onemy) / &
    (two - xi * onepy))
  x_minus = xb_minus / sqrt(one - xi) * sqrt ((two - xi * onepy) / &
    (two - xi * onemy))
  xi_plus = xi_tilde * (one - xb_plus)
  xi_minus = xi_tilde * (one - xb_minus)
  p_real(I_PLUS) = x_plus / xb_plus * p_born(I_PLUS)
  p_real(I_MINUS) = x_minus / xb_minus * p_born(I_MINUS)

```

```

!!! Fraction of momentum fractions in a collinear splitting
generator%isr_kinematics%z(I_PLUS) = (one - xi_plus)
generator%isr_kinematics%z(I_MINUS) = (one - xi_minus)

!!! Create radiation momentum in the real CMS
sqrts_real = generator%isr_kinematics%sqrts_born / sqrt (one - xi)
k0_np1 = sqrts_real * xi / two
p_real(nlegreal)%p(0) = k0_np1
p_real(nlegreal)%p(1) = k0_np1 * sqrt (one - y**2) * sin(phi)
p_real(nlegreal)%p(2) = k0_np1 * sqrt (one - y**2) * cos(phi)
p_real(nlegreal)%p(3) = k0_np1 * y

!!! Boosts the radiation from real CMS to the real LAB frame
call get_boost_parameters (p_real, beta_gamma, beta_vec)
lambda_longit = create_longitudinal_boost &
    (beta_gamma, beta_vec, inverse = .true.)
p_real(nlegreal) = lambda_longit * p_real(nlegreal)

call get_boost_parameters (p_born, beta_gamma, beta_vec)
lambda_longit = create_longitudinal_boost &
    (beta_gamma, beta_vec, inverse = .false.)
forall (i = 3 : nlegborn) p_real(i) = lambda_longit * p_born(i)

lambda_transv = create_transversal_boost (p_real(nlegreal), xi, sqrts_real)
forall (i = 3 : nlegborn) p_real(i) = lambda_transv * p_real(i)

lambda_longit_inv = create_longitudinal_boost &
    (beta_gamma, beta_vec, inverse = .true.)
forall (i = 3 : nlegborn) p_real(i) = lambda_longit_inv * p_real(i)

!!! Compute Jacobians
associate (jac => generator%real_kinematics%jac(i_phs))
!!! Additional 1 / (1 - xi) factor because in the real jacobian,
!!! there is s_real in the numerator
!!! We also have to adapt the flux factor, which is 1/(2s_real) for
!!! the real component
!!! The reweighting factor is s_born / s_real, cancelling the
!!! (1-xi) factor from above
jac%jac(1) = one / (one - xi)
jac%jac(2) = one
jac%jac(3) = one / (one - xi_plus)**2
jac%jac(4) = one / (one - xi_minus)**2
end associate
contains
subroutine get_boost_parameters (p, beta_gamma, beta_vec)
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(out) :: beta_gamma
    type(vector3_t), intent(out) :: beta_vec
    beta_vec = (p(1)%p(1:3) + p(2)%p(1:3)) / (p(1)%p(0) + p(2)%p(0))
    beta_gamma = beta_vec**1 / sqrt (one - beta_vec**2)
    beta_vec = beta_vec / beta_vec**1
end subroutine get_boost_parameters

```



```

function create_longitudinal_boost &
    (beta_gamma, beta_vec, inverse) result (lambda)
    real(default), intent(in) :: beta_gamma
    type(vector3_t), intent(in) :: beta_vec
    logical, intent(in) :: inverse
    type(lorentz_transformation_t) :: lambda
    if (inverse) then
        lambda = boost (beta_gamma, beta_vec)
    else
        lambda = boost (-beta_gamma, beta_vec)
    end if
end function create_longitudinal_boost

function create_transversal_boost (p_rad, xi, sqrts_real) result (lambda)
    type(vector4_t), intent(in) :: p_rad
    real(default), intent(in) :: xi, sqrts_real
    type(lorentz_transformation_t) :: lambda
    type(vector3_t) :: vec_transverse
    real(default) :: pt2, beta, beta_gamma
    pt2 = transverse_part (p_rad)**2
    beta = one / sqrt (one + sqrts_real**2 * (one - xi) / pt2)
    beta_gamma = beta / sqrt (one - beta**2)
    vec_transverse%p(1:2) = p_rad%p(1:2)
    vec_transverse%p(3) = zero
    vec_transverse = normalize (vec_transverse)
    lambda = boost (-beta_gamma, vec_transverse)
end function create_transversal_boost
end subroutine phs_fks_generator_generate_isr

```

<PHS fks: phs fks generator: TBP>+≡

```

procedure :: set_sqrts_hat => phs_fks_generator_set_sqrts_hat

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_set_sqrts_hat (generator, sqrts)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: sqrts
end subroutine phs_fks_generator_set_sqrts_hat

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generator_set_sqrts_hat (generator, sqrts)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: sqrts
    generator%sqrts = sqrts
end subroutine phs_fks_generator_set_sqrts_hat

```

<PHS fks: phs fks generator: TBP>+≡

```

procedure :: set_emitters => phs_fks_generator_set_emitters

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_set_emitters (generator, emitters)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in), dimension(:), allocatable :: emitters
end subroutine phs_fks_generator_set_emitters

```

```

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_set_emitters (generator, emitters)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in), dimension(:), allocatable :: emitters
    allocate (generator%emitters (size (emitters)))
    generator%emitters = emitters
  end subroutine phs_fks_generator_set_emitters

<PHS fks: phs fks generator: TBP>+≡
  procedure :: setup_masses => phs_fks_generator_setup_masses

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_setup_masses (generator, n_tot)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: n_tot
  end subroutine phs_fks_generator_setup_masses

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_setup_masses (generator, n_tot)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: n_tot
    if (.not. allocated (generator%m2)) then
      allocate (generator%is_massive (n_tot))
      allocate (generator%m2 (n_tot))
      generator%is_massive = .false.
      generator%m2 = zero
    end if
  end subroutine phs_fks_generator_setup_masses

<PHS fks: phs fks generator: TBP>+≡
  procedure :: set_xi_and_y_bounds => phs_fks_generator_set_xi_and_y_bounds

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_set_xi_and_y_bounds &
    (generator, fks_xi_min, fks_y_max)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in), optional :: fks_xi_min, fks_y_max
  end subroutine phs_fks_generator_set_xi_and_y_bounds

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_set_xi_and_y_bounds &
    (generator, fks_xi_min, fks_y_max)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in), optional :: fks_xi_min, fks_y_max
    real(default) :: xi_min, y_max
    xi_min = zero; y_max = one
    if (present (fks_xi_min)) xi_min = fks_xi_min
    if (present (fks_y_max)) y_max = fks_y_max
    generator%xi_min = min (one, max (xi_min, tiny_07))
    generator%y_max = min (abs (y_max), one)
  end subroutine phs_fks_generator_set_xi_and_y_bounds

Sets x in the isr_kinematics of the generator.

<PHS fks: phs fks generator: TBP>+≡
  procedure :: set_isr_kinematics => phs_fks_generator_set_isr_kinematics

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_set_isr_kinematics (generator, p)
  class(phs_fks_generator_t), intent(inout) :: generator
  type(vector4_t), dimension(2), intent(in) :: p
end subroutine phs_fks_generator_set_isr_kinematics

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generator_set_isr_kinematics (generator, p)
  class(phs_fks_generator_t), intent(inout) :: generator
  type(vector4_t), dimension(2), intent(in) :: p
  if (allocated (generator%isr_kinematics%beam_energy)) then
    select case (size (generator%isr_kinematics%beam_energy))
    case (1)
      generator%isr_kinematics%x = p%p(0) / &
        generator%isr_kinematics%beam_energy(1)
    case (2)
      generator%isr_kinematics%x = p%p(0) / &
        generator%isr_kinematics%beam_energy
    end select
  else
    generator%isr_kinematics%x = 0
  end if
end subroutine phs_fks_generator_set_isr_kinematics

```

<PHS fks: phs fks generator: TBP>+≡

```

procedure :: generate_radiation_variables => &
  phs_fks_generator_generate_radiation_variables

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_generator_generate_radiation_variables &
  (generator, r_in, p_born, phs_identifiers, threshold)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in), dimension(:) :: r_in
  type(vector4_t), intent(in), dimension(:) :: p_born
  type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
  logical, intent(in), optional :: threshold
end subroutine phs_fks_generator_generate_radiation_variables

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_generator_generate_radiation_variables &
  (generator, r_in, p_born, phs_identifiers, threshold)
  class(phs_fks_generator_t), intent(inout) :: generator
  real(default), intent(in), dimension(:) :: r_in
  type(vector4_t), intent(in), dimension(:) :: p_born
  type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
  logical, intent(in), optional :: threshold

  associate (rad_var => generator%real_kinematics)
    rad_var%phi = r_in (I_PHI) * twopi
    select case (generator%mode)
    case (GEN_REAL_PHASE_SPACE)
      rad_var%jac_rand = twopi
      call generator%compute_y_real_phs (r_in(I_Y), p_born, phs_identifiers, &
        rad_var%jac_rand, rad_var%y, threshold)
    case (GEN_SOFT_MISMATCH)

```

```

        rad_var%jac_mismatch = twopi
        call generator%compute_y_mismatch (r_in(I_Y), rad_var%jac_mismatch, &
            rad_var%y_mismatch, rad_var%y_soft)
    case default
        call generator%compute_y_test (rad_var%y)
    end select
    call generator%compute_xi_tilde (r_in(I_XI))
    call generator%set_masses (p_born, phs_identifiers)
end associate
end subroutine phs_fks_generator_generate_radiation_variables

```

(PHS fks: phs fks generator: TBP)+≡

```

procedure :: compute_xi_ref_momenta => &
    phs_fks_generator_compute_xi_ref_momenta

```

(PHS fks: sub interfaces)+≡

```

module subroutine phs_fks_generator_compute_xi_ref_momenta &
    (generator, p_born, resonance_contributors)
class(phs_fks_generator_t), intent(inout) :: generator
type(vector4_t), intent(in), dimension(:) :: p_born
type(resonance_contributors_t), intent(in), dimension(:), optional &
    :: resonance_contributors
end subroutine phs_fks_generator_compute_xi_ref_momenta

```

(PHS fks: procedures)+≡

```

module subroutine phs_fks_generator_compute_xi_ref_momenta &
    (generator, p_born, resonance_contributors)
class(phs_fks_generator_t), intent(inout) :: generator
type(vector4_t), intent(in), dimension(:) :: p_born
type(resonance_contributors_t), intent(in), dimension(:), optional &
    :: resonance_contributors
integer :: i_con, n_contributors
if (present (resonance_contributors)) then
    n_contributors = size (resonance_contributors)
    if (.not. allocated (generator%resonance_contributors)) &
        allocate (generator%resonance_contributors (n_contributors))
    do i_con = 1, n_contributors
        generator%real_kinematics%xi_ref_momenta(i_con) = &
            get_resonance_momentum (p_born, resonance_contributors(i_con)%c)
        generator%resonance_contributors(i_con) = &
            resonance_contributors(i_con)
    end do
else
    generator%real_kinematics%xi_ref_momenta(1) = &
        sum (p_born(1:generator%n_in))
end if
end subroutine phs_fks_generator_compute_xi_ref_momenta

```

(PHS fks: phs fks generator: TBP)+≡

```

procedure :: compute_xi_ref_momenta_threshold &
    => phs_fks_generator_compute_xi_ref_momenta_threshold

```

(PHS fks: sub interfaces)+≡

```

module subroutine phs_fks_generator_compute_xi_ref_momenta_threshold &
    (generator, p_born)

```

```

        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
    end subroutine phs_fks_generator_compute_xi_ref_momenta_threshold

<PHS fks: procedures>+≡
    module subroutine phs_fks_generator_compute_xi_ref_momenta_threshold &
        (generator, p_born)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
        generator%real_kinematics%xi_ref_momenta(1) = &
            p_born(THR_POS_WP) + p_born(THR_POS_B)
        generator%real_kinematics%xi_ref_momenta(2) = &
            p_born(THR_POS_WM) + p_born(THR_POS_BBAR)
    end subroutine phs_fks_generator_compute_xi_ref_momenta_threshold

<PHS fks: phs fks generator: TBP>+≡
    procedure :: compute_cms_energy => phs_fks_generator_compute_cms_energy

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_generator_compute_cms_energy (generator, p_born)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
    end subroutine phs_fks_generator_compute_cms_energy

<PHS fks: procedures>+≡
    module subroutine phs_fks_generator_compute_cms_energy (generator, p_born)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t) :: p_sum
        p_sum = sum (p_born (1 : generator%n_in))
        generator%real_kinematics%cms_energy2 = p_sum**2
    end subroutine phs_fks_generator_compute_cms_energy

<PHS fks: phs fks generator: TBP>+≡
    procedure :: compute_xi_max => phs_fks_generator_compute_xi_max

<PHS fks: sub interfaces>+≡
    module subroutine phs_fks_generator_compute_xi_max (generator, emitter, &
        i_phs, p, xi_max, i_con, y_in)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: i_phs, emitter
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(out) :: xi_max
        integer, intent(in), optional :: i_con
        real(default), intent(in), optional :: y_in
    end subroutine phs_fks_generator_compute_xi_max

<PHS fks: procedures>+≡
    module subroutine phs_fks_generator_compute_xi_max (generator, emitter, &
        i_phs, p, xi_max, i_con, y_in)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: i_phs, emitter
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(out) :: xi_max
        integer, intent(in), optional :: i_con
        real(default), intent(in), optional :: y_in

```

```

real(default) :: q0
type(vector4_t), dimension(:), allocatable :: pp, pp_decay
type(vector4_t) :: p_res
type(lorentz_transformation_t) :: L_to_resonance
real(default) :: y
if (.not. any (generator%emitters == emitter)) return
allocate (pp (size (p)))
associate (rad_var => generator%real_kinematics)
  if (present (i_con)) then
    q0 = rad_var%xi_ref_momenta(i_con)**1
  else
    q0 = energy (sum (p(1:generator%n_in)))
  end if
  if (present (y_in)) then
    y = y_in
  else
    y = rad_var%y(i_phs)
  end if
  if (present (i_con)) then
    p_res = rad_var%xi_ref_momenta(i_con)
    L_to_resonance = inverse (boost (p_res, q0))
    pp = L_to_resonance * p
  else
    pp = p
  end if
  if (emitter <= generator%n_in) then
    select case (generator%isr_kinematics%isr_mode)
    case (SQRTS_FIXED)
      if (generator%n_in > 1) then
        allocate (pp_decay (size (pp) - 1))
      else
        allocate (pp_decay (size (pp)))
      end if
      pp_decay (1) = sum (pp(1:generator%n_in))
      pp_decay (2 : ) = pp (generator%n_in + 1 : )
      xi_max = get_xi_max_isr_decay (pp_decay)
      deallocate (pp_decay)
    case (SQRTS_VAR)
      xi_max = get_xi_max_isr (generator%isr_kinematics%x, y)
    end select
  else
    if (generator%is_massive(emitter)) then
      xi_max = get_xi_max_fsr (pp, q0, emitter, generator%m2(emitter), y)
    else
      xi_max = get_xi_max_fsr (pp, q0, emitter)
    end if
  end if
  deallocate (pp)
end associate
end subroutine phs_fks_generator_compute_xi_max

```

(PHS fks: phs fks generator: TBP) +=

```

procedure :: compute_xi_max_isr_factorized &
=> phs_fks_generator_compute_xi_max_isr_factorized

```

```

(PHS fks: sub interfaces)+≡
  module subroutine phs_fks_generator_compute_xi_max_isr_factorized &
    (generator, i_phs, p)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine phs_fks_generator_compute_xi_max_isr_factorized

(PHS fks: procedures)+≡
  module subroutine phs_fks_generator_compute_xi_max_isr_factorized &
    (generator, i_phs, p)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p
    generator%real_kinematics%xi_max(i_phs) = get_xi_max_isr_decay (p)
  end subroutine phs_fks_generator_compute_xi_max_isr_factorized

(PHS fks: phs fks generator: TBP)+≡
  procedure :: set_masses => phs_fks_generator_set_masses

(PHS fks: sub interfaces)+≡
  module subroutine phs_fks_generator_set_masses &
    (generator, p, phs_identifiers)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine phs_fks_generator_set_masses

(PHS fks: procedures)+≡
  module subroutine phs_fks_generator_set_masses &
    (generator, p, phs_identifiers)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: emitter, i_phs
    do i_phs = 1, size (phs_identifiers)
      emitter = phs_identifiers(i_phs)%emitter
      if (any (generator%emitters == emitter) .and. emitter > 0) then
        if (generator%is_massive (emitter) .and. emitter > generator%n_in) &
          generator%m2(emitter) = p(emitter)**2
        end if
      end do
    end subroutine phs_fks_generator_set_masses

(PHS fks: public)+≡
  public :: compute_y_from_emitter

(PHS fks: sub interfaces)+≡
  module subroutine compute_y_from_emitter (r_y, p, n_in, emitter, &
    massive, y_max, jac_rand, y, contributors, threshold)
    real(default), intent(in) :: r_y
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: n_in
    integer, intent(in) :: emitter
    logical, intent(in) :: massive

```

```

    real(default), intent(in) :: y_max
    real(default), intent(inout) :: jac_rand
    real(default), intent(out) :: y
    integer, intent(in), dimension(:), allocatable, optional :: contributors
    logical, intent(in), optional :: threshold
end subroutine compute_y_from_emitter

```

(PHS fks: procedures)+≡

```

module subroutine compute_y_from_emitter (r_y, p, n_in, emitter, &
    massive, y_max, jac_rand, y, contributors, threshold)
    real(default), intent(in) :: r_y
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: n_in
    integer, intent(in) :: emitter
    logical, intent(in) :: massive
    real(default), intent(in) :: y_max
    real(default), intent(inout) :: jac_rand
    real(default), intent(out) :: y
    integer, intent(in), dimension(:), allocatable, optional :: contributors
    logical, intent(in), optional :: threshold
    logical :: thr, resonance
    type(vector4_t) :: p_res, p_em
    real(default) :: q0
    type(lorentz_transformation_t) :: boost_to_resonance
    integer :: i
    real(default) :: beta, one_m_beta, one_p_beta
    thr = .false.; if (present (threshold)) thr = threshold
    p_res = vector4_null
    if (present (contributors)) then
        resonance = allocated (contributors)
    else
        resonance = .false.
    end if
    if (massive) then
        if (resonance) then
            do i = 1, size (contributors)
                p_res = p_res + p(contributors(i))
            end do
        else if (thr) then
            p_res = p(ass_boson(thr_leg(emitter))) + p(ass_quark(thr_leg(emitter)))
        else
            p_res = sum (p(1:n_in))
        end if
        q0 = p_res**1
        boost_to_resonance = inverse (boost (p_res, q0))
        p_em = boost_to_resonance * p(emitter)
        beta = beta_emitter (q0, p_em)
        one_m_beta = one - beta
        one_p_beta = one + beta
        y = one / beta * (one - one_p_beta * &
            exp ( - r_y * log(one_p_beta / one_m_beta)))
        jac_rand = jac_rand * &
            (one - beta * y) * log(one_p_beta / one_m_beta) / beta
    else
        y = (one - two * r_y) * y_max
    end if
end module

```



```

        jac_rand = jac_rand * 3 * (one - y**2) * y_max
        y = 1.5_default * (y - y**3 / 3)
    end if
end subroutine compute_y_from_emitter

```

<PHS fks: phs fks generator: TBP>+≡

```

    procedure :: compute_y_real_phs => phs_fks_generator_compute_y_real_phs

```

<PHS fks: sub interfaces>+≡

```

    module subroutine phs_fks_generator_compute_y_real_phs &
        (generator, r_y, p, phs_identifiers, &
         jac_rand, y, threshold)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r_y
        type(vector4_t), intent(in), dimension(:) :: p
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(inout), dimension(:) :: jac_rand
        real(default), intent(out), dimension(:) :: y
        logical, intent(in), optional :: threshold
    end subroutine phs_fks_generator_compute_y_real_phs

```

<PHS fks: procedures>+≡

```

    module subroutine phs_fks_generator_compute_y_real_phs &
        (generator, r_y, p, phs_identifiers, &
         jac_rand, y, threshold)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r_y
        type(vector4_t), intent(in), dimension(:) :: p
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(inout), dimension(:) :: jac_rand
        real(default), intent(out), dimension(:) :: y
        logical, intent(in), optional :: threshold
        real(default) :: beta, one_p_beta, one_m_beta
        type(lorentz_transformation_t) :: boost_to_resonance
        real(default) :: q0
        type(vector4_t) :: p_res, p_em
        integer :: i, i_phs, emitter
        logical :: thr
        logical :: construct_massive_fsr
        construct_massive_fsr = .false.
        thr = .false.; if (present (threshold)) thr = threshold
        do i_phs = 1, size (phs_identifiers)
            emitter = phs_identifiers(i_phs)%emitter
            !!! We need this additional check because of decay phase spaces
            !!! t -> bW has a massive emitter at position 1, which should
            !!! not be treated here.
            construct_massive_fsr = emitter > generator%n_in
            if (construct_massive_fsr) construct_massive_fsr = &
                construct_massive_fsr .and. generator%is_massive (emitter)
            call compute_y_from_emitter (r_y, p, generator%n_in, &
                emitter, construct_massive_fsr, &
                generator%y_max, jac_rand(i_phs), y(i_phs), &
                phs_identifiers(i_phs)%contributors, threshold)
        end do
    end subroutine phs_fks_generator_compute_y_real_phs

```

```

<PHS fks: phs fks generator: TBP>+≡
  procedure :: compute_y_mismatch => phs_fks_generator_compute_y_mismatch

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_compute_y_mismatch &
    (generator, r_y, jac_rand, y, y_soft)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: r_y
    real(default), intent(inout) :: jac_rand
    real(default), intent(out) :: y
    real(default), intent(out), dimension(:) :: y_soft
  end subroutine phs_fks_generator_compute_y_mismatch

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_compute_y_mismatch &
    (generator, r_y, jac_rand, y, y_soft)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: r_y
    real(default), intent(inout) :: jac_rand
    real(default), intent(out) :: y
    real(default), intent(out), dimension(:) :: y_soft
    y = (one - two * r_y) * generator%y_max
    jac_rand = jac_rand * 3 * (one - y**2) * generator%y_max
    y = 1.5_default * (y - y**3 / 3)
    y_soft = y
  end subroutine phs_fks_generator_compute_y_mismatch

<PHS fks: phs fks generator: TBP>+≡
  procedure :: compute_y_test => phs_fks_generator_compute_y_test

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_compute_y_test (generator, y)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(out), dimension(:):: y
  end subroutine phs_fks_generator_compute_y_test

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_compute_y_test (generator, y)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(out), dimension(:):: y
    select case (generator%mode)
    case (GEN_SOFT_LIMIT_TEST)
      y = y_test_soft
    case (GEN_COLL_LIMIT_TEST)
      y = y_test_coll
    case (GEN_ANTI_COLL_LIMIT_TEST)
      y = - y_test_coll
    case (GEN_SOFT_COLL_LIMIT_TEST)
      y = y_test_coll
    case (GEN_SOFT_ANTI_COLL_LIMIT_TEST)
      y = - y_test_coll
    end select
  end subroutine phs_fks_generator_compute_y_test

```

```

<PHS fks: public>+≡
    public :: beta_emitter

<PHS fks: sub interfaces>+≡
    pure module function beta_emitter (q0, p) result (beta)
        real(default), intent(in) :: q0
        type(vector4_t), intent(in) :: p
        real(default) :: beta
    end function beta_emitter

<PHS fks: procedures>+≡
    pure module function beta_emitter (q0, p) result (beta)
        real(default), intent(in) :: q0
        type(vector4_t), intent(in) :: p
        real(default) :: beta
        real(default) :: m2, mrec2, k0_max
        m2 = p**2
        mrec2 = (q0 - p%p(0))**2 - p%p(1)**2 - p%p(2)**2 - p%p(3)**2
        k0_max = (q0**2 - mrec2 + m2) / (two * q0)
        beta = sqrt(one - m2 / k0_max**2)
    end function beta_emitter

<PHS fks: phs fks generator: TBP>+≡
    procedure :: compute_xi_tilde => phs_fks_generator_compute_xi_tilde

<PHS fks: sub interfaces>+≡
    pure module subroutine phs_fks_generator_compute_xi_tilde (generator, r)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r
    end subroutine phs_fks_generator_compute_xi_tilde

<PHS fks: procedures>+≡
    pure module subroutine phs_fks_generator_compute_xi_tilde (generator, r)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r
        real(default) :: deno
        associate (rad_var => generator%real_kinematics)
            select case (generator%mode)
            case (GEN_REAL_PHASE_SPACE)
                if (generator%singular_jacobian) then
                    rad_var%xi_tilde = (one - generator%xi_min) - (one - r)**2 * &
                        (one - two * generator%xi_min)
                    rad_var%jac_rand = rad_var%jac_rand * two * (one - r) * &
                        (one - two * generator%xi_min)
                else
                    rad_var%xi_tilde = generator%xi_min + r * (one - generator%xi_min)
                    rad_var%jac_rand = rad_var%jac_rand * (one - generator%xi_min)
                end if
            case (GEN_SOFT_MISMATCH)
                deno = one - r
                if (deno < tiny_13) deno = tiny_13
                rad_var%xi_mismatch = generator%xi_min + r / deno
                rad_var%jac_mismatch = rad_var%jac_mismatch / deno**2
            case (GEN_SOFT_LIMIT_TEST)
                rad_var%xi_tilde = r * two * xi_tilde_test_soft
                rad_var%jac_rand = two * xi_tilde_test_soft
            end case
        end associate
    end subroutine

```

```

      case (GEN_COLL_LIMIT_TEST)
        rad_var%xi_tilde = xi_tilde_test_coll
        rad_var%jac_rand = xi_tilde_test_coll
      case (GEN_ANTI_COLL_LIMIT_TEST)
        rad_var%xi_tilde = xi_tilde_test_coll
        rad_var%jac_rand = xi_tilde_test_coll
      case (GEN_SOFT_COLL_LIMIT_TEST)
        rad_var%xi_tilde = r * two * xi_tilde_test_soft
        rad_var%jac_rand = two * xi_tilde_test_soft
      case (GEN_SOFT_ANTI_COLL_LIMIT_TEST)
        rad_var%xi_tilde = r * two * xi_tilde_test_soft
        rad_var%jac_rand = two * xi_tilde_test_soft
      end select
    end associate
  end subroutine phs_fks_generator_compute_xi_tilde

```

(PHS fks: phs fks generator: TBP)+≡

```

  procedure :: prepare_generation => phs_fks_generator_prepare_generation

```

(PHS fks: sub interfaces)+≡

```

  module subroutine phs_fks_generator_prepare_generation (generator, &
    r_in, i_phs, emitter, p_born, phs_identifiers, contributors, i_con)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), dimension(3), intent(in) :: r_in
    integer, intent(in) :: i_phs, emitter
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
    type(resonance_contributors_t), intent(in), dimension(:), optional :: &
      contributors
    integer, intent(in), optional :: i_con
  end subroutine phs_fks_generator_prepare_generation

```

(PHS fks: procedures)+≡

```

  module subroutine phs_fks_generator_prepare_generation (generator, &
    r_in, i_phs, emitter, p_born, phs_identifiers, contributors, i_con)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), dimension(3), intent(in) :: r_in
    integer, intent(in) :: i_phs, emitter
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
    type(resonance_contributors_t), intent(in), dimension(:), optional :: &
      contributors
    integer, intent(in), optional :: i_con
    call generator%generate_radiation_variables (r_in, p_born, phs_identifiers)
    call generator%compute_xi_ref_momenta &
      (generator%real_kinematics%p_born_lab%phs_point(1)%get (), &
      contributors)
    call generator%compute_xi_max (emitter, i_phs, p_born, &
      generator%real_kinematics%xi_max(i_phs), i_con = i_con)
  end subroutine phs_fks_generator_prepare_generation

```

Get xi and y from an external routine (e.g. powheg) and generate an FSR phase space. Note that the flag supply_xi_max is set to .false. because it

is assumed that the upper bound on xi has already been taken into account during its generation.

```

(PHS fks: phs fks generator: TBP)+≡
  procedure :: generate_fsr_from_xi_and_y => &
    phs_fks_generator_generate_fsr_from_xi_and_y

(PHS fks: sub interfaces)+≡
  module subroutine phs_fks_generator_generate_fsr_from_xi_and_y &
    (generator, xi, y, &
     phi, emitter, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: xi, y, phi
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
  end subroutine phs_fks_generator_generate_fsr_from_xi_and_y

(PHS fks: procedures)+≡
  module subroutine phs_fks_generator_generate_fsr_from_xi_and_y &
    (generator, xi, y, &
     phi, emitter, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: xi, y, phi
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
    associate (rad_var => generator%real_kinematics)
      rad_var%supply_xi_max = .false.
      rad_var%xi_tilde = xi
      rad_var%y(i_phs) = y
      rad_var%phi = phi
    end associate
    call generator%set_sqrts_hat (p_born(1)%p(0) + p_born(2)%p(0))
    call generator%generate_fsr (emitter, i_phs, p_born, p_real)
  end subroutine phs_fks_generator_generate_fsr_from_xi_and_y

```

Get xi and y from an external routine (e.g. powheg) and generate the ISR phase space. For this, we need to overwrite all variables of the real kinematics dependent on (ξ, y, ϕ) that we need to compute p_{real} . From the `isr_kinematics` we just need `sqme_born` and `x`. Both do not depend on the real radiation so we can leave them as they are.

```

(PHS fks: phs fks generator: TBP)+≡
  procedure :: generate_isr_from_xi_and_y => &
    phs_fks_generator_generate_isr_from_xi_and_y

(PHS fks: sub interfaces)+≡
  module subroutine phs_fks_generator_generate_isr_from_xi_and_y &
    (generator, xi, xi_max, y, phi, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: xi, xi_max, y, phi
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
  end subroutine phs_fks_generator_generate_isr_from_xi_and_y

```

```

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_generate_isr_from_xi_and_y &
    (generator, xi, xi_max, y, phi, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: xi, xi_max, y, phi
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(out), dimension(:) :: p_real
    associate (rad_var => generator%real_kinematics)
      rad_var%xi_max(i_phs) = xi_max
      rad_var%xi_tilde = xi / xi_max
      rad_var%y(i_phs) = y
      rad_var%phi = phi
    end associate
    call generator%generate_isr (i_phs, p_born, p_real)
  end subroutine phs_fks_generator_generate_isr_from_xi_and_y

<PHS fks: phs fks generator: TBP>+≡
  procedure :: get_radiation_variables => &
    phs_fks_generator_get_radiation_variables

<PHS fks: sub interfaces>+≡
  pure module subroutine phs_fks_generator_get_radiation_variables &
    (generator, i_phs, xi, y, phi)
    class(phs_fks_generator_t), intent(in) :: generator
    integer, intent(in) :: i_phs
    real(default), intent(out) :: xi, y
    real(default), intent(out), optional :: phi
  end subroutine phs_fks_generator_get_radiation_variables

<PHS fks: procedures>+≡
  pure module subroutine phs_fks_generator_get_radiation_variables &
    (generator, i_phs, xi, y, phi)
    class(phs_fks_generator_t), intent(in) :: generator
    integer, intent(in) :: i_phs
    real(default), intent(out) :: xi, y
    real(default), intent(out), optional :: phi
    associate (rad_var => generator%real_kinematics)
      xi = rad_var%xi_max(i_phs) * rad_var%xi_tilde
      y = rad_var%y(i_phs)
      if (present (phi)) phi = rad_var%phi
    end associate
  end subroutine phs_fks_generator_get_radiation_variables

<PHS fks: phs fks generator: TBP>+≡
  procedure :: write => phs_fks_generator_write

<PHS fks: sub interfaces>+≡
  module subroutine phs_fks_generator_write (generator, unit)
    class(phs_fks_generator_t), intent(in) :: generator
    integer, intent(in), optional :: unit
  end subroutine phs_fks_generator_write

<PHS fks: procedures>+≡
  module subroutine phs_fks_generator_write (generator, unit)

```

```

class(phs_fks_generator_t), intent(in) :: generator
integer, intent(in), optional :: unit
integer :: u
type(string_t) :: massive_phsp
u = given_output_unit (unit); if (u < 0) return
if (generator%massive_phsp) then
    massive_phsp = " massive "
else
    massive_phsp = " massless "
end if
write (u, "(A)") char ("This is a generator for a" &
    // massive_phsp // "phase space")
if (associated (generator%real_kinematics)) then
    call generator%real_kinematics%write ()
else
    write (u, "(A)") "Warning: There are no real " // &
        "kinematics associated with this generator"
end if
call write_separator (u)
write (u, "(A," // FMT_17 // ",1X)") "sqrts      : ", generator%sqrts
write (u, "(A," // FMT_17 // ",1X)") "E_gluon    : ", generator%E_gluon
write (u, "(A," // FMT_17 // ",1X)") "mrec2      : ", generator%mrec2
end subroutine phs_fks_generator_write

```

<PHS fks: phs fks: TBP>+≡

```

procedure :: compute_isr_kinematics => phs_fks_compute_isr_kinematics

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_compute_isr_kinematics (phs, r)
    class(phs_fks_t), intent(inout) :: phs
    real(default), intent(in) :: r
end subroutine phs_fks_compute_isr_kinematics

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_compute_isr_kinematics (phs, r)
    class(phs_fks_t), intent(inout) :: phs
    real(default), intent(in) :: r
    if (.not. phs%config%lab_is_cm) then
        call phs%generator%compute_isr_kinematics &
            (r, phs%lt_cm_to_lab * phs%phs_wood_t%p)
    else
        call phs%generator%compute_isr_kinematics (r, phs%phs_wood_t%p)
    end if
end subroutine phs_fks_compute_isr_kinematics

```

<PHS fks: phs fks: TBP>+≡

```

procedure :: final => phs_fks_final

```

<PHS fks: sub interfaces>+≡

```

module subroutine phs_fks_final (object)
    class(phs_fks_t), intent(inout) :: object
end subroutine phs_fks_final

```

<PHS fks: procedures>+≡

```

module subroutine phs_fks_final (object)

```

```

class(phs_fks_t), intent(inout) :: object
call object%forest%final ()
call object%generator%final ()
end subroutine phs_fks_final

```

(PHS fks: procedures)+≡

```

subroutine filter_particles_from_resonances &
  (res_hist, exclusion_list, &
  model, res_hist_filtered)
  type(resonance_history_t), intent(in), dimension(:) :: res_hist
  type(string_t), intent(in), dimension(:) :: exclusion_list
  type(model_t), intent(in) :: model
  type(resonance_history_t), intent(out), dimension(:), allocatable :: &
    res_hist_filtered
  integer :: i_hist, i_flv, i_new, n_orig
  logical, dimension(size (res_hist)) :: to_filter
  type(flavor_t) :: flv
  to_filter = .false.
  n_orig = size (res_hist)
  do i_flv = 1, size (exclusion_list)
    call flv%init (exclusion_list (i_flv), model)
    do i_hist = 1, size (res_hist)
      if (res_hist(i_hist)%has_flavor (flv)) to_filter (i_hist) = .true.
    end do
  end do
  allocate (res_hist_filtered (n_orig - count (to_filter)))
  i_new = 1
  do i_hist = 1, size (res_hist)
    if (.not. to_filter (i_hist)) then
      res_hist_filtered (i_new) = res_hist (i_hist)
      i_new = i_new + 1
    end if
  end do
end subroutine filter_particles_from_resonances

```

(PHS fks: procedures)+≡

```

subroutine clean_resonance_histories &
  (res_hist, n_in, flv, res_hist_clean, success)
  type(resonance_history_t), intent(in), dimension(:) :: res_hist
  integer, intent(in) :: n_in
  integer, intent(in), dimension(:) :: flv
  type(resonance_history_t), intent(out), dimension(:), allocatable :: &
    res_hist_clean
  logical, intent(out) :: success
  integer :: i_hist
  type(resonance_history_t), dimension(:), allocatable :: &
    res_hist_colored, res_hist_contracted

  if (debug_on) call msg_debug (D_SUBTRACTION, "resonance_mapping_init")
  if (debug_active (D_SUBTRACTION)) then
    call msg_debug (D_SUBTRACTION, "Original resonances:")
    do i_hist = 1, size(res_hist)
      call res_hist(i_hist)%write ()
    end do
  end if

```



```

        end do
    end if

    call remove_uncolored_resonances ()
    call contract_resonances (res_hist_colored, res_hist_contracted)
    call remove_subresonances (res_hist_contracted, res_hist_clean)
    !!! Here, we are still not sure whether we actually would rather use
    !!! call remove_multiple_resonances (res_hist_contracted, res_hist_clean)
    if (debug_active (D_SUBTRACTION)) then
        call msg_debug (D_SUBTRACTION, "Resonances after removing uncolored and duplicates: ")
        do i_hist = 1, size (res_hist_clean)
            call res_hist_clean(i_hist)%write ()
        end do
    end if
    if (size (res_hist_clean) == 0) then
        call msg_warning ("No resonances found. Proceed in usual FKS mode.")
        success = .false.
    else
        success = .true.
    end if

contains
    subroutine remove_uncolored_resonances ()
        type(resonance_history_t), dimension(:), allocatable :: res_hist_tmp
        integer :: n_hist, nleg_out, n_removed
        integer :: i_res, i_hist
        n_hist = size (res_hist)
        nleg_out = size (flv) - n_in
        allocate (res_hist_tmp (n_hist))
        allocate (res_hist_colored (n_hist))
        do i_hist = 1, n_hist
            res_hist_tmp(i_hist) = res_hist(i_hist)
            call res_hist_tmp(i_hist)%add_offset (n_in)
            n_removed = 0
            do i_res = 1, res_hist_tmp(i_hist)%n_resonances
                associate (resonance => res_hist_tmp(i_hist)%resonances(i_res - n_removed))
                    if (.not. any (is_colored (flv (resonance%contributors%c))) &
                        .or. size (resonance%contributors%c) == nleg_out) then
                        call res_hist_tmp(i_hist)%remove_resonance (i_res - n_removed)
                        n_removed = n_removed + 1
                    end if
                end associate
            end do
            if (allocated (res_hist_tmp(i_hist)%resonances)) then
                if (any (res_hist_colored == res_hist_tmp(i_hist))) then
                    cycle
                else
                    do i_res = 1, res_hist_tmp(i_hist)%n_resonances
                        associate (resonance => res_hist_tmp(i_hist)%resonances(i_res))
                            call res_hist_colored(i_hist)%add_resonance (resonance)
                        end associate
                    end do
                end if
            end if
        end do
    end if
end if

```

```

        end do
end subroutine remove_uncolored_resonances

subroutine contract_resonances (res_history_in, res_history_out)
    type(resonance_history_t), intent(in), dimension(:) :: res_history_in
    type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
    logical, dimension(:), allocatable :: i_non_zero
    integer :: n_hist_non_zero, n_hist
    integer :: i_hist_new
    n_hist = size (res_history_in); n_hist_non_zero = 0
    allocate (i_non_zero (n_hist))
    i_non_zero = .false.
    do i_hist = 1, n_hist
        if (res_history_in(i_hist)%n_resonances /= 0) then
            n_hist_non_zero = n_hist_non_zero + 1
            i_non_zero(i_hist) = .true.
        end if
    end do
    allocate (res_history_out (n_hist_non_zero))
    i_hist_new = 1
    do i_hist = 1, n_hist
        if (i_non_zero (i_hist)) then
            res_history_out (i_hist_new) = res_history_in (i_hist)
            i_hist_new = i_hist_new + 1
        end if
    end do
end subroutine contract_resonances

subroutine remove_subresonances (res_history_in, res_history_out)
    type(resonance_history_t), intent(in), dimension(:) :: res_history_in
    type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
    logical, dimension(:), allocatable :: i_non_sub_res
    integer :: n_hist, n_hist_non_sub_res
    integer :: i_hist1, i_hist2
    logical :: is_not_subres
    n_hist = size (res_history_in); n_hist_non_sub_res = 0
    allocate (i_non_sub_res (n_hist)); i_non_sub_res = .false.
    do i_hist1 = 1, n_hist
        is_not_subres = .true.
        do i_hist2 = 1, n_hist
            if (i_hist1 == i_hist2) cycle
            is_not_subres = is_not_subres .and. &
                .not.(res_history_in(i_hist2) .contains. res_history_in(i_hist1))
        end do
        if (is_not_subres) then
            n_hist_non_sub_res = n_hist_non_sub_res + 1
            i_non_sub_res (i_hist1) = .true.
        end if
    end do

    allocate (res_history_out (n_hist_non_sub_res))
    i_hist2 = 1
    do i_hist1 = 1, n_hist
        if (i_non_sub_res (i_hist1)) then

```

```

        res_history_out (i_hist2) = res_history_in (i_hist1)
        i_hist2 = i_hist2 + 1
    end if
end do
end subroutine remove_subresonances

subroutine remove_multiple_resonances (res_history_in, res_history_out)
    type(resonance_history_t), intent(in), dimension(:) :: res_history_in
    type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
    integer :: n_hist, n_hist_single
    logical, dimension(:), allocatable :: i_hist_single
    integer :: i_hist, j
    n_hist = size (res_history_in)
    n_hist_single = 0
    allocate (i_hist_single (n_hist)); i_hist_single = .false.
    do i_hist = 1, n_hist
        if (res_history_in(i_hist)%n_resonances == 1) then
            n_hist_single = n_hist_single + 1
            i_hist_single(i_hist) = .true.
        end if
    end do

    allocate (res_history_out (n_hist_single))
    j = 1
    do i_hist = 1, n_hist
        if (i_hist_single(i_hist)) then
            res_history_out(j) = res_history_in(i_hist)
            j = j + 1
        end if
    end do
end subroutine remove_multiple_resonances
end subroutine clean_resonance_histories

```

<PHS fks: public>+≡

```
public :: get_filtered_resonance_histories
```

<PHS fks: sub interfaces>+≡

```

module subroutine get_filtered_resonance_histories &
    (phs_config, n_in, flv_state, model, excluded_resonances, &
    resonance_histories_filtered, success)
    type(phs_fks_config_t), intent(inout) :: phs_config
    integer, intent(in) :: n_in
    integer, intent(in), dimension(:,:), allocatable :: flv_state
    type(model_t), intent(in) :: model
    type(string_t), intent(in), dimension(:), allocatable :: &
    excluded_resonances
    type(resonance_history_t), intent(out), dimension(:), &
    allocatable :: resonance_histories_filtered
    logical, intent(out) :: success
end subroutine get_filtered_resonance_histories

```

<PHS fks: procedures>+≡

```

module subroutine get_filtered_resonance_histories &
    (phs_config, n_in, flv_state, model, excluded_resonances, &
    resonance_histories_filtered, success)

```

```

type(phs_fks_config_t), intent(inout) :: phs_config
integer, intent(in) :: n_in
integer, intent(in), dimension(:,:), allocatable :: flv_state
type(model_t), intent(in) :: model
type(string_t), intent(in), dimension(:), allocatable :: &
    excluded_resonances
type(resonance_history_t), intent(out), dimension(:), &
    allocatable :: resonance_histories_filtered
logical, intent(out) :: success
type(resonance_history_t), dimension(:), allocatable :: resonance_histories
type(resonance_history_t), dimension(:), allocatable :: &
    resonance_histories_clean!, resonance_histories_filtered
allocate (resonance_histories (size (phs_config%get_resonance_histories ())))
resonance_histories = phs_config%get_resonance_histories ()
call clean_resonance_histories (resonance_histories, &
    n_in, flv_state (:,1), resonance_histories_clean, success)
if (success .and. allocated (excluded_resonances)) then
    call filter_particles_from_resonances (resonance_histories_clean, &
        excluded_resonances, model, resonance_histories_filtered)
else
    allocate (resonance_histories_filtered (size (resonance_histories_clean)))
    resonance_histories_filtered = resonance_histories_clean
end if
end subroutine get_filtered_resonance_histories

```

19.13.3 Unit tests

Test module for FKS phase space, followed by the corresponding implementation module.

```
<phs_fks_ut.f90>≡
  <File header>

  module phs_fks_ut
    use unit_tests
    use phs_fks_uti

    <Standard module head>

    <PHS fks: public test>

    contains

    <PHS fks: test driver>

  end module phs_fks_ut
<phs_fks_uti.f90>≡
  <File header>

  module phs_fks_uti

    <Use kinds>
    use format_utils, only: write_separator, pac_fmt
    use format_defs, only: FMT_15, FMT_19
    use numeric_utils, only: nearly_equal
    use constants, only: tiny_07, zero, one, two
    use lorentz
    use phs_points, only: assignment(=)

    use physics_defs, only: THR_POS_B, THR_POS_BBAR, THR_POS_WP, THR_POS_WM, THR_POS_GLUON
    use physics_defs, only: thr_leg

    use resonances, only: resonance_contributors_t
    use phs_fks

    <Standard module head>

    <PHS fks: test declarations>

    contains

    <PHS fks: tests>

  end module phs_fks_uti
API: driver for the unit tests below.
<PHS fks: public test>≡
  public :: phs_fks_generator_test
<PHS fks: test driver>≡
  subroutine phs_fks_generator_test (u, results)
```

```

integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
call test(phs_fks_generator_1, "phs_fks_generator_1", &
  "Test the generation of FKS phase spaces", u, results)
call test(phs_fks_generator_2, "phs_fks_generator_2", &
  "Test the generation of an ISR FKS phase space", u, results)
call test(phs_fks_generator_3, "phs_fks_generator_3", &
  "Test the generation of a real phase space for decays", &
  u, results)
call test(phs_fks_generator_4, "phs_fks_generator_4", &
  "Test the generation of an FSR phase space with "&
  &"conserved invariant resonance masses", u, results)
call test(phs_fks_generator_5, "phs_fks_generator_5", &
  "Test on-shell projection of a Born phase space and the generation"&
  &" of a real phase-space from that", u, results)
call test(phs_fks_generator_6, "phs_fks_generator_6", &
  "Test the generation of a real phase space for 1 -> 3 decays", &
  u, results)
call test(phs_fks_generator_7, "phs_fks_generator_7", &
  "Test the generation of an ISR FKS phase space for fixed beam energy", &
  u, results)
end subroutine phs_fks_generator_test

```

<PHS fks: test declarations>≡

```
public :: phs_fks_generator_1
```

<PHS fks: tests>≡

```

subroutine phs_fks_generator_1 (u)
  integer, intent(in) :: u
  type(phs_fks_generator_t) :: generator
  type(vector4_t), dimension(:), allocatable :: p_born
  type(vector4_t), dimension(:), allocatable :: p_real
  integer :: emitter, i_phs
  real(default) :: x1, x2, x3
  real(default), parameter :: sqrts = 250.0_default
  type(phs_identifier_t), dimension(2) :: phs_identifiers
  write (u, "(A)") "* Test output: phs_fks_generator_1"
  write (u, "(A)") "* Purpose: Create massless fsr phase space"
  write (u, "(A)")

  allocate (p_born (4))
  p_born(1)%p(0) = 125.0_default
  p_born(1)%p(1:2) = 0.0_default
  p_born(1)%p(3) = 125.0_default
  p_born(2)%p(0) = 125.0_default
  p_born(2)%p(1:2) = 0.0_default
  p_born(2)%p(3) = -125.0_default
  p_born(3)%p(0) = 125.0_default
  p_born(3)%p(1) = -39.5618_default
  p_born(3)%p(2) = -20.0791_default
  p_born(3)%p(3) = -114.6957_default
  p_born(4)%p(0) = 125.0_default
  p_born(4)%p(1:3) = -p_born(3)%p(1:3)

```

```

allocate (generator%isr_kinematics)
generator%n_in = 2
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

call generator%set_sqrts_hat (sqrts)

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.75_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)

allocate (generator%emitters (2))
generator%emitters(1) = 3; generator%emitters(2) = 4
allocate (generator%m2 (4))
generator%m2 = zero
allocate (generator%is_massive (4))
generator%is_massive(1:2) = .false.
generator%is_massive(3:4) = .true.
phs_identifiers(1)%emitter = 3
phs_identifiers(2)%emitter = 4
call generator%compute_xi_ref_momenta (p_born)
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do
write (u, "(A)") &
    "* With these, the following radiation variables have been produced:"
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F3.2)") "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A,F3.2)") "y: ", rad_var%y(1)
    write (u, "(A,F3.2)") "phi: ", rad_var%phi
end associate
call write_separator (u)
write (u, "(A)") "Produce real momenta: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter

allocate (p_real (5))
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator (u)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_1"

```

```

end subroutine phs_fks_generator_1

<PHS fks: test declarations>+≡
  public :: phs_fks_generator_2

<PHS fks: tests>+≡
  subroutine phs_fks_generator_2 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator
    type(vector4_t), dimension(:), allocatable :: p_born
    type(vector4_t), dimension(:), allocatable :: p_real
    integer :: emitter, i_phs
    real(default) :: x1, x2, x3
    real(default), parameter :: sqrts_hadronic = 250.0_default
    type(phs_identifier_t), dimension(2) :: phs_identifiers
    write (u, "(A)") "* Test output: phs_fks_generator_2"
    write (u, "(A)") "* Purpose: Create massless ISR phase space"
    write (u, "(A)")

    allocate (p_born (4))
    p_born(1)%p(0) = 114.661_default
    p_born(1)%p(1:2) = 0.0_default
    p_born(1)%p(3) = 114.661_default
    p_born(2)%p(0) = 121.784_default
    p_born(2)%p(1:2) = 0.0_default
    p_born(2)%p(3) = -121.784_default
    p_born(3)%p(0) = 115.148_default
    p_born(3)%p(1) = -46.250_default
    p_born(3)%p(2) = -37.711_default
    p_born(3)%p(3) = 98.478_default
    p_born(4)%p(0) = 121.296_default
    p_born(4)%p(1:2) = -p_born(3)%p(1:2)
    p_born(4)%p(3) = -105.601_default

    phs_identifiers(1)%emitter = 1
    phs_identifiers(2)%emitter = 2

    allocate (generator%emitters (2))
    allocate (generator%isr_kinematics)
    generator%emitters(1) = 1; generator%emitters(2) = 2
    generator%sqrts = sqrts_hadronic
    allocate (generator%isr_kinematics%beam_energy(2))
    generator%isr_kinematics%beam_energy = sqrts_hadronic / two
    call generator%set_sqrts_hat (sqrts_hadronic)
    call generator%set_isr_kinematics (p_born)
    generator%n_in = 2
    generator%isr_kinematics%isr_mode = SQRTS_VAR
    call generator%set_xi_and_y_bounds ()
    write (u, "(A)") "* Use four-particle phase space containing: "
    call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
    write (u, "(A)") "*****"
    write (u, "(A)")

```



```

x1=0.5_default; x2=0.25_default; x3=0.65_default
write (u, "(A)" ) "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)" ) &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%m2 (2))
generator%m2(1) = 0._default; generator%m2(2) = 0._default
allocate (generator%is_massive (4))
generator%is_massive = .false.
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do
write (u, "(A)" ) &
    "* With these, the following radiation variables have been produced:"
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F3.2)" ) "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A,F3.2)" ) "y: " , rad_var%y(1)
    write (u, "(A,F3.2)" ) "phi: ", rad_var%phi
end associate
write (u, "(A)" ) "Initial-state momentum fractions: "
associate (xb => generator%isr_kinematics%x)
    write (u, "(A,F3.2)" ) "x_born_plus: ", xb(1)
    write (u, "(A,F3.2)" ) "x_born_minus: ", xb(2)
end associate
call write_separator (u)
write (u, "(A)" ) "Produce real momenta: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)" ) "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr (i_phs, p_born, p_real)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator (u)
write (u, "(A)" )
write (u, "(A)" ) "* Test output end: phs_fks_generator_2"

end subroutine phs_fks_generator_2

<PHS fks: test declarations>+≡
public :: phs_fks_generator_3

<PHS fks: tests>+≡
subroutine phs_fks_generator_3 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator
    type(vector4_t), dimension(:), allocatable :: p_born

```

```

type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
real(default) :: mB, mW, mT
integer :: i, emitter, i_phs
type(phs_identfier_t), dimension(2) :: phs_identifiers

write (u, "(A)") "* Test output: phs_fks_generator_3"
write (u, "(A)") "* Puropse: Create real phase space for particle decays"
write (u, "(A)")

allocate (p_born(3))
p_born(1)%p(0) = 172._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 0._default
p_born(2)%p(0) = 104.72866679_default
p_born(2)%p(1) = 45.028053213_default
p_born(2)%p(2) = 29.450337581_default
p_born(2)%p(3) = -5.910229156_default
p_born(3)%p(0) = 67.271333209_default
p_born(3)%p(1:3) = -p_born(2)%p(1:3)

generator%n_in = 1
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mT = 172._default

generator%sqrts = mT

write (u, "(A)") "* Use three-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (3, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%emitters(2))
generator%emitters(1) = 1
generator%emitters(2) = 3
allocate (generator%m2 (3), generator%is_massive(3))
generator%m2(1) = mT**2
generator%m2(2) = mW**2
generator%m2(3) = mB**2

```

```

generator%is_massive = .true.
phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 3

call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real (4))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
write (u, "(A)") "Produce real momenta via final-state emission: "
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_3"

end subroutine phs_fks_generator_3

<PHS fks: test declarations>+≡
public :: phs_fks_generator_4

<PHS fks: tests>+≡
subroutine phs_fks_generator_4 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator
    type(vector4_t), dimension(:), allocatable :: p_born
    type(vector4_t), dimension(:), allocatable :: p_real
    integer, dimension(:), allocatable :: emitters
    integer, dimension(:,,:), allocatable :: resonance_lists
    type(resonance_contributors_t), dimension(2) :: alr_contributors

```

```

real(default) :: x1, x2, x3
real(default), parameter :: sqrts = 250.0_default
integer, parameter :: nlegborn = 6
integer :: i_phs, i_con, emitter
real(default) :: m_inv_born, m_inv_real
character(len=7) :: fmt
type(phs_identif_t), dimension(2) :: phs_identifiers

call pac_fmt (fmt, FMT_19, FMT_15, .true.)

write (u, "(A)") "* Test output: phs_fks_generator_4"
write (u, "(A)") "* Purpose: Create FSR phase space with fixed resonances"
write (u, "(A)")

allocate (p_born (nlegborn))
p_born(1)%p(0) = 250._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 250._default
p_born(2)%p(0) = 250._default
p_born(2)%p(1) = 0._default
p_born(2)%p(2) = 0._default
p_born(2)%p(3) = -250._default
p_born(3)%p(0) = 145.91184486_default
p_born(3)%p(1) = 50.39727589_default
p_born(3)%p(2) = 86.74156041_default
p_born(3)%p(3) = -69.03608748_default
p_born(4)%p(0) = 208.1064784_default
p_born(4)%p(1) = -44.07610020_default
p_born(4)%p(2) = -186.34264578_default
p_born(4)%p(3) = 13.48038407_default
p_born(5)%p(0) = 26.25614471_default
p_born(5)%p(1) = -25.12258068_default
p_born(5)%p(2) = -1.09540228_default
p_born(5)%p(3) = -6.27703505_default
p_born(6)%p(0) = 119.72553196_default
p_born(6)%p(1) = 18.80140499_default
p_born(6)%p(2) = 100.69648766_default
p_born(6)%p(3) = 61.83273846_default

allocate (generator%isr_kinematics)
generator%n_in = 2
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

call generator%set_sqrts_hat (sqrts)

write (u, "(A)") "* Test process: e+ e- -> W+ W- b b~"
write (u, "(A)") "* Resonance pairs: (3,5) and (4,6)"
write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

```

```

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.75_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (nlegborn, 2, 2, 2)

allocate (generator%emitters (2))
generator%emitters(1) = 5; generator%emitters(2) = 6
allocate (generator%m2 (nlegborn))
generator%m2 = p_born**2
allocate (generator%is_massive (nlegborn))
generator%is_massive (1:2) = .false.
generator%is_massive (3:6) = .true.

phs_identifiers(1)%emitter = 5
phs_identifiers(2)%emitter = 6
do i_phs = 1, 2
    allocate (phs_identifiers(i_phs)%contributors (2))
end do
allocate (resonance_lists (2, 2))
resonance_lists (1,:) = [3,5]
resonance_lists (2,:) = [4,6]
!!! Here is obviously some redundancy. Surely we can improve on this.
do i_phs = 1, 2
    phs_identifiers(i_phs)%contributors = resonance_lists(i_phs,:)
end do
do i_con = 1, 2
    allocate (alr_contributors(i_con)%c (size (resonance_lists(i_con,:))))
    alr_contributors(i_con)%c = resonance_lists(i_con,:)
end do
call generator%generate_radiation_variables &
    ([x1, x2, x3], p_born, phs_identifiers)

allocate (p_real(nlegborn + 1))
call generator%compute_xi_ref_momenta (p_born, alr_contributors)
!!! Keep the distinction between i_phs and i_con because in general,
!!! they are not the same.
do i_phs = 1, 2
    i_con = i_phs
    emitter = phs_identifiers(i_phs)%emitter
    write (u, "(A,I1,1X,A,I1,A,I1,A)") &
        "* Generate FSR phase space for emitter ", emitter, &
        "and resonance pair (", resonance_lists (i_con, 1), ",", &
        resonance_lists (i_con, 2), ")"
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs), i_con = i_con)
    call generator%generate_fsr (emitter, i_phs, i_con, p_born, p_real)
    call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
    call write_separator(u)
    write (u, "(A)") "* Check if resonance masses are conserved: "
    m_inv_born = compute_resonance_mass (p_born, resonance_lists (i_con,:))
    m_inv_real = compute_resonance_mass (p_real, resonance_lists (i_con,:), 7)

```

```

write (u, "(A,1X, " // fmt // ")") "m_inv_born = ", m_inv_born
write (u, "(A,1X, " // fmt // ")") "m_inv_real = ", m_inv_real
if (abs (m_inv_born - m_inv_real) < tiny_07) then
  write (u, "(A)") " Success! "
else
  write (u, "(A)") " Failure! "
end if
call write_separator(u)
call write_separator(u)
end do
deallocate (p_real)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_4"
end subroutine phs_fks_generator_4

```

<PHS fks: test declarations>+≡

```
public :: phs_fks_generator_5
```

<PHS fks: tests>+≡

```

subroutine phs_fks_generator_5 (u)
  use ttv_formfactors, only: init_parameters
  integer, intent(in) :: u
  type(phs_fks_generator_t) :: generator
  type(vector4_t), dimension(:), allocatable :: p_born, pb1
  type(vector4_t), dimension(:), allocatable :: p_born_onshell, pb1_os
  type(vector4_t), dimension(:), allocatable :: p_real
  real(default) :: x1, x2, x3
  real(default) :: mB, mW, mtop, mcheck
  integer :: i, emitter, i_phs
  type(phs_identifier_t), dimension(2) :: phs_identifiers
  type(lorentz_transformation_t) :: L_to_cms
  real(default), parameter :: sqrts = 360._default
  real(default), parameter :: momentum_tolerance = 1E-10_default
  real(default) :: mpole, gam_out

  write (u, "(A)") "* Test output: phs_fks_generator_5"
  write (u, "(A)") "* Puropse: Perform threshold on-shell projection of "
  write (u, "(A)") "*           Born momenta and create a real phase-space "
  write (u, "(A)") "*           point from those. "
  write (u, "(A)")

  allocate (p_born(6), p_born_onshell(6))
  p_born(1)%p(0) = sqrts / two
  p_born(1)%p(1:2) = zero
  p_born(1)%p(3) = sqrts / two
  p_born(2)%p(0) = sqrts / two
  p_born(2)%p(1:2) = zero
  p_born(2)%p(3) = -sqrts / two
  p_born(3)%p(0) = 117.1179139230_default
  p_born(3)%p(1) = 56.91215483880_default
  p_born(3)%p(2) = -40.02386013017_default
  p_born(3)%p(3) = -49.07634310496_default
  p_born(4)%p(0) = 98.91904548743_default
  p_born(4)%p(1) = 56.02241403836_default

```

```

p_born(4)%p(2) = -8.302977504723_default
p_born(4)%p(3) = -10.50293716131_default
p_born(5)%p(0) = 62.25884689208_default
p_born(5)%p(1) = -60.00786540278_default
p_born(5)%p(2) = 4.753602375910_default
p_born(5)%p(3) = 15.32916731546_default
p_born(6)%p(0) = 81.70419369751_default
p_born(6)%p(1) = -52.92670347439_default
p_born(6)%p(2) = 43.57323525898_default
p_born(6)%p(3) = 44.25011295081_default

generator%n_in = 2
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mtop = 172._default

generator%sqrts = sqrts

!!! Dummy-initialization of the threshold model because generate_fsr_threshold
!!! uses mis_to_mpole to determine if it is above or below threshold.
call init_parameters (mpole, gam_out, mtop, one, one / 1.5_default, 125._default, &
    0.47_default, 0.118_default, 91._default, 80._default, 4.2_default, &
    one, one, one, one, zero, zero, zero, zero, zero, zero, .false., zero)

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
call vector4_check_momentum_conservation &
    (p_born, 2, unit = u, abs_smallness = momentum_tolerance, verbose = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

allocate (generator%real_kinematics)
call generator%real_kinematics%init (7, 2, 2, 2)
call generator%real_kinematics%init_onshell (7, 2)
generator%real_kinematics%p_born_cms%phs_point(1) = p_born

write (u, "(A)") "Get boost projection system -> CMS: "
L_to_cms = get_boost_for_threshold_projection (p_born, sqrts, mtop)
call L_to_cms%write (u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

write (u, "(A)") "* Perform onshell-projection:"
pb1 = generator%real_kinematics%p_born_cms%phs_point(1)
call threshold_projection_born (mtop, L_to_cms, pb1, p_born_onshell)
generator%real_kinematics%p_born_onshell%phs_point(1) = p_born_onshell

call generator%real_kinematics%p_born_onshell%write &
    (1, unit = u, testflag = .true., ultra = .true.)

```

```

pb1_os = generator%real_kinematics%p_born_onshell%phs_point(1)
call check_phsp (pb1_os, 0)

allocate (generator%emitters (2))
generator%emitters(1) = THR_POS_B; generator%emitters(2) = THR_POS_BBAR

allocate (generator%m2 (6), generator%is_massive(6))
generator%m2 = p_born**2
generator%is_massive (1:2) = .false.
generator%is_massive (3:6) = .true.

phs_identifiers(1)%emitter = THR_POS_B
phs_identifiers(2)%emitter = THR_POS_BBAR

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

call generator%generate_radiation_variables ([x1,x2,x3], p_born_onshell, phs_identifiers)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_ref_momenta_threshold (p_born_onshell)
    call generator%compute_xi_max (emitter, i_phs, p_born_onshell, &
        generator%real_kinematics%xi_max(i_phs), i_con = thr_leg(emitter))
end do
write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A)") "xi_max: "
    write (u, "(2F5.2)") rad_var%xi_max(1), rad_var%xi_max(2)
    write (u, "(A)") "y: "
    write (u, "(2F5.2)") rad_var%y(1), rad_var%y(2)
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "* Produce real momenta from on-shell phase space: "
allocate (p_real(7))
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    write (u, "(A,I1)") "emitter: ", emitter
    call generator%generate_fsr_threshold (emitter, i_phs, p_born_onshell, p_real)
    call check_phsp (p_real, emitter)
end do

call write_separator(u)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_5"

contains
subroutine check_phsp (p, emitter)

```



```

type(vector4_t), intent(inout), dimension(:) :: p
integer, intent(in) :: emitter
type(vector4_t) :: pp
real(default) :: E_tot
logical :: check
write (u, "(A)") "* Check momentum conservation: "
call vector4_check_momentum_conservation &
    (p, 2, unit = u, abs_smallness = momentum_tolerance, verbose = .true.)
write (u, "(A)") "* Check invariant masses: "
write (u, "(A)", advance = "no") "inv(W+, b, gl): "
pp = p(THR_POS_WP) + p(THR_POS_B)
if (emitter == THR_POS_B) pp = pp + p(THR_POS_GLUON)
if (nearly_equal (pp**1, mtop)) then
    write (u, "(A)") "CHECK"
else
    write (u, "(A,F7.3)") "FAIL: ", pp**1
end if
write (u, "(A)", advance = "no") "inv(W-, bbar): "
pp = p(THR_POS_WM) + p(THR_POS_BBAR)
if (emitter == THR_POS_BBAR) pp = pp + p(THR_POS_GLUON)
if (nearly_equal (pp**1, mtop)) then
    write (u, "(A)") "CHECK"
else
    write (u, "(A,F7.3)") "FAIL: ", pp**1
end if
write (u, "(A)") "* Sum of energies equal to sqrts?"
E_tot = sum(p(1:2)%p(0)); check = nearly_equal (E_tot, sqrts)
write (u, "(A,L1)") "Initial state: ", check
if (.not. check) write (u, "(A,F7.3)") "E_tot: ", E_tot
if (emitter > 0) then
    E_tot = sum(p(3:7)%p(0))
else
    E_tot = sum(p(3:6)%p(0))
end if
check = nearly_equal (E_tot, sqrts)
write (u, "(A,L1)") "Final state : ", check
if (.not. check) write (u, "(A,F7.3)") "E_tot: ", E_tot
call pacify (p, 1E-6_default)
call vector4_write_set (p, u, testflag = .true., ultra = .true.)

end subroutine check_phsp
end subroutine phs_fks_generator_5

```

<PHS fks: test declarations>+≡

```
public :: phs_fks_generator_6
```

<PHS fks: tests>+≡

```

subroutine phs_fks_generator_6 (u)
integer, intent(in) :: u
type(phs_fks_generator_t) :: generator
type(vector4_t), dimension(:), allocatable :: p_born
type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
real(default) :: mB, mW, mT

```

```

integer :: i, emitter, i_phs
type(phs_identifer_t), dimension(2) :: phs_identifiers

write (u, "(A)") "* Test output: phs_fks_generator_6"
write (u, "(A)") "* Puropse: Create real phase space for particle decays"
write (u, "(A)")

allocate (p_born(4))
p_born(1)%p(0) = 173.1_default
p_born(1)%p(1) = zero
p_born(1)%p(2) = zero
p_born(1)%p(3) = zero
p_born(2)%p(0) = 68.17074462929_default
p_born(2)%p(1) = -37.32578717617_default
p_born(2)%p(2) = 30.99675959336_default
p_born(2)%p(3) = -47.70321718398_default
p_born(3)%p(0) = 65.26639312326_default
p_born(3)%p(1) = -1.362927648502_default
p_born(3)%p(2) = -33.25327150840_default
p_born(3)%p(3) = 56.14324922494_default
p_born(4)%p(0) = 39.66286224745_default
p_born(4)%p(1) = 38.68871482467_default
p_born(4)%p(2) = 2.256511915049_default
p_born(4)%p(3) = -8.440032040958_default

generator%n_in = 1
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mT = 173.1_default

generator%sqrts = mT

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1=0.5_default; x2=0.25_default; x3=0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (3, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%emitters(2))
generator%emitters(1) = 1
generator%emitters(2) = 2
allocate (generator%m2 (4), generator%is_massive(4))

```

```

generator%m2(1) = mT**2
generator%m2(2) = mB**2
generator%m2(3) = zero
generator%m2(4) = zero
generator%is_massive(1:2) = .true.
generator%is_massive(3:4) = .false.
phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 2

call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
write (u, "(A)") "Produce real momenta via final-state emission: "
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_6"

end subroutine phs_fks_generator_6

```

```

<PHS fks: test declarations>+≡
public :: phs_fks_generator_7

<PHS fks: tests>+≡
subroutine phs_fks_generator_7 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator

```

```

type(vector4_t), dimension(:), allocatable :: p_born
type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
integer :: i, emitter, i_phs
type(phs_identifier_t), dimension(2) :: phs_identifiers
real(default), parameter :: sqrts = 1000.0_default

write (u, "(A)") "* Test output: phs_fks_generator_7"
write (u, "(A)") "* Puropse: Create real phase space for scattering ISR"
write (u, "(A)") "*           keeping the beam energy fixed."
write (u, "(A)")

allocate (p_born(4))
p_born(1)%p(0) = 500._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 500._default
p_born(2)%p(0) = 500._default
p_born(2)%p(1) = 0._default
p_born(2)%p(2) = 0._default
p_born(2)%p(3) = -500._default
p_born(3)%p(0) = 500._default
p_born(3)%p(1) = 11.275563070_default
p_born(3)%p(2) = -13.588797663_default
p_born(3)%p(3) = 486.93070588_default
p_born(4)%p(0) = 500._default
p_born(4)%p(1:3) = -p_born(3)%p(1:3)

phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 2

allocate (generator%emitters(2))
generator%n_in = 2
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()
generator%emitters(1) = 1; generator%emitters(2) = 2
generator%sqrts = sqrts

write (u, "(A)") "* Use 2 -> 2 phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%m2 (4))

```

```

generator%m2 = 0._default
allocate (generator%is_massive(4))
generator%is_massive = .false.
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_7"

end subroutine phs_fks_generator_7

```

19.14 Dispatch

`<dispatch_phase_space.f90>`≡
<File header>

module dispatch_phase_space

<Use kinds>

<Use strings>

use variables, only: var_list_t

use os_interface, only: os_data_t

```

    use sf_mappings, only: sf_channel_t
    use beam_structures, only: beam_structure_t
    use dispatch_beams, only: sf_prop_t, strfun_mode

    use mappings
    use phs_forests, only: phs_parameters_t
    use phs_base

    <Standard module head>

    <Dispatch phs: public>

    interface
    <Dispatch phs: sub interfaces>
    end interface

    end module dispatch_phase_space

    <dispatch_phase_space_sub.f90>≡
    <File header>

    submodule (dispatch_phase_space) dispatch_phase_space_s

        use io_units, only: free_unit
        use diagnostics
        use phs_none
        use phs_single
        use phs_rambo
        use phs_wood
        use phs_fks

        implicit none

    contains

    <Dispatch phs: procedures>

    end submodule dispatch_phase_space_s

```

Allocate a phase-space object according to the variable \$phs_method.

```

    <Dispatch phs: public>≡
        public :: dispatch_phs

    <Dispatch phs: sub interfaces>≡
        module subroutine dispatch_phs (phs, var_list, os_data, process_id, &
            mapping_defaults, phs_par, phs_method_in)
            class(phs_config_t), allocatable, intent(inout) :: phs
            type(var_list_t), intent(in) :: var_list
            type(os_data_t), intent(in) :: os_data
            type(string_t), intent(in) :: process_id
            type(mapping_defaults_t), intent(in), optional :: mapping_defaults
            type(phs_parameters_t), intent(in), optional :: phs_par
            type(string_t), intent(in), optional :: phs_method_in
        end subroutine dispatch_phs

```

<Dispatch phs: procedures>≡

```

module subroutine dispatch_phs (phs, var_list, os_data, process_id, &
    mapping_defaults, phs_par, phs_method_in)
    class(phs_config_t), allocatable, intent(inout) :: phs
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: process_id
    type(mapping_defaults_t), intent(in), optional :: mapping_defaults
    type(phs_parameters_t), intent(in), optional :: phs_par
    type(string_t), intent(in), optional :: phs_method_in
    type(string_t) :: phs_method, phs_file, run_id
    logical :: use_equivalences, vis_channels, fatal_beam_decay
    integer :: u_phs
    logical :: exist
    if (present (phs_method_in)) then
        phs_method = phs_method_in
    else
        phs_method = &
            var_list%get_sval (var_str ("phs_method"))
    end if
    phs_file = &
        var_list%get_sval (var_str ("phs_file"))
    use_equivalences = &
        var_list%get_lval (var_str ("use_vamp_equivalences"))
    vis_channels = &
        var_list%get_lval (var_str ("vis_channels"))
    fatal_beam_decay = &
        var_list%get_lval (var_str ("fatal_beam_decay"))
    run_id = &
        var_list%get_sval (var_str ("run_id"))
    select case (char (phs_method))
    case ("none")
        allocate (phs_none_config_t :: phs)
    case ("single")
        allocate (phs_single_config_t :: phs)
        if (vis_channels) then
            call msg_warning ("Visualizing phase space channels not " // &
                "available for method 'single'.")
        end if
    case ("rambo")
        allocate (phs_rambo_config_t :: phs)
        if (vis_channels) &
            call msg_warning ("Visualizing phase space channels not " // &
                "available for method 'rambo'.")
    case ("fks")
        allocate (phs_fks_config_t :: phs)
        if (use_equivalences) then
            select type (phs)
            type is (phs_fks_config_t)
                call phs%enable_equivalences ()
            end select
        end if
    case ("wood", "default", "fast_wood")
        call dispatch_wood ()

```

```

    case default
        call msg_fatal ("Phase space: parameterization method '" &
            // char (phs_method) // "' not implemented")
    end select
contains
<Dispatch phs: dispatch phs: procedures>
end subroutine dispatch_phs

```

```

<Dispatch phs: dispatch phs: procedures>≡
subroutine dispatch_wood ()
    allocate (phs_wood_config_t :: phs)
    select type (phs)
    type is (phs_wood_config_t)
        if (phs_file /= "") then
            inquire (file = char (phs_file), exist = exist)
            if (exist) then
                call msg_message ("Phase space: reading configuration from '" &
                    // char (phs_file) // "'")
                u_phs = free_unit ()
                open (u_phs, file = char (phs_file), &
                    action = "read", status = "old")
                call phs%set_input (u_phs)
            else
                call msg_fatal ("Phase space: configuration file '" &
                    // char (phs_file) // "' not found")
            end if
        end if
        if (present (phs_par)) &
            call phs%set_parameters (phs_par)
        if (use_equivalences) &
            call phs%enable_equivalences ()
        if (present (mapping_defaults)) &
            call phs%set_mapping_defaults (mapping_defaults)
        if (phs_method == "fast_wood") phs%use_cascades2 = .true.
        phs%vis_channels = vis_channels
        phs%fatal_beam_decay = fatal_beam_decay
        phs%os_data = os_data
        phs%run_id = run_id
    end select
end subroutine dispatch_wood

```

Configure channel mappings, using some conditions from the phase space configuration. If there are no structure functions, we enable a default setup with a single (dummy) structure-function channel. Otherwise, we look at the channel collection that we got from the phase-space configuration step. Each entry should be translated into an independent structure-function channel, where typically there is one default entry, which could be mapped using a standard s-channel mapping if the structure function setup recommends this, and other entries with s-channel resonances. The latter need to be translated into global mappings from the structure-function chain.

```

<Dispatch phs: public>+≡
    public :: dispatch_sf_channels

```


(Dispatch phs: sub interfaces)+≡

```

module subroutine dispatch_sf_channels (sf_channel, sf_string, sf_prop, &
    coll, var_list, sqrts, beam_structure)
    type(sf_channel_t), dimension(:), allocatable, intent(out) :: sf_channel
    type(string_t), intent(out) :: sf_string
    type(sf_prop_t), intent(in) :: sf_prop
    type(phs_channel_collection_t), intent(in) :: coll
    type(var_list_t), intent(in) :: var_list
    real(default), intent(in) :: sqrts
    type(beam_structure_t), intent(in) :: beam_structure
end subroutine dispatch_sf_channels

```

(Dispatch phs: procedures)+≡

```

module subroutine dispatch_sf_channels (sf_channel, sf_string, sf_prop, &
    coll, var_list, sqrts, beam_structure)
    type(sf_channel_t), dimension(:), allocatable, intent(out) :: sf_channel
    type(string_t), intent(out) :: sf_string
    type(sf_prop_t), intent(in) :: sf_prop
    type(phs_channel_collection_t), intent(in) :: coll
    type(var_list_t), intent(in) :: var_list
    real(default), intent(in) :: sqrts
    type(beam_structure_t), intent(in) :: beam_structure
    type(beam_structure_t) :: beam_structure_tmp
    class(channel_prop_t), allocatable :: prop
    integer :: n_strfun, n_sf_channel, i
    logical :: sf_allow_s_mapping, circe1_map, circe1_generate
    logical :: s_mapping_enable, endpoint_mapping, power_mapping
    logical :: single_parameter
    integer, dimension(:), allocatable :: s_mapping, single_mapping
    real(default) :: s_mapping_power
    real(default) :: circe1_mapping_slope, endpoint_mapping_slope
    real(default) :: power_mapping_eps
    beam_structure_tmp = beam_structure
    call beam_structure_tmp%expand (strfun_mode)
    n_strfun = beam_structure_tmp%get_n_record ()
    sf_string = beam_structure_tmp%to_string (sf_only = .true.)
    sf_allow_s_mapping = &
        var_list%get_lval (var_str ("?sf_allow_s_mapping"))
    circe1_generate = &
        var_list%get_lval (var_str ("?circe1_generate"))
    circe1_map = &
        var_list%get_lval (var_str ("?circe1_map"))
    circe1_mapping_slope = &
        var_list%get_rval (var_str ("circe1_mapping_slope"))
    s_mapping_enable = .false.
    s_mapping_power = 1
    endpoint_mapping = .false.
    endpoint_mapping_slope = 1
    power_mapping = .false.
    single_parameter = .false.
    select case (char (sf_string))
    case ("", "[any particles]")
    case ("pdf_builtin, none", &
        "pdf_builtin_photon, none", &
        "none, pdf_builtin", &

```

```

"none, pdf_builtin_photon", &
"lhpdf, none", &
"lhpdf_photon, none", &
"none, lhpdf", &
"none, lhpdf_photon")
single_parameter = .true.
case ("pdf_builtin, none => none, pdf_builtin", &
"pdf_builtin, none => none, pdf_builtin_photon", &
"pdf_builtin_photon, none => none, pdf_builtin", &
"pdf_builtin_photon, none => none, pdf_builtin_photon", &
"lhpdf, none => none, lhpdf", &
"lhpdf, none => none, lhpdf_photon", &
"lhpdf_photon, none => none, lhpdf", &
"lhpdf_photon, none => none, lhpdf_photon")
allocate (s_mapping (2), source = [1, 2])
s_mapping_enable = .true.
s_mapping_power = 2
case ("pdf_builtin, none => none, pdf_builtin => epa, none => none, epa", &
"pdf_builtin, none => none, pdf_builtin => ewa, none => none, ewa", &
"pdf_builtin, none => none, pdf_builtin => ewa, none => none, epa", &
"pdf_builtin, none => none, pdf_builtin => epa, none => none, ewa")
allocate (s_mapping (2), source = [1, 2])
s_mapping_enable = .true.
s_mapping_power = 2
case ("isr, none", &
"none, isr")
allocate (single_mapping (1), source = [1])
single_parameter = .true.
case ("isr, none => none, isr")
allocate (s_mapping (2), source = [1, 2])
power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("isr, none => none, isr => epa, none => none, epa", &
"isr, none => none, isr => ewa, none => none, ewa", &
"isr, none => none, isr => ewa, none => none, epa", &
"isr, none => none, isr => epa, none => none, ewa")
allocate (s_mapping (2), source = [1, 2])
power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe1 => isr, none => none, isr => epa, none => none, epa", &
"circe1 => isr, none => none, isr => ewa, none => none, ewa", &
"circe1 => isr, none => none, isr => ewa, none => none, epa", &
"circe1 => isr, none => none, isr => epa, none => none, ewa")
if (circe1_generate) then
allocate (s_mapping (2), source = [2, 3])
else
allocate (s_mapping (3), source = [1, 2, 3])
endpoint_mapping = .true.
endpoint_mapping_slope = circe1_mapping_slope
end if
power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("pdf_builtin, none => none, isr", &
"pdf_builtin_photon, none => none, isr", &

```

```

        "lhpdf, none => none, isr", &
        "lhpdf_photon, none => none, isr")
    allocate (single_mapping (1), source = [2])
case ("isr, none => none, pdf_builtin", &
    "isr, none => none, pdf_builtin_photon", &
    "isr, none => none, lhpdf", &
    "isr, none => none, lhpdf_photon")
    allocate (single_mapping (1), source = [1])
case ("epa, none", &
    "none, epa")
    allocate (single_mapping (1), source = [1])
    single_parameter = .true.
case ("epa, none => none, epa")
    allocate (single_mapping (2), source = [1, 2])
case ("epa, none => none, isr", &
    "isr, none => none, epa", &
    "ewa, none => none, isr", &
    "isr, none => none, ewa")
    allocate (single_mapping (2), source = [1, 2])
case ("pdf_builtin, none => none, epa", &
    "pdf_builtin_photon, none => none, epa", &
    "lhpdf, none => none, epa", &
    "lhpdf_photon, none => none, epa")
    allocate (single_mapping (1), source = [2])
case ("pdf_builtin, none => none, ewa", &
    "pdf_builtin_photon, none => none, ewa", &
    "lhpdf, none => none, ewa", &
    "lhpdf_photon, none => none, ewa")
    allocate (single_mapping (1), source = [2])
case ("epa, none => none, pdf_builtin", &
    "epa, none => none, pdf_builtin_photon", &
    "epa, none => none, lhpdf", &
    "epa, none => none, lhpdf_photon")
    allocate (single_mapping (1), source = [1])
case ("ewa, none => none, pdf_builtin", &
    "ewa, none => none, pdf_builtin_photon", &
    "ewa, none => none, lhpdf", &
    "ewa, none => none, lhpdf_photon")
    allocate (single_mapping (1), source = [1])
case ("ewa, none", &
    "none, ewa")
    allocate (single_mapping (1), source = [1])
    single_parameter = .true.
case ("ewa, none => none, ewa")
    allocate (single_mapping (2), source = [1, 2])
case ("energy_scan, none => none, energy_scan")
    allocate (s_mapping (2), source = [1, 2])
case ("sf_test_1, none => none, sf_test_1")
    allocate (s_mapping (2), source = [1, 2])
case ("circe1")
    if (circe1_generate) then
        !!! no mapping
    else if (circe1_map) then
        allocate (s_mapping (1), source = [1])

```

```

        endpoint_mapping = .true.
        endpoint_mapping_slope = circe1_mapping_slope
    else
        allocate (s_mapping (1), source = [1])
        s_mapping_enable = .true.
    end if
case ("circe1 => isr, none => none, isr")
    if (circe1_generate) then
        allocate (s_mapping (2), source = [2, 3])
    else
        allocate (s_mapping (3), source = [1, 2, 3])
        endpoint_mapping = .true.
        endpoint_mapping_slope = circe1_mapping_slope
    end if
    power_mapping = .true.
    power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe1 => isr, none", &
    "circe1 => none, isr")
    allocate (single_mapping (1), source = [2])
case ("circe1 => epa, none => none, epa")
    if (circe1_generate) then
        allocate (single_mapping (2), source = [2, 3])
    else
        call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
            &only")
    end if
case ("circe1 => ewa, none => none, ewa")
    if (circe1_generate) then
        allocate (single_mapping (2), source = [2, 3])
    else
        call msg_fatal ("CIRCE/EWA: supported with ?circe1_generate=true &
            &only")
    end if
case ("circe1 => epa, none", &
    "circe1 => none, epa")
    if (circe1_generate) then
        allocate (single_mapping (1), source = [2])
    else
        call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
            &only")
    end if
case ("circe1 => epa, none => none, isr", &
    "circe1 => isr, none => none, epa", &
    "circe1 => ewa, none => none, isr", &
    "circe1 => isr, none => none, ewa")
    if (circe1_generate) then
        allocate (single_mapping (2), source = [2, 3])
    else
        call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
            &only")
    end if
case ("circe2", &
    "gaussian", &
    "beam_events")

```

```

!!! no mapping
case ("circe2 => isr, none => none, isr", &
"gaussian => isr, none => none, isr", &
"beam_events => isr, none => none, isr")
allocate (s_mapping (2), source = [2, 3])
power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe2 => isr, none", &
"circe2 => none, isr", &
"gaussian => isr, none", &
"gaussian => none, isr", &
"beam_events => isr, none", &
"beam_events => none, isr")
allocate (single_mapping (1), source = [2])
case ("circe2 => epa, none => none, epa", &
"gaussian => epa, none => none, epa", &
"beam_events => epa, none => none, epa")
allocate (single_mapping (2), source = [2, 3])
case ("circe2 => epa, none", &
"circe2 => none, epa", &
"circe2 => ewa, none", &
"circe2 => none, ewa", &
"gaussian => epa, none", &
"gaussian => none, epa", &
"gaussian => ewa, none", &
"gaussian => none, ewa", &
"beam_events => epa, none", &
"beam_events => none, epa", &
"beam_events => ewa, none", &
"beam_events => none, ewa")
allocate (single_mapping (1), source = [2])
case ("circe2 => epa, none => none, isr", &
"circe2 => isr, none => none, epa", &
"circe2 => ewa, none => none, isr", &
"circe2 => isr, none => none, ewa", &
"gaussian => epa, none => none, isr", &
"gaussian => isr, none => none, epa", &
"gaussian => ewa, none => none, isr", &
"gaussian => isr, none => none, ewa", &
"beam_events => epa, none => none, isr", &
"beam_events => isr, none => none, epa", &
"beam_events => ewa, none => none, isr", &
"beam_events => isr, none => none, ewa")
allocate (single_mapping (2), source = [2, 3])
case ("energy_scan")
case default
call msg_fatal ("Beam structure: " &
// char (sf_string) // " not supported")
end select
if (sf_allow_s_mapping .and. coll%n > 0) then
n_sf_channel = coll%n
allocate (sf_channel (n_sf_channel))
do i = 1, n_sf_channel
call sf_channel(i)%init (n_strfun)

```

```

if (allocated (single_mapping)) then
  call sf_channel(i)%activate_mapping (single_mapping)
end if
if (allocated (prop)) deallocate (prop)
call coll%get_entry (i, prop)
if (allocated (prop)) then
  if (endpoint_mapping .and. power_mapping) then
    select type (prop)
    type is (resonance_t)
      call sf_channel(i)%set_eir_mapping (s_mapping, &
        a = endpoint_mapping_slope, eps = power_mapping_eps, &
        m = prop%mass / sqrts, w = prop%width / sqrts)
    type is (on_shell_t)
      call sf_channel(i)%set_eio_mapping (s_mapping, &
        a = endpoint_mapping_slope, eps = power_mapping_eps, &
        m = prop%mass / sqrts)
    end select
  else if (endpoint_mapping) then
    select type (prop)
    type is (resonance_t)
      call sf_channel(i)%set_epr_mapping (s_mapping, &
        a = endpoint_mapping_slope, &
        m = prop%mass / sqrts, w = prop%width / sqrts)
    type is (on_shell_t)
      call sf_channel(i)%set_epo_mapping (s_mapping, &
        a = endpoint_mapping_slope, &
        m = prop%mass / sqrts)
    end select
  else if (power_mapping) then
    select type (prop)
    type is (resonance_t)
      call sf_channel(i)%set_ipr_mapping (s_mapping, &
        eps = power_mapping_eps, &
        m = prop%mass / sqrts, w = prop%width / sqrts)
    type is (on_shell_t)
      call sf_channel(i)%set_ipo_mapping (s_mapping, &
        eps = power_mapping_eps, &
        m = prop%mass / sqrts)
    end select
  else if (allocated (s_mapping)) then
    select type (prop)
    type is (resonance_t)
      call sf_channel(i)%set_res_mapping (s_mapping, &
        m = prop%mass / sqrts, w = prop%width / sqrts, &
        single = single_parameter)
    type is (on_shell_t)
      call sf_channel(i)%set_os_mapping (s_mapping, &
        m = prop%mass / sqrts, &
        single = single_parameter)
    end select
  else if (allocated (single_mapping)) then
    select type (prop)
    type is (resonance_t)
      call sf_channel(i)%set_res_mapping (single_mapping, &

```

```

        m = prop%mass / sqrts, w = prop%width / sqrts, &
        single = single_parameter)
    type is (on_shell_t)
        call sf_channel(i)%set_os_mapping (single_mapping, &
            m = prop%mass / sqrts, &
            single = single_parameter)
    end select
end if
else if (endpoint_mapping .and. power_mapping) then
    call sf_channel(i)%set_ei_mapping (s_mapping, &
        a = endpoint_mapping_slope, eps = power_mapping_eps)
else if (endpoint_mapping .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_ep_mapping (s_mapping, &
        a = endpoint_mapping_slope)
else if (power_mapping .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_ip_mapping (s_mapping, &
        eps = power_mapping_eps)
else if (s_mapping_enable .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_s_mapping (s_mapping, &
        power = s_mapping_power)
end if
end do
else if (sf_allow_s_mapping) then
    allocate (sf_channel (1))
    call sf_channel(1)%init (n_strfun)
    if (allocated (single_mapping)) then
        call sf_channel(1)%activate_mapping (single_mapping)
    else if (endpoint_mapping .and. power_mapping) then
        call sf_channel(i)%set_ei_mapping (s_mapping, &
            a = endpoint_mapping_slope, eps = power_mapping_eps)
    else if (endpoint_mapping) then
        call sf_channel(1)%set_ep_mapping (s_mapping, &
            a = endpoint_mapping_slope)
    else if (power_mapping) then
        call sf_channel(1)%set_ip_mapping (s_mapping, &
            eps = power_mapping_eps)
    else if (s_mapping_enable) then
        call sf_channel(1)%set_s_mapping (s_mapping, &
            power = s_mapping_power)
    end if
else
    allocate (sf_channel (1))
    call sf_channel(1)%init (n_strfun)
    if (allocated (single_mapping)) then
        call sf_channel(1)%activate_mapping (single_mapping)
    end if
end if
end subroutine dispatch_sf_channels

```

19.14.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_phs_ut.f90>≡
  <File header>

  module dispatch_phs_ut
    use unit_tests
    use dispatch_phs_util

    <Standard module head>

    <Dispatch phs: public test>

    contains

    <Dispatch phs: test driver>

  end module dispatch_phs_ut
<dispatch_phs_util.f90>≡
  <File header>

  module dispatch_phs_util

    <Use kinds>
    <Use strings>
    use variables
    use io_units, only: free_unit
    use os_interface, only: os_data_t
    use process_constants
    use model_data
    use models
    use phs_base
    use phs_none
    use phs_forests
    use phs_wood
    use mappings
    use dispatch_phase_space

    <Standard module head>

    <Dispatch phs: test declarations>

    contains

    <Dispatch phs: tests>

  end module dispatch_phs_util
API: driver for the unit tests below.
<Dispatch phs: public test>≡
  public :: dispatch_phs_test
<Dispatch phs: test driver>≡
  subroutine dispatch_phs_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Dispatch phs: execute tests>

```



```
end subroutine dispatch_phs_test
```

Select type: phase-space configuration object

```

<Dispatch phs: execute tests>≡
  call test (dispatch_phs_1, "dispatch_phs_1", &
    "phase-space configuration", &
    u, results)

<Dispatch phs: test declarations>≡
  public :: dispatch_phs_1

<Dispatch phs: tests>≡
  subroutine dispatch_phs_1 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    class(phs_config_t), allocatable :: phs
    type(phs_parameters_t) :: phs_par
    type(os_data_t) :: os_data
    type(mapping_defaults_t) :: mapping_defs

    write (u, "(A)")  "* Test output: dispatch_phs_1"
    write (u, "(A)")  "* Purpose: select phase-space configuration method"
    write (u, "(A)")

    call var_list%init_defaults (0)

    write (u, "(A)")  "* Allocate PHS as phs_none_t"
    write (u, "(A)")

    call var_list%set_string (&
      var_str ("phs_method"), &
      var_str ("none"), is_known = .true.)
    call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))
    call phs%write (u)

    call phs%final ()
    deallocate (phs)

    write (u, "(A)")
    write (u, "(A)")  "* Allocate PHS as phs_single_t"
    write (u, "(A)")

    call var_list%set_string (&
      var_str ("phs_method"), &
      var_str ("single"), is_known = .true.)
    call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))
    call phs%write (u)

    call phs%final ()
    deallocate (phs)

    write (u, "(A)")
    write (u, "(A)")  "* Allocate PHS as phs_wood_t"

```

```

write (u, "(A)")

call var_list%set_string (&
    var_str ("phs_method"), &
    var_str ("wood"), is_known = .true.)
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))
call phs%write (u)

call phs%final ()
deallocate (phs)

write (u, "(A)")
write (u, "(A)")  "* Setting parameters for phs_wood_t"
write (u, "(A)")

phs_par%m_threshold_s = 123
phs_par%m_threshold_t = 456
phs_par%t_channel = 42
phs_par%off_shell = 17
phs_par%keep_nonresonant = .false.
mapping_defs%energy_scale = 987
mapping_defs%invariant_mass_scale = 654
mapping_defs%momentum_transfer_scale = 321
mapping_defs%step_mapping = .false.
mapping_defs%step_mapping_exp = .false.
mapping_defs%enable_s_mapping = .true.
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"), &
    mapping_defs, phs_par)
call phs%write (u)

call phs%final ()

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_phs_1"

end subroutine dispatch_phs_1

```

Phase-space configuration with file

```

<Dispatch phs: execute tests>+≡
    call test (dispatch_phs_2, "dispatch_phs_2", &
        "configure phase space using file", &
        u, results)

<Dispatch phs: test declarations>+≡
    public :: dispatch_phs_2

<Dispatch phs: tests>+≡
    subroutine dispatch_phs_2 (u)
        use phs_base_ut, only: init_test_process_data
        use phs_wood_ut, only: write_test_phs_file
        use phs_forests

```

```

integer, intent(in) :: u
type(var_list_t) :: var_list
type(os_data_t) :: os_data
type(process_constants_t) :: process_data
type(model_list_t) :: model_list
type(model_t), pointer :: model
class(phs_config_t), allocatable :: phs
integer :: u_phs

write (u, "(A)")  "* Test output: dispatch_phs_2"
write (u, "(A)")  "* Purpose: select 'wood' phase-space &
    &for a test process"
write (u, "(A)")  "*               and read phs configuration from file"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process"
write (u, "(A)")

call var_list%init_defaults (0)
call os_data%init ( )
call syntax_model_file_init ( )
call model_list%read_model &
    (var_str ("Test"), var_str ("Test.mdl"), os_data, model)

call syntax_phs_forest_init ( )

call init_test_process_data (var_str ("dispatch_phs_2"), process_data)

write (u, "(A)")  "* Write phase-space file"

u_phs = free_unit ( )
open (u_phs, file = "dispatch_phs_2.phs", action = "write", status = "replace")
call write_test_phs_file (u_phs, var_str ("dispatch_phs_2"))
close (u_phs)

write (u, "(A)")
write (u, "(A)")  "* Allocate PHS as phs_wood_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("phs_method"), &
    var_str ("wood"), is_known = .true.)
call var_list%set_string (&
    var_str ("phs_file"), &
    var_str ("dispatch_phs_2.phs"), is_known = .true.)
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_2"))

call phs%init (process_data, model)
call phs%configure (sqrt_s = 1000._default)

call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_config_t)

```

```

        call phs%write_forest (u)
    end select

    call phs%final ()

    call var_list%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: dispatch_phs_2"

end subroutine dispatch_phs_2

```

Chapter 20

VEGAS Integration

The backbone integrator of WHIZARD is an object-oriented implemetation of the VEGAS algorithm.

```
<vegas.f90>≡  
  <File header>  
  
  module vegas  
    <Use kinds>  
    <Vegas: modules>  
  
    <Standard module head>  
  
    <Vegas: public>  
  
    <Vegas: parameters>  
  
    <Vegas: types>  
  
    <Vegas: interfaces>  
  
    interface  
      <Vegas: sub interfaces>  
    end interface  
  
    contains  
  
    <Vegas: main procedures>  
  
  end module vegas  
  
<vegas_sub.f90>≡  
  <File header>  
  
  submodule (vegas) vegas_s  
  
    implicit none  
  
    contains
```

```
⟨Vegas: procedures⟩
```

```
end submodule vegas_s
```

```
⟨Vegas: modules⟩≡
  use diagnostics
  use io_units
  use format_utils, only: write_indent
  use format_defs, only: FMT_17
  use rng_base, only: rng_t
  use rng_stream, only: rng_stream_t
```

MPI Module.

```
⟨MPI: Vegas: modules⟩≡
  use request_callback, only: request_handler_t
  use mpi_f08 !NODEP!
```

20.1 Integration modes

VEGAS operates in three different modes: `vegas_mode_importance_only`, `vegas_mode_importance` or `vegas_mode_stratified`. The default mode is `vegas_mode_importance`, where the algorithm decides whether if it is possible to use importance sampling or stratified sampling. In low dimensions VEGAS uses strict stratified sampling.

```
⟨Vegas: parameters⟩≡
  integer, parameter, public :: VEGAS_MODE_IMPORTANCE = 0, &
    & VEGAS_MODE_STRATIFIED = 1, VEGAS_MODE_IMPORTANCE_ONLY = 2
```

20.2 Type: `vegas_func_t`

We define a abstract `func` type which only gives an interface to an `evaluate` procedure. The inside of implementation and also the optimization of are not a concern of the `vegas` implementation.

```
⟨Vegas: public⟩≡
  public :: vegas_func_t

⟨Vegas: types⟩≡
  type, abstract :: vegas_func_t
  !
  contains
    procedure(vegas_func_evaluate), deferred, pass, public :: evaluate
  end type vegas_func_t
```

The only procedure called in `vegas` is `vegas_func_evaluate`. It takes a real value `x` and returns a real value `f`.

```
⟨Vegas: interfaces⟩≡
  abstract interface
    real(default) function vegas_func_evaluate (self, x) result (f)
    import :: default, vegas_func_t
    class(vegas_func_t), intent(inout) :: self
```

```

        real(default), dimension(:), intent(in) :: x
    end function vegas_func_evaluate
end interface

```

20.3 Type: vegas_config_t

We store the complete configuration in a transparent container. The `vegas_config_t` object inside VEGAS must not be directly accesible. We provide a get method which returns a copy of the `vegas_config_t` object.

Apart from the options which can be set by the constructor of `vegas_t` object, we store the run-time configuration `n_calls`, `calls_per_box`, `n_bins` and `n_boxes`. Those are calculated and set accordingly by VEGAS.

```

<Vegas: public>+≡
    public :: vegas_config_t

<Vegas: types>+≡
    type :: vegas_config_t
        integer :: n_dim = 0
        real(default) :: alpha = 1.5_default
        integer :: n_bins_max = 50
        integer :: iterations = 5
        integer :: mode = VEGAS_MODE_STRATIFIED
        integer :: calls_per_box = 0
        integer :: n_calls = 0
        integer :: n_calls_min = 20
        integer :: n_boxes = 1
        integer :: n_bins = 1
    contains
        <Vegas: vegas config: TBP>
    end type vegas_config_t

```

Write out the configuration of the grid.

```

<Vegas: vegas config: TBP>≡
    procedure, public :: write => vegas_config_write

<Vegas: sub interfaces>≡
    module subroutine vegas_config_write (self, unit, indent)
        class(vegas_config_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
    end subroutine vegas_config_write

<Vegas: procedures>≡
    module subroutine vegas_config_write (self, unit, indent)
        class(vegas_config_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &

```

```

        & "Number of dimensions" = ", self%n_dim
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Adaption power (alpha)" = ", self%alpha
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Max. number of bins (per dim.)" = ", self%n_bins_max
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Number of iterations" = ", self%iterations
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Mode (stratified or importance)" = ", self%mode
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Calls per box" = ", self%calls_per_box
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Number of calls" = ", self%n_calls
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Min. number of calls" = ", self%n_calls_min
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Number of bins" = ", self%n_bins
call write_indent (u, ind)
write (u, "(2x,A,I0)") &
        & "Number of boxes" = ", self%n_boxes
end subroutine vegas_config_write

```

20.4 Type: vegas_grid_t

We provide a simple and transparent grid container. The container can then later be used, to export the actual grid.

```

<Vegas: public>+≡
    public :: vegas_grid_t

<Vegas: types>+≡
    type :: vegas_grid_t
        integer :: n_dim = 1
        integer :: n_bins = 1
        real(default), dimension(:), allocatable :: x_lower
        real(default), dimension(:), allocatable :: x_upper
        real(default), dimension(:), allocatable :: delta_x
        real(default), dimension(:,:), allocatable :: xi
    contains
        <Vegas: vegas_grid: TBP>
    end type vegas_grid_t

```

Initialise grid.

```

<Vegas: interfaces>+≡

```



```

interface vegas_grid_t
  module procedure vegas_grid_init
end interface vegas_grid_t

<Vegas: sub interfaces>+≡
  module function vegas_grid_init (n_dim, n_bins_max) result (self)
    type(vegas_grid_t) :: self
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_bins_max
  end function vegas_grid_init

<Vegas: procedures>+≡
  module function vegas_grid_init (n_dim, n_bins_max) result (self)
    type(vegas_grid_t) :: self
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_bins_max
    self%n_dim = n_dim
    self%n_bins = 1
    allocate (self%x_upper(n_dim), source=1.0_default)
    allocate (self%x_lower(n_dim), source=0.0_default)
    allocate (self%delta_x(n_dim), source=1.0_default)
    allocate (self%xi((n_bins_max + 1), n_dim), source=0.0_default)
  end function vegas_grid_init

```

Output.

```

<Vegas: vegas_grid: TBP>≡
  procedure, public :: write => vegas_grid_write

<Vegas: sub interfaces>+≡
  module subroutine vegas_grid_write (self, unit, pacify)
    class(vegas_grid_t), intent(in) :: self
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
  end subroutine vegas_grid_write

<Vegas: procedures>+≡
  module subroutine vegas_grid_write (self, unit, pacify)
    class(vegas_grid_t), intent(in) :: self
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical :: pac
    integer :: u, i, j
    pac = .false.; if (present (pacify)) pac = pacify
    u = given_output_unit (unit)
    write (u, descr_fmt) "begin vegas_grid_t"
    write (u, integer_fmt) "n_dim = ", self%n_dim
    write (u, integer_fmt) "n_bins = ", self%n_bins
    write (u, descr_fmt) "begin x_lower"
    if (allocated (self%x_lower)) then
      do j = 1, self%n_dim
        if (pac) then
          write (u, double_array_pac_fmt) j, self%x_lower(j)
        else
          write (u, double_array_fmt) j, self%x_lower(j)
        end if
      end do
    end if
  end subroutine vegas_grid_write

```

```

        end do
    end if
    write (u, descr_fmt) "end x_lower"
    write (u, descr_fmt) "begin x_upper"
    if (allocated (self%x_upper)) then
        do j = 1, self%n_dim
            if (pac) then
                write (u, double_array_pac_fmt) j, self%x_upper(j)
            else
                write (u, double_array_fmt) j, self%x_upper(j)
            end if
        end do
    end if
    write (u, descr_fmt) "end x_upper"
    write (u, descr_fmt) "begin delta_x"
    if (allocated (self%delta_x)) then
        do j = 1, self%n_dim
            if (pac) then
                write (u, double_array_pac_fmt) j, self%delta_x(j)
            else
                write (u, double_array_fmt) j, self%delta_x(j)
            end if
        end do
    end if
    write (u, descr_fmt) "end delta_x"
    write (u, descr_fmt) "begin xi"
    if (allocated (self%xi)) then
        do j = 1, self%n_dim
            do i = 1, self%n_bins + 1
                if (pac) then
                    write (u, double_array2_pac_fmt) i, j, self%xi(i, j)
                else
                    write (u, double_array2_fmt) i, j, self%xi(i, j)
                end if
            end do
        end do
    end if
    write (u, descr_fmt) "end xi"
    write (u, descr_fmt) "end vegas_grid_t"
end subroutine vegas_grid_write

```

Compare two grids, if they match up to an given precision.

```

<Vegas: public>+≡
    public :: operator (==)

<Vegas: interfaces>+≡
    interface operator (==)
        module procedure vegas_grid_equal
    end interface operator (==)

<Vegas: sub interfaces>+≡
    module function vegas_grid_equal (grid_a, grid_b) result (yorn)
        logical :: yorn
        type(vegas_grid_t), intent(in) :: grid_a, grid_b
    end function vegas_grid_equal

```

```

<Vegas: procedures>+≡
  module function vegas_grid_equal (grid_a, grid_b) result (yorn)
    logical :: yorn
    type(vegas_grid_t), intent(in) :: grid_a, grid_b
    yorn = .true.
    yorn = yorn .and. (grid_a%n_dim == grid_b%n_dim)
    yorn = yorn .and. (grid_a%n_bins == grid_b%n_bins)
    yorn = yorn .and. all (grid_a%x_lower == grid_b%x_lower)
    yorn = yorn .and. all (grid_a%x_upper == grid_b%x_upper)
    yorn = yorn .and. all (grid_a%delta_x == grid_b%delta_x)
    yorn = yorn .and. all (grid_a%xi == grid_b%xi)
  end function vegas_grid_equal

```

Resize each bin accordingly to its corresponding weight w . Can be used to resize the grid to a new size of bins or refinement.

The procedure expects two arguments, firstly, `n_bins` and, secondly, the refinement weights w . If `n_bins` differs from the internally stored one, we resize the grid under consideration of w . If each element of w equals one, then the bins are resized preserving their original bin density.

Anytime else, we refine the grid accordingly to w .

```

<Vegas: vegas_grid: TBP>+≡
  procedure, private :: resize => vegas_grid_resize

<Vegas: sub interfaces>+≡
  module subroutine vegas_grid_resize (self, n_bins, w)
    class(vegas_grid_t), intent(inout) :: self
    integer, intent(in) :: n_bins
    real(default), dimension(:, :), intent(in) :: w
  end subroutine vegas_grid_resize

<Vegas: procedures>+≡
  module subroutine vegas_grid_resize (self, n_bins, w)
    class(vegas_grid_t), intent(inout) :: self
    integer, intent(in) :: n_bins
    real(default), dimension(:, :), intent(in) :: w
    real(default), dimension(size(self%xi)) :: xi_new
    integer :: i, j, k
    real(default) :: pts_per_bin
    real(default) :: d_width
    do j = 1, self%n_dim
      if (self%n_bins /= n_bins) then
        pts_per_bin = real(self%n_bins, default) / real(n_bins, default)
        self%n_bins = n_bins
      else
        if (all (w(:, j) == 0.)) then
          call msg_bug ("[VEGAS] grid_resize: resize weights are zero.")
        end if
        pts_per_bin = sum(w(:, j)) / self%n_bins
      end if
      d_width = 0.
      k = 0
      do i = 2, self%n_bins
        do while (pts_per_bin > d_width)
          k = k + 1

```

```

        d_width = d_width + w(k, j)
    end do
    d_width = d_width - pts_per_bin
    associate (x_upper => self%xi(k + 1, j), x_lower => self%xi(k, j))
        xi_new(i) = x_upper - (x_upper - x_lower) * d_width / w(k, j)
    end associate
    end do
    self%xi(:, j) = 0. ! Reset grid explicitly
    self%xi(2:n_bins, j) = xi_new(2:n_bins)
    self%xi(n_bins + 1, j) = 1.
end do
end subroutine vegas_grid_resize

```

Find the probability for a given x in the unit hypercube.

For the case $n_bins < N_BINARY_SEARCH$, we utilize linear search which is faster for short arrays. Else we make use of a binary search. Furthermore, we calculate the inverse of the probability and invert the result only at the end (saving some time on division).

```

<Vegas: vegas_grid: TBP>+≡
    procedure, public :: get_probability => vegas_grid_get_probability

<Vegas: sub interfaces>+≡
    module function vegas_grid_get_probability (self, x) result (g)
        class(vegas_grid_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: g
    end function vegas_grid_get_probability

<Vegas: procedures>+≡
    module function vegas_grid_get_probability (self, x) result (g)
        class(vegas_grid_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: g
        integer :: j, i_lower, i_higher, i_mid
        real(default), dimension(size(x)) :: y
        g = 1
        y = (x - self%x_lower) / self%delta_x
        if (any (y < 0 .or. y > 1)) then
            g = 0; return
        end if
        ndim: do j = 1, self%n_dim
            i_lower = 1
            i_higher = self%n_bins + 1
            !! Left-most search
            search: do while (i_lower < i_higher - 1)
                i_mid = floor ((i_higher + i_lower) / 2.)
                if (y(j) > self%xi(i_mid, j)) then
                    i_lower = i_mid
                else
                    i_higher = i_mid
                end if
            end do search
            g = g * (self%delta_x(j) * &
                & self%n_bins * (self%xi(i_lower + 1, j) - self%xi(i_lower, j)))
        end do
    end function

```

```

end do ndim
! Move division to the end, which is more efficient.
if (g /= 0) g = 1 / g
end function vegas_grid_get_probability

```

Broadcast the grid information. As safety measure, we get the actual grid object from VEGAS (correctly allocated, but for non-root unfilled) and broadcast the root object. On success, we set grid into VEGAS.

We use the non-blocking broadcast routine, because we have to send quite a bunch of integers and reals.

We have to be very careful with `n_bins`, the number of bins can actually change during different iterations. If we reuse a grid, we have to take that, every grid uses the same `n_bins`. We expect, that the number of dimension does not change, which is in principle possible, but will be checked onto in `vegas_set_grid`.

```

<MPI: Vegas: vegas_grid: TBP>≡
  procedure, public :: broadcast => vegas_grid_broadcast

<MPI: Vegas: sub interfaces>≡
  module subroutine vegas_grid_broadcast (self, comm)
    class(vegas_grid_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
  end subroutine vegas_grid_broadcast

<MPI: Vegas: procedures>≡
  module subroutine vegas_grid_broadcast (self, comm)
    class(vegas_grid_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
    integer :: j, ierror
    type(MPI_Request), dimension(self%n_dim + 4) :: status
    ! Blocking
    call MPI_Bcast (self%n_bins, 1, MPI_INTEGER, 0, comm)
    ! Non blocking
    call MPI_Ibcast (self%n_dim, 1, MPI_INTEGER, 0, comm, status(1))
    call MPI_Ibcast (self%x_lower, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(2))
    call MPI_Ibcast (self%x_upper, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(3))
    call MPI_Ibcast (self%delta_x, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(4))
    ndim: do j = 1, self%n_dim
      call MPI_Ibcast (self%xi(1:self%n_bins + 1, j), self%n_bins + 1, &
        & MPI_DOUBLE_PRECISION, 0, comm, status(4 + j))
    end do ndim
    call MPI_Waitall (self%n_dim + 4, status, MPI_STATUSES_IGNORE)
  end subroutine vegas_grid_broadcast

```

20.5 Type: vegas_result_t

We store the result of the latest iteration(s) in a transparent container. The `vegas_result_t` object inside VEGAS must not be directly accessible. We export the a copy of the result via a get-method of the `vegas_t` object.

We store latest event weight in `evt_weight` and a (possible) event weight excess in `evt_weight_excess`, if the event weight is larger than `max_abs_f`.

```

<Vegas: public>+≡
    public :: vegas_result_t

<Vegas: types>+≡
    type :: vegas_result_t
        integer :: it_start = 0
        integer :: it_num = 0
        integer :: samples = 0
        real(default) :: sum_int_wgtd = 0._default
        real(default) :: sum_wgts
        real(default) :: sum_chi = 0._default
        real(default) :: chi2 = 0._default
        real(default) :: efficiency = 0._default
        real(default) :: efficiency_pos = 0._default
        real(default) :: efficiency_neg = 0._default
        real(default) :: max_abs_f = 0._default
        real(default) :: max_abs_f_pos = 0._default
        real(default) :: max_abs_f_neg = 0._default
        real(default) :: result = 0._default
        real(default) :: std = 0._default
        real(default) :: evt_weight = 0._default
        real(default) :: evt_weight_excess = 0._default
    contains
    <Vegas: vegas result: TBP>
end type vegas_result_t

```

Write out the current status of the integration result.

```

<Vegas: vegas result: TBP>≡
    procedure, public :: write => vegas_result_write

<Vegas: sub interfaces>+≡
    module subroutine vegas_result_write (self, unit, indent)
        class(vegas_result_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
    end subroutine vegas_result_write

<Vegas: procedures>+≡
    module subroutine vegas_result_write (self, unit, indent)
        class(vegas_result_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Start iteration" = ", self%it_start
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Iteration number" = ", self%it_num
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &

```

```

        & "Sample number" = ", self%samples
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Sum of weighted integrals" = ", self%sum_int_wgtd
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Sum of weights" = ", self%sum_wgts
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Sum of chi" = ", self%sum_chi
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "chi2" = ", self%chi2
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Overall efficiency" = ", self%efficiency
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "f-positive efficiency" = ", self%efficiency_pos
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "f-negative efficiency" = ", self%efficiency_neg
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Maximum absolute overall value" = ", self%max_abs_f
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Maximum absolute positive value" = ", self%max_abs_f_pos
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Maximum absolute negative value" = ", self%max_abs_f_neg
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Integral (of latest iteration)" = ", self%result
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Standard deviation" = ", self%std
write (u, "(2x,A," // FMT_17 // ")") &
        & "Event weight" = ", self%evt_weight
write (u, "(2x,A," // FMT_17 // ")") &
        & "Event weight excess" = ", self%evt_weight_excess
end subroutine vegas_result_write

```

Update results and efficiency.

We define

$$\max_x w(x) = \frac{f(x)}{p(x)} \Delta_{\text{jac}}. \quad (20.1)$$

In the implementation we have to factor out `n_calls` in the jacobian. Also, during event generation.

$\langle \text{Vegas: vegas result: TBP} \rangle + \equiv$

```

procedure, public :: update => vegas_result_update
procedure, public :: update_efficiency => vegas_result_update_efficiency

```

```

{ Vegas: sub interfaces } +=
  module subroutine vegas_result_update (result, integral, variance)
    class(vegas_result_t), intent(inout) :: result
    real(default), intent(in) :: integral
    real(default), intent(in) :: variance
  end subroutine vegas_result_update
  module subroutine vegas_result_update_efficiency (result, &
    n_calls, max_pos, max_neg, sum_pos, sum_neg)
    class(vegas_result_t), intent(inout) :: result
    integer, intent(in) :: n_calls
    real(default), intent(in) :: max_pos
    real(default), intent(in) :: max_neg
    real(default), intent(in) :: sum_pos
    real(default), intent(in) :: sum_neg
  end subroutine vegas_result_update_efficiency

{ Vegas: procedures } +=
  module subroutine vegas_result_update (result, integral, variance)
    class(vegas_result_t), intent(inout) :: result
    real(default), intent(in) :: integral
    real(default), intent(in) :: variance
    real(default) :: guarded_variance, sq_integral
    real(default) :: wgt, chi
    !! Guard against zero (or negative) variance.
    !! \Delta = I * \epsilon -> I = \Delta.
    if (variance < &
      max ((epsilon (integral) * integral)**2, tiny(integral))) then
      guarded_variance = &
        max ((epsilon (integral) * integral)**2, &
          tiny (integral))
    else
      guarded_variance = variance
    end if
    wgt = 1._default / guarded_variance
    sq_integral = integral**2
    result%result = integral
    result%std = sqrt (guarded_variance)
    result%samples = result%samples + 1
    if (result%samples == 1) then
      result%chi2 = 0._default
    else
      chi = integral
      if (result%sum_wgts > 0) then
        chi = chi - result%sum_int_wgtd / result%sum_wgts
      end if
      result%chi2 = result%chi2 * (result%samples - 2.0_default)
      result%chi2 = (wgt / (1._default + (wgt / result%sum_wgts))) &
        & * chi**2
      result%chi2 = result%chi2 / (result%samples - 1._default)
    end if
    result%sum_wgts = result%sum_wgts + wgt
    result%sum_int_wgtd = result%sum_int_wgtd + (integral * wgt)
    result%sum_chi = result%sum_chi + (sq_integral * wgt)
  end subroutine vegas_result_update

```



```

module subroutine vegas_result_update_efficiency (result, &
    n_calls, max_pos, max_neg, sum_pos, sum_neg)
    class(vegas_result_t), intent(inout) :: result
    integer, intent(in) :: n_calls
    real(default), intent(in) :: max_pos
    real(default), intent(in) :: max_neg
    real(default), intent(in) :: sum_pos
    real(default), intent(in) :: sum_neg
    result%max_abs_f_pos = n_calls * max_pos
    result%max_abs_f_neg = n_calls * max_neg
    result%max_abs_f = &
        & max (result%max_abs_f_pos, result%max_abs_f_neg)
    result%efficiency_pos = 0
    if (max_pos > 0) then
        result%efficiency_pos = &
            & sum_pos / max_pos
    end if
    result%efficiency_neg = 0
    if (max_neg > 0) then
        result%efficiency_neg = &
            & sum_neg / max_neg
    end if
    result%efficiency = 0
    if (result%max_abs_f > 0.) then
        result%efficiency = (sum_pos + sum_neg) &
            & / result%max_abs_f
    end if
end subroutine vegas_result_update_efficiency

```

Reset results.

```

< Vegas: vegas result: TBP >+≡
    procedure, public :: reset => vegas_result_reset

< Vegas: sub interfaces >+≡
    module subroutine vegas_result_reset (result)
        class(vegas_result_t), intent(inout) :: result
        end subroutine vegas_result_reset

< Vegas: procedures >+≡
    module subroutine vegas_result_reset (result)
        class(vegas_result_t), intent(inout) :: result
        result%sum_int_wgtd = 0
        result%sum_wgts = 0
        result%sum_chi = 0
        result%it_num = 0
        result%samples = 0
        result%chi2 = 0
        result%efficiency = 0
        result%efficiency_pos = 0
        result%efficiency_neg = 0
        result%max_abs_f = 0
        result%max_abs_f_pos = 0
        result%max_abs_f_neg = 0
    end subroutine vegas_result_reset

```

Send the result object to specified rank, internally in a non-blocking way.

We do not need to handle the event results, because each event result is atomic.

(MPI: Vegas: vegas result: TBP)≡

```
procedure, public :: send => vegas_result_send
```

(MPI: Vegas: sub interfaces)+≡

```
module subroutine vegas_result_send (self, receiver, tag, comm, request)
  class(vegas_result_t), intent(in) :: self
  integer, intent(in) :: receiver
  integer, intent(in) :: tag
  type(MPI_COMM), intent(in) :: comm
  type(MPI_Request), dimension(:), intent(inout) :: request
end subroutine vegas_result_send
```

(MPI: Vegas: procedures)+≡

```
module subroutine vegas_result_send (self, receiver, tag, comm, request)
  class(vegas_result_t), intent(in) :: self
  integer, intent(in) :: receiver
  integer, intent(in) :: tag
  type(MPI_COMM), intent(in) :: comm
  type(MPI_Request), dimension(:), intent(inout) :: request
  if (size(request) /= self%get_n_requests()) &
    call msg_bug ("VEGAS: number of requests does not match.")
  call MPI_Isend (self%it_start, 1, MPI_INTEGER, receiver, tag + 1,&
    & comm, request(1))
  call MPI_Isend (self%it_num, 1, MPI_INTEGER, receiver, tag + 2,&
    & comm, request(2))
  call MPI_Isend (self%samples, 1, MPI_INTEGER, receiver, tag + 3,&
    & comm, request(3))
  call MPI_Isend (self%sum_int_wgtd, 1, MPI_DOUBLE_PRECISION, receiver, tag + 4,&
    & comm, request(4))
  call MPI_Isend (self%sum_wgts, 1, MPI_DOUBLE_PRECISION, receiver, tag + 5,&
    & comm, request(5))
  call MPI_Isend (self%sum_chi, 1, MPI_DOUBLE_PRECISION, receiver, tag + 6,&
    & comm, request(6))
  call MPI_Isend (self%chi2, 1, MPI_DOUBLE_PRECISION, receiver, tag + 7,&
    & comm, request(7))
  call MPI_Isend (self%efficiency, 1, MPI_DOUBLE_PRECISION, receiver, tag + 8,&
    & comm, request(8))
  call MPI_Isend (self%efficiency_pos, 1, MPI_DOUBLE_PRECISION, receiver, tag + 9,&
    & comm, request(9))
  call MPI_Isend (self%efficiency_neg, 1, MPI_DOUBLE_PRECISION, receiver, tag + 10,&
    & comm, request(10))
  call MPI_Isend (self%max_abs_f, 1, MPI_DOUBLE_PRECISION, receiver, tag + 11,&
    & comm, request(11))
  call MPI_Isend (self%max_abs_f_pos, 1, MPI_DOUBLE_PRECISION, receiver, tag + 12,&
    & comm, request(12))
  call MPI_Isend (self%max_abs_f_neg, 1, MPI_DOUBLE_PRECISION, receiver, tag + 13,&
    & comm, request(13))
  call MPI_Isend (self%result, 1, MPI_DOUBLE_PRECISION, receiver, tag + 14,&
    & comm, request(14))
  call MPI_Isend (self%std, 1, MPI_DOUBLE_PRECISION, receiver, tag + 15,&
    & comm, request(15))
end subroutine vegas_result_send
```

Receive the result object from a specified rank, internally in a non-blocking way.

(MPI: Vegas: vegas result: TBP)+≡

```
procedure, public :: receive => vegas_result_receive
```

(MPI: Vegas: sub interfaces)+≡

```
module subroutine vegas_result_receive (self, sender, tag, comm, request)
  class(vegas_result_t), intent(inout) :: self
  integer, intent(in) :: sender
  integer, intent(in) :: tag
  type(MPI_COMM), intent(in) :: comm
  type(MPI_REQUEST), dimension(:), intent(inout) :: request
end subroutine vegas_result_receive
```

(MPI: Vegas: procedures)+≡

```
module subroutine vegas_result_receive (self, sender, tag, comm, request)
  class(vegas_result_t), intent(inout) :: self
  integer, intent(in) :: sender
  integer, intent(in) :: tag
  type(MPI_COMM), intent(in) :: comm
  type(MPI_REQUEST), dimension(:), intent(inout) :: request
  if (size (request) /= self%get_n_requests ()) &
    call msg_bug ("VEGAS: number of requests does not match.")
  call MPI_Irecv (self%it_start, 1, MPI_INTEGER, sender, tag + 1,&
    & comm, request(1))
  call MPI_Irecv (self%it_num, 1, MPI_INTEGER, sender, tag + 2,&
    & comm, request(2))
  call MPI_Irecv (self%samples, 1, MPI_INTEGER, sender, tag + 3,&
    & comm, request(3))
  call MPI_Irecv (self%sum_int_wgtd, 1, MPI_DOUBLE_PRECISION, sender, tag + 4,&
    & comm, request(4))
  call MPI_Irecv (self%sum_wgts, 1, MPI_DOUBLE_PRECISION, sender, tag + 5,&
    & comm, request(5))
  call MPI_Irecv (self%sum_chi, 1, MPI_DOUBLE_PRECISION, sender, tag + 6,&
    & comm, request(6))
  call MPI_Irecv (self%chi2, 1, MPI_DOUBLE_PRECISION, sender, tag + 7,&
    & comm, request(7))
  call MPI_Irecv (self%efficiency, 1, MPI_DOUBLE_PRECISION, sender, tag + 8,&
    & comm, request(8))
  call MPI_Irecv (self%efficiency_pos, 1, MPI_DOUBLE_PRECISION, sender, tag + 9,&
    & comm, request(9))
  call MPI_Irecv (self%efficiency_neg, 1, MPI_DOUBLE_PRECISION, sender, tag + 10,&
    & comm, request(10))
  call MPI_Irecv (self%max_abs_f, 1, MPI_DOUBLE_PRECISION, sender, tag + 11,&
    & comm, request(11))
  call MPI_Irecv (self%max_abs_f_pos, 1, MPI_DOUBLE_PRECISION, sender, tag + 12,&
    & comm, request(12))
  call MPI_Irecv (self%max_abs_f_neg, 1, MPI_DOUBLE_PRECISION, sender, tag + 13,&
    & comm, request(13))
  call MPI_Irecv (self%result, 1, MPI_DOUBLE_PRECISION, sender, tag + 14,&
    & comm, request(14))
  call MPI_Irecv (self%std, 1, MPI_DOUBLE_PRECISION, sender, tag + 15,&
    & comm, request(15))
end subroutine vegas_result_receive
```

```

<MPI: Vegas: vegas result: TBP>+≡
    procedure, private :: get_n_requests => vegas_result_get_n_requests

<MPI: Vegas: sub interfaces>+≡
    pure module function vegas_result_get_n_requests (result) result (n_requests)
        class(vegas_result_t), intent(in) :: result
        integer :: n_requests
    end function vegas_result_get_n_requests

<MPI: Vegas: procedures>+≡
    pure module function vegas_result_get_n_requests (result) result (n_requests)
        class(vegas_result_t), intent(in) :: result
        integer :: n_requests
        n_requests = 15
    end function vegas_result_get_n_requests

```

20.6 Type: vegas_handler_t

Callback handler for VEGAS result and grid.

```

<MPI: Vegas: public>≡
    public :: vegas_handler_t

<MPI: Vegas: types>≡
    type, extends(request_handler_t) :: vegas_handler_t
        type(vegas_result_t), pointer :: result => null ()
        real(default), dimension(:, :), pointer :: d => null ()
    contains
        <Vegas: vegas handler: TBP>
    end type vegas_handler_t

```

Provide the actual communication between master and client.

The communication for `vegas_result_t` is done in a separate procedure, where we only have to pass the MPI requests. Collecting of the distribution array is done directly.

```

<MPI: Vegas: vegas handler: TBP>≡
    procedure :: init => vegas_handler_init
    procedure :: write => vegas_handler_write
    procedure :: handle => vegas_handler_handle
    procedure :: client_handle => vegas_handler_client_handle
    final :: vegas_handler_final

<MPI: Vegas: sub interfaces>+≡
    module subroutine vegas_handler_init (handler, handler_id, result, d)
        class(vegas_handler_t), intent(inout) :: handler
        integer, intent(in) :: handler_id
        type(vegas_result_t), intent(in), target :: result
        real(default), dimension(:, :), intent(in), target :: d
    end subroutine vegas_handler_init
    module subroutine vegas_handler_write (handler, unit)
        class(vegas_handler_t), intent(in) :: handler
        integer, intent(in), optional :: unit
    end subroutine vegas_handler_write
    module subroutine vegas_handler_client_handle (handler, dest_rank, comm)
        class(vegas_handler_t), intent(inout) :: handler

```

```

        integer, intent(in) :: dest_rank
        type(MPI_COMM), intent(in) :: comm
    end subroutine vegas_handler_client_handle
module subroutine vegas_handler_handle (handler, source_rank, comm)
    class(vegas_handler_t), intent(inout) :: handler
    integer, intent(in) :: source_rank
    type(MPI_COMM), intent(in) :: comm
end subroutine vegas_handler_handle
module subroutine vegas_handler_final (handler)
    type(vegas_handler_t), intent(inout) :: handler
end subroutine vegas_handler_final

<MPI: Vegas: procedures>+≡
module subroutine vegas_handler_init (handler, handler_id, result, d)
    class(vegas_handler_t), intent(inout) :: handler
    integer, intent(in) :: handler_id
    type(vegas_result_t), intent(in), target :: result
    real(default), dimension(:, :), intent(in), target :: d
    integer :: n_requests, tag_offset
    handler%result => result
    handler%d => d
    handler%finished = .false.
    !! Add one request for handling of the distribution d.
    n_requests = result%get_n_requests () + 1
    tag_offset = max(handler_id - 1, 0) * n_requests
    call handler%allocate (n_requests, tag_offset)
end subroutine vegas_handler_init

module subroutine vegas_handler_write (handler, unit)
    class(vegas_handler_t), intent(in) :: handler
    integer, intent(in), optional :: unit
    integer :: u, j
    u = given_output_unit (unit)
    write (u, "(A)") "[VEGAS_HANDLER]"
    call handler%base_write (unit)
    call handler%result%write (u)
    write (u, "(A)") "BEGIN D"
    do j = 1, size (handler%d, dim=2)
        write (u, "(1X,I3,999(1X," // FMT_17 // "))" j, handler%d(:, j))
    end do
    write (u, "(A)") "END D"
end subroutine vegas_handler_write

module subroutine vegas_handler_handle (handler, source_rank, comm)
    class(vegas_handler_t), intent(inout) :: handler
    integer, intent(in) :: source_rank
    type(MPI_COMM), intent(in) :: comm
    !! Take the complete contiguous array memory.
    call MPI_Irecv (handler%d, size (handler%d), &
        & MPI_DOUBLE_PRECISION, source_rank, handler%tag_offset, comm, &
        & handler%request(1))
    call handler%result%receive (source_rank, handler%tag_offset, comm, &
        handler%request(2:))
    handler%activated = .true.
    handler%finished = .false.

```

```

end subroutine vegas_handler_handle

module subroutine vegas_handler_client_handle (handler, dest_rank, comm)
  class(vegas_handler_t), intent(inout) :: handler
  integer, intent(in) :: dest_rank
  type(MPI_COMM), intent(in) :: comm
  !! Take the complete contiguous array memory.
  call MPI_Isend (handler%d, size (handler%d), &
    & MPI_DOUBLE_PRECISION, dest_rank, handler%tag_offset, comm, &
    & handler%request(1))
  call handler%result%send (dest_rank, handler%tag_offset, comm, &
    handler%request(2))
  handler%activated = .true.
  handler%finished = .false.
end subroutine vegas_handler_client_handle

!> Finalize vegas_handler_t.
!!
!! Nullify pointer to object.
module subroutine vegas_handler_final (handler)
  type(vegas_handler_t), intent(inout) :: handler
  nullify (handler%result)
  nullify (handler%d)
end subroutine vegas_handler_final

```

20.7 Type: vegas_t

The VEGAS object contains the methods for integration and grid resize- and refinement. We store the grid configuration and the (current) result in transparent containers alongside with the actual grid and the distribution.

The values of the distribution depend on the chosen mode whether the function value or the variance is stored. The distribution is used after each iteration to refine the grid.

```

< Vegas: public > +=
  public :: vegas_t

< Vegas: types > +=
  type :: vegas_t
    private
    type(vegas_config_t) :: config
    real(default) :: hypercube_volume = 0._default
    real(default) :: jacobian = 0._default
    real(default), dimension(:, :), allocatable :: d
    type(vegas_grid_t) :: grid
    integer, dimension(:), allocatable :: bin
    integer, dimension(:), allocatable :: box
    type(vegas_result_t) :: result
  < Vegas: vegas: type >
  contains
  < Vegas: vegas: TBP >
end type vegas_t

```

Add members for MPI communication and parallel mode. Must be set before calling to `vegas_integrate`, likewise `vegas_set_calls`.

```
(MPI: Vegas: vegas: type)≡
  type(MPI_COMM) :: comm
  logical :: parallel_mode = .false.
```

We overload the type constructor of `vegas_t` which initialises the mandatory argument `n_dim` and allocate memory for the grid.

```
(Vegas: interfaces)+≡
  interface vegas_t
    module procedure vegas_init
  end interface vegas_t

(Vegas: sub interfaces)+≡
  module function vegas_init &
    (n_dim, alpha, n_bins_max, iterations, mode) result (self)
    type(vegas_t) :: self
    integer, intent(in) :: n_dim
    integer, intent(in), optional :: n_bins_max
    real(default), intent(in), optional :: alpha
    integer, intent(in), optional :: iterations
    integer, intent(in), optional :: mode
  end function vegas_init

(Vegas: procedures)+≡
  module function vegas_init &
    (n_dim, alpha, n_bins_max, iterations, mode) result (self)
    type(vegas_t) :: self
    integer, intent(in) :: n_dim
    integer, intent(in), optional :: n_bins_max
    real(default), intent(in), optional :: alpha
    integer, intent(in), optional :: iterations
    integer, intent(in), optional :: mode
    self%config%n_dim = n_dim
    if (present (alpha)) self%config%alpha = alpha
    if (present (n_bins_max)) self%config%n_bins_max = n_bins_max
    if (present (iterations)) self%config%iterations = iterations
    if (present (mode)) self%config%mode = mode
    self%grid = vegas_grid_t (n_dim, self%config%n_bins_max)
    allocate (self%d(self%config%n_bins_max, n_dim), source=0.0_default)
    allocate (self%box(n_dim), source=1)
    allocate (self%bin(n_dim), source=1)
    self%config%n_bins = 1
    self%config%n_boxes = 1
    call self%set_limits (self%grid%x_lower, self%grid%x_upper)
    call self%reset_grid ()
    call self%reset_result ()
  (Vegas: vegas init)
  end function vegas_init
```

```
(Vegas: vegas init)≡
```

Prepare VEGAS to be run in parallel modues (when compiled with MPI).

```
(MPI: Vegas: vegas init)≡
  call self%prepare_parallel_integrate (MPI_COMM_WORLD, &
```

```

        duplicate_comm = .false., &
        parallel_mode = .true.)

```

Finalize the grid. Deallocate grid memory.

```

< Vegas: vegas: TBP >≡
    procedure, public :: final => vegas_final

< Vegas: sub interfaces >+≡
    module subroutine vegas_final (self)
        class(vegas_t), intent(inout) :: self
    end subroutine vegas_final

< Vegas: procedures >+≡
    module subroutine vegas_final (self)
        class(vegas_t), intent(inout) :: self
        deallocate (self%grid%x_upper)
        deallocate (self%grid%x_lower)
        deallocate (self%grid%delta_x)
        deallocate (self%d)
        deallocate (self%grid%xi)
        deallocate (self%box)
        deallocate (self%bin)
    end subroutine vegas_final

```

20.8 Get-/Set-methods

The VEGAS object prohibits direct access from outside. Communication is handle via get- or set-methods. Set the limits of integration. The defaults limits corresponsing the n -dimensional unit hypercube.

Remark: After setting the limits, the grid is initialised, again. Previous results are lost due to recalculation of the overall jacobian.

```

< Vegas: vegas: TBP >+≡
    procedure, public :: set_limits => vegas_set_limits

< Vegas: sub interfaces >+≡
    module subroutine vegas_set_limits (self, x_lower, x_upper)
        class(vegas_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x_lower
        real(default), dimension(:), intent(in) :: x_upper
    end subroutine vegas_set_limits

< Vegas: procedures >+≡
    module subroutine vegas_set_limits (self, x_lower, x_upper)
        class(vegas_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x_lower
        real(default), dimension(:), intent(in) :: x_upper
        if (size (x_lower) /= self%config%n_dim &
            & .or. size (x_upper) /= self%config%n_dim) then
            write (msg_buffer, "(A, I5, A, I5, A, I5)") &
                "VEGAS: [set_limits] n_dim of new lower/upper integration limit&
                & does not match previously set n_dim. ", self%config%n_dim, " /=&
                & ", size (x_lower), " /= ", size (x_upper)
            call msg_fatal ()
        end if
        if (any(x_upper < x_lower)) then

```



```

        call msg_fatal ("VEGAS: [set_limits] upper limits are smaller than lower limits.")
    end if
    if (any((x_upper - x_lower) > huge(0._default))) then
        call msg_fatal ("VEGAS: [set_limits] upper and lower limits exceed rendering.")
    end if
    self%grid%x_upper = x_upper
    self%grid%x_lower = x_lower
    self%grid%delta_x = self%grid%x_upper - self%grid%x_lower
    self%hypercube_volume = product (self%grid%delta_x)
    call self%reset_result ()
end subroutine vegas_set_limits

```

Set the number of calls. If the number of calls changed during different passes, we resize the grid preserving the probability density. We should reset the results after changing the number of calls which change the size of the grid and the running mode of VEGAS. But, this is a set method only for the number of calls.

```

<Vegas: vegas: TBP>+≡
    procedure, public :: set_calls => vegas_set_n_calls
<Vegas: sub interfaces>+≡
    module subroutine vegas_set_n_calls (self, n_calls)
        class(vegas_t), intent(inout) :: self
        integer, intent(in) :: n_calls
    end subroutine vegas_set_n_calls
<Vegas: procedures>+≡
    module subroutine vegas_set_n_calls (self, n_calls)
        class(vegas_t), intent(inout) :: self
        integer, intent(in) :: n_calls
        if (.not. (n_calls > 0)) then
            write (msg_buffer, "(A, I5)") &
                "VEGAS: [set_calls] number of calls must be a positive number. Keep&
                & number of calls = ", self%config%n_calls
            call msg_warning ()
        else
            self%config%n_calls = max (n_calls, self%config%n_calls_min)
            if (self%config%n_calls /= n_calls) then
                write (msg_buffer, "(A,I5)") &
                    "VEGAS: [set calls] number of calls is too few, reset to ", self%config%n_calls
                call msg_warning ()
            end if
            call self%init_grid ()
        end if
    end subroutine vegas_set_n_calls

```

Get the grid object and set `n_bins`, `n_dim` inside grid container.

```

<Vegas: vegas: TBP>+≡
    procedure, public :: get_grid => vegas_get_grid
<Vegas: sub interfaces>+≡
    module function vegas_get_grid (self) result (grid)
        class(vegas_t), intent(in) :: self
        type(vegas_grid_t) :: grid
    end function vegas_get_grid

```

```

<Vegas: procedures>+≡
  module function vegas_get_grid (self) result (grid)
    class(vegas_t), intent(in) :: self
    type(vegas_grid_t) :: grid
    grid = self%grid
    grid%n_dim = self%config%n_dim
    grid%n_bins = self%config%n_bins
  end function vegas_get_grid

```

Set grid. We need a set method for the parallelisation. We do some additional checks before copying the object. Be careful, we do not check on `n_bins`, because the number of bins can change after setting `n_calls`. We remind you, that you will loose all your current progress, if you use set the grid. Hence, it will only be used when compiled with MPI.

```

<MPI: Vegas: vegas: TBP>≡
  procedure, public :: set_grid => vegas_set_grid

<MPI: Vegas: sub interfaces>+≡
  module subroutine vegas_set_grid (self, grid)
    class(vegas_t), intent(inout) :: self
    type(vegas_grid_t), intent(in) :: grid
  end subroutine vegas_set_grid

<MPI: Vegas: procedures>+≡
  module subroutine vegas_set_grid (self, grid)
    class(vegas_t), intent(inout) :: self
    type(vegas_grid_t), intent(in) :: grid
    integer :: j
    logical :: success
    success = .true.
    success = (success .and. (grid%n_dim .eq. self%config%n_dim))
    success = (success .and. all (grid%x_lower .eq. self%grid%x_lower))
    success = (success .and. all (grid%x_upper .eq. self%grid%x_upper))
    success = (success .and. all (grid%delta_x .eq. self%grid%delta_x))
    if (success) then
      self%config%n_bins = grid%n_bins
      do j = 1, self%config%n_dim
        self%grid%xi(1, j) = 0._default
        self%grid%xi(2:self%config%n_bins, j) = grid%xi(2:grid%n_bins, j)
        self%grid%xi(self%config%n_bins + 1, j) = 1._default
      end do
    else
      call msg_bug ("VEGAS: set grid: boundary conditions do not match.")
    end if
  end subroutine vegas_set_grid

```

Prepare a parallel integration.

A parallel integration requires a communicator, which may be duplicated in order to provide a safe communication context for the current VEGAS instance. Furthermore, given an optional parameter, the behavior with regards to the parallel evaluation can be changed (e.g. embbed integration).

```

<MPI: Vegas: vegas: TBP>+≡
  procedure, public :: prepare_parallel_integrate => &
    vegas_prepare_parallel_integrate

```

```

<MPI: Vegas: sub interfaces>+≡
  module subroutine vegas_prepare_parallel_integrate &
    (self, comm, duplicate_comm, parallel_mode)
    class(vegas_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
    logical, intent(in), optional :: duplicate_comm
    logical, intent(in), optional :: parallel_mode
  end subroutine vegas_prepare_parallel_integrate
<MPI: Vegas: procedures>+≡
  module subroutine vegas_prepare_parallel_integrate &
    (self, comm, duplicate_comm, parallel_mode)
    class(vegas_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
    logical, intent(in), optional :: duplicate_comm
    logical, intent(in), optional :: parallel_mode
    logical :: flag
    flag = .true.; if (present (duplicate_comm)) flag = duplicate_comm
    if (duplicate_comm) then
      call MPI_COMM_DUP (comm, self%comm)
    else
      self%comm = comm
    end if
    self%parallel_mode = .true.; if (present (parallel_mode)) &
      self%parallel_mode = parallel_mode
  end subroutine vegas_prepare_parallel_integrate

```

We check if it is senseful to parallelize the actual grid. In simple, this means that `n_boxes` has to be larger than 2. With the result that we could have an actual superimposed stratified grid. In advance, we can give the size of communicator `n_size` and check whether we have enough boxes to distribute.

```

<MPI: Vegas: vegas: TBP>+≡
  procedure, public :: is_parallelizable => vegas_is_parallelizable
<MPI: Vegas: sub interfaces>+≡
  elemental module function vegas_is_parallelizable &
    (self, opt_n_size) result (flag)
    class(vegas_t), intent(in) :: self
    logical :: flag
    integer, intent(in), optional :: opt_n_size
  end function vegas_is_parallelizable
<MPI: Vegas: procedures>+≡
  elemental module function vegas_is_parallelizable &
    (self, opt_n_size) result (flag)
    class(vegas_t), intent(in) :: self
    logical :: flag
    integer, intent(in), optional :: opt_n_size
    integer :: n_size
    n_size = 2; if (present (opt_n_size)) n_size = opt_n_size
    flag = (self%config%n_boxes**floor (self%config%n_dim / 2.) >= n_size)
  end function vegas_is_parallelizable

```

Get the config object.

```

<Vegas: vegas: TBP>+≡

```

```

        procedure, public :: get_config => vegas_get_config
    <Vegas: sub interfaces>+≡
        module subroutine vegas_get_config (self, config)
            class(vegas_t), intent(in) :: self
            type(vegas_config_t), intent(out) :: config
        end subroutine vegas_get_config
    <Vegas: procedures>+≡
        module subroutine vegas_get_config (self, config)
            class(vegas_t), intent(in) :: self
            type(vegas_config_t), intent(out) :: config
            config = self%config
        end subroutine vegas_get_config

```

Set non-runtime dependent configuration. It will no be possible to change `n_bins_max`.

```

    <Vegas: vegas: TBP>+≡
        procedure, public :: set_config => vegas_set_config
    <Vegas: sub interfaces>+≡
        module subroutine vegas_set_config (self, config)
            class(vegas_t), intent(inout) :: self
            class(vegas_config_t), intent(in) :: config
        end subroutine vegas_set_config
    <Vegas: procedures>+≡
        module subroutine vegas_set_config (self, config)
            class(vegas_t), intent(inout) :: self
            class(vegas_config_t), intent(in) :: config
            self%config%alpha = config%alpha
            self%config%iterations = config%iterations
            self%config%mode = config%mode
            self%config%n_calls_min = config%n_calls_min
        end subroutine vegas_set_config

```

Get the result object.

```

    <Vegas: vegas: TBP>+≡
        procedure, public :: get_result => vegas_get_result
    <Vegas: sub interfaces>+≡
        module function vegas_get_result (self) result (result)
            type(vegas_result_t) :: result
            class(vegas_t), intent(in) :: self
        end function vegas_get_result
    <Vegas: procedures>+≡
        module function vegas_get_result (self) result (result)
            type(vegas_result_t) :: result
            class(vegas_t), intent(in) :: self
            result = self%result
        end function vegas_get_result

```

Set the result object. Be reminded, that you will loose your current results, if you are not careful! Hence, it will only be avaiable during usage with MPI.

```

    <MPI: Vegas: vegas: TBP>+≡
        procedure, public :: set_result => vegas_set_result

```

```

<MPI: Vegas: sub interfaces>+≡
  module subroutine vegas_set_result (self, result)
    class(vegas_t), intent(inout) :: self
    type(vegas_result_t), intent(in) :: result
  end subroutine vegas_set_result

```

```

<MPI: Vegas: procedures>+≡
  module subroutine vegas_set_result (self, result)
    class(vegas_t), intent(inout) :: self
    type(vegas_result_t), intent(in) :: result
    self%result = result
  end subroutine vegas_set_result

```

Get (actual) number of calls.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: get_calls => vegas_get_n_calls

<Vegas: sub interfaces>+≡
  elemental module function vegas_get_n_calls (self) result (n_calls)
    class(vegas_t), intent(in) :: self
    real(default) :: n_calls
  end function vegas_get_n_calls

<Vegas: procedures>+≡
  elemental module function vegas_get_n_calls (self) result (n_calls)
    class(vegas_t), intent(in) :: self
    real(default) :: n_calls
    n_calls = self%config%n_calls
  end function vegas_get_n_calls

```

Get the cumulative result of the integration. Recalculate weighted average of the integration.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: get_integral => vegas_get_integral

<Vegas: sub interfaces>+≡
  elemental module function vegas_get_integral (self) result (integral)
    class(vegas_t), intent(in) :: self
    real(default) :: integral
  end function vegas_get_integral

<Vegas: procedures>+≡
  elemental module function vegas_get_integral (self) result (integral)
    class(vegas_t), intent(in) :: self
    real(default) :: integral
    integral = 0.
    if (self%result%sum_wgts > 0.) then
      integral = self%result%sum_int_wgtd / self%result%sum_wgts
    end if
  end function vegas_get_integral

```

Get the cumulative variance of the integration. Recalculate the variance.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: get_variance => vegas_get_variance

```

```

<Vegas: sub interfaces>+≡
    elemental module function vegas_get_variance (self) result (variance)
        class(vegas_t), intent(in) :: self
        real(default) :: variance
    end function vegas_get_variance

<Vegas: procedures>+≡
    elemental module function vegas_get_variance (self) result (variance)
        class(vegas_t), intent(in) :: self
        real(default) :: variance
        variance = 0.
        if (self%result%sum_wgts > 0.) then
            variance = 1.0 / self%result%sum_wgts
        end if
    end function vegas_get_variance

Get efficiency.

<Vegas: vegas: TBP>+≡
    procedure, public :: get_efficiency => vegas_get_efficiency

<Vegas: sub interfaces>+≡
    elemental module function vegas_get_efficiency (self) result (efficiency)
        class(vegas_t), intent(in) :: self
        real(default) :: efficiency
    end function vegas_get_efficiency

<Vegas: procedures>+≡
    elemental module function vegas_get_efficiency (self) result (efficiency)
        class(vegas_t), intent(in) :: self
        real(default) :: efficiency
        efficiency = 0.
        if (self%result%efficiency > 0. ) then
            efficiency = self%result%efficiency
        end if
    end function vegas_get_efficiency

Get f_max.

<Vegas: vegas: TBP>+≡
    procedure, public :: get_max_abs_f => vegas_get_max_abs_f

<Vegas: sub interfaces>+≡
    elemental module function vegas_get_max_abs_f (self) result (max_abs_f)
        class(vegas_t), intent(in) :: self
        real(default) :: max_abs_f
    end function vegas_get_max_abs_f

<Vegas: procedures>+≡
    elemental module function vegas_get_max_abs_f (self) result (max_abs_f)
        class(vegas_t), intent(in) :: self
        real(default) :: max_abs_f
        max_abs_f = 0.
        if (self%result%max_abs_f > 0.) then
            max_abs_f = self%result%max_abs_f
        end if
    end function vegas_get_max_abs_f

```

Get sum of absolute (positive and negative) values.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: get_sum_abs_f_pos => vegas_get_sum_abs_f_pos
  procedure, public :: get_sum_abs_f_neg => vegas_get_sum_abs_f_neg

<Vegas: sub interfaces>+≡
  elemental module function vegas_get_sum_abs_f_pos (self) result (sum_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: sum_abs_f
  end function vegas_get_sum_abs_f_pos
  elemental module function vegas_get_sum_abs_f_neg (self) result (sum_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: sum_abs_f
  end function vegas_get_sum_abs_f_neg

<Vegas: procedures>+≡
  elemental module function vegas_get_sum_abs_f_pos (self) result (sum_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: sum_abs_f
    sum_abs_f = self%result%efficiency_pos * self%result%max_abs_f_pos
  end function vegas_get_sum_abs_f_pos

  elemental module function vegas_get_sum_abs_f_neg (self) result (sum_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: sum_abs_f
    sum_abs_f = self%result%efficiency_neg * self%result%max_abs_f_neg
  end function vegas_get_sum_abs_f_neg

```

Get f_max_pos.

```

<Vegas: sub interfaces>+≡

<Vegas: vegas: TBP>+≡
  procedure, public :: get_max_abs_f_pos => vegas_get_max_abs_f_pos

<Vegas: sub interfaces>+≡
  elemental module function vegas_get_max_abs_f_pos (self) result (max_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: max_abs_f
  end function vegas_get_max_abs_f_pos

<Vegas: procedures>+≡
  elemental module function vegas_get_max_abs_f_pos (self) result (max_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: max_abs_f
    max_abs_f = 0.
    if (self%result%max_abs_f_pos > 0.) then
      max_abs_f = self%result%max_abs_f_pos
    end if
  end function vegas_get_max_abs_f_pos

```

Get f_max_neg.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: get_max_abs_f_neg => vegas_get_max_abs_f_neg

```

```

{ Vegas: sub interfaces } +=
  elemental module function vegas_get_max_abs_f_neg (self) result (max_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: max_abs_f
  end function vegas_get_max_abs_f_neg

```

```

{ Vegas: procedures } +=
  elemental module function vegas_get_max_abs_f_neg (self) result (max_abs_f)
    class(vegas_t), intent(in) :: self
    real(default) :: max_abs_f
    max_abs_f = 0.
    if (self%result%max_abs_f_neg > 0.) then
      max_abs_f = self%result%max_abs_f_neg
    end if
  end function vegas_get_max_abs_f_neg

```

Get event weight and excess.

```

{ Vegas: vegas: TBP } +=
  procedure, public :: get_evt_weight => vegas_get_evt_weight
  procedure, public :: get_evt_weight_excess => vegas_get_evt_weight_excess

{ Vegas: sub interfaces } +=
  module function vegas_get_evt_weight (self) result (evt_weight)
    class(vegas_t), intent(in) :: self
    real(default) :: evt_weight
  end function vegas_get_evt_weight
  module function vegas_get_evt_weight_excess (self) result (evt_weight_excess)
    class(vegas_t), intent(in) :: self
    real(default) :: evt_weight_excess
  end function vegas_get_evt_weight_excess

```

```

{ Vegas: procedures } +=
  module function vegas_get_evt_weight (self) result (evt_weight)
    class(vegas_t), intent(in) :: self
    real(default) :: evt_weight
    evt_weight = self%result%evt_weight
  end function vegas_get_evt_weight

  module function vegas_get_evt_weight_excess (self) result (evt_weight_excess)
    class(vegas_t), intent(in) :: self
    real(default) :: evt_weight_excess
    evt_weight_excess = self%result%evt_weight_excess
  end function vegas_get_evt_weight_excess

```

Get and set distribution.

We allow the distribution to be manipulated by an external call. The integration result cannot be changed by this, however, the error behavior may worsen and the efficiency may fall pretty low. But, also, the opposite is possible, see `vamp2_equivalences`.

```

{ Vegas: vegas: TBP } +=
  procedure, public :: get_distribution => vegas_get_distribution
  procedure, public :: set_distribution => vegas_set_distribution

```



```

<Vegas: sub interfaces>+=
  module function vegas_get_distribution (self) result (d)
    class(vegas_t), intent(in) :: self
    real(default), dimension(:, :), allocatable :: d
  end function vegas_get_distribution
  module subroutine vegas_set_distribution (self, d)
    class(vegas_t), intent(inout) :: self
    real(default), dimension(:, :), intent(in) :: d
  end subroutine vegas_set_distribution

<Vegas: procedures>+=
  module function vegas_get_distribution (self) result (d)
    class(vegas_t), intent(in) :: self
    real(default), dimension(:, :), allocatable :: d
    d = self%d
  end function vegas_get_distribution

  module subroutine vegas_set_distribution (self, d)
    class(vegas_t), intent(inout) :: self
    real(default), dimension(:, :), intent(in) :: d
    if (size (d, dim = 2) /= self%config%n_dim) then
      call msg_bug ("[VEGAS] set_distribution: new distribution has wrong size of dimension")
    end if
    if (size (d, dim = 1) /= self%config%n_bins_max) then
      call msg_bug ("[VEGAS] set_distribution: new distribution has wrong number of bins")
    end if
    self%d = d
  end subroutine vegas_set_distribution

```

Allocate result handler from VEGAS integrator object. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MPI: Vegas: vegas: TBP>+=
  procedure, public :: allocate_handler => vegas_allocate_handler

<MPI: Vegas: main procedures>=
  subroutine vegas_allocate_handler (self, handler_id, handler)
    class(vegas_t), intent(in), target :: self
    integer, intent(in) :: handler_id
    class(request_handler_t), pointer, intent(out) :: handler
    allocate (vegas_handler_t :: handler)
    select type (handler)
      type is (vegas_handler_t)
        call handler%init (handler_id, result = self%result, d = self%d)
    end select
  end subroutine vegas_allocate_handler

```

20.9 Grid resize- and refinement

Before integration the grid itself must be initialised. Given the number of `n_calls` and `n_dim` we prepare the grid for the integration.

The grid is binned according to the VEGAS mode and `n_calls`. If the mode is not set to `vegas_importance_only`, the grid is divided in to equal boxes. We

try for 2 calls per box

$$boxes = \sqrt[n_{dim}]{\frac{calls}{2}}. \quad (20.2)$$

If the numbers of boxes exceeds the number of bins, which is the case for low dimensions, the algorithm switches to stratified sampling. Otherwise, we are still using importance sampling, but keep the boxes for book keeping. If the number of bins changes from the previous invocation, bins are expanded or contracted accordingly, while preserving bin density.

```

(Vegas: vegas: TBP)+≡
  procedure, private :: init_grid => vegas_init_grid

(Vegas: sub interfaces)+≡
  module subroutine vegas_init_grid (self)
    class(vegas_t), intent(inout) :: self
  end subroutine vegas_init_grid

(Vegas: procedures)+≡
  module subroutine vegas_init_grid (self)
    class(vegas_t), intent(inout) :: self
    integer :: n_bins, n_boxes, box_per_bin, n_total_boxes
    real(default), dimension(:, :), allocatable :: w
    n_bins = self%config%n_bins_max
    n_boxes = 1
    if (self%config%mode /= VEGAS_MODE_IMPORTANCE_ONLY) then
      ! We try for 2 calls per box
      n_boxes = max (floor ((self%config%n_calls / 2.)*(1. / self%config%n_dim)), 1)
      self%config%mode = VEGAS_MODE_IMPORTANCE
      if (2 * n_boxes >= self%config%n_bins_max) then
        ! if n_bins/box < 2
        box_per_bin = max (n_boxes / self%config%n_bins_max, 1)
        n_bins = min (n_boxes / box_per_bin, self%config%n_bins_max)
        n_boxes = box_per_bin * n_bins
        self%config%mode = VEGAS_MODE_STRATIFIED
      end if
    end if
    n_total_boxes = n_boxes**self%config%n_dim
    self%config%calls_per_box = max (floor (real (self%config%n_calls) / n_total_boxes), 2)
    self%config%n_calls = self%config%calls_per_box * n_total_boxes
    ! Total volume of x-space/(average n_calls per bin)
    self%jacobian = self%hypercube_volume * real(n_bins, default)&
      &***self%config%n_dim / real(self%config%n_calls, default)
    self%config%n_boxes = n_boxes
    if (n_bins /= self%config%n_bins) then
      allocate (w(self%config%n_bins, self%config%n_dim), source=1.0_default)
      call self%grid%resize (n_bins, w)
      self%config%n_bins = n_bins
    end if
  end subroutine vegas_init_grid

```

Reset the cumulative result, and efficiency and max. grid values.

```

(Vegas: vegas: TBP)+≡
  procedure, public :: reset_result => vegas_reset_result

```

```

<Vegas: sub interfaces>+≡
  module subroutine vegas_reset_result (self)
    class(vegas_t), intent(inout) :: self
    end subroutine vegas_reset_result

```

```

<Vegas: procedures>+≡
  module subroutine vegas_reset_result (self)
    class(vegas_t), intent(inout) :: self
    call self%result%reset ()
  end subroutine vegas_reset_result

```

Reset the grid. Purge the adapted grid and the distribution. Furthermore, reset the results. The maximal size of the grid remains.

Note: Handle `vegas_reset_grid` with great care! Instead of reusing an old object, create a new one.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: reset_grid => vegas_reset_grid

```

```

<Vegas: sub interfaces>+≡
  module subroutine vegas_reset_grid (self)
    class(vegas_t), intent(inout) :: self
    end subroutine vegas_reset_grid

```

```

<Vegas: procedures>+≡
  module subroutine vegas_reset_grid (self)
    class(vegas_t), intent(inout) :: self
    self%config%n_bins = 1
    self%d = 0._default
    self%grid%xi = 0._default
    self%grid%xi(1, :) = 0._default
    self%grid%xi(2, :) = 1._default
    call self%reset_result ()
  end subroutine vegas_reset_grid

```

Refine the grid to match the distribution `d`.

Average the distribution over neighbouring bins, then contract or expand the bins. The averaging dampens high fluctuations among the integrand or the variance.

We make the type-bound procedure public accessible because the multi-channel integration refines each grid after integration over all grids.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: refine => vegas_refine_grid

```

```

<Vegas: sub interfaces>+≡
  module subroutine vegas_refine_grid (self, average)
    class(vegas_t), intent(inout) :: self
    logical, intent(in), optional :: average
    end subroutine vegas_refine_grid

```

```

<Vegas: procedures>+≡
  module subroutine vegas_refine_grid (self, average)
    class(vegas_t), intent(inout) :: self
    logical, intent(in), optional :: average
    logical :: opt_average
    opt_average = .true.; if (present (average)) opt_average = average

```

```

    if (opt_average) call self%average_distribution ()
    call self%grid%resize (self%config%n_bins, self%d(:self%config%n_bins, :))
end subroutine vegas_refine_grid

```

We average the collected values d of the (sq.) weighted f over neighbouring bins. The averaged d are then again damped by a logarithm to enhance numerical stability. The results are then the refinement weights w .

We have to take care of the special case where we have a very low sampling rate. In those cases we can not be sure that the distribution is satisfying filled, although we have already averaged over neighbouring bins. This will lead to a squashing of the unfilled bins and such the boundaries of those will be pushed together. We circumvent this problem by setting those unfilled bins to the smallest representable value of a default real.

The problem becomes very annoying in the multi-channel formulae where have to look up via binary search the corresponding probability of x and if the width is zero, the point will be neglected.

Another issue arises when NaNs appear during sampling. A single NaN may spoil the complete adaption as the refinement depends on all weights for a single axis, c.f. `vegas_grid_resize` for the details of the mechanism. Therefore, if we find a single (or more) NaNs in the distribution of an axis, then we won't adapt that specific axis by setting the weights to one. Hence, we skip the adaption for parts of the grid, where NaN appeared during evaluation.

```

{ Vegas: vegas: TBP } +=
  procedure, private :: average_distribution => vegas_average_distribution

{ Vegas: sub interfaces } +=
  module subroutine vegas_average_distribution (self)
    class(vegas_t), intent(inout) :: self
  end subroutine vegas_average_distribution

{ Vegas: procedures } +=
  module subroutine vegas_average_distribution (self)
    !! use, intrinsic :: ieee_arithmetic, only: ieee_is_nan
    class(vegas_t), intent(inout) :: self
    integer :: j
    ndim: do j = 1, self%config%n_dim
      associate (d => self%d(:self%config%n_bins, j), &
        n_bins => self%config%n_bins)
        !! Non-portable and compiler-flag sensitive test, may replace with ieee_is_nan
        if (any (d /= d)) then
          d = 1.0_default
          cycle ndim
        end if
        if (n_bins > 2) then
          d(1) = (d(1) + d(2)) / 2.0_default
          d(2:n_bins - 1) = (d(1:n_bins - 2) + d(2:n_bins - 1) + d(3:n_bins)) / &
            & 3.0_default
          d(n_bins) = d(n_bins - 1) + d(n_bins) / 2.0_default
        end if
        if (all (d < tiny (d))) then
          d = 1.0_default; cycle ndim
        end if
      end do
      d = d / sum (d)
    end do
  end subroutine vegas_average_distribution

```

```

      where (d < tiny (1.0_default))
        d = tiny (1.0_default)
      end where
      where (d /= 1.0_default)
        d = ((d - 1.0_default) / log(d))**self%config%alpha
      elsewhere
        ! Analytic limes for d -> 1
        d = 1.0_default
      end where
    end associate
  end do ndim
end subroutine vegas_average_distribution

```

20.10 Integration

Integrate `func`, in the previous set bounds `x_lower` to `x_upper`, with `n_calls`. Use results from previous invocations of `integrate` with `opt_reset_result = .false.` and better with subsequent calls.

Before we walk through the hybercube, we initialise the grid (at a central position).

We step through the (equidistant) boxes which ensure we do not miss any place in the n -dim. hypercube. In each box we sample `calls_per_box` random points and transform them to bin coordinates. The total integral and the total (sample) variance over each box i is then calculated by

$$E(I)_i = \sum_j^{\text{calls per box}} I_{i,j},$$

$$V(I)_i = \text{calls per box} \frac{\sum_j^{\text{calls per box}} I_{i,j}^2}{I} - \left(\sum_j^{\text{calls per box}} I_{i,j} \right)^2 * 2 \frac{\text{calls per box}}{\text{calls per box} - 1}.$$

The stratification of the n -dimensional hybercube allows a simple parallelisation of the algorithm (R. Kreckel, "Parallelization of adaptive MC integrators", Computer Physics Communications, vol. 106, no. 3, pp. 258–266, Nov. 1997.). We have to ensure that all boxes are sampled, but the number of boxes to distribute is too large. We allow each thread to sample a fraction r of all boxes k such that $r \ll k$. Furthermore, we constrain that the number of process p is much smaller than r .

The overall constraint is

$$p \ll r \ll k. \quad (20.3)$$

We divide the integration into a parallel and a perpendicular subspace. The number of parallel dimensions is $D_{\parallel} = \lfloor \frac{D}{2} \rfloor$.

`< Vegas: vegas: TBP > +=`

```

  procedure, public :: integrate => vegas_integrate

```

`< Vegas: sub interfaces > +=`

```

  module subroutine vegas_integrate (self, func, rng, iterations, reset_result, &
    refine_grid, verbose, result, abserr)
    class(vegas_t), intent(inout) :: self

```

```

class(vegas_func_t), intent(inout) :: func
class(rng_t), intent(inout) :: rng
integer, intent(in), optional :: iterations
logical, intent(in), optional :: reset_result
logical, intent(in), optional :: refine_grid
logical, intent(in), optional :: verbose
real(default), optional, intent(out) :: result, abserr
end subroutine vegas_integrate

< Vegas: procedures >+≡
module subroutine vegas_integrate (self, func, rng, iterations, reset_result, &
    refine_grid, verbose, result, abserr)
class(vegas_t), intent(inout) :: self
class(vegas_func_t), intent(inout) :: func
class(rng_t), intent(inout) :: rng
integer, intent(in), optional :: iterations
logical, intent(in), optional :: reset_result
logical, intent(in), optional :: refine_grid
logical, intent(in), optional :: verbose
real(default), optional, intent(out) :: result, abserr
integer :: it, k
real(default), dimension(self%config%n_dim) :: x
real(default) :: fval, fval_sq, bin_volume
real(default) :: fval_box, fval_sq_box
real(default) :: total_integral, total_sq_integral
real(default) :: cumulative_int, cumulative_std
real(default) :: sum_abs_f_pos, max_abs_f_pos
real(default) :: sum_abs_f_neg, max_abs_f_neg
logical :: opt_reset_result
logical :: opt_refine_grid
logical :: opt_verbose
integer :: n_size
integer :: n_dim_par
logical :: box_success
< Vegas: vegas_integrate: variables >
call set_options ()
call self%init_grid ()
if (opt_reset_result) call self%result%reset ()
self%result%it_start = self%result%it_num
cumulative_int = 0.
cumulative_std = 0.
n_dim_par = floor (self%config%n_dim / 2.)
n_size = 1
< Vegas: vegas_integrate: init >
if (opt_verbose) then
    call msg_message ("Results: [it, calls, integral, error, chi^2, eff.]")
end if
iteration: do it = 1, self%config%iterations
    self%result%it_num = self%result%it_start + it
    self%d = 0.
    self%box = 1
    self%bin = 1
    total_integral = 0.
    total_sq_integral = 0.
    sum_abs_f_pos = 0.

```

```

max_abs_f_pos = 0.
sum_abs_f_neg = 0.
max_abs_f_neg = 0.
box_success = .true.
select type (rng)
type is (rng_stream_t)
    call rng%next_substream ()
end select
< Vegas: vegas integrate: presampling >
loop_over_par_boxes: do while (box_success)
    loop_over_perp_boxes: do while (box_success)
        fval_box = 0._default
        fval_sq_box = 0._default
        do k = 1, self%config%calls_per_box
            call self%random_point (rng, x, bin_volume)
            ! Call the function, yeah, call it...
            fval = self%jacobian * bin_volume * func%evaluate (x)
            fval_sq = fval**2
            fval_box = fval_box + fval
            fval_sq_box = fval_sq_box + fval_sq
            if (fval > 0.) then
                max_abs_f_pos = max(abs (fval), max_abs_f_pos)
                sum_abs_f_pos = sum_abs_f_pos + abs(fval)
            else
                max_abs_f_neg = max(abs (fval), max_abs_f_neg)
                sum_abs_f_neg = sum_abs_f_neg + abs(fval)
            end if
            if (self%config%mode /= VEGAS_MODE_STRATIFIED) then
                call self%accumulate_distribution (fval_sq)
            end if
        end do
        fval_sq_box = sqrt (fval_sq_box * self%config%calls_per_box)
        ! (a - b) * (a + b) = a**2 - b**2
        fval_sq_box = (fval_sq_box - fval_box) * (fval_sq_box + fval_box)
        if (fval_sq_box <= 0.0) fval_sq_box = fval_box**2 * epsilon (1.0_default)
        total_integral = total_integral + fval_box
        total_sq_integral = total_sq_integral + fval_sq_box
        if (self%config%mode == VEGAS_MODE_STRATIFIED) then
            call self%accumulate_distribution (fval_sq_box)
        end if
        call increment_box_coord (self%box(n_dim_par + 1:self%config&
            &%n_dim), box_success)
    end do loop_over_perp_boxes
    shift: do k = 1, n_size
        call increment_box_coord (self%box(1:n_dim_par), box_success)
        if (.not. box_success) exit shift
    end do shift
< Vegas: vegas integrate: loop >
end do loop_over_par_boxes
< Vegas: vegas integrate: postsampling >
associate (result => self%result)
! Compute final results for this iterations
call result%update (total_integral, variance = &
    total_sq_integral / (self%config%calls_per_box - 1._default))

```

```

        call result%update_efficiency (n_calls = self%config%n_calls, &
            max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
            sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
        cumulative_int = result%sum_int_wgtd / result%sum_wgts
        cumulative_std = sqrt (1 / result%sum_wgts)
    end associate
    if (opt_verbose) then
        write (msg_buffer, "(I0,1x,I0,1x, 4(E24.16E4,1x))" ) &
            & it, self%config%n_calls, cumulative_int, cumulative_std, &
            & self%result%chi2, self%result%efficiency
        call msg_message ()
    end if
    if (opt_refine_grid) then
        call self%refine (average = .true.)
    else
        !! Skip grid refinement, but average the (grid) distribution.
        !! \note Now, we always average and dampen the distribution,
        !!     even when not adapting (e.g. final pass).
        call self%average_distribution ()
    end if
end do iteration
if (present(result)) result = cumulative_int
if (present(abserr)) abserr = abs(cumulative_std)
contains
< Vegas: vegas integrate: procedures >
end subroutine vegas_integrate

```

Set optional arguments of vegas_integrate.

```

< Vegas: vegas integrate: procedures >≡
subroutine set_options ()
    if (present (iterations)) self%config%iterations = iterations
    opt_reset_result = .true.
    if (present (reset_result)) opt_reset_result = reset_result
    opt_refine_grid = .true.
    if (present (refine_grid)) opt_refine_grid = refine_grid
    opt_verbose = .false.
    if (present (verbose)) opt_verbose = verbose
end subroutine set_options

```

We define additional chunk, which will be used later on for inserting MPI/general MPI code. The code is then removed by additional noweb filter if not compiled with the correspondig compiler flag.

Overall variables, some additionally introduced due to the MPI parallelization and needed in sequentiell verison.

```

< Vegas: vegas integrate: variables >≡

```

Overall initialization.

```

< Vegas: vegas integrate: init >≡

```

Reset all last-iteration results before sampling.

```

< Vegas: vegas integrate: presampling >≡

```

Adjust rng between parallel and perpendicular loops.

```

< Vegas: vegas integrate: loop >≡

```


<Vegas: vegas integrate: postsampling>≡

Increment the box coordinates by 1. If we reach the largest value for the current axis (starting with the largest dimension number), we reset the counter to 1 and increment the next axis counter by 1. And so on, until we reach the maximum counter value of the axis with the lowest dimension, then we set **success** to false and the box coord is set to 1.

<Vegas: vegas integrate: procedures>+≡

```
subroutine increment_box_coord (box, success)
  integer, dimension(:), intent(inout) :: box
  logical, intent(out) :: success
  integer :: j
  success = .true.
  do j = size (box), 1, -1
    box(j) = box(j) + 1
    if (box(j) <= self%config%n_boxes) return
    box(j) = 1
  end do
  success = .false.
end subroutine increment_box_coord
```

We parallelize **VEGAS** in simple forward manner. The hyper-cube is dissambled in to equidistant boxes in which we sample the integrand **calls_per_box** times. The workload of calculating those boxes is distributed along the worker.

The number of dimensions which will be parallelised are $\lfloor \frac{D}{2} \rfloor$, such MPI Variables for **vegas_integrate**. We have to duplicate all buffers for **MPI_Ireduce**, because we cannot use the same send or receive buffer.

We temporarily store a (empty) grid, before communicating.

<MPI: Vegas: vegas integrate: variables>≡

```
integer :: rank
logical :: parallel_mode
type(vegas_grid_t) :: grid
```

MPI procedure-specific initialization.

Allow for (external) veto on parallel mode.

<MPI: Vegas: vegas integrate: init>≡

```
parallel_mode = self%parallel_mode .and. self%is_parallelizable ()
if (parallel_mode) then
  call MPI_Comm_size (self%comm, n_size)
  call MPI_Comm_rank (self%comm, rank)
else
  n_size = 1
  rank = 0
end if
```

Pre-sampling communication.

We make a copy of the (actual) grid, which is unfilled when non-root. The actual grid is then broadcasted among the workers and inserted into the **VEGAS** object.

<MPI: Vegas: vegas integrate: presampling>≡

```
if (parallel_mode) then
  grid = self%get_grid ()
  call grid%broadcast (self%comm)
  call self%set_grid (grid)
```

Start index of the boxes for different ranks. If the random number generator is RngStream, we can advance the current stream in such a way, that we will get matching numbers. If `n_boxes` is larger than 2, otherwise parallelization is useless.

```

(MPI: Vegas: vegas integrate: presampling)+≡
  do k = 1, rank
    call increment_box_coord (self%box(1:n_dim_par), box_success)
    if (.not. box_success) exit
  end do
  select type (rng)
  type is (rng_stream_t)
    call rng%advance_state (self%config%n_dim * self%config%calls_per_box&
      & * self%config%n_boxes**(self%config%n_dim - n_dim_par) * rank)
  end select
end if

```

Increment `n_size` times the box coordinates.

```

(MPI: Vegas: vegas integrate: loop)≡
  if (parallel_mode) then
    select type (rng)
    type is (rng_stream_t)
      call rng%advance_state (self%config%n_dim * self%config%calls_per_box&
        & * self%config%n_boxes**(self%config%n_dim - n_dim_par) * (n_size - 1))
    end select
  end if

```

Call to `vegas_integrate_collect`.

```

(MPI: Vegas: vegas integrate: postsampling)≡
  if (parallel_mode) then
    call vegas_integrate_collect ()
    if (rank /= 0) cycle iteration
  end if

```

Reduce (in an non-blocking fashion) all sampled information via `MPI_SUM` or `MPI_MAX`.

```

(MPI: Vegas: vegas integrate: procedures)≡
  subroutine vegas_integrate_collect ()
    integer :: j
    real(default) :: root_total_integral, root_total_sq_integral
    real(default) :: root_sum_abs_f_pos, root_max_abs_f_pos
    real(default) :: root_sum_abs_f_neg, root_max_abs_f_neg
    real(default), dimension(self%config%n_bins_max, self%config%n_dim) :: root_d
    type(MPI_Request), dimension(self%config%n_dim + 6) :: status
    root_d = 0._default
    root_sum_abs_f_pos = 0._default
    root_sum_abs_f_neg = 0._default
    root_max_abs_f_pos = 0._default
    root_max_abs_f_neg = 0._default
    root_total_integral = 0._default
    root_total_sq_integral = 0._default
    call MPI_Ireduce (sum_abs_f_pos, root_sum_abs_f_pos, 1, MPI_DOUBLE_PRECISION,&
      & MPI_SUM, 0, self%comm, status(1))
    call MPI_Ireduce (sum_abs_f_neg, root_sum_abs_f_neg, 1, MPI_DOUBLE_PRECISION,&
      & MPI_SUM, 0, self%comm, status(2))
    call MPI_Ireduce (max_abs_f_pos, root_max_abs_f_pos, 1, MPI_DOUBLE_PRECISION,&

```

```

        & MPI_MAX, 0, self%comm, status(3))
call MPI_Ireduce (max_abs_f_neg, root_max_abs_f_neg, 1, MPI_DOUBLE_PRECISION,&
    & MPI_MAX, 0, self%comm, status(4))
call MPI_Ireduce (total_integral, root_total_integral, 1, MPI_DOUBLE_PRECISION,&
    & MPI_SUM, 0, self%comm, status(5))
call MPI_Ireduce (total_sq_integral, root_total_sq_integral, 1,&
    & MPI_DOUBLE_PRECISION, MPI_SUM, 0, self%comm, status(6))
do j = 1, self%config%n_dim
    call MPI_Ireduce (self%d(1:self%config%n_bins, j), root_d(1:self%config&
        &n_bins, j), self%config%n_bins, MPI_DOUBLE_PRECISION, MPI_SUM, 0,&
        & self%comm, status(6 + j))
end do
call MPI_Waitall (self%config%n_dim + 6, status, MPI_STATUSES_IGNORE)
if (rank == 0) sum_abs_f_pos = root_sum_abs_f_pos
if (rank == 0) sum_abs_f_neg = root_sum_abs_f_neg
if (rank == 0) max_abs_f_pos = root_max_abs_f_pos
if (rank == 0) max_abs_f_neg = root_max_abs_f_neg
if (rank == 0) total_integral = root_total_integral
if (rank == 0) total_sq_integral = root_total_sq_integral
if (rank == 0) self%d = root_d
end subroutine vegas_integrate_collect

```

Obtain a random point inside the n -dimensional hypercube, transform onto the correct interval and calculate the bin volume. The additional factor `n_bins` is already applied to the jacobian (per dimension).

(Vegas: vegas: TBP)+≡

```

    procedure, private :: random_point => vegas_random_point

```

(Vegas: sub interfaces)+≡

```

    module subroutine vegas_random_point (self, rng, x, bin_volume)
        class(vegas_t), intent(inout) :: self
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        real(default), intent(out) :: bin_volume
    end subroutine vegas_random_point

```

(Vegas: procedures)+≡

```

    module subroutine vegas_random_point (self, rng, x, bin_volume)
        class(vegas_t), intent(inout) :: self
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        real(default), intent(out) :: bin_volume
        integer :: j
        real(default) :: r, y, z, bin_width
        bin_volume = 1.
        ndim: do j = 1, self%config%n_dim
            call rng%generate (r)
            z = ((self%box(j) - 1 + r) / self%config%n_boxes) * self%config%n_bins + 1
            self%bin(j) = max (min (int (z), self%config%n_bins), 1)
            if (self%bin(j) == 1) then
                bin_width = self%grid%xi(2, j)
                y = (z - self%bin(j)) * bin_width
            else
                bin_width = self%grid%xi(self%bin(j) + 1, j) - self%grid%xi(self%bin(j), j)
                y = self%grid%xi(self%bin(j), j) + (z - self%bin(j)) * bin_width
            end if
        end do ndim
        x = self%grid%xi(self%bin(1), 1) + y
        bin_volume = bin_volume * self%grid%xi(self%bin(1), 1)
    end subroutine vegas_random_point

```

```

        end if
        x(j) = self%grid%x_lower(j) + y * self%grid%delta_x(j)
        bin_volume = bin_volume * bin_width
    end do ndim
end subroutine vegas_random_point

```

Obtain a random point inside the n -dimensional hyper-cube. We neglect stratification and generate the random point in the most simple way. Hence, we do not need to know in which box we are actually sampling. This is useful for only for event generation.

```

<Vegas: vegas: TBP>+≡
    procedure, private :: simple_random_point => vegas_simple_random_point

<Vegas: sub interfaces>+≡
    module subroutine vegas_simple_random_point (self, rng, x, bin_volume)
        class(vegas_t), intent(inout) :: self
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        real(default), intent(out) :: bin_volume
    end subroutine vegas_simple_random_point

<Vegas: procedures>+≡
    module subroutine vegas_simple_random_point (self, rng, x, bin_volume)
        class(vegas_t), intent(inout) :: self
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        real(default), intent(out) :: bin_volume
        integer :: j, k
        real(default) :: r, y, z, bin_width
        bin_volume = 1.
        ndim: do j = 1, self%config%n_dim
            call rng%generate (r)
            z = r * self%config%n_bins + 1
            k = max (min (int (z), self%config%n_bins), 1)
            if (k == 1) then
                bin_width = self%grid%xi(2, j)
                y = (z - 1) * bin_width
            else
                bin_width = self%grid%xi(k + 1, j) - self%grid%xi(k, j)
                y = self%grid%xi(k, j) + (z - k) * bin_width
            end if
            x(j) = self%grid%x_lower(j) + y * self%grid%delta_x(j)
            bin_volume = bin_volume * bin_width
        end do ndim
    end subroutine vegas_simple_random_point

<Vegas: vegas: TBP>+≡
    procedure, private :: accumulate_distribution => vegas_accumulate_distribution

<Vegas: sub interfaces>+≡
    module subroutine vegas_accumulate_distribution (self, y)
        class(vegas_t), intent(inout) :: self
        real(default), intent(in) :: y
    end subroutine vegas_accumulate_distribution

```

```

<Vegas: procedures>+≡
module subroutine vegas_accumulate_distribution (self, y)
  class(vegas_t), intent(inout) :: self
  real(default), intent(in) :: y
  integer :: j
  do j = 1, self%config%n_dim
    self%d(self%bin(j), j) = self%d(self%bin(j), j) + y
  end do
end subroutine vegas_accumulate_distribution

```

Generate weighted random event.

The weight given by the overall jacobian

$$\Delta_{\text{jac}} = \prod_{j=1}^d (x_j^+ - x_j^-) \frac{N_{\text{bins}}^d}{N_{\text{calls}}} \quad (20.4)$$

includes the overall non-changing factors $\frac{1}{N_{\text{calls}}}$ -factor (divisions are expensive) and N_{bins}^d , the latter combined with `bin_volume` gives rise to the probability, see `vegas_init_grid` for details. We have to factor out N_{calls} to retrieve the correct weight.

```

<Vegas: vegas: TBP>+≡
  procedure :: generate_weighted => vegas_generate_weighted_event
<Vegas: sub interfaces>+≡
  module subroutine vegas_generate_weighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(inout) :: x
  end subroutine vegas_generate_weighted_event
<Vegas: procedures>+≡
  module subroutine vegas_generate_weighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(inout) :: x
    real(default) :: bin_volume
    call self%simple_random_point (rng, x, bin_volume)
    ! Cancel n_calls from jacobian with n_calls
    self%result%evt_weight = self%config%n_calls * self%jacobian * bin_volume &
      & * func%evaluate (x)
  end subroutine vegas_generate_weighted_event

```

Generate random event. We accept on the rate

$$\frac{|f(x)|}{\max_x |f(x)|}. \quad (20.5)$$

We keep separate maximum weights for positive and negative weights, and use them, accordingly. In the case of unweighted event generation, if the current weight exceeds the the maximum weight, we update the maximum, accordingly.

```

<Vegas: vegas: TBP>+≡
  procedure, public :: generate_unweighted=> vegas_generate_unweighted_event

```

```

< Vegas: sub interfaces > +=
  module subroutine vegas_generate_unweighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
  end subroutine vegas_generate_unweighted_event

< Vegas: procedures > +=
  module subroutine vegas_generate_unweighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
    real(default) :: bin_volume
    real(default) :: r
    associate (result => self%result)
      generate: do
        call self%generate_weighted (func, rng, x)
        if (abs(result%evt_weight) > result%max_abs_f) then
          result%evt_weight_excess = &
            & abs(result%evt_weight) / result%max_abs_f - 1._default
          exit generate
        end if
        call rng%generate (r)
        ! Do not use division, because max_abs_f could be zero.
        if (result%max_abs_f * r <= abs(result%evt_weight)) then
          exit generate
        end if
      end do generate
    end associate
  end subroutine vegas_generate_unweighted_event

```

20.11 I/O operation

Write grid to file. We use the original VAMP formatter.

```

< Vegas: parameters > +=
  character(len=*), parameter, private :: &
    descr_fmt = "(1X,A)", &
    integer_fmt = "(1X,A18,1X,I15)", &
    integer_array_fmt = "(1X,I18,1X,I15)", &
    logical_fmt = "(1X,A18,1X,L1)", &
    double_fmt = "(1X,A18,1X,E24.16E4)", &
    double_array_fmt = "(1X,I18,1X,E24.16E4)", &
    double_array_pac_fmt = "(1X,I18,1X,E16.8E4)", &
    double_array2_fmt = "(1X,2(1X,I8),1X,E24.16E4)", &
    double_array2_pac_fmt = "(1X,2(1X,I8),1X,E16.8E4)"

< Vegas: vegas: TBP > +=
  procedure, public :: write_grid => vegas_write_grid

```

{ Vegas: sub interfaces } +=

```

module subroutine vegas_write_grid (self, unit)
  class(vegas_t), intent(in) :: self
  integer, intent(in), optional :: unit
end subroutine vegas_write_grid

```

{ Vegas: procedures } +=

```

module subroutine vegas_write_grid (self, unit)
  class(vegas_t), intent(in) :: self
  integer, intent(in), optional :: unit
  integer :: u
  integer :: i, j
  u = given_output_unit (unit)
  write (u, descr_fmt) "begin type(vegas_t)"
  write (u, integer_fmt) "n_dim =", self%config%n_dim
  write (u, integer_fmt) "n_bins_max =", self%config%n_bins_max
  write (u, double_fmt) "alpha =", self%config%alpha
  write (u, integer_fmt) "iterations =", self%config%iterations
  write (u, integer_fmt) "mode =", self%config%mode
  write (u, integer_fmt) "calls_per_box =", self%config%calls_per_box
  write (u, integer_fmt) "n_calls =", self%config%n_calls
  write (u, integer_fmt) "n_calls_min =", self%config%n_calls_min
  write (u, integer_fmt) "n_boxes =", self%config%n_boxes
  write (u, integer_fmt) "n_bins =", self%config%n_bins
  write (u, integer_fmt) "it_start =", self%result%it_start
  write (u, integer_fmt) "it_num =", self%result%it_num
  write (u, integer_fmt) "samples =", self%result%samples
  write (u, double_fmt) "sum_int_wgtd =", self%result%sum_int_wgtd
  write (u, double_fmt) "sum_wgts =", self%result%sum_wgts
  write (u, double_fmt) "sum_chi =", self%result%sum_chi
  write (u, double_fmt) "chi2 =", self%result%chi2
  write (u, double_fmt) "efficiency =", self%result%efficiency
  write (u, double_fmt) "efficiency =", self%result%efficiency_pos
  write (u, double_fmt) "efficiency =", self%result%efficiency_neg
  write (u, double_fmt) "max_abs_f =", self%result%max_abs_f
  write (u, double_fmt) "max_abs_f_pos =", self%result%max_abs_f_pos
  write (u, double_fmt) "max_abs_f_neg =", self%result%max_abs_f_neg
  write (u, double_fmt) "result =", self%result%result
  write (u, double_fmt) "std =", self%result%std
  write (u, double_fmt) "hypercube_volume =", self%hypercube_volume
  write (u, double_fmt) "jacobian =", self%jacobian
  write (u, descr_fmt) "begin x_lower"
  do j = 1, self%config%n_dim
    write (u, double_array_fmt) j, self%grid%x_lower(j)
  end do
  write (u, descr_fmt) "end x_lower"
  write (u, descr_fmt) "begin x_upper"
  do j = 1, self%config%n_dim
    write (u, double_array_fmt) j, self%grid%x_upper(j)
  end do
  write (u, descr_fmt) "end x_upper"
  write (u, descr_fmt) "begin delta_x"
  do j = 1, self%config%n_dim
    write (u, double_array_fmt) j, self%grid%delta_x(j)
  end do

```

```

write (u, descr_fmt) "end delta_x"
write (u, integer_fmt) "n_bins =", self%config%n_bins
write (u, descr_fmt) "begin bin"
do j = 1, self%config%n_dim
    write (u, integer_array_fmt) j, self%bin(j)
end do
write (u, descr_fmt) "end n_bin"
write (u, integer_fmt) "n_boxes =", self%config%n_boxes
write (u, descr_fmt) "begin box"
do j = 1, self%config%n_dim
    write (u, integer_array_fmt) j, self%box(j)
end do
write (u, descr_fmt) "end box"
write (u, descr_fmt) "begin d"
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max
        write (u, double_array2_fmt) i, j, self%d(i, j)
    end do
end do
write (u, descr_fmt) "end d"
write (u, descr_fmt) "begin xi"
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max + 1
        write (u, double_array2_fmt) i, j, self%grid%xi(i, j)
    end do
end do
write (u, descr_fmt) "end xi"
write (u, descr_fmt) "end type(vegas_t)"
end subroutine vegas_write_grid

```

Read grid configuration from file.

```

<Vegas: vegas: TBP>+≡
    procedure, public :: read_grid => vegas_read_grid

<Vegas: sub interfaces>+≡
    module subroutine vegas_read_grid (self, unit)
        class(vegas_t), intent(out) :: self
        integer, intent(in) :: unit
    end subroutine vegas_read_grid

<Vegas: procedures>+≡
    module subroutine vegas_read_grid (self, unit)
        class(vegas_t), intent(out) :: self
        integer, intent(in) :: unit
        integer :: i, j
        character(len=80) :: buffer
        integer :: ibuffer, jbuffer
        read (unit, descr_fmt) buffer
        read (unit, integer_fmt) buffer, ibuffer
        read (unit, integer_fmt) buffer, jbuffer
        select type(self)
        type is (vegas_t)
            self = vegas_t (n_dim = ibuffer, n_bins_max = jbuffer)
        end select
        read (unit, double_fmt) buffer, self%config%alpha
    end subroutine

```



```

read (unit, integer_fmt) buffer, self%config%iterations
read (unit, integer_fmt) buffer, self%config%mode
read (unit, integer_fmt) buffer, self%config%calls_per_box
read (unit, integer_fmt) buffer, self%config%n_calls
read (unit, integer_fmt) buffer, self%config%n_calls_min
read (unit, integer_fmt) buffer, self%config%n_boxes
read (unit, integer_fmt) buffer, self%config%n_bins
self%grid%n_bins = self%config%n_bins
read (unit, integer_fmt) buffer, self%result%it_start
read (unit, integer_fmt) buffer, self%result%it_num
read (unit, integer_fmt) buffer, self%result%samples
read (unit, double_fmt) buffer, self%result%sum_int_wgtd
read (unit, double_fmt) buffer, self%result%sum_wgts
read (unit, double_fmt) buffer, self%result%sum_chi
read (unit, double_fmt) buffer, self%result%chi2
read (unit, double_fmt) buffer, self%result%efficiency
read (unit, double_fmt) buffer, self%result%efficiency_pos
read (unit, double_fmt) buffer, self%result%efficiency_neg
read (unit, double_fmt) buffer, self%result%max_abs_f
read (unit, double_fmt) buffer, self%result%max_abs_f_pos
read (unit, double_fmt) buffer, self%result%max_abs_f_neg
read (unit, double_fmt) buffer, self%result%result
read (unit, double_fmt) buffer, self%result%std
read (unit, double_fmt) buffer, self%hypercube_volume
read (unit, double_fmt) buffer, self%jacobian
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%x_lower(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%x_upper(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%delta_x(j)
end do
read (unit, descr_fmt) buffer
read (unit, integer_fmt) buffer, self%config%n_bins
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, integer_array_fmt) jbuffer, self%bin(j)
end do
read (unit, descr_fmt) buffer
read (unit, integer_fmt) buffer, self%config%n_boxes
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, integer_array_fmt) jbuffer, self%box(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim

```

```

        do i = 1, self%config%n_bins_max
            read (unit, double_array2_fmt) ibuffer, jbuffer, self%d(i, j)
        end do
    end do
    read (unit, descr_fmt) buffer
    read (unit, descr_fmt) buffer
    do j = 1, self%config%n_dim
        do i = 1, self%config%n_bins_max + 1
            read (unit, double_array2_fmt) ibuffer, jbuffer, self%grid%xi(i, j)
        end do
    end do
    read (unit, descr_fmt) buffer
    read (unit, descr_fmt) buffer
end subroutine vegas_read_grid

```

Read and write a grid from an unformatted file.

```

{ Vegas: vegas: TBP } +=
    procedure :: write_binary_grid => vegas_write_binary_grid
    procedure :: read_binary_grid => vegas_read_binary_grid

{ Vegas: sub interfaces } +=
    module subroutine vegas_write_binary_grid (self, unit)
        class(vegas_t), intent(in) :: self
        integer, intent(in) :: unit
    end subroutine vegas_write_binary_grid
    module subroutine vegas_read_binary_grid (self, unit)
        class(vegas_t), intent(out) :: self
        integer, intent(in) :: unit
    end subroutine vegas_read_binary_grid

{ Vegas: procedures } +=
    module subroutine vegas_write_binary_grid (self, unit)
        class(vegas_t), intent(in) :: self
        integer, intent(in) :: unit
        integer :: i, j
        write (unit) self%config%n_dim
        write (unit) self%config%n_bins_max
        write (unit) self%config%alpha
        write (unit) self%config%iterations
        write (unit) self%config%mode
        write (unit) self%config%calls_per_box
        write (unit) self%config%n_calls
        write (unit) self%config%n_calls_min
        write (unit) self%config%n_boxes
        write (unit) self%config%n_bins
        write (unit) self%result%it_start
        write (unit) self%result%it_num
        write (unit) self%result%samples
        write (unit) self%result%sum_int_wgtd
        write (unit) self%result%sum_wgts
        write (unit) self%result%sum_chi
        write (unit) self%result%chi2
        write (unit) self%result%efficiency
        write (unit) self%result%efficiency_pos
        write (unit) self%result%efficiency_neg
    end subroutine vegas_write_binary_grid

```

```

write (unit) self%result%max_abs_f
write (unit) self%result%max_abs_f_pos
write (unit) self%result%max_abs_f_neg
write (unit) self%result%result
write (unit) self%result%std
write (unit) self%hypercube_volume
write (unit) self%jacobian
do j = 1, self%config%n_dim
  write (unit) j, self%grid%x_lower(j)
end do
do j = 1, self%config%n_dim
  write (unit) j, self%grid%x_upper(j)
end do
do j = 1, self%config%n_dim
  write (unit) j, self%grid%delta_x(j)
end do
write (unit) self%config%n_bins
do j = 1, self%config%n_dim
  write (unit) j, self%bin(j)
end do
write (unit) self%config%n_boxes
do j = 1, self%config%n_dim
  write (unit) j, self%box(j)
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max
    write (unit) i, j, self%d(i, j)
  end do
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max + 1
    write (unit) i, j, self%grid%xi(i, j)
  end do
end do
end subroutine vegas_write_binary_grid

module subroutine vegas_read_binary_grid (self, unit)
  class(vegas_t), intent(out) :: self
  integer, intent(in) :: unit
  integer :: i, j
  integer :: ibuffer, jbuffer
  read (unit) ibuffer
  read (unit) jbuffer
  select type(self)
  type is (vegas_t)
    self = vegas_t (n_dim = ibuffer, n_bins_max = jbuffer)
  end select
  read (unit) self%config%alpha
  read (unit) self%config%iterations
  read (unit) self%config%mode
  read (unit) self%config%calls_per_box
  read (unit) self%config%n_calls
  read (unit) self%config%n_calls_min
  read (unit) self%config%n_boxes

```

```

read (unit) self%config%n_bins
self%grid%n_bins = self%config%n_bins
read (unit) self%result%it_start
read (unit) self%result%it_num
read (unit) self%result%samples
read (unit) self%result%sum_int_wgtd
read (unit) self%result%sum_wgts
read (unit) self%result%sum_chi
read (unit) self%result%chi2
read (unit) self%result%efficiency
read (unit) self%result%efficiency_pos
read (unit) self%result%efficiency_neg
read (unit) self%result%max_abs_f
read (unit) self%result%max_abs_f_pos
read (unit) self%result%max_abs_f_neg
read (unit) self%result%result
read (unit) self%result%std
read (unit) self%hypercube_volume
read (unit) self%jacobian
do j = 1, self%config%n_dim
  read (unit) jbuffer, self%grid%x_lower(j)
end do
do j = 1, self%config%n_dim
  read (unit) jbuffer, self%grid%x_upper(j)
end do
do j = 1, self%config%n_dim
  read (unit) jbuffer, self%grid%delta_x(j)
end do
read (unit) self%config%n_bins
do j = 1, self%config%n_dim
  read (unit) jbuffer, self%bin(j)
end do
read (unit) self%config%n_boxes
do j = 1, self%config%n_dim
  read (unit) jbuffer, self%box(j)
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max
    read (unit) ibuffer, jbuffer, self%d(i, j)
  end do
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max + 1
    read (unit) ibuffer, jbuffer, self%grid%xi(i, j)
  end do
end do
end subroutine vegas_read_binary_grid

```

20.12 Unit tests

Test module, followed by the corresponding implementation module.

```

<vegas_ut.f90>≡
  <File header>

  module vegas_ut
    use unit_tests
    use vegas_util

    <Standard module head>

    <Vegas: public test>

    contains
    <Vegas: test driver>
  end module vegas_ut

<vegas_util.f90>≡
  <File header>

  module vegas_util
    <Use kinds>
    use io_units
    use constants, only: pi
    use format_defs, only: FMT_10, FMT_12
    use rng_base
    use rng_stream
    use vegas

    <Standard module head>

    <Vegas: test declaration>

    <Vegas: test types>

    contains
    <Vegas: tests>
  end module vegas_util
API: driver for the unit tests below.
<Vegas: public test>≡
  public :: vegas_test
<Vegas: test driver>≡
  subroutine vegas_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Vegas: execute tests>
  end subroutine vegas_test

```

Test function

We use the example from the Monte Carlo Examples of the GSL library

$$I = \int_{-pi}^{+pi} dk_x / (2pi) \int_{-pi}^{+pi} dk_y / (2pi) \int_{-pi}^{+pi} dk_z / (2pi) 1 / (1 - \cos(k_x) \cos(k_y) \cos(k_z)). \quad (20.6)$$

The integral is reduced to region $(0,0,0) \rightarrow (\pi, \pi, \pi)$ and multiplied by 8.

```

<Vegas: test types>≡
  type, extends (vegas_func_t) :: vegas_test_func_t
  !
  contains
    <Vegas: vegas test func: TBP>
  end type vegas_test_func_t

```

Evaluate the integrand.

```

<Vegas: vegas test func: TBP>≡
  procedure, public :: evaluate => vegas_test_func_evaluate

<Vegas: tests>≡
  real(default) function vegas_test_func_evaluate (self, x) result (f)
    class(vegas_test_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    f = 1.0 / (pi**3)
    f = f / ( 1.0 - cos (x(1)) * cos (x(2)) * cos (x(3)))
  end function vegas_test_func_evaluate

```

The second test function is the normalised n-dim. gaussian distribution.

```

<Vegas: test types>+≡
  type, extends (vegas_func_t) :: vegas_gaussian_test_func_t
  !
  contains
    <Vegas: vegas gaussian test func: TBP>
  end type vegas_gaussian_test_func_t

```

Evaluate the integrand.

```

<Vegas: vegas gaussian test func: TBP>≡
  procedure, public :: evaluate => vegas_gaussian_evaluate

<Vegas: tests>+≡
  real(default) function vegas_gaussian_evaluate (self, x) result (f)
    class(vegas_gaussian_test_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    real(default), parameter :: inv_sqrt_pi = 1._default / sqrt(pi)
    f = inv_sqrt_pi**size (x)
    f = f * exp (- dot_product(x, x))
  end function vegas_gaussian_evaluate

```

The third test function is a three-dimensional polynomial function which factorises. The function is defined in such a way that the integral in the unit range is normalised to zero.

$$f(x) = -\frac{8}{3}(x+1)*(y-1)*z \quad (20.7)$$

```

<Vegas: test types>+≡
  type, extends (vegas_func_t) :: vegas_polynomial_func_t
  !
  contains
    <Vegas: vegas polynomial func: TBP>
  end type vegas_polynomial_func_t

```

```

<Vegas: vegas polynomial func: TBP>≡
  procedure, public :: evaluate => vegas_polynomial_evaluate

<Vegas: tests>+≡
  real(default) function vegas_polynomial_evaluate (self, x) result (f)
    class(vegas_polynomial_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    f = - 8. / 3. * (x(1) + 1.) * (x(2) - 1.) * x(3)
  end function vegas_polynomial_evaluate

```

MC Integrator check

Initialise the VEGAS MC integrator and call to `vegas_init_grid` for the initialisation of the grid.

```

<Vegas: execute tests>≡
  call test (vegas_1, "vegas_1", "VEGAS initialisation and&
    & grid preparation", u, results)

<Vegas: test declaration>≡
  public :: vegas_1

<Vegas: tests>+≡
  subroutine vegas_1 (u)
    integer, intent(in) :: u
    type(vegas_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vegas_func_t), allocatable :: func
    real(default), dimension(3), parameter :: x_lower = 0., &
      x_upper = pi
    real(default) :: result, abserr

    write (u, "(A)") "* Test output: vegas_1"
    write (u, "(A)") "* Purpose: initialise the VEGAS MC integrator and the grid"
    write (u, "(A)")

    write (u, "(A)") "* Initialise random number generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
    write (u, "(A)")

    allocate (vegas_test_func_t :: func)
    mc_integrator = vegas_t (3)

    write (u, "(A)")
    write (u, "(A)") "* Initialise grid with n_calls = 10000"
    write (u, "(A)")

```

```

call mc_integrator%set_limits (x_lower, x_upper)
call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vegas_1

```

Configuration and result check

Initialise the MC integrator. Get and write the config object, also the (empty) result object.

```

<Vegas: execute tests>+≡
    call test (vegas_2, "vegas_2", "VEGAS configuration and result object", u, results)
<Vegas: test declaration>+≡
    public :: vegas_2
<Vegas: tests>+≡
    subroutine vegas_2 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_result_t) :: mc_integrator_result

        write (u, "(A)") "* Test output: vegas_2"
        write (u, "(A)") "* Purpose: use transparent containers for&
            & configuration and result."
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 10"
        write (u, "(A)")

        mc_integrator = vegas_t (10)

```



```

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 10000 (Importance Sampling)"
write (u, "(A)")

call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS config object and write out"
write (u, "(A)")

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS empty result object and write out"
write (u, "(A)")

mc_integrator_result = mc_integrator%get_result ()
call mc_integrator_result%write (u)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_2

```

Grid check

Initialise the MC integrator. Get and write the config object. Integrate the gaussian distribution. Get and write the result object. Before and after integration get the grid object and output both. Repeat with different number of dimensions.

```

<Vegas: execute tests>+≡
    call test (vegas_3, "vegas_3", "VEGAS integration of multi-dimensional gaussian", u, results)
<Vegas: test declaration>+≡
    public :: vegas_3
<Vegas: tests>+≡
    subroutine vegas_3 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower_3 = -10._default, &
            x_upper_3 = 10._default
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_grid_t) :: mc_integrator_grid
        type(vegas_result_t) :: mc_integrator_result

        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_3"
        write (u, "(A)") "* Purpose: Integrate gaussian distribution."

```

```

write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_gaussian_test_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 10000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS config object and write out"
write (u, "(A)")

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS grid object and write out"
write (u, "(A)")

mc_integrator_grid = mc_integrator%get_grid ()
call mc_integrator_grid%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Get VEGAS result object and write out"
write (u, "(A)")

mc_integrator_result = mc_integrator%get_result ()
call mc_integrator_result%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS grid object and write out"
write (u, "(A)")

mc_integrator_grid = mc_integrator%get_grid ()
call mc_integrator_grid%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_3

```

Three-dimensional integration with polynomial function

Initialise the MC integrator. Get and write the config object. Integrate the factorisable polynomial function. Get and write the result object. Repeat with different number of dimensions.

```

<Vegas: execute tests>+=
  call test (vegas_4, "vegas_4", "VEGAS integration of three&
    &-dimensional factorisable polynomial function", u, results)

<Vegas: test declaration>+=
  public :: vegas_4

<Vegas: tests>+=
  subroutine vegas_4 (u)
    integer, intent(in) :: u
    type(vegas_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vegas_func_t), allocatable :: func
    real(default), dimension(3), parameter :: x_lower_3 = 0._default, &
      x_upper_3 = 1._default
    type(vegas_config_t) :: mc_integrator_config
    type(vegas_result_t) :: mc_integrator_result

    real(default) :: result, abserr

    write (u, "(A)") "* Test output: vegas_4"
    write (u, "(A)") "* Purpose: Integrate gaussian distribution."
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

```

```

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_polynomial_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 2000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (2000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (20000)

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_4

```

Event generation

Initialise the MC integrator. Integrate the gaussian distribution. Get and write the result object. Finally, generate events in accordance to the adapted grid

and print them out.

```

<Vegas: execute tests>+≡
    call test (vegas_5, "vegas_5", "VEGAS integration and event&
        & generation of multi-dimensional gaussian", u, results)

<Vegas: test declaration>+≡
    public :: vegas_5

<Vegas: tests>+≡
    subroutine vegas_5 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(1), parameter :: x_lower_1 = -10._default, &
            x_upper_1 = 10._default
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_result_t) :: mc_integrator_result

        integer :: i, u_event
        real(default), dimension(1) :: event, mean, delta, M2
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_5"
        write (u, "(A)") "* Purpose: Integrate gaussian distribution."
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 1"
        write (u, "(A)")

        allocate (vegas_gaussian_test_func_t :: func)
        mc_integrator = vegas_t (1)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 20000"
        write (u, "(A)")

        call mc_integrator%set_limits (x_lower_1, x_upper_1)
        call mc_integrator%set_calls (20000)

        write (u, "(A)")
        write (u, "(A)") "* Integrate with n_it = 3 (Adaptation)"
        write (u, "(A)")

        call mc_integrator%integrate (func, rng, 3, verbose=.true., result=result, abserr=abserr)
        call mc_integrator%get_config (mc_integrator_config)
        call mc_integrator_config%write (u)
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") &
            & "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, verbose=.true., result=result, abserr=abserr)
call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") &
    & "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Generate 10000 events based on the adaptation and&
    & calculate mean and variance"
write (u, "(A)")

mean = 0._default
M2 = 0._default
do i = 1, 10000
    call mc_integrator%generate_unweighted (func, rng, event)
    delta = event - mean
    mean = mean + delta / i
    M2 = M2 + delta * (event - mean)
end do

write (u, "(2X,A)") "Result:"
write (u, "(4X,A," // FMT_12 // ")") &
    & "mean          = ", mean
write (u, "(4X,A," // FMT_12 // ")") &
    & "(sample) std. dev. = ", sqrt (M2 / (9999))

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_5

```

Grid I/O

Initialise the MC integrator. Get and write the config object. Integrate the factorisable polynomial function. Get and write the result object. Write grid to file and start with fresh grid.

```

<Vegas: execute tests>+≡
    call test (vegas_6, "vegas_6", "VEGAS integrate and write grid, &
        & read grid and continue", u, results)

<Vegas: test declaration>+≡
    public :: vegas_6

<Vegas: tests>+≡
    subroutine vegas_6 (u)
        integer, intent(in) :: u

```

```

type(vegas_t) :: mc_integrator
class(rng_t), allocatable :: rng
class(vegas_func_t), allocatable :: func
real(default), dimension(3), parameter :: x_lower_3 = 0._default, &
      x_upper_3 = 1._default
type(vegas_config_t) :: mc_integrator_config
type(vegas_result_t) :: mc_integrator_result

real(default) :: result, abserr
integer :: unit

write (u, "(A)") "* Test output: vegas_6"
write (u, "(A)") "* Purpose: Write and read grid, and continue."
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_polynomial_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 2000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (2000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Write grid to file vegas_io.grid"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vegas_io.grid", &
      action = "write", status = "replace")

```

```

call mc_integrator%write_grid (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Read grid from file vegas_io.grid"
write (u, "(A)")

call mc_integrator%final ()
open (unit, file = "vegas_io.grid", &
      action = "read", status = "old")
call mc_integrator%read_grid (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (20000)

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_6

```

Numeric stability

We wrap a previous testing function to produce a single NaN.

```

⟨Vegas: test types⟩+≡
  type, extends (vegas_test_func_t) :: vegas_nan_test_func_t
  private
  logical :: evaluate_to_nan = .true.
  contains
  ⟨Vegas: vegas nan test func: TBP⟩
end type vegas_nan_test_func_t

```

Evaluate the integrand.

```

⟨Vegas: vegas nan test func: TBP⟩≡
  procedure, public :: evaluate => vegas_nan_test_func_evaluate

⟨Vegas: tests⟩+≡
  real(default) function vegas_nan_test_func_evaluate (self, x) result (f)
  use, intrinsic :: ieee_arithmetic, only: ieee_value, ieee_quiet_nan
  class(vegas_nan_test_func_t), intent(inout) :: self

```



```

real(default), dimension(:), intent(in) :: x
if (self%evaluate_to_nan) then
    f = ieee_value(1.0_default, ieee_quiet_nan)
    self%evaluate_to_nan = .false.
else
    f = self%vegas_test_func_t%evaluate (x)
end if
end function vegas_nan_test_func_evaluate

```

Initialise the VEGAS MC integrator. Run a integration pass and insert a single NaN that leads to a NaN result. However, the integration grid will be fine.

Proceed with a second pass, and get the correct result.

```

< Vegas: execute tests >+≡
    !!! Disabled for the moment as NAGFOR stops execution on NaNs as intended
    ! call test (vegas_7, "vegas_7", "VEGAS NaN stability test", u, results)

< Vegas: test declaration >+≡
    public :: vegas_7

< Vegas: tests >+≡
    subroutine vegas_7 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower = 0., &
            x_upper = pi
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_7"
        write (u, "(A)") "* Purpose: initialise the VEGAS MC integrator and the grid"
        write (u, "(A)")

        write (u, "(A)") "* Initialise random number generator (default seed)"
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
        write (u, "(A)")

        allocate (vegas_nan_test_func_t :: func)
        mc_integrator = vegas_t (3)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 10000"
        write (u, "(A)")

        call mc_integrator%set_limits (x_lower, x_upper)
        call mc_integrator%set_calls (10000)

```

```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vegas_7

```

20.13 VAMP2

We concentrate all configuration and run-time data in a derived-type, such that, `mci_t` can span each time a distinctive MCI VEGAS integrator object.

```
<vamp2.f90>≡  
  <File header>  
  
  module vamp2  
  
    <Use kinds>  
    use diagnostics  
    use rng_base  
  
    use vegas  
  
    <VAMP2: modules>  
  
    <Standard module head>  
  
    <VAMP2: public>  
  
    <VAMP2: parameters>  
  
    <VAMP2: types>  
  
    <VAMP2: interfaces>  
  
    interface  
    <VAMP2: sub interfaces>  
    end interface  
  
    contains  
  
    <VAMP2: main procedures>  
  
  end module vamp2  
  
<vamp2_sub.f90>≡  
  <File header>  
  
  submodule (vamp2) vamp2_s  
  
    use io_units  
    use format_utils, only: pac_fmt  
    use format_utils, only: write_separator, write_indent  
    use format_defs, only: FMT_17  
    use iterator  
    use rng_stream, only: rng_stream_t  
  
    implicit none  
  
    contains  
  
    <VAMP2: procedures>
```

```
end submodule vamp2_s
```

```
<VAMP2: modules>≡
```

```
<MPI: VAMP2: modules>≡
```

```
  use request_base
  use request_simple
  use request_caller
  use balancer_base
  use request_callback
  use mpi_f08 !NODEP!
```

20.13.1 Type: vamp2_func_t

We extend `vegas_func_t` with the multi-channel weights and the `vegas_grid_t`, such that, the overall multi-channel weight can be calculated by the function itself.

We add an additional logical `valid_x`, if it is set to `.false.`, we do not compute weighted function and just set the weighted integrand to zero. This behavior is in particular very useful, if a mapping is prohibited or fails. Or in the case of WHIZARD, a phase cut is applied.

```
<VAMP2: public>≡
```

```
  public :: vamp2_func_t
```

```
<VAMP2: types>≡
```

```
  type, abstract, extends(vegas_func_t) :: vamp2_func_t
    integer :: current_channel = 0
    integer :: n_dim = 0
    integer :: n_channel = 0
    integer :: n_calls = 0
    logical :: valid_x = .false.
    real(default), dimension(:, :), allocatable :: xi
    real(default), dimension(:, :), allocatable :: det
    real(default), dimension(:, :), allocatable :: wi
    real(default), dimension(:, :), allocatable :: gi
    type(vegas_grid_t), dimension(:, :), allocatable :: grids
    real(default) :: g = 0._default
  contains
    <VAMP2: vamp2_func: TBP>
  end type vamp2_func_t
```

Init.

```
<VAMP2: vamp2_func: TBP>≡
```

```
  procedure, public :: init => vamp2_func_init
```

```
<VAMP2: sub interfaces>≡
```

```
  module subroutine vamp2_func_init (self, n_dim, n_channel)
    class(vamp2_func_t), intent(out) :: self
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
  end subroutine vamp2_func_init
```

```

<VAMP2: procedures>≡
  module subroutine vamp2_func_init (self, n_dim, n_channel)
    class(vamp2_func_t), intent(out) :: self
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    self%n_dim = n_dim
    self%n_channel = n_channel
    allocate (self%xi(n_dim, n_channel), source=0._default)
    allocate (self%det(n_channel), source=1._default)
    allocate (self%wi(n_channel), source=0._default)
    allocate (self%gi(n_channel), source=0._default)
    allocate (self%grids(n_channel))
  end subroutine vamp2_func_init

Set current channel.
<VAMP2: vamp2 func: TBP>+≡
  procedure, public :: set_channel => vamp2_func_set_channel
<VAMP2: sub interfaces>+≡
  module subroutine vamp2_func_set_channel (self, channel)
    class(vamp2_func_t), intent(inout) :: self
    integer, intent(in) :: channel
  end subroutine vamp2_func_set_channel
<VAMP2: procedures>+≡
  module subroutine vamp2_func_set_channel (self, channel)
    class(vamp2_func_t), intent(inout) :: self
    integer, intent(in) :: channel
    self%current_channel = channel
  end subroutine vamp2_func_set_channel

Get number of function calls for which  $f \neq 0$ .
<VAMP2: vamp2 func: TBP>+≡
  procedure, public :: get_n_calls => vamp2_func_get_n_calls
<VAMP2: sub interfaces>+≡
  module function vamp2_func_get_n_calls (self) result (n_calls)
    class(vamp2_func_t), intent(in) :: self
    integer :: n_calls
  end function vamp2_func_get_n_calls
<VAMP2: procedures>+≡
  module function vamp2_func_get_n_calls (self) result (n_calls)
    class(vamp2_func_t), intent(in) :: self
    integer :: n_calls
    n_calls = self%n_calls
  end function vamp2_func_get_n_calls

Reset number of calls.
<VAMP2: vamp2 func: TBP>+≡
  procedure, public :: reset_n_calls => vamp2_func_reset_n_calls
<VAMP2: sub interfaces>+≡
  module subroutine vamp2_func_reset_n_calls (self)
    class(vamp2_func_t), intent(inout) :: self
  end subroutine vamp2_func_reset_n_calls

```

```

<VAMP2: procedures>+≡
  module subroutine vamp2_func_reset_n_calls (self)
    class(vamp2_func_t), intent(inout) :: self
    self%n_calls = 0
  end subroutine vamp2_func_reset_n_calls

```

Evaluate mappings. We defer this method to be implemented by the user. The result must be written to `xi` and `det`.

The mapping is defined by $\phi : U \rightarrow M$. We map $x \in M$ to the different mappings of the hypercube U_i , such that $x_i \in U_i$.

The mapping should determine, whether `x` is a valid point, e.g. can be mapped, or is restricted otherwise.

```

<VAMP2: vamp2_func: TBP>+≡
  procedure(vamp2_func_evaluate_maps), deferred :: evaluate_maps

<VAMP2: interfaces>≡
  abstract interface
    subroutine vamp2_func_evaluate_maps (self, x)
      import :: vamp2_func_t, default
      class(vamp2_func_t), intent(inout) :: self
      real(default), dimension(:), intent(in) :: x
    end subroutine vamp2_func_evaluate_maps
  end interface

```

Evaluate channel weights.

The calling procedure must handle the case of a vanishing overall probability density where either a channel weight or a channel probability vanishes.

```

<VAMP2: vamp2_func: TBP>+≡
  procedure, private :: evaluate_weight => vamp2_func_evaluate_weight

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_func_evaluate_weight (self)
    class(vamp2_func_t), intent(inout) :: self
  end subroutine vamp2_func_evaluate_weight

<VAMP2: procedures>+≡
  module subroutine vamp2_func_evaluate_weight (self)
    class(vamp2_func_t), intent(inout) :: self
    integer :: ch
    self%g = 0
    self%gi = 0
    !$OMP PARALLEL DO PRIVATE(ch) SHARED(self)
    do ch = 1, self%n_channel
      if (self%wi(ch) /= 0) then
        self%gi(ch) = self%grids(ch)%get_probability (self%xi(:, ch))
      end if
    end do
    !$OMP END PARALLEL DO
    if (self%gi(self%current_channel) /= 0) then
      do ch = 1, self%n_channel
        if (self%wi(ch) /= 0 .and. self%det(ch) /= 0) then
          self%g = self%g + self%wi(ch) * self%gi(ch) / self%det(ch)
        end if
      end do
    end do
  end subroutine vamp2_func_evaluate_weight

```

```

        self%g = self%g / self%gi(self%current_channel)
    end if
end subroutine vamp2_func_evaluate_weight

```

Evaluate function at x. We call this procedure in `vamp2_func_evaluate`.

```

<VAMP2: vamp2_func: TBP>+≡
    procedure(vamp2_func_evaluate_func), deferred :: evaluate_func

<VAMP2: interfaces>+≡
    abstract interface
        real(default) function vamp2_func_evaluate_func (self, x) result (f)
            import :: vamp2_func_t, default
            class(vamp2_func_t), intent(in) :: self
            real(default), dimension(:), intent(in) :: x
        end function vamp2_func_evaluate_func
    end interface

<VAMP2: vamp2_func: TBP>+≡
    procedure, public :: evaluate => vamp2_func_evaluate

<VAMP2: sub interfaces>+≡
    module function vamp2_func_evaluate (self, x) result (f)
        class(vamp2_func_t), intent(inout) :: self
        real(default) :: f
        real(default), dimension(:), intent(in) :: x
    end function vamp2_func_evaluate

<VAMP2: procedures>+≡
    module function vamp2_func_evaluate (self, x) result (f)
        class(vamp2_func_t), intent(inout) :: self
        real(default) :: f
        real(default), dimension(:), intent(in) :: x
        call self%evaluate_maps (x)
        f = 0.
        self%gi = 0.
        self%g = 1
        if (self%valid_x) then
            call self%evaluate_weight ()
            if (self%g /= 0) then
                f = self%evaluate_func (x) / self%g
                self%n_calls = self%n_calls + 1
            end if
        end if
    end function vamp2_func_evaluate

```

20.13.2 Type: `vamp2_config_t`

This is a transparent container which incorporates and extends the definitions in `vegas_config`. The parent object can then be used to parametrise the VEGAS grids directly, where the new parameters are exclusively used in the multi-channel implementation of VAMP2. `n_calls_min` is calculated by

`n_calls_min_per_channel` and `n_channel`. The channels weights (and the result `n_calls` for each channel) are calculated regarding `n_calls_threshold`.

```

(VAMP2: public)+≡
    public :: vamp2_config_t

(VAMP2: types)+≡
    type, extends(vegas_config_t) :: vamp2_config_t
        integer :: n_channel = 0
        integer :: n_calls_min_per_channel = 20
        integer :: n_calls_threshold = 10
        integer :: n_chains = 0
        logical :: stratified = .true.
        logical :: equivalences = .false.
        real(default) :: beta = 0.5_default
        real(default) :: accuracy_goal = 0._default
        real(default) :: error_goal = 0._default
        real(default) :: rel_error_goal = 0._default
    contains
        (VAMP2: vamp2 config: TBP)
    end type vamp2_config_t

```

Write.

```

(VAMP2: vamp2 config: TBP)≡
    procedure, public :: write => vamp2_config_write

(VAMP2: sub interfaces)+≡
    module subroutine vamp2_config_write (self, unit, indent)
        class(vamp2_config_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
    end subroutine vamp2_config_write

(VAMP2: procedures)+≡
    module subroutine vamp2_config_write (self, unit, indent)
        class(vamp2_config_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call self%vegas_config_t%write (unit, indent)
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Number of channels" = ", self%n_channel
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Min. number of calls per channel (setting calls) = ", &
            & self%n_calls_min_per_channel
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Threshold number of calls (adapting weights) = ", &
            & self%n_calls_threshold
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Number of chains" = ", self%n_chains
    end subroutine vamp2_config_write

```



```

call write_indent (u, ind)
write (u, "(2x,A,L1)" &
      & "Stratified" = ", self%stratified
call write_indent (u, ind)
write (u, "(2x,A,L1)" &
      & "Equivalences" = ", self%equivalences
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
      & "Adaption power (beta)" = ", self%beta
if (self%accuracy_goal > 0) then
  call write_indent (u, ind)
  write (u, "(2x,A," // FMT_17 // ")") &
      & "accuracy_goal" = ", self%accuracy_goal
end if
if (self%error_goal > 0) then
  call write_indent (u, ind)
  write (u, "(2x,A," // FMT_17 // ")") &
      & "error_goal" = ", self%error_goal
end if
if (self%rel_error_goal > 0) then
  call write_indent (u, ind)
  write (u, "(2x,A," // FMT_17 // ")") &
      & "rel_error_goal" = ", self%rel_error_goal
end if
end subroutine vamp2_config_write

```

20.13.3 Type: vamp2_result_t

This is a transparent container which incorporates and extends the definitions of `vegas_result_t`.

```

<VAMP2: public>+≡
  public :: vamp2_result_t

<VAMP2: types>+≡
  type, extends(vegas_result_t) :: vamp2_result_t
  contains
  <VAMP2: vamp2 result: TBP>
  end type vamp2_result_t

```

Output.

```

<VAMP2: vamp2 result: TBP>≡
  procedure, public :: write => vamp2_result_write

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_result_write (self, unit, indent)
    class(vamp2_result_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
  end subroutine vamp2_result_write

<VAMP2: procedures>+≡
  module subroutine vamp2_result_write (self, unit, indent)
    class(vamp2_result_t), intent(in) :: self

```

```

integer, intent(in), optional :: unit
integer, intent(in), optional :: indent
integer :: u, ind
u = given_output_unit (unit)
ind = 0; if (present (indent)) ind = indent
call self%vegas_result_t%write (unit, indent)
end subroutine vamp2_result_write

```

20.13.4 Type: vamp2_equivalences_t

<VAMP2: parameters>≡

```

integer, parameter, public :: &
    VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3

```

Channel equivalences. Store retrieving and sourcing channel.

<VAMP2: types>+≡

```

type :: vamp2_equi_t
    integer :: ch
    integer :: ch_src
    integer, dimension(:), allocatable :: perm
    integer, dimension(:), allocatable :: mode
contains
    <VAMP2: vamp2_equi: TBP>
end type vamp2_equi_t

```

Write equivalence.

<VAMP2: vamp2_equi: TBP>≡

```

procedure :: write => vamp2_equi_write

```

<VAMP2: sub interfaces>+≡

```

module subroutine vamp2_equi_write (self, unit, indent)
    class(vamp2_equi_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
end subroutine vamp2_equi_write

```

<VAMP2: procedures>+≡

```

module subroutine vamp2_equi_write (self, unit, indent)
    class(vamp2_equi_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(2(A,1X,I0))") "src:", self%ch_src, "-> dest:", self%ch
    call write_indent (u, ind)
    write (u, "(A,99(1X,I0))") "Perm: ", self%perm
    call write_indent (u, ind)
    write (u, "(A,99(1X,I0))") "Mode: ", self%mode
end subroutine vamp2_equi_write

```

```

<VAMP2: public>+≡
  public :: vamp2_equivalences_t

<VAMP2: types>+≡
  type :: vamp2_equivalences_t
    private
      integer :: n_eqv = 0
      integer :: n_channel = 0
      integer :: n_dim = 0
      type(vamp2_equi_t), dimension(:), allocatable :: eqv
      integer, dimension(:), allocatable :: map
      integer, dimension(:), allocatable :: multiplicity
      integer, dimension(:), allocatable :: symmetry
      logical, dimension(:), allocatable :: independent
      integer, dimension(:), allocatable :: equivalent_to_ch
      logical, dimension(:, :), allocatable :: dim_is_invariant
    contains
      <VAMP2: vamp2 equivalences: TBP>
    end type vamp2_equivalences_t

```

Constructor.

```

<VAMP2: interfaces>+≡
  interface vamp2_equivalences_t
    module procedure vamp2_equivalences_init
  end interface vamp2_equivalences_t

<VAMP2: sub interfaces>+≡
  module function vamp2_equivalences_init (n_eqv, n_channel, &
    n_dim) result (eqv)
    type(vamp2_equivalences_t) :: eqv
    integer, intent(in) :: n_eqv, n_channel, n_dim
  end function vamp2_equivalences_init

<VAMP2: procedures>+≡
  module function vamp2_equivalences_init (n_eqv, n_channel, &
    n_dim) result (eqv)
    type(vamp2_equivalences_t) :: eqv
    integer, intent(in) :: n_eqv, n_channel, n_dim
    eqv%n_eqv = n_eqv
    eqv%n_channel = n_channel
    eqv%n_dim = n_dim
    allocate (eqv%eqv(n_eqv))
    allocate (eqv%map(n_channel), source = 0)
    allocate (eqv%multiplicity(n_channel), source = 0)
    allocate (eqv%symmetry(n_channel), source = 0)
    allocate (eqv%independent(n_channel), source = .true.)
    allocate (eqv%equivalent_to_ch(n_channel), source = 0)
    allocate (eqv%dim_is_invariant(n_dim, n_channel), source = .false.)
  end function vamp2_equivalences_init

```

Write equivalences.

```

<VAMP2: vamp2 equivalences: TBP>≡
  procedure :: write => vamp2_equivalences_write

```

```

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_equivalences_write (self, unit, indent)
    class(vamp2_equivalences_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
  end subroutine vamp2_equivalences_write

<VAMP2: procedures>+≡
  module subroutine vamp2_equivalences_write (self, unit, indent)
    class(vamp2_equivalences_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind, i_eqv, ch
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    write (u, "(A)") "Inequivalent channels:"
    if (allocated (self%independent)) then
      do ch = 1, self%n_channel
        if (self%independent(ch)) then
          write (u, "(2X,A,1x,I0,A,4x,A,I0,4x,A,I0,4x,A,999(L1))") &
            "Channel", ch, ":", &
            "Mult. = ", self%multiplicity(ch), &
            "Symm. = ", self%symmetry(ch), &
            "Invar.: ", self%dim_is_invariant(:, ch)
        end if
      end do
    else
      write (u, "(A)") "[not allocated]"
    end if
    write (u, "(A)") "Equivalence list:"
    if (allocated (self%eqv)) then
      do i_eqv = 1, self%n_eqv
        write (u, "(2X,A,1X,I0)") "i_eqv:", i_eqv
        call self%eqv(i_eqv)%write (unit, indent = ind + 4)
      end do
    else
      write (u, "(A)") "[not allocated]"
    end if
  end subroutine vamp2_equivalences_write

```

Is allocated.

```

<VAMP2: vamp2 equivalences: TBP>+≡
  procedure, public :: is_allocated => vamp2_equivalences_is_allocated

<VAMP2: sub interfaces>+≡
  module function vamp2_equivalences_is_allocated (self) result (yorn)
    class(vamp2_equivalences_t), intent(in) :: self
    logical :: yorn
  end function vamp2_equivalences_is_allocated

<VAMP2: procedures>+≡
  module function vamp2_equivalences_is_allocated (self) result (yorn)
    class(vamp2_equivalences_t), intent(in) :: self
    logical :: yorn
    yorn = allocated (self%eqv)
  end function vamp2_equivalences_is_allocated

```

```
end function vamp2_equivalences_is_allocated
```

Get source channel and destination channel for given equivalence.

```
{VAMP2: vamp2 equivalences: TBP}+≡
```

```
procedure, public :: get_channels => vamp2_equivalences_get_channels
```

```
{VAMP2: sub interfaces}+≡
```

```
module subroutine vamp2_equivalences_get_channels (eqv, i_eqv, dest, src)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, intent(out) :: dest, src
end subroutine vamp2_equivalences_get_channels
```

```
{VAMP2: procedures}+≡
```

```
module subroutine vamp2_equivalences_get_channels (eqv, i_eqv, dest, src)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, intent(out) :: dest, src
  dest = eqv%eqv(i_eqv)%ch
  src = eqv%eqv(i_eqv)%ch_src
end subroutine vamp2_equivalences_get_channels
```

```
{VAMP2: vamp2 equivalences: TBP}+≡
```

```
procedure, public :: get_mode => vamp2_equivalences_get_mode
```

```
procedure, public :: get_perm => vamp2_equivalences_get_perm
```

```
{VAMP2: sub interfaces}+≡
```

```
module function vamp2_equivalences_get_mode (eqv, i_eqv) result (mode)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, dimension(:), allocatable :: mode
end function vamp2_equivalences_get_mode
module function vamp2_equivalences_get_perm (eqv, i_eqv) result (perm)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, dimension(:), allocatable :: perm
end function vamp2_equivalences_get_perm
```

```
{VAMP2: procedures}+≡
```

```
module function vamp2_equivalences_get_mode (eqv, i_eqv) result (mode)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, dimension(:), allocatable :: mode
  mode = eqv%eqv(i_eqv)%mode
end function vamp2_equivalences_get_mode
```

```
module function vamp2_equivalences_get_perm (eqv, i_eqv) result (perm)
  class(vamp2_equivalences_t), intent(in) :: eqv
  integer, intent(in) :: i_eqv
  integer, dimension(:), allocatable :: perm
  perm = eqv%eqv(i_eqv)%perm
end function vamp2_equivalences_get_perm
```

```

(VAMP2: vamp2 equivalences: TBP)+≡
  procedure, public :: set_equivalence => &
    vamp2_equivalences_set_equivalence

(VAMP2: sub interfaces)+≡
  module subroutine vamp2_equivalences_set_equivalence &
    (eqv, i_eqv, dest, src, perm, mode)
    class(vamp2_equivalences_t), intent(inout) :: eqv
    integer, intent(in) :: i_eqv
    integer, intent(in) :: dest, src
    integer, dimension(:), intent(in) :: perm, mode
  end subroutine vamp2_equivalences_set_equivalence

(VAMP2: procedures)+≡
  module subroutine vamp2_equivalences_set_equivalence &
    (eqv, i_eqv, dest, src, perm, mode)
    class(vamp2_equivalences_t), intent(inout) :: eqv
    integer, intent(in) :: i_eqv
    integer, intent(in) :: dest, src
    integer, dimension(:), intent(in) :: perm, mode
    integer :: i
    if (dest < 1 .or. dest > eqv%n_channel) call msg_bug &
      ("VAMP2: set_equivalences: destination channel out of range.")
    if (src < 1 .or. src > eqv%n_channel) call msg_bug &
      ("VAMP2: set_equivalences: source channel out of range.")
    if (size(perm) /= eqv%n_dim) call msg_bug &
      ("VAMP2: set_equivalences: size(perm) does not match n_dim.")
    if (size(mode) /= eqv%n_dim) call msg_bug &
      ("VAMP2: set_equivalences: size(mode) does not match n_dim.")
    eqv%eqv(i_eqv)%ch = dest
    eqv%eqv(i_eqv)%ch_src = src
    allocate (eqv%eqv(i_eqv)%perm (size (perm)))
    do i = 1, size (perm)
      eqv%eqv(i_eqv)%perm(i) = perm(i)
    end do
    allocate (eqv%eqv(i_eqv)%mode (size (mode)))
    do i = 1, size (mode)
      eqv%eqv(i_eqv)%mode(i) = mode(i)
    end do
  end subroutine vamp2_equivalences_set_equivalence

```

Freeze equivalences.

```

(VAMP2: vamp2 equivalences: TBP)+≡
  procedure, public :: freeze => vamp2_equivalences_freeze

(VAMP2: sub interfaces)+≡
  module subroutine vamp2_equivalences_freeze (self)
    class(vamp2_equivalences_t), intent(inout) :: self
  end subroutine vamp2_equivalences_freeze

(VAMP2: procedures)+≡
  module subroutine vamp2_equivalences_freeze (self)
    class(vamp2_equivalences_t), intent(inout) :: self
    integer :: i_eqv, ch, upper, lower
    ch = 0
    do i_eqv = 1, self%n_eqv

```

```

        if (ch /= self%eqv(i_eqv)%ch) then
            ch = self%eqv(i_eqv)%ch
            self%map(ch) = i_eqv
        end if
    end do
do ch = 1, self%n_channel
    lower = self%map(ch)
    if (ch == self%n_channel) then
        upper = self%n_eqv
    else
        upper = self%map(ch + 1) - 1
    end if
    associate (eqv => self%eqv, n_eqv => size (self%eqv(lower:upper)))
        if (.not. all(eqv(lower:upper)%ch == ch) .or. &
            eqv(lower)%ch_src > ch) then
            do i_eqv = lower, upper
                call self%eqv(i_eqv)%write ()
            end do
            call msg_bug ("VAMP2: vamp2_equivalences_freeze: &
                &equivalence order is not correct.")
        end if
        self%symmetry(ch) = count (eqv(lower:upper)%ch_src == ch)
        if (mod (n_eqv, self%symmetry(ch)) /= 0) then
            do i_eqv = lower, upper
                call self%eqv(i_eqv)%write ()
            end do
            call msg_bug ("VAMP2: vamp2_equivalences_freeze: &
                &permutation count is not correct.")
        end if
        self%multiplicity(ch) = n_eqv / self%symmetry(ch)
        self%independent(ch) = all (eqv(lower:upper)%ch_src >= ch)
        self%equivalent_to_ch(ch) = eqv(lower)%ch_src
        self%dim_is_invariant(:, ch) = eqv(lower)%mode == VEQ_INVARIANT
    end associate
end do
end subroutine vamp2_equivalences_freeze

```

20.13.5 Type: vamp2_t

```

<VAMP2: public>+≡
    public :: vamp2_t

<VAMP2: types>+≡
    type :: vamp2_t
        private
        type(vamp2_config_t) :: config
        type(vegas_t), dimension(:), allocatable :: integrator
        integer, dimension(:), allocatable :: chain
        real(default), dimension(:), allocatable :: weight
        real(default), dimension(:), allocatable :: integral
        real(default), dimension(:), allocatable :: variance
        real(default), dimension(:), allocatable :: efficiency
        type(vamp2_result_t) :: result

```

```

        type(vamp2_equivalences_t) :: equivalences
        logical :: event_prepared
        real(default), dimension(:), allocatable :: event_weight
    <VAMP2: vamp2: type>
    contains
    <VAMP2: vamp2: TBP>
end type vamp2_t

<MPI: VAMP2: vamp2: type>≡
    class(request_base_t), allocatable :: request

<VAMP2: interfaces>+≡
    interface vamp2_t
        module procedure vamp2_init
    end interface vamp2_t

```

Constructor.

```

<VAMP2: sub interfaces>+≡
    module function vamp2_init (n_channel, n_dim, alpha, beta, n_bins_max,&
        & n_calls_min_per_channel, iterations, mode) result (self)
        type(vamp2_t) :: self
        integer, intent(in) :: n_channel
        integer, intent(in) :: n_dim
        integer, intent(in), optional :: n_bins_max
        integer, intent(in), optional :: n_calls_min_per_channel
        real(default), intent(in), optional :: alpha
        real(default), intent(in), optional :: beta
        integer, intent(in), optional :: iterations
        integer, intent(in), optional :: mode
    end function vamp2_init

<VAMP2: procedures>+≡
    module function vamp2_init (n_channel, n_dim, alpha, beta, n_bins_max,&
        & n_calls_min_per_channel, iterations, mode) result (self)
        type(vamp2_t) :: self
        integer, intent(in) :: n_channel
        integer, intent(in) :: n_dim
        integer, intent(in), optional :: n_bins_max
        integer, intent(in), optional :: n_calls_min_per_channel
        real(default), intent(in), optional :: alpha
        real(default), intent(in), optional :: beta
        integer, intent(in), optional :: iterations
        integer, intent(in), optional :: mode
        integer :: ch
        self%config%n_dim = n_dim
        self%config%n_channel = n_channel
        call set_options ()
        allocate (self%chain(n_channel), source=0)
        allocate (self%integrator(n_channel))
        allocate (self%weight(n_channel), source=0._default)
        do ch = 1, n_channel
            self%integrator(ch) = vegas_t (n_dim, alpha, n_bins_max, 1, mode)
        end do
        self%weight = 1._default / self%config%n_channel
        call self%reset_result ()
    end function vamp2_init

```



```

        allocate (self%event_weight(self%config%n_channel), source = 0._default)
        self%event_prepared = .false.
contains
    subroutine set_options ()
        if (present (n_bins_max)) self%config%n_bins_max = n_bins_max
        if (present (n_calls_min_per_channel)) &
            self%config%n_calls_min_per_channel = n_calls_min_per_channel
        if (present (alpha)) self%config%alpha = alpha
        if (present (beta)) self%config%beta = beta
        if (present (iterations)) self%config%iterations = iterations
        if (present (mode)) self%config%mode = mode
    end subroutine set_options
end function vamp2_init

<VAMP2: vamp2: TBP>≡
    procedure, public :: final => vamp2_final

<VAMP2: sub interfaces>+≡
    module subroutine vamp2_final (self)
        class(vamp2_t), intent(inout) :: self
    end subroutine vamp2_final

<VAMP2: procedures>+≡
    module subroutine vamp2_final (self)
        class(vamp2_t), intent(inout) :: self
        integer :: ch
        do ch = 1, self%config%n_channel
            call self%integrator(ch)%final ()
        end do
    end subroutine vamp2_final

```

Output.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: write => vamp2_write

<VAMP2: sub interfaces>+≡
    module subroutine vamp2_write (self, unit, indent)
        class(vamp2_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
    end subroutine vamp2_write

<VAMP2: procedures>+≡
    module subroutine vamp2_write (self, unit, indent)
        class(vamp2_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind, ch
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, ind)
        write (u, "(A)") "VAMP2: VEGAS AMPlified 2"
        call write_indent (u, ind)
        call self%config%write (unit, indent)
        call self%result%write (unit, indent)
    end subroutine vamp2_write

```

```
end subroutine vamp2_write
```

Get the config object.

```
<VAMP2: vamp2: TBP>+≡
  procedure, public :: get_config => vamp2_get_config

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_get_config (self, config)
    class(vamp2_t), intent(in) :: self
    type(vamp2_config_t), intent(out) :: config
  end subroutine vamp2_get_config

<VAMP2: procedures>+≡
  module subroutine vamp2_get_config (self, config)
    class(vamp2_t), intent(in) :: self
    type(vamp2_config_t), intent(out) :: config
    config = self%config
  end subroutine vamp2_get_config
```

Set non-runtime dependent configuration. It will no be possible to change `n_bins_max`.

```
<VAMP2: vamp2: TBP>+≡
  procedure, public :: set_config => vamp2_set_config

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_set_config (self, config)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_config_t), intent(in) :: config
  end subroutine vamp2_set_config

<VAMP2: procedures>+≡
  module subroutine vamp2_set_config (self, config)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_config_t), intent(in) :: config
    integer :: ch
    self%config%equivalences = config%equivalences
    self%config%n_calls_min_per_channel = config%n_calls_min_per_channel
    self%config%n_calls_threshold = config%n_calls_threshold
    self%config%n_calls_min = config%n_calls_min
    self%config%beta = config%beta
    self%config%accuracy_goal = config%accuracy_goal
    self%config%error_goal = config%error_goal
    self%config%rel_error_goal = config%rel_error_goal
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%set_config (config)
    end do
  end subroutine vamp2_set_config
```

Set the overall number of calls. The number of calls each channel is scaled by the channel weights

$$N_i = \alpha_i N. \quad (20.8)$$

```
<VAMP2: vamp2: TBP>+≡
  procedure, public :: set_calls => vamp2_set_n_calls
```

```

<VAMP2: sub interfaces>+=
  module subroutine vamp2_set_n_calls (self, n_calls)
    class(vamp2_t), intent(inout) :: self
    integer, intent(in) :: n_calls
  end subroutine vamp2_set_n_calls

<VAMP2: procedures>+=
  module subroutine vamp2_set_n_calls (self, n_calls)
    class(vamp2_t), intent(inout) :: self
    integer, intent(in) :: n_calls
    integer :: ch
    self%config%n_calls_min = self%config%n_calls_min_per_channel &
      & * self%config%n_channel
    self%config%n_calls = max(n_calls, self%config%n_calls_min)
    if (self%config%n_calls > n_calls) then
      write (msg_buffer, "(A,I0)") "VAMP2: [set_calls] number of calls too few,&
        & reset to = ", self%config%n_calls
      call msg_message ()
    end if
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%set_calls (max (nint (self%config%n_calls *&
        & self%weight(ch)), self%config%n_calls_min_per_channel))
    end do
  end subroutine vamp2_set_n_calls

```

Set limits. We only support same limits for all channels.

```

<VAMP2: vamp2: TBP>+=
  procedure, public :: set_limits => vamp2_set_limits

<VAMP2: sub interfaces>+=
  module subroutine vamp2_set_limits (self, x_upper, x_lower)
    class(vamp2_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x_upper
    real(default), dimension(:), intent(in) :: x_lower
  end subroutine vamp2_set_limits

<VAMP2: procedures>+=
  module subroutine vamp2_set_limits (self, x_upper, x_lower)
    class(vamp2_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x_upper
    real(default), dimension(:), intent(in) :: x_lower
    integer :: ch
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%set_limits (x_upper, x_lower)
    end do
  end subroutine vamp2_set_limits

```

Set `n_chains` and the (actual) chains. `chain` must have size `n_channels` and each elements must store an index to a corresponding chain. This means, that channels with equal index correspond to the same chain, and we refer to those as chained weights, where we average the contributions of the chained weights in `vamp2_adapt_weights`.

```

<VAMP2: vamp2: TBP>+=
  procedure, public :: set_chain => vamp2_set_chain

```

```

<VAMP2: sub interfaces>+≡
    module subroutine vamp2_set_chain (self, n_chains, chain)
        class(vamp2_t), intent(inout) :: self
        integer, intent(in) :: n_chains
        integer, dimension(:), intent(in) :: chain
    end subroutine vamp2_set_chain

<VAMP2: procedures>+≡
    module subroutine vamp2_set_chain (self, n_chains, chain)
        class(vamp2_t), intent(inout) :: self
        integer, intent(in) :: n_chains
        integer, dimension(:), intent(in) :: chain
        if (size (chain) /= self%config%n_channel) then
            call msg_bug ("VAMP2: set chain: size of chain array does not match n_channel.")
        else
            call msg_message ("VAMP2: set chain: use chained weights.")
        end if
        self%config%n_chains = n_chains
        self%chain = chain
    end subroutine vamp2_set_chain

```

Set channel equivalences.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: set_equivalences => vamp2_set_equivalences

<VAMP2: sub interfaces>+≡
    module subroutine vamp2_set_equivalences (self, equivalences)
        class(vamp2_t), intent(inout) :: self
        type(vamp2_equivalences_t), intent(in) :: equivalences
    end subroutine vamp2_set_equivalences

<VAMP2: procedures>+≡
    module subroutine vamp2_set_equivalences (self, equivalences)
        class(vamp2_t), intent(inout) :: self
        type(vamp2_equivalences_t), intent(in) :: equivalences
        self%equivalences = equivalences
    end subroutine vamp2_set_equivalences

```

Move allocated (and prepared!) request object into VAMP2. Gfortran 7/8/9 bug, has to remain in the main module.

```

<MPI: VAMP2: vamp2: TBP>≡
    generic, public :: allocate_request => allocate_request_by_method, &
        allocate_request_by_object
    procedure, private :: allocate_request_by_method => vamp2_allocate_request_by_method
    procedure, private :: allocate_request_by_object => vamp2_allocate_request_by_object

<MPI: VAMP2: main procedures>≡
    subroutine vamp2_allocate_request_by_method (self, method)
        class(vamp2_t), intent(inout) :: self
        character(len=*), intent(in) :: method
        class(request_base_t), allocatable :: request
        select case (trim(method))
        case("simple", "Simple", "SIMPLE")
            allocate (request_simple_t :: request)
        case("load", "Load", "LOAD")

```

```

        allocate (request_caller_t :: request)
    case default
        call msg_bug ("VAMP2: Unknown method for MPI request module.")
    end select
    select type (request)
    type is (request_simple_t)
        call request%init (MPI_COMM_WORLD, n_channels = self%config%n_channel)
    type is (request_caller_t)
        call request%init (MPI_COMM_WORLD, n_channels = self%config%n_channel)
    end select
    call self%allocate_request_by_object (request)
end subroutine vamp2_allocate_request_by_method

subroutine vamp2_allocate_request_by_object (self, request)
    class(vamp2_t), intent(inout) :: self
    class(request_base_t), allocatable, intent(inout) :: request
    !! Only output in case of "parallel" integration.
    if (request%has_workers ()) then
        select type (request)
        type is (request_simple_t)
            call msg_message ("VAMP2: Simple Request Balancing.")
        type is (request_caller_t)
            call msg_message ("VAMP2: Request with load balancing.")
        class default
            call msg_bug ("VAMP2: Unknown extension of request_base.")
        end select
    end if
    call move_alloc (request, self%request)
end subroutine vamp2_allocate_request_by_object

```

Get `n_calls` calculated by VEGAS.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: get_n_calls => vamp2_get_n_calls

<VAMP2: sub interfaces>+≡
    elemental module function vamp2_get_n_calls (self) result (n_calls)
        class(vamp2_t), intent(in) :: self
        real(default) :: n_calls
    end function vamp2_get_n_calls

<VAMP2: procedures>+≡
    elemental module function vamp2_get_n_calls (self) result (n_calls)
        class(vamp2_t), intent(in) :: self
        real(default) :: n_calls
        n_calls = sum (self%integrator%get_calls ())
    end function vamp2_get_n_calls

```

Get the cumulative result of the integration. Recalculate weighted average of the integration.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: get_integral => vamp2_get_integral

<VAMP2: sub interfaces>+≡
    elemental module function vamp2_get_integral (self) result (integral)

```

```

        class(vamp2_t), intent(in) :: self
        real(default) :: integral
    end function vamp2_get_integral
<VAMP2: procedures>+≡
    elemental module function vamp2_get_integral (self) result (integral)
        class(vamp2_t), intent(in) :: self
        real(default) :: integral
        integral = 0.
        if (self%result%sum_wgts > 0.) then
            integral = self%result%sum_int_wgtd / self%result%sum_wgts
        end if
    end function vamp2_get_integral

```

Get the cumulative variance of the integration. Recalculate the variance.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: get_variance => vamp2_get_variance
<VAMP2: sub interfaces>+≡
    elemental module function vamp2_get_variance (self) result (variance)
        class(vamp2_t), intent(in) :: self
        real(default) :: variance
    end function vamp2_get_variance
<VAMP2: procedures>+≡
    elemental module function vamp2_get_variance (self) result (variance)
        class(vamp2_t), intent(in) :: self
        real(default) :: variance
        variance = 0
        if (self%result%sum_wgts > 0.) then
            variance = 1.0 / self%result%sum_wgts
        end if
    end function vamp2_get_variance

```

Get efficiency.

```

<VAMP2: vamp2: TBP>+≡
    procedure, public :: get_efficiency => vamp2_get_efficiency
<VAMP2: sub interfaces>+≡
    elemental module function vamp2_get_efficiency (self) result (efficiency)
        class(vamp2_t), intent(in) :: self
        real(default) :: efficiency
    end function vamp2_get_efficiency
<VAMP2: procedures>+≡
    elemental module function vamp2_get_efficiency (self) result (efficiency)
        class(vamp2_t), intent(in) :: self
        real(default) :: efficiency
        efficiency = 0.
        if (self%result%efficiency > 0.) then
            efficiency = self%result%efficiency
        end if
    end function vamp2_get_efficiency

```

Get event weight and event weight excess.

```

(VAMP2: vamp2: TBP)+≡
  procedure :: get_evt_weight => vamp2_get_evt_weight
  procedure :: get_evt_weight_excess => vamp2_get_evt_weight_excess
(VAMP2: sub interfaces)+≡
  module function vamp2_get_evt_weight (self) result (evt_weight)
    class(vamp2_t), intent(in) :: self
    real(default) :: evt_weight
  end function vamp2_get_evt_weight
  module function vamp2_get_evt_weight_excess (self) result (evt_weight_excess)
    class(vamp2_t), intent(in) :: self
    real(default) :: evt_weight_excess
  end function vamp2_get_evt_weight_excess
(VAMP2: procedures)+≡
  module function vamp2_get_evt_weight (self) result (evt_weight)
    class(vamp2_t), intent(in) :: self
    real(default) :: evt_weight
    evt_weight = self%result%evt_weight
  end function vamp2_get_evt_weight

  module function vamp2_get_evt_weight_excess (self) result (evt_weight_excess)
    class(vamp2_t), intent(in) :: self
    real(default) :: evt_weight_excess
    evt_weight_excess = self%result%evt_weight_excess
  end function vamp2_get_evt_weight_excess

```

Get procedure to retrieve channel-th grid.

```

(VAMP2: vamp2: TBP)+≡
  procedure :: get_grid => vamp2_get_grid
(VAMP2: sub interfaces)+≡
  module function vamp2_get_grid (self, channel) result (grid)
    class(vamp2_t), intent(in) :: self
    type(vegas_grid_t) :: grid
    integer, intent(in) :: channel
  end function vamp2_get_grid
(VAMP2: procedures)+≡
  module function vamp2_get_grid (self, channel) result (grid)
    class(vamp2_t), intent(in) :: self
    type(vegas_grid_t) :: grid
    integer, intent(in) :: channel
    if (channel < 1 .or. channel > self%config%n_channel) &
      call msg_bug ("VAMP2: vamp2_get_grid: channel index < 1 or > n_channel.")
    grid = self%integrator(channel)%get_grid ()
  end function vamp2_get_grid

```

Adapt. We adapt the weights due the contribution of variances with $\beta > 0$.

$$\alpha_i = \frac{\alpha_i V_i^\beta}{\sum_i \alpha_i V_i^\beta} \quad (20.9)$$

If `n_calls_threshold` is set, we rescale the weights in such a way, that the `n_calls` for each channel are greater than `n_calls_threshold`. We calculate

the distance of the weights to the `weight_min` and reset those weights which are less than `weight_mins` to this value. The other values are accordingly resized to fit the boundary condition of the partition of unity.

```

<VAMP2: vamp2: TBP>+=
  procedure, private :: adapt_weights => vamp2_adapt_weights
<VAMP2: sub interfaces>+=
  module subroutine vamp2_adapt_weights (self)
    class(vamp2_t), intent(inout) :: self
    end subroutine vamp2_adapt_weights
<VAMP2: procedures>+=
  module subroutine vamp2_adapt_weights (self)
    class(vamp2_t), intent(inout) :: self
    integer :: n_weights_underflow
    real(default) :: weight_min, sum_weights_underflow
    self%weight = self%weight * self%integrator%get_variance ()**self%config%beta
    if (sum (self%weight) == 0) self%weight = real(self%config%n_calls, default)
    if (self%config%n_chains > 0) then
      call chain_weights ()
    end if
    self%weight = self%weight / sum(self%weight)
    if (self%config%n_calls_threshold /= 0) then
      weight_min = real(self%config%n_calls_threshold, default) &
        & / self%config%n_calls
      sum_weights_underflow = sum (self%weight, self%weight < weight_min)
      n_weights_underflow = count (self%weight < weight_min)
      where (self%weight < weight_min)
        self%weight = weight_min
      elsewhere
        self%weight = self%weight * (1. - n_weights_underflow * weight_min) &
          & / (1. - sum_weights_underflow)
      end where
    end if
    call self%set_calls (self%config%n_calls)
  contains
    <VAMP2: vamp2 adapt weights: procedures>
  end subroutine vamp2_adapt_weights

```

We average the weights over their respective chain members.

```

<VAMP2: vamp2 adapt weights: procedures>=
  subroutine chain_weights ()
    integer :: ch
    real(default) :: average
    do ch = 1, self%config%n_chains
      average = max (sum (self%weight, self%chain == ch), 0._default)
      if (average /= 0) then
        average = average / count (self%chain == ch)
        where (self%chain == ch)
          self%weight = average
        end where
      end if
    end do
  end subroutine chain_weights

```



```

<VAMP2: vamp2: TBP>+=
  procedure, private :: apply_equivalences => vamp2_apply_equivalences

<VAMP2: sub interfaces>+=
  module subroutine vamp2_apply_equivalences (self)
    class(vamp2_t), intent(inout) :: self
  end subroutine vamp2_apply_equivalences

<VAMP2: procedures>+=
  module subroutine vamp2_apply_equivalences (self)
    class(vamp2_t), intent(inout) :: self
    integer :: ch, ch_src, j, j_src, i_eqv
    real(default), dimension(:, :, :), allocatable :: d
    real(default), dimension(:, :), allocatable :: d_src
    integer, dimension(:), allocatable :: mode, perm
    if (.not. self%equivalences%is_allocated ()) then
      call msg_bug ("VAMP2: vamp2_apply_equivalences: &
        &cannot apply not-allocated equivalences.")
    end if
    allocate (d(self%config%n_bins_max, self%config%n_dim, &
      self%config%n_channel), source=0._default)
    associate (eqv => self%equivalences, nb => self%config%n_bins_max)
      do i_eqv = 1, self%equivalences%n_eqv
        call eqv%get_channels (i_eqv, ch, ch_src)
        d_src = self%integrator(ch_src)%get_distribution ()
        mode = eqv%get_mode (i_eqv)
        perm = eqv%get_perm (i_eqv)
        do j = 1, self%config%n_dim
          select case (mode (j))
            case (VEQ_IDENTITY)
              d(:, j, ch) = d(:, j, ch) + &
                d_src(:, perm(j))
            case (VEQ_INVERT)
              d(:, j, ch) = d(:, j, ch) + &
                d_src(nb:1:-1, perm(j))
            case (VEQ_SYMMETRIC)
              d(:, j, ch) = d(:, j, ch) + &
                d_src(:, perm(j)) / 2. + &
                d_src(nb:1:-1, perm(j)) / 2.
            case (VEQ_INVARIANT)
              d(:, j, ch) = 1._default
          end select
        end do
      end do
    end associate
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%set_distribution (d(:, :, ch))
    end do
  end subroutine vamp2_apply_equivalences

```

Reset the cumulative result.

```

<VAMP2: vamp2: TBP>+=
  procedure, public :: reset_result => vamp2_reset_result

<VAMP2: sub interfaces>+=

```

```

module subroutine vamp2_reset_result (self)
  class(vamp2_t), intent(inout) :: self
end subroutine vamp2_reset_result
<VAMP2: procedures>+≡
module subroutine vamp2_reset_result (self)
  class(vamp2_t), intent(inout) :: self
  call self%result%reset ()
end subroutine vamp2_reset_result

```

Integrate. We integrate each channel separately and combine the results

$$I = \sum_i \alpha_i I_i, \quad (20.10)$$

$$\sigma^2 = \sum_i \alpha_i^2 \sigma_i^2. \quad (20.11)$$

Although, the (population) variance is given by

$$\begin{aligned}
\sigma^2 &= \frac{1}{N} \left(\sum_i \alpha_i I_i^2 - I^2 \right) \\
&= \frac{1}{N-1} \left(\sum_i (N_i \sigma_i^2 + I_i^2) - I^2 \right) \\
&= \frac{1}{N-1} \left(\sum_i \alpha_i \sigma_i^2 + \alpha_i I_i^2 - I^2 \right),
\end{aligned} \quad (20.12)$$

where we used $\sigma_i^2 = \frac{1}{N} (\langle I_i^2 \rangle - \langle I_i \rangle^2)$, we use the approximation for numeric stability. The population variance relates to sample variance

$$s^2 = \frac{n}{n-1} \sigma^2, \quad (20.13)$$

which gives an unbiased error estimate.

Beside those adaption to multichannel, the overall processing of `total_integral`, `total_sq_integral` and `total_variance` is the same as in `vegas_integrate`.

```

<VAMP2: vamp2: TBP>+≡
  procedure, public :: integrate => vamp2_integrate
<VAMP2: sub interfaces>+≡
  module subroutine vamp2_integrate (self, func, rng, iterations, &
    reset_result, refine_grids, adapt_weights, verbose, result, abserr)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    integer, intent(in), optional :: iterations
    logical, intent(in), optional :: reset_result
    logical, intent(in), optional :: refine_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: verbose
    real(default), optional, intent(out) :: result, abserr
  end subroutine vamp2_integrate

```

```

<VAMP2: procedures>+≡
  module subroutine vamp2_integrate (self, func, rng, iterations, &
    reset_result, refine_grids, adapt_weights, verbose, result, abserr)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    integer, intent(in), optional :: iterations
    logical, intent(in), optional :: reset_result
    logical, intent(in), optional :: refine_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: verbose
    real(default), optional, intent(out) :: result, abserr
    integer :: it, ch
    type(iterator_t) :: channel_iterator
    real(default) :: cumulative_int, cumulative_std
    logical :: opt_reset_result
    logical :: opt_adapt_weights
    logical :: opt_refine_grids
    logical :: opt_verbose
  <VAMP2: vamp2 integrate: variables>
    call set_options ()
    if (opt_verbose) then
      call msg_message ("Results: [it, calls, integral, error, chi^2, eff.]")
    end if
    if (opt_reset_result) call self%reset_result ()
  <VAMP2: vamp2 integrate: init>
    iteration: do it = 1, self%config%iterations
      call channel_iterator%init (1, self%config%n_channel)
      call self%prepare_integrate_iteration (func)
    <VAMP2: vamp2 integrate: presampling>
    channel: do
      <VAMP2: vamp2 integrate: sampling>
      call func%set_channel (ch)
      call self%integrator(ch)%integrate ( &
        & func, rng, iterations, refine_grid = .false., verbose = .false.)
      <VAMP2: vamp2 integrate: callback>
      call channel_iterator%next_step ()
    end do channel
    <VAMP2: vamp2 integrate: postsampling>
    call self%compute_result_and_efficiency ()
    associate (result => self%result)
      cumulative_int = result%sum_int_wgtd / result%sum_wgts
      cumulative_std = sqrt (1 / result%sum_wgts)
      if (opt_verbose) then
        write (msg_buffer, "(I0,1x,I0,1x, 4(E24.16E4,1x))" ) &
          & it, self%config%n_calls, cumulative_int, cumulative_std, &
          & result%chi2, result%efficiency
        call msg_message ()
      end if
    end associate
    if (opt_adapt_weights) then
      call self%adapt_weights ()
    end if
    if (opt_refine_grids) then

```

```

        if (self%config%equivalences .and. self%equivalences%is_allocated ()) then
            call self%apply_equivalences ()
        end if
        do ch = 1, self%config%n_channel
            !! When we apply the grid refinement outside of VEGAS, then we do not average over di
            !! as VEGAS averaged the distribution internally.
            call self%integrator(ch)%refine (average = .false.)
        end do
    end if
end do iteration
if (present (result)) result = cumulative_int
if (present (abserr)) abserr = abs (cumulative_std)
contains
<VAMP2: vamp2 integrate: procedures>
end subroutine vamp2_integrate

```

Set optional parameters.

```

<VAMP2: vamp2 integrate: procedures>≡
subroutine set_options ()
    if (present (iterations)) self%config%iterations = iterations
    opt_reset_result = .true.
    if (present (reset_result)) opt_reset_result = reset_result
    opt_adapt_weights = .true.
    if (present (adapt_weights)) opt_adapt_weights = adapt_weights
    opt_refine_grids = .true.
    if (present (refine_grids)) opt_refine_grids = refine_grids
    opt_verbose = .false.
    if (present (verbose)) opt_verbose = verbose
end subroutine set_options

```

We define additional chunks, which we use to insert parallel/MPI code.

```

<VAMP2: vamp2 integrate: variables>≡

```

```

<VAMP2: vamp2 integrate: init>≡

```

```

<VAMP2: vamp2 integrate: presampling>≡

```

Conditional handling. We introduce a different behavior for the MPI-/non-MPI variant.

```

<NOMPI: VAMP2: vamp2 integrate: sampling>≡
    if (.not. channel_iterator%is_iterable ()) exit channel
    ch = channel_iterator%get_current ()

```

```

<VAMP2: vamp2 integrate: callback>≡

```

```

<VAMP2: vamp2 integrate: postsampling>≡

```

```

<MPI: VAMP2: vamp2 integrate: variables>≡
    type(request_t) :: request

```

Verify that we have an allocated request object, else fallback to simple method. Be aware that we keep the fallback silent (!) in order to keep any possible testing output uninterrupted.

```

<MPI: VAMP2: vamp2 integrate: init>≡
    if (.not. allocated (self%request)) then
        call self%allocate_request_by_method ("simple")
    end if

```

```

(MPI: VAMP2: vamp2 integrate: presampling)≡
  if (self%request%is_master ()) then
    select type (req => self%request)
    type is (request_caller_t)
      request%terminate = .true.
      call update_iter_and_rng (request, channel_iterator, rng)
      !! channel_iter is already drained for master.
      !! Do not descent into channel integration (later on).
      call req%handle_workload ()
    end select
  end if

```

Conditional handling for the MPI-version of sampling.

We have a request object and an advanced `channel_iterator` and have to consider three cases:

1. `channel_iterator` drained,
2. request terminated,
3. request received.

When the `channel_iterator` is drained by `update_iter_and_rng`, we send a terminate request to the master and await in the next cycle of channel loop the terminated request. When the request is terminated, we can gracefully exit the channel loop as `channel_iterator` and `rng` are already advanced by `update_iter_and_rng`. When we received a genuine request, then, we proceed as prophesied.

```

(MPI: VAMP2: vamp2 integrate: sampling)≡
  select type (req => self%request)
  type is (request_caller_t)
    if (self%request%is_master ()) exit channel
  end select
  call self%request%request_workload (request)
  call update_iter_and_rng (request, channel_iterator, rng)
  if (request%terminate) then
    exit channel
  else if (.not. channel_iterator%is_iterable ()) then
    select type (req => self%request)
    type is (request_caller_t)
      call req%request_terminate ()
      cycle channel
    class is (request_base_t)
      exit channel
    end select
  end if
  if (request%group) call MPI_BARRIER (request%comm)
  ch = request%handler_id
  call self%integrator(ch)%prepare_parallel_integrate(request%comm, &
    duplicate_comm = .false., &
    parallel_mode = request%group)

```

```

(MPI: VAMP2: vamp2 integrate: callback)≡
  if (request%group_master) then
    if (.not. self%request%is_master ()) &

```

```

        call allocate_handler (self%request, ch)
        call self%request%handle_and_release_workload (request)
    else
        call self%request%release_workload (request)
    end if

<MPI: VAMP2: vamp2 integrate: postsampling>≡
    call reduce_func_calls (func)
    call self%request%await_handler ()
    call self%request%barrier ()
    if (.not. self%request%is_master ()) cycle

<MPI: VAMP2: vamp2 integrate: procedures>≡
    subroutine allocate_handler (req, ch)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: ch
        class(request_handler_t), pointer :: vegas_result_handler
        call self%integrator(ch)%allocate_handler (&
            handler_id = ch,&
            handler = vegas_result_handler)
        call req%add_handler (ch, vegas_result_handler)
    end subroutine allocate_handler

    !! Advance the random number generator for the skipped channels.
    !!
    !! We set current_channel = request%handler_id, hence, we need to advance
    !! the random number generator until th iterator returns the same channel.
    subroutine update_iter_and_rng (request, iter, rng)
        type(request_t), intent(in) :: request
        type(iterator_t), intent(inout) :: iter
        class(rng_t), intent(inout) :: rng
        advance: do while (iter%is_iterable ())
            !! Advance up to iterator%end when in terminate mode,
            !! else advance until we hit the previous channel (i.e. request%handler_id - 1):
            !! Proof: current_channel <= request%handler_id - 1
            if (.not. request%terminate) then
                if (iter%get_current () >= request%handler_id) &
                    exit advance
            end if
            select type (rng)
            type is (rng_stream_t)
                call rng%next_substream ()
            end select
            call iter%next_step ()
        end do advance
    end subroutine update_iter_and_rng

    subroutine reduce_func_calls (func)
        class(vamp2_func_t), intent(inout) :: func
        type(MPI_COMM) :: comm
        integer :: root_n_calls
        call self%request%get_external_comm (comm)
        call MPI_reduce (func%n_calls, root_n_calls, 1, MPI_INTEGER, &
            MPI_SUM, 0, comm)
        if (self%request%is_master ()) then

```

```

        func%n_calls = root_n_calls
    else
        call func%reset_n_calls ()
    end if
end subroutine reduce_func_calls

```

Prepeare current integration's iteration.

Prepare iteration, i.e. provide weights and grids to function object. Gfortran 7/8/9 bug, only for the MPI version, has to remain in the main module:

```

<VAMP2: vamp2: TBP>+=
    procedure, private :: prepare_integrate_iteration => &
        vamp2_prepare_integrate_iteration

<VAMP2: main procedures>=
    subroutine vamp2_prepare_integrate_iteration (self, func)
        class(vamp2_t), intent(inout) :: self
        class(vamp2_func_t), intent(inout) :: func
    <VAMP2: vamp2 prepare integrate iteration: body>
        call fill_func_with_weights_and_grids (func)
    contains
        subroutine fill_func_with_weights_and_grids (func)
            class(vamp2_func_t), intent(inout) :: func
            integer :: ch
            do ch = 1, self%config%n_channel
                func%wi(ch) = self%weight(ch)
                !! \todo Use pointers instead of a deep copy.
                func%grids(ch) = self%integrator(ch)%get_grid ()
            end do
        end subroutine fill_func_with_weights_and_grids
    <VAMP2: vamp2 prepare integrate iteration: procedures>
    end subroutine vamp2_prepare_integrate_iteration

<VAMP2: vamp2 prepare integrate iteration: body>=
<VAMP2: vamp2 prepare integrate iteration: procedures>=
<MPI: VAMP2: vamp2 prepare integrate iteration: body>=
    if (.not. allocated (self%request)) then
        call msg_bug ("VAMP2: prepare integration iteration failed: unallocated request.")
    end if
    call broadcast_weights_and_grids ()
    select type (req => self%request)
    type is (request_simple_t)
        call req%update (self%integrator%is_parallelizable ())
        call init_all_handler (req)
        call call_all_handler (req)
        !! Add all handlers, call all handlers.
    type is (request_caller_t)
        if (req%is_master ()) then
            call req%update_balancer (self%weight, self%integrator%is_parallelizable ())
            call init_all_handler (req)
        else
            call self%request%reset ()
        end if
    class default

```

```

        call msg_bug ("VAMP2: prepare integration iteration failed: unknown request type.")
    end select

<MPI: VAMP2: vamp2 prepare integrate iteration: procedures>≡
subroutine broadcast_weights_and_grids ()
    type(vegas_grid_t) :: grid
    type(MPI_COMM) :: comm
    integer :: ch
    call self%request%get_external_comm (comm)
    call MPI_BCAST (self%weight, self%config%n_channel, &
        MPI_DOUBLE_PRECISION, 0, comm)
    do ch = 1, self%config%n_channel
        grid = self%integrator(ch)%get_grid ()
        call grid%broadcast (comm)
        call self%integrator(ch)%set_grid (grid)
    end do
    call self%set_calls (self%config%n_calls)
end subroutine broadcast_weights_and_grids

subroutine init_all_handler (req)
    class(request_base_t), intent(inout) :: req
    class(request_handler_t), pointer :: vegas_result_handler
    integer :: ch
    !! The master worker needs always all handler (callback objects)
    !! in order to perform the communication to the client handler (callbacks).
    if (.not. req%is_master ()) return
    do ch = 1, self%config%n_channel
        call self%integrator(ch)%allocate_handler (&
            handler_id = ch,&
            handler = vegas_result_handler)
        call req%add_handler (ch, vegas_result_handler)
    end do
end subroutine init_all_handler

subroutine call_all_handler (req)
    class(request_base_t), intent(inout) :: req
    integer :: ch
    if (.not. req%is_master ()) return
    do ch = 1, self%config%n_channel
        select type (req)
            type is (request_simple_t)
                call req%call_handler (handler_id = ch, &
                    source_rank = req%get_request_master (ch))
        end select
    end do
end subroutine call_all_handler

Compute the result and efficiency of the current status of the integrator.
<VAMP2: vamp2: TBP>+≡
    procedure, private :: compute_result_and_efficiency => &
        vamp2_compute_result_and_efficiency

<VAMP2: sub interfaces>+≡
    module subroutine vamp2_compute_result_and_efficiency (self)
        class(vamp2_t), intent(inout) :: self
    end subroutine vamp2_compute_result_and_efficiency

```


<VAMP2: procedures>+≡

```

module subroutine vamp2_compute_result_and_efficiency (self)
  class(vamp2_t), intent(inout) :: self
  real(default) :: total_integral, total_variance
  real(default) :: max_abs_f_pos, max_abs_f_neg, &
    sum_abs_f_pos, sum_abs_f_neg
  call compute_integral_and_variance (total_integral, total_variance)
  call self%result%update (total_integral, total_variance)
  call compute_efficiency (max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
    sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
  !! Do not average of number of calls, we have already averaged the efficiencies of all channel
  call self%result%update_efficiency (n_calls = 1, &
    max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
    sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
contains
  subroutine compute_integral_and_variance (integral, variance)
    real(default), intent(out) :: integral, variance
    real(default) :: sq_integral
    integral = dot_product (self%weight, self%integrator%get_integral ())
    sq_integral = dot_product (self%weight, self%integrator%get_integral ()**2)
    variance = self%config%n_calls * dot_product (self%weight**2, self%integrator%get_variance ())
    variance = sqrt (variance + sq_integral)
    variance = 1._default / self%config%n_calls * &
      (variance + integral) * (variance - integral)
  end subroutine compute_integral_and_variance

  !> We compute the weight-averaged sum and maximum of the channel (integration) weights \f$w_{i,j}$.
  !!
  !! The averaged integration weight and maximum are
  !! \f[
  !! \langle w \rangle = \sum_i \alpha_i \frac{\sum_j w_{i,j}}{N_i},
  !! \f]
  !! \f[
  !! \langle \max w \rangle = \sum_i \alpha_i |\max_j w_{i,j}|.
  !! \f]
  subroutine compute_efficiency (max_pos, max_neg, &
    sum_pos, sum_neg)
    real(default), intent(out) :: max_pos, max_neg
    real(default), intent(out) :: sum_pos, sum_neg
    max_abs_f_pos = dot_product (self%weight, self%integrator%get_max_abs_f_pos ())
    max_abs_f_neg = dot_product (self%weight, self%integrator%get_max_abs_f_neg ())
    sum_abs_f_pos = dot_product (self%weight, &
      self%integrator%get_sum_abs_f_pos () / self%integrator%get_calls ())
    sum_abs_f_neg = dot_product (self%weight, &
      self%integrator%get_sum_abs_f_neg () / self%integrator%get_calls ())
  end subroutine compute_efficiency
end subroutine vamp2_compute_result_and_efficiency

```

Generate event from multi-channel weight $w(x) = f(x)/g(x)$.

We select a channel using the a-priori weights and f_i^{\max} , to flatten possible unbalanced channel weight(s).

An additional rescale factor `opt_event_rescale` is applied to `f_max`, iff set.

<VAMP2: vamp2: TBP>+≡

```

    procedure, public :: generate_weighted => vamp2_generate_weighted_event
<VAMP2: sub interfaces>+≡
    module subroutine vamp2_generate_weighted_event (self, func, rng, x)
        class(vamp2_t), intent(inout) :: self
        class(vamp2_func_t), intent(inout) :: func
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
    end subroutine vamp2_generate_weighted_event
<VAMP2: procedures>+≡
    module subroutine vamp2_generate_weighted_event (self, func, rng, x)
        class(vamp2_t), intent(inout) :: self
        class(vamp2_func_t), intent(inout) :: func
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        integer :: ch, i
        real(default) :: r
        if (.not. self%event_prepared) then
            call prepare_event ()
        else
            if (.not. allocated (func%grids)) then
                call prepare_event ()
            else
                if (any ([(.not. allocated (func%grids(i)%xi),i=1,size(func%grids))])) then
                    call prepare_event ()
                end if
            end if
        end if
        call rng%generate (r)
        nchannel: do ch = 1, self%config%n_channel
            r = r - self%event_weight(ch)
            if (r <= 0._default) exit nchannel
        end do nchannel
        ch = min (ch, self%config%n_channel)
        call func%set_channel (ch)
        call self%integrator(ch)%generate_weighted (func, rng, x)
        ! Norm weight by f_max, hidden in event_weight(ch), else by 1
        self%result%evt_weight = self%integrator(ch)%get_evt_weight () &
            * self%weight(ch) / self%event_weight(ch)
    contains
    <VAMP2: vamp2 generate event: procedures>
    end subroutine vamp2_generate_weighted_event

```

Generate unweighted events.

After selecting a channel ch by the inversion method using a random number $r \in [0, 1]$

$$F^{-1}(r) := \inf\{c \in \{1, \dots, N_c\} | F(c) \geq r\}, F(c) = \sum_{c' \leq c} \alpha'_{c'}, \quad (20.14)$$

we try for an event from the previously selected channel. If the event is rejected, we also reject the selected channel.

The inversion method is implemented as a loop over the channel weights α_i until $\sum_c^{c^{prime}} \alpha_c - r \leq 0$, the last value of the loop index `ch` is then c' .

(VAMP2: vamp2: TBP)+≡

```
procedure, public :: generate_unweighted => &
    vamp2_generate_unweighted_event
```

(VAMP2: sub interfaces)+≡

```
module subroutine vamp2_generate_unweighted_event (self, func, rng, &
    x, opt_event_rescale)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
    real(default), intent(in), optional :: opt_event_rescale
end subroutine vamp2_generate_unweighted_event
```

(VAMP2: procedures)+≡

```
module subroutine vamp2_generate_unweighted_event (self, func, rng, &
    x, opt_event_rescale)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
    real(default), intent(in), optional :: opt_event_rescale
    integer :: ch, i
    real(default) :: r, max_abs_f, event_rescale
    event_rescale = 1._default
    if (present (opt_event_rescale)) then
        event_rescale = opt_event_rescale
    end if
    if (.not. self%event_prepared) then
        call prepare_event ()
    else
        if (.not. allocated (func%grids)) then
            call prepare_event ()
        else
            if (any ([(.not. allocated (func%grids(i)%xi), i=1, size(func%grids))])) then
                call prepare_event ()
            end if
        end if
    end if
    generate: do
        call rng%generate (r)
        nchannel: do ch = 1, self%config%n_channel
            r = r - self%event_weight(ch)
            if (r <= 0._default) exit nchannel
        end do nchannel
        ch = min (ch, self%config%n_channel)
        call func%set_channel (ch)
        call self%integrator(ch)%generate_weighted (func, rng, x)
        self%result%evt_weight = self%integrator(ch)%get_evt_weight ()
        max_abs_f = self%integrator(ch)%get_max_abs_f ()
        self%result%evt_weight_excess = 0._default
        if (abs(self%result%evt_weight) > max_abs_f) then
            self%result%evt_weight_excess = abs(self%result%evt_weight) / max_abs_f - 1._default
        end if
    end generate
end subroutine
```

```

        exit generate
    end if
    call rng%generate (r)
    ! Do not use division, because max_abs_f could be zero.
    if (event_rescale * max_abs_f * r <= abs(self%result%evt_weight)) then
        exit generate
    end if
end do generate
contains
<VAMP2: vamp2 generate event: procedures>
end subroutine vamp2_generate_unweighted_event

```

Prepare event generation. We have to set the channel weights and the grids for the integrand's object.

We use an ansatz proposed by T. Ohl in the original VAMP code where we do not have to accept on

$$\frac{w_i(x)}{\sum_i \alpha_i \max_x w_i(x)},$$

after we have selected a channel by the weights α_i . But rather, we use a more efficient way where we rescale the channel weights α_i

$$\alpha_i \rightarrow \alpha_i \frac{\max_x w_i(x)}{\sum_i \alpha_i \max_x w_i(x)}.$$

The overall magic is to insert a "1" and to move the uneasy part into the channel selection, such that we can generate events likewise in the single channel mode. We generate an unweighted event by

$$\frac{w_i(x)}{\max_x w_i x},$$

after we have selected a channel by the rescaled event channel weights. The overall normalization $\max_{i,x}$ is not needed because we normalize the event channel weights to one and therefore the overall normalization cancels.

```

<VAMP2: vamp2 generate event: procedures>≡
subroutine prepare_event ()
    integer :: i
    self%event_prepared = .false.
    do i = 1, self%config%n_channel
        func%wi(i) = self%weight(i)
        func%grids(i) = self%integrator(i)%get_grid ()
    end do
    if (any (self%integrator%get_max_abs_f () > 0)) then
        self%event_weight = self%weight * self%integrator%get_max_abs_f ()
    else
        self%event_weight = self%weight
    end if
    self%event_weight = self%event_weight / sum (self%event_weight)
    self%event_prepared = .true.
end subroutine prepare_event

```

Write grids to unit.

```

<VAMP2: parameters>+=
  character(len=*), parameter, private :: &
    descr_fmt = "(1X,A)", &
    integer_fmt = "(1X,A18,1X,I15)", &
    integer_array_fmt = "(1X,I18,1X,I15)", &
    logical_fmt = "(1X,A18,1X,L1)", &
    double_fmt = "(1X,A18,1X,E24.16E4)", &
    double_array_fmt = "(1X,I18,1X,E24.16E4)", &
    double_array_pac_fmt = "(1X,I18,1X,E16.8E4)", &
    double_array2_fmt = "(1X,2(1X,I8),1X,E24.16E4)", &
    double_array2_pac_fmt = "(1X,2(1X,I8),1X,E16.8E4)"

<VAMP2: vamp2: TBP>+=
  procedure, public :: write_grids => vamp2_write_grids

<VAMP2: sub interfaces>+=
  module subroutine vamp2_write_grids (self, unit)
    class(vamp2_t), intent(in) :: self
    integer, intent(in), optional :: unit
  end subroutine vamp2_write_grids

<VAMP2: procedures>+=
  module subroutine vamp2_write_grids (self, unit)
    class(vamp2_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer :: u
    integer :: ch
    u = given_output_unit (unit)
    write (u, descr_fmt) "begin type(vamp2_t)"
    write (u, integer_fmt) "n_channel =", self%config%n_channel
    write (u, integer_fmt) "n_dim =", self%config%n_dim
    write (u, integer_fmt) "n_calls_min_ch =", self%config%n_calls_min_per_channel
    write (u, integer_fmt) "n_calls_thres =", self%config%n_calls_threshold
    write (u, integer_fmt) "n_chains =", self%config%n_chains
    write (u, logical_fmt) "stratified =", self%config%stratified
    write (u, double_fmt) "alpha =", self%config%alpha
    write (u, double_fmt) "beta =", self%config%beta
    write (u, integer_fmt) "n_bins_max =", self%config%n_bins_max
    write (u, integer_fmt) "iterations =", self%config%iterations
    write (u, integer_fmt) "n_calls =", self%config%n_calls
    write (u, integer_fmt) "it_start =", self%result%it_start
    write (u, integer_fmt) "it_num =", self%result%it_num
    write (u, integer_fmt) "samples =", self%result%samples
    write (u, double_fmt) "sum_int_wgtd =", self%result%sum_int_wgtd
    write (u, double_fmt) "sum_wgts =", self%result%sum_wgts
    write (u, double_fmt) "sum_chi =", self%result%sum_chi
    write (u, double_fmt) "chi2 =", self%result%chi2
    write (u, double_fmt) "efficiency =", self%result%efficiency
    write (u, double_fmt) "efficiency_pos =", self%result%efficiency_pos
    write (u, double_fmt) "efficiency_neg =", self%result%efficiency_neg
    write (u, double_fmt) "max_abs_f =", self%result%max_abs_f
    write (u, double_fmt) "max_abs_f_pos =", self%result%max_abs_f_pos
    write (u, double_fmt) "max_abs_f_neg =", self%result%max_abs_f_neg
    write (u, double_fmt) "result =", self%result%result
    write (u, double_fmt) "std =", self%result%std

```

```

write (u, descr_fmt) "begin weight"
do ch = 1, self%config%n_channel
  write (u, double_array_fmt) ch, self%weight(ch)
end do
write (u, descr_fmt) "end weight"
if (self%config%n_chains > 0) then
  write (u, descr_fmt) "begin chain"
  do ch = 1, self%config%n_channel
    write (u, integer_array_fmt) ch, self%chain(ch)
  end do
  write (u, descr_fmt) "end chain"
end if
write (u, descr_fmt) "begin integrator"
do ch = 1, self%config%n_channel
  call self%integrator(ch)%write_grid (unit)
end do
write (u, descr_fmt) "end integrator"
write (u, descr_fmt) "end type(vamp2_t)"
end subroutine vamp2_write_grids

```

Read grids from unit.

```

(VAMP2: vamp2: TBP)+≡
  procedure, public :: read_grids => vamp2_read_grids
(VAMP2: sub interfaces)+≡
  module subroutine vamp2_read_grids (self, unit)
    class(vamp2_t), intent(out) :: self
    integer, intent(in), optional :: unit
  end subroutine vamp2_read_grids
(VAMP2: procedures)+≡
  module subroutine vamp2_read_grids (self, unit)
    class(vamp2_t), intent(out) :: self
    integer, intent(in), optional :: unit
    integer :: u
    integer :: ibuffer, jbuffer, ch
    character(len=80) :: buffer
    read (unit, descr_fmt) buffer
    read (unit, integer_fmt) buffer, ibuffer
    read (unit, integer_fmt) buffer, jbuffer
    select type (self)
    type is (vamp2_t)
      self = vamp2_t (n_channel = ibuffer, n_dim = jbuffer)
    end select
    read (unit, integer_fmt) buffer, self%config%n_calls_min_per_channel
    read (unit, integer_fmt) buffer, self%config%n_calls_threshold
    read (unit, integer_fmt) buffer, self%config%n_chains
    read (unit, logical_fmt) buffer, self%config%stratified
    read (unit, double_fmt) buffer, self%config%alpha
    read (unit, double_fmt) buffer, self%config%beta
    read (unit, integer_fmt) buffer, self%config%n_bins_max
    read (unit, integer_fmt) buffer, self%config%iterations
    read (unit, integer_fmt) buffer, self%config%n_calls
    read (unit, integer_fmt) buffer, self%result%it_start
    read (unit, integer_fmt) buffer, self%result%it_num

```

```

read (unit, integer_fmt) buffer, self%result%samples
read (unit, double_fmt) buffer, self%result%sum_int_wgtd
read (unit, double_fmt) buffer, self%result%sum_wgts
read (unit, double_fmt) buffer, self%result%sum_chi
read (unit, double_fmt) buffer, self%result%chi2
read (unit, double_fmt) buffer, self%result%efficiency
read (unit, double_fmt) buffer, self%result%efficiency_pos
read (unit, double_fmt) buffer, self%result%efficiency_neg
read (unit, double_fmt) buffer, self%result%max_abs_f
read (unit, double_fmt) buffer, self%result%max_abs_f_pos
read (unit, double_fmt) buffer, self%result%max_abs_f_neg
read (unit, double_fmt) buffer, self%result%result
read (unit, double_fmt) buffer, self%result%std
read (unit, descr_fmt) buffer
do ch = 1, self%config%n_channel
    read (unit, double_array_fmt) ibuffer, self%weight(ch)
end do
read (unit, descr_fmt) buffer
if (self%config%n_chains > 0) then
    read (unit, descr_fmt) buffer
    do ch = 1, self%config%n_channel
        read (unit, integer_array_fmt) ibuffer, self%chain(ch)
    end do
    read (unit, descr_fmt) buffer
end if
read (unit, descr_fmt) buffer
do ch = 1, self%config%n_channel
    call self%integrator(ch)%read_grid (unit)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
end subroutine vamp2_read_grids

```

Read and write grids from an unformatted file.

```

<VAMP2: vamp2: TBP>+≡
  procedure :: write_binary_grids => vamp2_write_binary_grids
  procedure :: read_binary_grids => vamp2_read_binary_grids

<VAMP2: sub interfaces>+≡
  module subroutine vamp2_write_binary_grids (self, unit)
    class(vamp2_t), intent(in) :: self
    integer, intent(in) :: unit
  end subroutine vamp2_write_binary_grids
  module subroutine vamp2_read_binary_grids (self, unit)
    class(vamp2_t), intent(out) :: self
    integer, intent(in) :: unit
  end subroutine vamp2_read_binary_grids

<VAMP2: procedures>+≡
  module subroutine vamp2_write_binary_grids (self, unit)
    class(vamp2_t), intent(in) :: self
    integer, intent(in) :: unit
    integer :: ch
    write (unit)
    write (unit) self%config%n_channel

```

```

write (unit) self%config%n_dim
write (unit) self%config%n_calls_min_per_channel
write (unit) self%config%n_calls_threshold
write (unit) self%config%n_chains
write (unit) self%config%stratified
write (unit) self%config%alpha
write (unit) self%config%beta
write (unit) self%config%n_bins_max
write (unit) self%config%iterations
write (unit) self%config%n_calls
write (unit) self%result%it_start
write (unit) self%result%it_num
write (unit) self%result%samples
write (unit) self%result%sum_int_wgtd
write (unit) self%result%sum_wgts
write (unit) self%result%sum_chi
write (unit) self%result%chi2
write (unit) self%result%efficiency
write (unit) self%result%efficiency_pos
write (unit) self%result%efficiency_neg
write (unit) self%result%max_abs_f
write (unit) self%result%max_abs_f_pos
write (unit) self%result%max_abs_f_neg
write (unit) self%result%result
write (unit) self%result%std
do ch = 1, self%config%n_channel
    write (unit) ch, self%weight(ch)
end do
if (self%config%n_chains > 0) then
    do ch = 1, self%config%n_channel
        write (unit) ch, self%chain(ch)
    end do
end if
do ch = 1, self%config%n_channel
    call self%integrator(ch)%write_binary_grid (unit)
end do
end subroutine vamp2_write_binary_grids

module subroutine vamp2_read_binary_grids (self, unit)
    class(vamp2_t), intent(out) :: self
    integer, intent(in) :: unit
    integer :: ch, ibuffer, jbuffer
    read (unit)
    read (unit) ibuffer
    read (unit) jbuffer
    select type (self)
    type is (vamp2_t)
        self = vamp2_t (n_channel = ibuffer, n_dim = jbuffer)
    end select
    read (unit) self%config%n_calls_min_per_channel
    read (unit) self%config%n_calls_threshold
    read (unit) self%config%n_chains
    read (unit) self%config%stratified
    read (unit) self%config%alpha

```



```

read (unit) self%config%beta
read (unit) self%config%n_bins_max
read (unit) self%config%iterations
read (unit) self%config%n_calls
read (unit) self%result%it_start
read (unit) self%result%it_num
read (unit) self%result%samples
read (unit) self%result%sum_int_wgtd
read (unit) self%result%sum_wgts
read (unit) self%result%sum_chi
read (unit) self%result%chi2
read (unit) self%result%efficiency
read (unit) self%result%efficiency_pos
read (unit) self%result%efficiency_neg
read (unit) self%result%max_abs_f
read (unit) self%result%max_abs_f_pos
read (unit) self%result%max_abs_f_neg
read (unit) self%result%result
read (unit) self%result%std
do ch = 1, self%config%n_channel
  read (unit) ibuffer, self%weight(ch)
end do
if (self%config%n_chains > 0) then
  do ch = 1, self%config%n_channel
    read (unit) ibuffer, self%chain(ch)
  end do
end if
do ch = 1, self%config%n_channel
  call self%integrator(ch)%read_binary_grid (unit)
end do
end subroutine vamp2_read_binary_grids

```

20.14 Unit tests

Test module, followed by the corresponding implementation module.

<vamp2_ut.f90>≡
<File header>

```

module vamp2_ut
  use unit_tests
  use vamp2_uti

```

<Standard module head>

<VAMP2: public test>

```

contains
<VAMP2: test driver>
end module vamp2_ut

```

<vamp2_uti.f90>≡
<File header>

```

module vamp2_util

  <Use kinds>
    use io_units
    use constants, only: pi
    use numeric_utils, only: nearly_equal
    use format_defs, only: FMT_12
    use rng_base
    use rng_stream
    use vegas, only: vegas_func_t, vegas_grid_t, operator(==)
    use vamp2

  <Standard module head>

  <VAMP2: test declaration>

  <VAMP2: test types>

  contains
  <VAMP2: tests>
end module vamp2_util

API: driver for the unit tests below.

<VAMP2: public test>≡
  public :: vamp2_test

<VAMP2: test driver>≡
  subroutine vamp2_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <VAMP2: execute tests>
  end subroutine vamp2_test

```

Test function

We use the example from the Monte Carlo Examples of the GSL library

$$I = \int_{-pi}^{+pi} dk_x / (2pi) \int_{-pi}^{+pi} dk_y / (2pi) \int_{-pi}^{+pi} dk_z / (2pi) 1 / (1 - \cos(k_x) \cos(k_y) \cos(k_z)). \quad (20.15)$$

The integral is reduced to region (0,0,0) → (π, π, π) and multiplied by 8.

```

<VAMP2: test types>≡
  type, extends (vamp2_func_t) :: vamp2_test_func_t
  !
  contains
  <VAMP2: vamp2 test func: TBP>
end type vamp2_test_func_t

<VAMP2: vamp2 test func: TBP>≡
  procedure, public :: evaluate_maps => vamp2_test_func_evaluate_maps

```

```

⟨VAMP2: tests⟩≡
  subroutine vamp2_test_func_evaluate_maps (self, x)
    class(vamp2_test_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    self%xi(:, 1) = x
    self%det(1) = 1
    self%valid_x = .true.
  end subroutine vamp2_test_func_evaluate_maps

```

Evaluate the integrand.

```

⟨VAMP2: vamp2 test func: TBP⟩+≡
  procedure, public :: evaluate_func => vamp2_test_func_evaluate

⟨VAMP2: tests⟩+≡
  real(default) function vamp2_test_func_evaluate (self, x) result (f)
    class(vamp2_test_func_t), intent(in) :: self
    real(default), dimension(:), intent(in) :: x
    f = 1.0 / (pi**3)
    f = f / ( 1.0 - cos (x(1)) * cos (x(2)) * cos (x(3)))
  end function vamp2_test_func_evaluate

```

The second test function implements

$$f(\vec{x}) = 4 \sin^2(\pi x_1) \sin^2(\pi x_2) + 2 \sin^2(\pi v), \quad (20.16)$$

where

$$x = u^v y = u^{1-v} \quad (20.17)$$

$$u = xyv = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log(xy)} \right). \quad (20.18)$$

The jacobian is $\frac{\partial(x,y)}{\partial(u,v)}$.

```

⟨VAMP2: test types⟩+≡
  type, extends(vamp2_func_t) :: vamp2_test_func_2_t
  !
  contains
    ⟨VAMP2: vamp2 test func 2: TBP⟩
  end type vamp2_test_func_2_t

```

Evaluate maps.

```

⟨VAMP2: vamp2 test func 2: TBP⟩≡
  procedure :: evaluate_maps => vamp2_test_func_2_evaluate_maps

⟨VAMP2: tests⟩+≡
  subroutine vamp2_test_func_2_evaluate_maps (self, x)
    class(vamp2_test_func_2_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    select case (self%current_channel)
    case (1)
      self%xi(:, 1) = x
      self%xi(1, 2) = x(1) * x(2)
      self%xi(2, 2) = 0.5 * ( 1. + log(x(1) / x(2)) / log(x(1) * x(2)))

```

```

case (2)
  self%xi(1, 1) = x(1)**x(2)
  self%xi(2, 1) = x(1)**(1. - x(2))
  self%xi(:, 2) = x
end select
self%det(1) = 1.
self%det(2) = abs (log(self%xi(1, 2)))
self%valid_x = .true.
end subroutine vamp2_test_func_2_evaluate_maps

```

Evaluate func.

```

⟨VAMP2: vamp2 test func 2: TBP⟩+≡
  procedure :: evaluate_func => vamp2_test_func_2_evaluate_func

⟨VAMP2: tests⟩+≡
  real(default) function vamp2_test_func_2_evaluate_func (self, x) result (f)
    class(vamp2_test_func_2_t), intent(in) :: self
    real(default), dimension(:), intent(in) :: x
    f = 4. * sin(pi * self%xi(1, 1))**2 * sin(pi * self%xi(2, 1))**2 &
      + 2. * sin(pi * self%xi(2, 2))**2
  end function vamp2_test_func_2_evaluate_func

```

The third test function implements

$$f(\vec{x}) = 5x_1^4 + 5(1 - x_1)^4, \quad (20.19)$$

where

$$x_1 = u^{1/5} \quad \vee \quad x_1 = 1 - v^{1/5} \quad (20.20)$$

The jacobians are $\frac{\partial x_1}{\partial u} = \frac{1}{5}u^{-\frac{4}{5}}$ and $\frac{\partial x_1}{\partial v} = \frac{1}{5}v^{-\frac{4}{5}}$.

```

⟨VAMP2: test types⟩+≡
  type, extends(vamp2_func_t) :: vamp2_test_func_3_t
  !
  contains
    ⟨VAMP2: vamp2 test func 3: TBP⟩
  end type vamp2_test_func_3_t

```

Evaluate maps.

```

⟨VAMP2: vamp2 test func 3: TBP⟩≡
  procedure :: evaluate_maps => vamp2_test_func_3_evaluate_maps

⟨VAMP2: tests⟩+≡
  subroutine vamp2_test_func_3_evaluate_maps (self, x)
    class(vamp2_test_func_3_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    real(default) :: u, v, xx
    select case (self%current_channel)
    case (1)
      u = x(1)
      xx = u**0.2_default
      v = (1 - xx)**5._default
    case (2)
      v = x(1)

```

```

        xx = 1 - v**0.2_default
        u = xx**5._default
    end select
    self%det(1) = 0.2_default * u**(-0.8_default)
    self%det(2) = 0.2_default * v**(-0.8_default)
    self%xi(:, 1) = [u]
    self%xi(:, 2) = [v]
    self%valid_x = .true.
end subroutine vamp2_test_func_3_evaluate_maps

```

Evaluate func.

```

<VAMP2: vamp2 test func 3: TBP>+≡
    procedure :: evaluate_func => vamp2_test_func_3_evaluate_func

<VAMP2: tests>+≡
    real(default) function vamp2_test_func_3_evaluate_func (self, x) result (f)
        class(vamp2_test_func_3_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: xx
        select case (self%current_channel)
        case (1)
            xx = x(1)**0.2_default
        case (2)
            xx = 1 - x(1)**0.2_default
        end select
        f = 5 * xx**4 + 5 * (1 - xx)**4
    end function vamp2_test_func_3_evaluate_func

```

MC Integrator check

We reproduce the first test case of VEGAS. Initialise the VAMP2 MC integrator and call to `vamp2_init_grid` for the initialisation of the grid.

```

<VAMP2: execute tests>≡
    call test (vamp2_1, "vamp2_1", "VAMP2 initialisation and&
        & grid preparation", u, results)

<VAMP2: test declaration>≡
    public :: vamp2_1

<VAMP2: tests>+≡
    subroutine vamp2_1 (u)
        integer, intent(in) :: u
        type(vamp2_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vamp2_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower = 0., &
            x_upper = pi
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vamp2_1"
        write (u, "(A)") "* Purpose: initialise the VAMP2 MC integrator and the grid"
        write (u, "(A)")
    end subroutine vamp2_1

```

```

write (u, "(A)") "* Initialise random number generator (default seed)"
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
write (u, "(A)")

allocate (vamp2_test_func_t :: func)
call func%init (n_dim = 3, n_channel = 1)
mc_integrator = vamp2_t (1, 3)
call mc_integrator%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 10000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower, x_upper)
call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_1

```

Integrate a function with two-dimensional argument and two channels.

```

<VAMP2: execute tests>+≡
  call test (vamp2_2, "vamp2_2", "VAMP2 intgeration of two-dimensional &
    & function with two channels", u, results)

<VAMP2: test declaration>+≡
  public :: vamp2_2

```

<VAMP2: tests>+≡

```

subroutine vamp2_2 (u)
  integer, intent(in) :: u
  type(vamp2_t) :: mc_integrator
  class(rng_t), allocatable :: rng
  class(vamp2_func_t), allocatable :: func
  real(default), dimension(2), parameter :: x_lower = 0., &
    x_upper = 1.
  real(default) :: result, abserr

  write (u, "(A)") "* Test output: vamp2_2"
  write (u, "(A)") "* Purpose: integration of two-dimensional &
    & function with two channels"
  write (u, "(A)")

  write (u, "(A)") "* Initialise random number generator (default seed)"
  write (u, "(A)")

  allocate (rng_stream_t :: rng)
  call rng%init ()

  call rng%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
  write (u, "(A)")

  allocate (vamp2_test_func_2_t :: func)
  call func%init (n_dim = 2, n_channel = 2)
  mc_integrator = vamp2_t (2, 2)
  call mc_integrator%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise grid with n_calls = 10000"
  write (u, "(A)")

  call mc_integrator%set_limits (x_lower, x_upper)
  call mc_integrator%set_calls (1000)

  write (u, "(A)")
  write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
  write (u, "(A)")

  call mc_integrator%integrate (func, rng, 3, verbose = .true., result=result, abserr=abserr)
  write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

  write (u, "(A)")
  write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
  write (u, "(A)")

  call mc_integrator%set_calls (200)
  call mc_integrator%integrate (func, rng, 3, verbose = .true., result=result, abserr=abserr)
  write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_2

```

Integrate a function with two-dimensional argument and two channels.

```

<VAMP2: execute tests>+≡
  call test (vamp2_3, "vamp2_3", "VAMP2 intgeration of two-dimensional &
    & function with two channels", u, results)

<VAMP2: test declaration>+≡
  public :: vamp2_3

<VAMP2: tests>+≡
  subroutine vamp2_3 (u)
    integer, intent(in) :: u
    type(vamp2_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vamp2_func_t), allocatable :: func
    real(default), dimension(2), parameter :: x_lower = 0., &
      x_upper = 1.
    real(default) :: result, abserr
    integer :: unit

    write (u, "(A)") "* Test output: vamp2_3"
    write (u, "(A)") "* Purpose: intgeration of two-dimensional &
      & function with two channels"
    write (u, "(A)")

    write (u, "(A)") "* Initialise random number generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
    write (u, "(A)")

    allocate (vamp2_test_func_2_t :: func)
    call func%init (n_dim = 2, n_channel = 2)
    mc_integrator = vamp2_t (2, 2)
    call mc_integrator%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise grid with n_calls = 20000"
    write (u, "(A)")

    call mc_integrator%set_limits (x_lower, x_upper)
    call mc_integrator%set_calls (20000)

```



```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Write grid to file vamp2_3.grids"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vamp2_3.grids", &
      action = "write", status = "replace")
call mc_integrator%write_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Read grid from file vamp2_3.grids"
write (u, "(A)")

call mc_integrator%final ()

unit = free_unit ()
open (unit, file = "vamp2_3.grids", &
      action = "read", status = "old")
call mc_integrator%read_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (5000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_3

```

Integrate a function with two-dimensional argument and two channels. Use chained weights, although we average over each weight itself.

```

<VAMP2: execute tests>+≡
  call test (vamp2_4, "vamp2_4", "VAMP2 intgeration of two-dimensional &
    & function with two channels with chains", u, results)

<VAMP2: test declaration>+≡
  public :: vamp2_4

```

<VAMP2: tests>+≡

```

subroutine vamp2_4 (u)
  integer, intent(in) :: u
  type(vamp2_t) :: mc_integrator
  class(rng_t), allocatable :: rng
  class(vamp2_func_t), allocatable :: func
  real(default), dimension(2), parameter :: x_lower = 0., &
    x_upper = 1.
  real(default) :: result, abserr
  integer :: unit

  write (u, "(A)") "* Test output: vamp2_4"
  write (u, "(A)") "* Purpose: integration of two-dimensional &
    & function with two channels with chains"
  write (u, "(A)")

  write (u, "(A)") "* Initialise random number generator (default seed)"
  write (u, "(A)")

  allocate (rng_stream_t :: rng)
  call rng%init ()

  call rng%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise MC integrator with n_channel = 2 and n_dim = 2"
  write (u, "(A)")

  allocate (vamp2_test_func_2_t :: func)
  call func%init (n_dim = 2, n_channel = 2)
  mc_integrator = vamp2_t (2, 2)
  call mc_integrator%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise grid with n_calls = 20000 and set chains"
  write (u, "(A)")

  call mc_integrator%set_limits (x_lower, x_upper)
  call mc_integrator%set_calls (20000)
  call mc_integrator%set_chain (2, [1, 2])

  write (u, "(A)")
  write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
  write (u, "(A)")

  call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
  write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

  write (u, "(A)")
  write (u, "(A)") "* Write grid to file vamp2_4.grids"
  write (u, "(A)")

  unit = free_unit ()
  open (unit, file = "vamp2_4.grids", &

```

```

        action = "write", status = "replace")
    call mc_integrator%write_grids (unit)
    close (unit)

    write (u, "(A)")
    write (u, "(A)") "* Read grid from file vamp2_4.grids"
    write (u, "(A)")

    call mc_integrator%final ()

    unit = free_unit ()
    open (unit, file = "vamp2_4.grids", &
        action = "read", status = "old")
    call mc_integrator%read_grids (unit)
    close (unit)

    write (u, "(A)")
    write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
    write (u, "(A)")

    call mc_integrator%set_calls (5000)
    call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
    write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

    write (u, "(A)")
    write (u, "(A)") "* Cleanup"

    call mc_integrator%final ()
    call rng%final ()
    deallocate (rng)
end subroutine vamp2_4

```

```

<VAMP2: execute tests>+≡
    call test (vamp2_5, "vamp2_5", "VAMP2 intgeration of two-dimensional &
        & function with two channels with equivalences", u, results)

```

```

<VAMP2: test declaration>+≡
    public :: vamp2_5

```

```

<VAMP2: tests>+≡
    subroutine vamp2_5 (u)
        integer, intent(in) :: u
        type(vamp2_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vamp2_func_t), allocatable :: func
        real(default), dimension(1), parameter :: x_lower = 0., &
            x_upper = 1.
        real(default) :: result, abserr
        integer :: unit
        type(vamp2_config_t) :: config
        type(vamp2_equivalences_t) :: eqv
        type(vegas_grid_t), dimension(2) :: grid

        write (u, "(A)") "* Test output: vamp2_5"
        write (u, "(A)") "* Purpose: intgeration of two-dimensional &

```

```

        & function with two channels with equivalences"
write (u, "(A)")

write (u, "(A)") "* Initialise random number generator (default seed)"
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_channel = 2 and n_dim = 1"
write (u, "(A)")

allocate (vamp2_test_func_3_t :: func)
call func%init (n_dim = 1, n_channel = 2)
config%equivalences = .true.
mc_integrator = vamp2_t (n_channel = 2, n_dim = 1)
call mc_integrator%set_config (config)
call mc_integrator%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 20000 and set chains"
write (u, "(A)")

call mc_integrator%set_limits (x_lower, x_upper)
call mc_integrator%set_calls (20000)

write (u, "(A)")
write (u, "(A)") "* Initialise equivalences"
write (u, "(A)")

eqv = vamp2_equivalences_t (n_eqv = 4, n_channel = 2, n_dim = 1)
call eqv%set_equivalence &
    (i_eqv = 1, dest = 2, src = 1, perm = [1], mode = [VEQ_IDENTITY])
call eqv%set_equivalence &
    (i_eqv = 2, dest = 1, src = 2, perm = [1], mode = [VEQ_IDENTITY])
call eqv%set_equivalence &
    (i_eqv = 3, dest = 1, src = 1, perm = [1], mode = [VEQ_IDENTITY])
call eqv%set_equivalence &
    (i_eqv = 4, dest = 2, src = 2, perm = [1], mode = [VEQ_IDENTITY])
call eqv%write (u)
call mc_integrator%set_equivalences (eqv)

write (u, "(A)")
write (u, "(A)") &
    "* Integrate with n_it = 3 and n_calls = 10000 (Grid-only Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, &
    adapt_weights = .false., result=result, abserr=abserr)
if (nearly_equal &
    (result, 2.000_default, rel_smallness = 0.003_default)) then

```

```

        write (u, "(2x,A)") "Result: 2.000 [ok]"
    else
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ",A)") &
            "Result: ", result, " +/- ", abserr, " [not ok]"
    end if

    write (u, "(A)")
    write (u, "(A)") "* Compare the grids of both channels"
    write (u, "(A)")

    grid(1) = mc_integrator%get_grid(channel = 1)
    grid(2) = mc_integrator%get_grid(channel = 2)

    write (u, "(2X,A,1X,L1)") "Equal grids =", (grid(1) == grid(2))

    write (u, "(A)")
    write (u, "(A)") "* Write grid to file vamp2_5.grids"
    write (u, "(A)")

    unit = free_unit ()
    open (unit, file = "vamp2_5.grids", &
        action = "write", status = "replace")
    call mc_integrator%write_grids (unit)
    close (unit)

    write (u, "(A)")
    write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
    write (u, "(A)")

    call mc_integrator%set_calls (5000)
    call mc_integrator%integrate (func, rng, 3, adapt_weights = .false., &
        refine_grids = .false., result=result, abserr=abserr)
    if (nearly_equal &
        (result, 2.000_default, rel_smallness = 0.003_default)) then
        write (u, "(2x,A)") "Result: 2.000 [ok]"
    else
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ",A)") &
            "Result: ", result, " +/- ", abserr, " [not ok]"
    end if

    write (u, "(A)")
    write (u, "(A)") "* Cleanup"

    call mc_integrator%final ()
    call rng%final ()
    deallocate (rng)
end subroutine vamp2_5

```

20.15 MPI Request

Request Direct interface for requests.

Balancer Subliary interfaces and types for implementation into **request**.

Callback Direct interface for non-blocking communication in callback fashion used in subsidiary in **request**.

20.15.1 Request Base

request Container type for current request, contains handler index and status of request.

request group cache Caching for communicator groups, tries to reduce the costly calls to `MPI_CREATE_COMM_GROUP`.

request base Base type for request handling, defines procedures and basic request scheme for direct implementation into **VAMP2**.

When a data type has an associated communicator field, it always must duplicate the communicator in order to ensure communication encapsulation. Only in special case (e.g. outside of object communication is required) the parent communicator should be directly used. For example, that is the case for the group cache, as it exports its newly created communicator to the outside of the request library.

```
<request_base.f90>≡  
  <File header>  
  module request_base  
  
    use balancer_base  
    use request_callback  
    use mpi_f08 !NODEP!  
  
    <Standard module head>  
  
    <Request base: public>  
  
    <Request base: types>  
  
    <Request base: interfaces>  
  
    interface  
    <Request base: sub interfaces>  
    end interface  
  
  end module request_base  
  
<request_base_sub.f90>≡  
  <File header>  
  
  submodule (request_base) request_base_s  
  
    use io_units  
    use diagnostics  
  
    implicit none
```

```

contains

<Request base: procedures>

end submodule request_base_s

<Request base: public>≡
    public :: request_t

<Request base: types>≡
    type :: request_t
        integer :: handler_id = 0
        logical :: terminate = .false.
        logical :: group = .false.
        logical :: group_master = .false.
        logical :: callback = .false.
        type(MPI_COMM) :: comm
    end type request_t

<Request base: types>+≡
    type :: request_group_cache_t
        private
        type(MPI_COMM) :: parent_comm
        type(MPI_GROUP) :: parent_group
        type(MPI_COMM) :: comm
        type(MPI_GROUP) :: group
        integer, dimension(:), allocatable :: rank
    contains
        <Request base: group cache: TBP>
    end type request_group_cache_t

```

Base type for requesting and back calling.

A short remark on the semantics of point-to-point communication (as its intended use in this implementation): MPI is strict regarding the order of the messages (for blocking communication), as those can not overtake each other, p. 41. For non-blocking communication, the standard extends it such that the order depends on "the execution order of the calls that initiate the communication". The non-overtaking requirement is then extended to this definition of order.

Color method for tracking communication? We restrict each slave to a single callback (at once), which can communicate during the next request computation. Before handling the next (current) callback, the former one has to finish (with a wait call on the client-side). On the server-side, we only test on the finishing, reporting a communication failure.

Furthermore, the implementation has to take care that the order of the communication calls on the master and slave code always matches!

Therefore, we need to secure the order of communication calls. First, we let the master initiate all callback communication **before** polling. This fixates the order. Second, we require that the implementation of the polling honors this order.

```

<Request base: public>+≡
    public :: request_base_t

```

```

<Request base: types>+≡
  type, abstract :: request_base_t
    type(MPI_COMM) :: comm
    type(MPI_COMM) :: external_comm !! communicator for use outside of request, however, just a d
    class(balancer_base_t), allocatable :: balancer
    type(request_group_cache_t) :: cache
    type(request_handler_manager_t) :: handler
  contains
    <Request base: base: TBP>
  end type request_base_t

```

```

<Request base: interfaces>≡
  !> The basic idea behind the request mechanism is that each associated worker can request a work
  !!
  !! We note that it is not necessary to differentiate between master and worker on this level of
  !! Hence, the request interface ignores any notion regarding a possible parallelization concept.
  abstract interface
    subroutine request_base_deferred_write (req, unit)
      import :: request_base_t
      class(request_base_t), intent(in) :: req
      integer, intent(in), optional :: unit
    end subroutine request_base_deferred_write

    !> Verify if request object has workers.
    !!
    !! An implementation shall return if there at least two workers, or otherwise stated,
    !! one master and one slave at least, when both are used as computing ranks.
    logical function request_base_has_workers (req) result (flag)
      import :: request_base_t
      class(request_base_t), intent(in) :: req
    end function request_base_has_workers
  end interface

```

```

<Request base: interfaces>+≡
  !> Request workload and returns an request_t object.
  !!
  !! The request_t object has an associated handler_id and provide several ways
  !! to indicate whether the execution is to be terminated, or the request has an associated co
  !! Finally, whether we expect that the handler id will be connected to an callback.
  !!
  !! \param[out] request Request container.
  abstract interface
    subroutine request_base_request_workload (req, request)
      import :: request_base_t, request_t
      class(request_base_t), intent(inout) :: req
      type(request_t), intent(out) :: request
    end subroutine request_base_request_workload
  end interface

```

```

<Request base: interfaces>+≡
  !> Release workload with the information from the request container.
  !!

```



```

!! The release procedure may notify the master about the finishing of the workload associated
!! Or, it may just bookkeep whether the workload has finished.
!! Additionally, if request%callback was true, it could handle the callback (from client side)
abstract interface
  subroutine request_base_release_workload (req, request)
    import :: request_base_t, request_t
    class(request_base_t), intent(inout) :: req
    type(request_t), intent(in) :: request
  end subroutine request_base_release_workload
end interface

<Request base: interfaces>+≡
  !> Handle associated callback and release workload with the information from the request cont
  !!
  !! The procedure must call the associated callback handler using the handler_id.
  !! Remark: The callback manager is quite squishy regarding a missing handler (silent failure)
  !! The procedure has to take care whether the callback was actually successful.
  !! The further release of the workload can then be deferred to the release_workload procedure
  !! \param[in] request.
abstract interface
  subroutine request_base_handle_and_release_workload (req, request)
    import :: request_base_t, request_t
    class(request_base_t), intent(inout) :: req
    type(request_t), intent(in) :: request
  end subroutine request_base_handle_and_release_workload
end interface

<Request base: group cache: TBP>≡
  procedure :: init => request_group_cache_init

<Request base: sub interfaces>≡
  module subroutine request_group_cache_init (cache, comm)
    class(request_group_cache_t), intent(inout) :: cache
    type(MPI_COMM), intent(in) :: comm
  end subroutine request_group_cache_init

<Request base: procedures>≡
  module subroutine request_group_cache_init (cache, comm)
    class(request_group_cache_t), intent(inout) :: cache
    type(MPI_COMM), intent(in) :: comm
    call MPI_COMM_DUP (comm, cache%parent_comm)
    !! Local operation.
    call MPI_COMM_GROUP (cache%parent_comm, cache%parent_group)
    cache%group = MPI_GROUP_EMPTY
    cache%comm = MPI_COMM_NULL
  end subroutine request_group_cache_init

<Request base: group cache: TBP>+≡
  procedure :: reset => request_group_cache_reset

<Request base: sub interfaces>+≡
  module subroutine request_group_cache_reset (cache)
    class(request_group_cache_t), intent(inout) :: cache
  end subroutine request_group_cache_reset

```

```

<Request base: procedures>+≡
  module subroutine request_group_cache_reset (cache)
    class(request_group_cache_t), intent(inout) :: cache
    cache%group = MPI_GROUP_EMPTY
    cache%comm = MPI_COMM_NULL
  end subroutine request_group_cache_reset

<Request base: group cache: TBP>+≡
  procedure :: update => request_group_cache_update

<Request base: sub interfaces>+≡
  module subroutine request_group_cache_update (cache, tag, rank)
    class(request_group_cache_t), intent(inout) :: cache
    integer, intent(in) :: tag
    integer, dimension(:), allocatable, intent(inout) :: rank
  end subroutine request_group_cache_update

<Request base: procedures>+≡
  module subroutine request_group_cache_update (cache, tag, rank)
    class(request_group_cache_t), intent(inout) :: cache
    integer, intent(in) :: tag
    integer, dimension(:), allocatable, intent(inout) :: rank
    type(MPI_GROUP) :: group
    integer :: result, error
    call move_alloc (rank, cache%rank)
    call MPI_GROUP_INCL (cache%parent_group, size (cache%rank), cache%rank, group)
    call MPI_GROUP_COMPARE (cache%group, group, result)
    if (result /= MPI_IDENT) then
      cache%group = group
      if (cache%comm /= MPI_COMM_NULL) call MPI_COMM_FREE (cache%comm)
      !! Group-local operation. However, time consuming.
      call MPI_COMM_CREATE_GROUP (cache%parent_comm, cache%group, tag, &
        cache%comm, error)
      if (error /= 0) then
        call msg_bug ("Error occurred during communicator creation...")
      end if
    ! else
      ! call msg_message ("CACHE UPDATE: GROUPS ARE (NEARLY) IDENTICAL")
    end if
  end subroutine request_group_cache_update

<Request base: group cache: TBP>+≡
  procedure :: get_comm => request_group_cache_get_comm

<Request base: sub interfaces>+≡
  module subroutine request_group_cache_get_comm (cache, comm)
    class(request_group_cache_t), intent(in) :: cache
    type(MPI_COMM), intent(out) :: comm
  end subroutine request_group_cache_get_comm

<Request base: procedures>+≡
  module subroutine request_group_cache_get_comm (cache, comm)
    class(request_group_cache_t), intent(in) :: cache
    type(MPI_COMM), intent(out) :: comm
    comm = cache%comm

```

```

end subroutine request_group_cache_get_comm

<Request base: group cache: TBP>+≡
  procedure :: is_master => request_group_cache_is_master
<Request base: sub interfaces>+≡
  module function request_group_cache_is_master (cache) result (flag)
    class(request_group_cache_t), intent(in) :: cache
    integer :: rank, error
    logical :: flag
  end function request_group_cache_is_master
<Request base: procedures>+≡
  module function request_group_cache_is_master (cache) result (flag)
    class(request_group_cache_t), intent(in) :: cache
    integer :: rank, error
    logical :: flag
    call MPI_COMM_RANK (cache%comm, rank, error)
    if (error /= 0) then
      call msg_bug ("Error: Could not retrieve group rank.")
    end if
    flag = (rank == 0)
  end function request_group_cache_is_master

<Request base: base: TBP>≡
  procedure :: base_init => request_base_init
<Request base: sub interfaces>+≡
  module subroutine request_base_init (req, comm)
    class(request_base_t), intent(out) :: req
    type(MPI_COMM), intent(in) :: comm
  end subroutine request_base_init
<Request base: procedures>+≡
  !! =====
  !! request_base_t
  !! =====

  !> Initialize request base with parent communicator.
  !!
  !! In order to separate the communication between different parts of the request library,
  !! duplicate the parent communicator using MPI_COMM_DUP, also done by cache and handler objects.
  !!
  !! \param[in] comm Parent MPI communicator for overall library.
  module subroutine request_base_init (req, comm)
    class(request_base_t), intent(out) :: req
    type(MPI_COMM), intent(in) :: comm
    call MPI_COMM_DUP (comm, req%comm)
    call MPI_COMM_DUP (comm, req%external_comm)
    call req%cache%init (comm)
    call req%handler%init (comm)
  end subroutine request_base_init

<Request base: base: TBP>+≡
  procedure :: base_write => request_base_write
  procedure(request_base_deferred_write), deferred :: write

```

```

<Request base: sub interfaces>+≡
    module subroutine request_base_write (req, unit)
        class(request_base_t), intent(in) :: req
        integer, intent(in), optional :: unit
    end subroutine request_base_write

<Request base: procedures>+≡
    module subroutine request_base_write (req, unit)
        class(request_base_t), intent(in) :: req
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (allocated (req%balancer)) then
            call req%balancer%write (u)
        else
            write (u, "(A)") "[BALANCER]"
            write (u, "(A)") "=> Not allocated"
        end if
        call req%handler%write (u)
    end subroutine request_base_write

<Request base: base: TBP>+≡
    procedure :: is_master => request_base_is_master
    procedure(request_base_has_workers), deferred :: has_workers

<Request base: sub interfaces>+≡
    module function request_base_is_master (req) result (flag)
        class(request_base_t), intent(in) :: req
        integer :: rank, ierr
        logical :: flag
    end function request_base_is_master

<Request base: procedures>+≡
    !> Check whether current worker is master rank in object communicator.
    !!
    !! Do not confuse with a group's master !!!
    !! Proof: rank == 0
    module function request_base_is_master (req) result (flag)
        class(request_base_t), intent(in) :: req
        integer :: rank, ierr
        logical :: flag
        call MPI_COMM_RANK(req%comm, rank, ierr)
        if (ierr /= 0) then
            write (*, "(A,1X,I0)") "MPI Error: request_base_is_master", ierr
            stop 1
        end if
        flag = (rank == 0)
    end function request_base_is_master

<Request base: base: TBP>+≡
    procedure :: get_external_comm => request_base_get_external_comm

<Request base: sub interfaces>+≡
    module subroutine request_base_get_external_comm (req, comm)
        class(request_base_t), intent(in) :: req

```

```

        type(MPI_COMM), intent(out) :: comm
    end subroutine request_base_get_external_comm

<Request base: procedures>+≡
    !> Provide external communicator.
    !!
    !! The external communicator is just a duplicate of request%comm,
    !! in order to provide the same group of workers to external communication,
    !! however, in a different context, such that communication from outside does not interfere with
    module subroutine request_base_get_external_comm (req, comm)
        class(request_base_t), intent(in) :: req
        type(MPI_COMM), intent(out) :: comm
        comm = req%external_comm
    end subroutine request_base_get_external_comm

<Request base: base: TBP>+≡
    procedure :: add_balancer => request_base_add_balancer

<Request base: sub interfaces>+≡
    module subroutine request_base_add_balancer (req, balancer)
        class(request_base_t), intent(inout) :: req
        class(balancer_base_t), allocatable, intent(inout) :: balancer
    end subroutine request_base_add_balancer

<Request base: procedures>+≡
    !> Add balancer to request.
    !!
    !! \param[inout] balancer
    module subroutine request_base_add_balancer (req, balancer)
        class(request_base_t), intent(inout) :: req
        class(balancer_base_t), allocatable, intent(inout) :: balancer
        if (allocated (req%balancer)) deallocate (req%balancer)
        call move_alloc (balancer, req%balancer)
    end subroutine request_base_add_balancer

<Request base: base: TBP>+≡
    procedure :: add_handler => request_base_add_handler

<Request base: sub interfaces>+≡
    module subroutine request_base_add_handler (req, handler_id, handler)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        class(request_handler_t), pointer, intent(in) :: handler
    end subroutine request_base_add_handler

<Request base: procedures>+≡
    !> Add request handler with handler_id.
    !!
    !! \param[in] handler_id
    !! \param[in] handler Pointer to handler object.
    module subroutine request_base_add_handler (req, handler_id, handler)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        class(request_handler_t), pointer, intent(in) :: handler
        call req%handler%add (handler_id, handler)
    end subroutine request_base_add_handler

```

```

<Request base: base: TBP>+≡
    procedure :: reset => request_base_reset

<Request base: sub interfaces>+≡
    module subroutine request_base_reset (req, deallocate_balancer)
        class(request_base_t), intent(inout) :: req
        logical, intent(in), optional :: deallocate_balancer
        logical :: flag
    end subroutine request_base_reset

<Request base: procedures>+≡
    !> Reset request.
    !! Clear handler manager from associated callbacks,
    !! deallocate balancer, iff allocated, and reset communicator cache.
    module subroutine request_base_reset (req, deallocate_balancer)
        class(request_base_t), intent(inout) :: req
        logical, intent(in), optional :: deallocate_balancer
        logical :: flag
        flag = .false.; if (present (deallocate_balancer)) &
            flag = deallocate_balancer
        if (flag .and. allocated (req%balancer)) then
            deallocate (req%balancer)
        end if
        call req%handler%clear ()
        call req%cache%reset ()
    end subroutine request_base_reset

<Request base: base: TBP>+≡
    procedure :: call_handler => request_base_call_handler

<Request base: sub interfaces>+≡
    module subroutine request_base_call_handler &
        (req, handler_id, source_rank)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        integer, intent(in) :: source_rank
    end subroutine request_base_call_handler

<Request base: procedures>+≡
    !> Call handler for master communication for handler_id.
    !!
    !! \param[in] handler_id The associated key of the callback object.
    !! \param[in] source_rank The rank of the result's source.
    module subroutine request_base_call_handler &
        (req, handler_id, source_rank)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        integer, intent(in) :: source_rank
        call req%handler%callback (handler_id, source_rank)
    end subroutine request_base_call_handler

<Request base: base: TBP>+≡
    procedure :: call_client_handler => request_base_call_client_handler

```

```

<Request base: sub interfaces>+≡
    module subroutine request_base_call_client_handler (req, handler_id)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
    end subroutine request_base_call_client_handler

<Request base: procedures>+≡
    !> Call handler for slave communication for handler_id.
    !!
    !! \param[in] handler_id The associated key of the callback object.
    module subroutine request_base_call_client_handler (req, handler_id)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        call req%handler%client_callback (handler_id, 0)
    end subroutine request_base_call_client_handler

<Request base: base: TBP>+≡
    procedure :: await_handler => request_base_await_handler

<Request base: sub interfaces>+≡
    module subroutine request_base_await_handler (req)
        class(request_base_t), intent(inout) :: req
    end subroutine request_base_await_handler

<Request base: procedures>+≡
    !> Wait on all handler in request handler manager to finish communication.
    module subroutine request_base_await_handler (req)
        class(request_base_t), intent(inout) :: req
        call req%handler%waitall ()
    end subroutine request_base_await_handler

<Request base: base: TBP>+≡
    procedure :: barrier => request_base_barrier
    procedure(request_base_request_workload), deferred :: request_workload
    procedure(request_base_release_workload), deferred :: release_workload
    procedure(request_base_handle_and_release_workload), deferred :: handle_and_release_workload

<Request base: sub interfaces>+≡
    module subroutine request_base_barrier (req)
        class(request_base_t), intent(in) :: req
        integer :: error
    end subroutine request_base_barrier

<Request base: procedures>+≡
    module subroutine request_base_barrier (req)
        class(request_base_t), intent(in) :: req
        integer :: error
        call MPI_BARRIER (req%comm, error)
        if (error /= MPI_SUCCESS) then
            call msg_fatal ("Request: Error occured during MPI_BARRIER synchronisation.")
        end if
    end subroutine request_base_barrier

```

20.15.2 Request Simple

We implement a local request scheme, without any additional communication, except the callback communication.

```
(request_simple.f90)≡
  <File header>
  module request_simple

    use array_list

    use balancer_base
    use balancer_simple
    use request_base

    use mpi_f08 !NODEP!

    <Standard module head>

    <Request simple: public>

    <Request simple: types>

    interface
    <Request simple: sub interfaces>
    end interface

    contains

    <Request simple: main procedures>

  end module request_simple
(request_simple_sub.f90)≡
  <File header>

  submodule (request_simple) request_simple_s

    use io_units
    use diagnostics

    implicit none

    contains

    <Request simple: procedures>

  end submodule request_simple_s

  <Request simple: public>≡
    public :: request_simple_t
  <Request simple: types>≡
    type, extends (request_base_t) :: request_simple_t
      integer :: n_workers = 0
      integer :: n_channels = 0
```



```

        logical, dimension(:), allocatable :: parallel_grid
contains
    <Request simple: simple: TBP>
end type request_simple_t

```

Gfortran 7/8/9 bug, has to remain in main module:

```

<Request simple: simple: TBP>≡
    procedure :: init => request_simple_init

<Request simple: main procedures>≡
    module subroutine request_simple_init (req, comm, n_channels)
        class(request_simple_t), intent(out) :: req
        type(MPI_COMM), intent(in) :: comm
        integer, intent(in) :: n_channels
        integer :: n_workers
        call req%base_init (comm)
        call MPI_COMM_SIZE (req%comm, req%n_workers)
        req%n_channels = n_channels
        allocate (req%parallel_grid (n_channels), source = .false.)
        call allocate_balancer ()
contains
        subroutine allocate_balancer ()
            class(balancer_base_t), allocatable :: balancer
            allocate (balancer_simple_t :: balancer)
            select type (balancer)
            type is (balancer_simple_t)
                call balancer%init (n_workers = req%n_workers, n_resources = req%n_channels)
            end select
            call req%add_balancer (balancer)
        end subroutine allocate_balancer
    end subroutine request_simple_init

```

Update number of channels and parallel grids. The simple request object does not utilize the request balancer, as the complexity of the request balancer is not required for the simple approach. The simple approach assigns each worker several channel by a modular mapping from the set of workers $\{0, \dots, N\}$ to the set of channels $\{1, \dots, N_c\}$. Vetoing on those channel which have a parallel grid (check the definition in `vegas.f90`), where all workers are assigned.

$$w = \phi(c) = (c - 1) \mod N, \text{ if not } P(c), \text{ else } \forall w \rightarrow c.$$

The information is stored in a dynamic-sized array list, which is filled, reversed and then used in a stack-like manner keeping track of the unassigned channels. Assigned and finished channels are then moved to the finished stack.

```

<Request simple: simple: TBP>+≡
    procedure :: update => request_simple_update

<Request simple: sub interfaces>≡
    module subroutine request_simple_update (req, parallel_grid)
        class(request_simple_t), intent(inout) :: req
        logical, dimension(:), intent(in) :: parallel_grid
    end subroutine request_simple_update

```

```

<Request simple: procedures>+=
  module subroutine request_simple_update (req, parallel_grid)
    class(request_simple_t), intent(inout) :: req
    logical, dimension(:), intent(in) :: parallel_grid
    integer :: me, worker
    call req%reset ()
    call MPI_COMM_RANK (req%comm, me)
    worker = SHIFT_RANK_TO_WORKER(me)
    select type (balancer => req%balancer)
    type is (balancer_simple_t)
      call balancer%update_state (worker, parallel_grid)
    end select
    req%parallel_grid = parallel_grid
  end subroutine request_simple_update

<Request simple: simple: TBP>+=
  procedure :: write => request_simple_write

<Request simple: sub interfaces>+=
  module subroutine request_simple_write (req, unit)
    class(request_simple_t), intent(in) :: req
    integer, intent(in), optional :: unit
  end subroutine request_simple_write

<Request simple: procedures>+=
  module subroutine request_simple_write (req, unit)
    class(request_simple_t), intent(in) :: req
    integer, intent(in), optional :: unit
    integer :: u, n_size
    u = given_output_unit (unit)
    write (u, "(A)") "[REQUEST_SIMPLE]"
    write (u, "(A,1X,I0)") "N_CHANNELS", req%n_channels
    write (u, "(A,1X,I0)") "N_WORKERS", req%n_workers
    n_size = min (25, req%n_channels)
    write (u, "(A,25(1X,L1))") "PARALLEL_GRID", req%parallel_grid(:n_size)
    call req%base_write (u)
  end subroutine request_simple_write

<Request simple: simple: TBP>+=
  procedure :: has_workers => request_simple_has_workers

<Request simple: sub interfaces>+=
  module function request_simple_has_workers (req) result (flag)
    class(request_simple_t), intent(in) :: req
    logical :: flag
  end function request_simple_has_workers

<Request simple: procedures>+=
  module function request_simple_has_workers (req) result (flag)
    class(request_simple_t), intent(in) :: req
    logical :: flag
    flag = (req%n_workers > 1)
  end function request_simple_has_workers

```

```

<Request simple: simple: TBP>+≡
    procedure :: get_request_master => request_simple_get_request_master

<Request simple: sub interfaces>+≡
    module function request_simple_get_request_master &
        (req, channel) result (rank)
        class(request_simple_t), intent(in) :: req
        integer, intent(in) :: channel
        integer :: rank
    end function request_simple_get_request_master

<Request simple: procedures>+≡
    module function request_simple_get_request_master &
        (req, channel) result (rank)
        class(request_simple_t), intent(in) :: req
        integer, intent(in) :: channel
        integer :: rank
        if (.not. allocated (req%balancer)) then
            call msg_bug ("Error: Balancer is not allocated.")
        end if
        rank = shift_worker_to_rank (req%balancer%get_resource_master (channel))
        !! "Caveat emptor" hits here:
        !! The balancer returns either a valid worker id or (-1) depending on the associated resource
        !! We have to check whether returned worker index is plausible.
    end function request_simple_get_request_master

<Request simple: simple: TBP>+≡
    !! deferred.
    procedure :: request_workload => request_simple_request_workload

<Request simple: sub interfaces>+≡
    module subroutine request_simple_request_workload (req, request)
        class(request_simple_t), intent(inout) :: req
        type(request_t), intent(out) :: request
    end subroutine request_simple_request_workload

<Request simple: procedures>+≡
    !> Request workload.
    !!
    !! Depending on parallel_grid, we fill the request object differently.
    !! First, we do not set communicator for .not. parallel_grid (group and group master are set to
    !! And the callback needs to be executed.
    !! Second, for parallel_grid, we set req%comm to the associated communicator and set group to .t
    !! However, the overall master has the grid's result, therefore, only the master needs to the ca
    !! Remark: We can actually intercept the callback for the master to himself; the results are alr
    module subroutine request_simple_request_workload (req, request)
        class(request_simple_t), intent(inout) :: req
        type(request_t), intent(out) :: request
        integer :: rank, worker_id
        call MPI_COMM_RANK (req%comm, rank)
        worker_id = shift_rank_to_worker (rank)
        if (.not. req%balancer%is_pending () &
            .or. .not. req%balancer%is_assignable (worker_id)) then
            request%terminate = .true.
            return
        end if

```

```

call req%balancer%assign_worker (worker_id, request%handler_id)
associate (channel => request%handler_id)
  if (req%parallel_grid (channel)) then
    request%comm = req%external_comm
    request%group = .true.
    !! The object communicator is master.
    request%group_master = &
      (req%get_request_master (channel) == rank)
    request%callback = req%is_master ()
  else
    request%comm = req%external_comm
    request%group = .false.
    request%group_master = .true.
    request%callback = .true.
  end if
end associate
end subroutine request_simple_request_workload

```

<Request simple: simple: TBP>+≡

```

procedure :: release_workload => request_simple_release_workload

```

<Request simple: sub interfaces>+≡

```

module subroutine request_simple_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
end subroutine request_simple_release_workload

```

<Request simple: procedures>+≡

```

module subroutine request_simple_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
  integer :: rank, worker_id
  call MPI_COMM_RANK (req%comm, rank)
  worker_id = shift_rank_to_worker (rank)
  call req%balancer%free_worker (worker_id, request%handler_id)
end subroutine request_simple_release_workload

```

<Request simple: simple: TBP>+≡

```

procedure :: handle_and_release_workload => &
  request_simple_handle_and_release_workload

```

<Request simple: sub interfaces>+≡

```

module subroutine request_simple_handle_and_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
end subroutine request_simple_handle_and_release_workload

```

<Request simple: procedures>+≡

```

module subroutine request_simple_handle_and_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
  call req%call_client_handler (request%handler_id)
  call req%release_workload (request)
end subroutine request_simple_handle_and_release_workload

```

20.15.3 Request Caller

We implement an global queue approach, requiring permanent communication between a governor and the worker.

```
<request_caller.f90>≡
  <File header>
  module request_caller

    <Use kinds>
    use diagnostics

    use request_base
    use balancer_base
    use balancer_channel
    use request_state
    use request_callback

    use mpi_f08 !NODEP!

    <Standard module head>

    <Request caller: public>

    <Request caller: types>

    interface
    <Request caller: sub interfaces>
    end interface

    contains

    <Request caller: main procedures>

  end module request_caller

<request_caller_sub.f90>≡
  <File header>

  submodule (request_caller) request_caller_s

    use io_units

    implicit none

    contains

    <Request caller: procedures>

  end submodule request_caller_s

  <Request caller: public>≡
    public :: request_caller_t

  <Request caller: types>≡
    type, extends (request_base_t):: request_caller_t
```

```

    private
    integer :: n_channels = 0
    integer :: n_workers = 0
    type(request_state_t) :: state
contains
    <Request caller: caller: TBP>
end type request_caller_t

```

Gfortran 7/8/9 bug, has to remain in the main module:

```

<Request caller: caller: TBP>≡
    procedure :: init => request_caller_init

<Request caller: main procedures>≡
    subroutine request_caller_init (req, comm, n_channels)
    class(request_caller_t), intent(out) :: req
    type(MPI_COMM), intent(in) :: comm
    integer, intent(in) :: n_channels
    call req%base_init (comm)
    call MPI_COMM_SIZE (req%comm, req%n_workers)
    !! Exclude master rank (0) from set of workers.
    req%n_workers = req%n_workers - 1
    if (.not. req%has_workers ()) then
        call msg_warning ("Must not handle less than 3 ranks in a master/slave global queue.")
        call MPI_ABORT (req%comm, 1)
    end if
    req%n_channels = n_channels
    call req%state%init (comm, req%n_workers)
    if (req%is_master ()) then
        call allocate_balancer ()
    end if
contains
    subroutine allocate_balancer ()
    class(balancer_base_t), allocatable :: balancer
    allocate (balancer_channel_t :: balancer)
    select type (balancer)
    type is (balancer_channel_t)
        call balancer%init (n_workers = req%n_workers, n_resources = req%n_channels)
    end select
    call req%add_balancer (balancer)
    end subroutine allocate_balancer
end subroutine request_caller_init

<Request caller: caller: TBP>+≡
    procedure :: write => request_caller_write

<Request caller: sub interfaces>≡
    module subroutine request_caller_write (req, unit)
    class(request_caller_t), intent(in) :: req
    integer, intent(in), optional :: unit
    end subroutine request_caller_write

<Request caller: procedures>≡
    module subroutine request_caller_write (req, unit)
    class(request_caller_t), intent(in) :: req

```

```

integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
write (u, "(A)") "[REQUEST_CALLER]"
call req%base_write (u)
if (req%is_master ()) &
    call req%state%write (u)
end subroutine request_caller_write

<Request caller: caller: TBP>+≡
    procedure :: has_workers => request_caller_has_workers

<Request caller: sub interfaces>+≡
    module function request_caller_has_workers (req) result (flag)
        class(request_caller_t), intent(in) :: req
        logical :: flag
    end function request_caller_has_workers

<Request caller: procedures>+≡
    module function request_caller_has_workers (req) result (flag)
        class(request_caller_t), intent(in) :: req
        logical :: flag
        !! n_workers excludes the master rank.
        flag = (req%n_workers > 1)
    end function request_caller_has_workers

<Request caller: caller: TBP>+≡
    procedure :: update_balancer => request_caller_update_balancer

<Request caller: sub interfaces>+≡
    module subroutine request_caller_update_balancer (req, weight, parallel_grid)
        class(request_caller_t), intent(inout) :: req
        real(default), dimension(:), intent(in) :: weight
        logical, dimension(:), intent(in) :: parallel_grid
    end subroutine request_caller_update_balancer

<Request caller: procedures>+≡
    module subroutine request_caller_update_balancer (req, weight, parallel_grid)
        class(request_caller_t), intent(inout) :: req
        real(default), dimension(:), intent(in) :: weight
        logical, dimension(:), intent(in) :: parallel_grid
        !! \note bug if not allocated?
        if (.not. allocated (req%balancer)) return
        call req%state%reset ()
        call req%reset ()
        select type (balancer => req%balancer)
        type is (balancer_channel_t)
            call balancer%update_state(weight, parallel_grid)
        end select
    end subroutine request_caller_update_balancer

<Request caller: caller: TBP>+≡
    procedure :: handle_workload => request_caller_handle_workload

```

```

<Request caller: sub interfaces>+≡
    module subroutine request_caller_handle_workload (req)
        class(request_caller_t), intent(inout) :: req
        end subroutine request_caller_handle_workload

<Request caller: procedures>+≡
    module subroutine request_caller_handle_workload (req)
        class(request_caller_t), intent(inout) :: req
        integer :: handler, tag, source, worker_id
        if (.not. allocated (req%balancer)) then
            call msg_warning ("Request: Error occured, load balancer not allocated.&
                & Terminate all workers.")
            !! We postpone to stop the program here so we can terminate all workers gracefully.
            !! First, we receive their requests, then we overwrite their "original" tag to MPI_TAG_TERM
            !! Second, we iterate this, until all workers are terminated and return without doing any b
        end if
        call req%state%init_request ()
        call req%state%receive_request ()
        do while (.not. req%state%is_terminated ())
            call req%state%await_request ()
            do while (req%state%has_request ())
                call req%state%get_request (source, tag, handler)
                !! Formally differentiate between worker_id and source.
                worker_id = source
                if (.not. allocated (req%balancer)) tag = MPI_TAG_TERMINATE
                select case (tag)
                    case (MPI_TAG_REQUEST)
                        if (req%balancer%is_assignable (worker_id)) then
                            call req%balancer%assign_worker (worker_id, handler)
                            if (.not. req%balancer%has_resource_group (handler)) then
                                call req%state%update_request (source, MPI_TAG_ASSIGN_SINGLE, handler)
                            else
                                call req%state%update_request (source, MPI_TAG_ASSIGN_GROUP, handler)
                                call provide_request_group (handler, source)
                            end if
                        else
                            call req%state%terminate (source)
                        end if
                    case (MPI_TAG_HANDLER_AND_RELEASE)
                        call req%call_handler (handler, source_rank = source)
                        call req%balancer%free_worker (worker_id, handler)
                    case (MPI_TAG_RELEASE)
                        call req%balancer%free_worker (worker_id, handler)
                    case (MPI_TAG_TERMINATE)
                        call req%state%terminate (source)
                    case (MPI_TAG_CLIENT_TERMINATE)
                        !! Allow workers to request their own termination.
                        call req%state%terminate (source)
                    case default
                        call msg_warning ()
                end select
            end do
            call req%state%receive_request ()
        end do
        !! If we are here, there should be no leftover communication.

```



```

    !! Hence, we must check whether there is no left-over communication call (from server-side).
    call req%state%free_request ()
contains
    subroutine provide_request_group (handler_id, dest_rank)
        integer, intent(in) :: handler_id
        integer, intent(in) :: dest_rank
        integer, dimension(:), allocatable :: rank
        !! Rank indices and worker indices are identical, as we skip the master worker deliberately,
        !! we can reuse the worker indices as rank indices.
        call req%balancer%get_resource_group (handler_id, rank)
        call req%state%provide_request_group (dest_rank, rank)
    end subroutine provide_request_group
end subroutine request_caller_handle_workload

<Request caller: caller: TBP>+≡
    procedure :: request_workload => request_caller_request_workload

<Request caller: sub interfaces>+≡
    module subroutine request_caller_request_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(out) :: request
    end subroutine request_caller_request_workload

<Request caller: procedures>+≡
    module subroutine request_caller_request_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(out) :: request
        type(MPI_STATUS) :: status
        call req%state%client_serve (request%handler_id, status)
        request%terminate = .false.
        request%group = .false.
        request%callback = .false.
        request%comm = MPI_COMM_NULL
        select case (status%MPI_TAG)
        case (MPI_TAG_ASSIGN_SINGLE)
            !! Default to req's communicator.
            request%comm = req%external_comm
            request%group_master = .true.
            request%callback = .true.
        case (MPI_TAG_ASSIGN_GROUP)
            request%group = .true.
            call retrieve_request_group (request%handler_id)
            call req%cache%get_comm (request%comm)
            request%group_master = req%cache%is_master ()
            request%callback = req%cache%is_master ()
        case (MPI_TAG_TERMINATE)
            request%terminate = status%MPI_TAG == MPI_TAG_TERMINATE
        end select
contains
    subroutine retrieve_request_group (handler_id)
        integer, intent(in) :: handler_id
        integer, dimension(:), allocatable :: rank
        !! Here, worker and rank indices are interchangeable.
        call req%state%retrieve_request_group (rank)
        call req%cache%update (handler_id, rank)

```

```

        end subroutine retrieve_request_group
    end subroutine request_caller_request_workload

<Request caller: caller: TBP>+≡
    procedure :: release_workload => request_caller_release_workload

<Request caller: sub interfaces>+≡
    module subroutine request_caller_release_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(in) :: request
    end subroutine request_caller_release_workload

<Request caller: procedures>+≡
    module subroutine request_caller_release_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(in) :: request
        call req%state%client_free (request%handler_id, &
            has_callback = request%group_master)
    end subroutine request_caller_release_workload

<Request caller: caller: TBP>+≡
    procedure :: handle_and_release_workload => &
        request_caller_handle_and_release_workload

<Request caller: sub interfaces>+≡
    module subroutine request_caller_handle_and_release_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(in) :: request
    end subroutine request_caller_handle_and_release_workload

<Request caller: procedures>+≡
    module subroutine request_caller_handle_and_release_workload (req, request)
        class(request_caller_t), intent(inout) :: req
        type(request_t), intent(in) :: request
        if (.not. req%handler%has_handler (request%handler_id)) then
            call msg_bug ("Request: Handler is not registered for this worker.")
        end if
        call req%release_workload (request)
        call req%call_client_handler (request%handler_id)
    end subroutine request_caller_handle_and_release_workload

<Request caller: caller: TBP>+≡
    procedure :: request_terminate => request_caller_request_terminate

<Request caller: sub interfaces>+≡
    module subroutine request_caller_request_terminate (req)
        class(request_caller_t), intent(inout) :: req
    end subroutine request_caller_request_terminate

<Request caller: procedures>+≡
    module subroutine request_caller_request_terminate (req)
        class(request_caller_t), intent(inout) :: req
        if (req%is_master ()) return
        call req%state%client_terminate ()
    end subroutine request_caller_request_terminate

```

Request Caller State

We implement the complete communication for `request_caller` into a state (or in WK's nomenclature, instance) object.

```
<request_state.f90>≡
  <File header>
  module request_state

    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT
    use iterator

    use mpi_f08 !NODEP!

    <Standard module head>

    <Request state: public>

    <Request state: parameters>

    <Request state: types>

    interface
    <Request state: sub interfaces>
    end interface

  end module request_state

<request_state_sub.f90>≡
  <File header>

  submodule (request_state) request_state_s

    use diagnostics

    implicit none

    contains

    <Request state: procedures>

  end submodule request_state_s

<Request state: parameters>≡
  integer, parameter, public :: MPI_EMPTY_HANDLER = 0

  integer, parameter, public :: MPI_TAG_NULL = 0, &
    MPI_TAG_REQUEST = 1, &
    MPI_TAG_RELEASE = 2, &
    MPI_TAG_HANDLER_AND_RELEASE = 4, &
    MPI_TAG_TERMINATE = 8, &
    MPI_TAG_CLIENT_TERMINATE = 16, &
    MPI_TAG_ASSIGN_SINGLE = 32, &
    MPI_TAG_ASSIGN_GROUP = 64, &
    MPI_TAG_COMMUNICATOR_GROUP = 128
```

```

integer, parameter :: MPI_STATE_ERR = 1

<Request state: public>≡
  public :: request_state_t

<Request state: types>≡
  type :: request_state_t
  private
  type(MPI_COMM) :: comm
  integer :: n_workers = 0
  integer :: n_workers_done = 0
  !! From MPI-3.1 book
  !! i \in {1, N_workes_done}, max size = N_workers
  type(MPI_Request), dimension(:), allocatable :: request
  type(MPI_Status), dimension(:), allocatable :: status
  integer, dimension(:), allocatable :: indices
  !! i \in {1, N_workers}
  integer, dimension(:), allocatable :: handler
  logical, dimension(:), allocatable :: terminated
  type(iterator_t) :: request_iterator
  contains
  <Request state: state: TBP>
end type request_state_t

<Request state: state: TBP>≡
  procedure :: init => request_state_init

<Request state: sub interfaces>≡
  module subroutine request_state_init (state, comm, n_workers)
    class(request_state_t), intent(out) :: state
    type(MPI_COMM), intent(in) :: comm
    integer, intent(in) :: n_workers
  end subroutine request_state_init

<Request state: procedures>≡
  module subroutine request_state_init (state, comm, n_workers)
    class(request_state_t), intent(out) :: state
    type(MPI_COMM), intent(in) :: comm
    integer, intent(in) :: n_workers
    integer :: rank
    call MPI_COMM_DUP (comm, state%comm)
    state%n_workers = n_workers
    state%n_workers_done = n_workers
    call state%request_iterator%init (1, n_workers)
    allocate (state%request(state%n_workers), source = MPI_REQUEST_NULL)
    allocate (state%status(state%n_workers), source = MPI_STATUS_IGNORE)
    allocate (state%handler(state%n_workers), source = MPI_EMPTY_HANDLER)
    allocate (state%indices(state%n_workers), source = 0)
    allocate (state%terminated(state%n_workers), source = .false.)
    state%indices = [(rank, rank = 1, n_workers)]
  end subroutine request_state_init

<Request state: state: TBP>+≡
  procedure :: write => request_state_write

```

```

<Request state: sub interfaces>+=
    module subroutine request_state_write (state, unit)
        class(request_state_t), intent(in) :: state
        integer, intent(in), optional :: unit
    end subroutine request_state_write

<Request state: procedures>+=
    module subroutine request_state_write (state, unit)
        class(request_state_t), intent(in) :: state
        integer, intent(in), optional :: unit
        integer :: u, i
        u = ERROR_UNIT; if (present (unit)) u = unit
        write (u, "(A)") "[REQUEST_STATE]"
        write (u, "(A,1X,I0)") "N_WORKERS", state%n_workers
        write (u, "(A,1X,I0)") "N_WORKERS_DONE", state%n_workers_done
        write (u, "(A)") "RANK | SOURCE | TAG | ERROR | REQUEST_NULL"
        do i = 1, state%n_workers_done
            write (u, "(A,4(1X,I0),1X,L1)") "REQUEST", state%indices(i), &
                state%status(i)%MPI_SOURCE, &
                state%status(i)%MPI_TAG, &
                state%status(i)%MPI_ERROR, &
                (state%request(i) == MPI_REQUEST_NULL)
        end do
        write (u, "(A,999(1X,I0))") "HANDLER", state%handler
        write (u, "(A,999(1X,L1))") "TERMINATED", state%terminated
    end subroutine request_state_write

<Request state: state: TBP>+=
    procedure :: reset => request_state_reset

<Request state: sub interfaces>+=
    module subroutine request_state_reset (state)
        class(request_state_t), intent(inout) :: state
    end subroutine request_state_reset

<Request state: procedures>+=
    module subroutine request_state_reset (state)
        class(request_state_t), intent(inout) :: state
        integer :: rank
        state%n_workers_done = state%n_workers
        call state%request_iterator%init (1, state%n_workers)
        state%handler = MPI_EMPTY_HANDLER
        state%indices = [(rank, rank = 1, state%n_workers)]
        state%terminated = .false.
    end subroutine request_state_reset

<Request state: state: TBP>+=
    procedure :: is_terminated => request_state_is_terminated

<Request state: sub interfaces>+=
    module function request_state_is_terminated (state) result (flag)
        class(request_state_t), intent(in) :: state
        logical :: flag
    end function request_state_is_terminated

```

```

<Request state: procedures>+≡
! pure module function request_state_is_terminated (state) result (flag)
module function request_state_is_terminated (state) result (flag)
  class(request_state_t), intent(in) :: state
  logical :: flag
  flag = all (state%terminated)
end function request_state_is_terminated

```

Set rank to be terminated (however, do not communicate it). This is an EVIL procedure, as it operates only locally on the master and does not communicate its purpose. However, in order to allow termination requests from client-side we need to manipulate the specific rank states.

```

<Request state: state: TBP>+≡
  procedure, private :: set_terminated => request_state_set_terminated

```

```

<Request state: sub interfaces>+≡
  module subroutine request_state_set_terminated (state, rank)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
  end subroutine request_state_set_terminated

```

```

<Request state: procedures>+≡
  module subroutine request_state_set_terminated (state, rank)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
    state%terminated(rank) = .true.
  end subroutine request_state_set_terminated

```

```

<Request state: state: TBP>+≡
  procedure :: terminate => request_state_terminate

```

```

<Request state: sub interfaces>+≡
  module subroutine request_state_terminate (state, rank)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
  end subroutine request_state_terminate

```

```

<Request state: procedures>+≡
  module subroutine request_state_terminate (state, rank)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
    integer :: error
    call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
      rank, MPI_TAG_TERMINATE, state%comm, error)
    if (error /= 0) then
      write (msg_buffer, "(A,1X,I3)") "Request: Error occurred " // &
        "during terminate, RANK", rank
      call msg_bug ()
    end if
    call state%set_terminated (rank)
  end subroutine request_state_terminate

```

```

<Request state: state: TBP>+≡
  procedure :: client_terminate => request_state_client_terminate

```

<Request state: sub interfaces>+≡

```
module subroutine request_state_client_terminate (state)
  class(request_state_t), intent(in) :: state
end subroutine request_state_client_terminate
```

<Request state: procedures>+≡

```
module subroutine request_state_client_terminate (state)
  class(request_state_t), intent(in) :: state
  integer :: error
  call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
    0, MPI_TAG_CLIENT_TERMINATE, state%comm, error)
  if (error /= 0) then
    write (msg_buffer, "(A,1X,I3)") "Request: Error occurred " // &
      "during client-sided terminate"
    call msg_bug ()
  end if
end subroutine request_state_client_terminate
```

Init persistent requests. Must be called before first `receive_request`. `Free_request` must be called after `is_terminated` returns true.

<Request state: state: TBP>+≡

```
procedure :: init_request => request_state_init_request
```

<Request state: sub interfaces>+≡

```
module subroutine request_state_init_request (state)
  class(request_state_t), intent(inout) :: state
end subroutine request_state_init_request
```

<Request state: procedures>+≡

```
module subroutine request_state_init_request (state)
  class(request_state_t), intent(inout) :: state
  integer :: i, rank, error
  do i = 1, state%n_workers_done
    rank = state%indices(i)
    call MPI_RECV_INIT (state%handler(rank), 1, MPI_INTEGER, &
      rank, MPI_ANY_TAG, state%comm, state%request(rank), error)
    if (error /= 0) then
      write (msg_buffer, "(A,2(A,1X,I0))") "Request: Error occurred during receive init, &
        & RANK", rank, "HANDLER", state%handler(rank)
      call msg_message ()
      call MPI_ABORT (state%comm, MPI_STATE_ERR)
    end if
  end do
end subroutine request_state_init_request
```

Receive requests from non-terminated workers. Before receiving new requests, sanitize arrays of received ranks from terminated ones.

<Request state: state: TBP>+≡

```
procedure :: receive_request => request_state_receive_request
```

<Request state: sub interfaces>+≡

```
module subroutine request_state_receive_request (state)
  class(request_state_t), intent(inout) :: state
end subroutine request_state_receive_request
```

<Request state: procedures>+≡

```

module subroutine request_state_receive_request (state)
  class(request_state_t), intent(inout) :: state
  integer :: i, rank
  integer :: error
  if (state%is_terminated ()) return
  call sanitize_from_terminated_ranks ()
  !! Receive new requests from (still active) workers.
  do i = 1, state%n_workers_done
    rank = state%indices(i)
    call MPI_START (state%request(rank), error)
    if (error /= 0) then
      write (msg_buffer, "(A,2(A,1X,I6))") "Request: Error occured during receive request, &
        & RANK", rank, "HANDLER", state%handler(rank)
      call msg_message ()
      call MPI_ABORT (state%comm, MPI_STATE_ERR)
    end if
  end do
contains
  subroutine sanitize_from_terminated_ranks ()
    integer :: n_workers_done
    integer, dimension(:), allocatable :: indices
    !! Remove terminated ranks from done workers.
    indices = pack(state%indices(:state%n_workers_done), &
      .not. state%terminated(state%indices(:state%n_workers_done)))
    state%n_workers_done = size (indices)
    state%indices(:state%n_workers_done) = indices
  end subroutine sanitize_from_terminated_ranks
end subroutine request_state_receive_request

```

<Request state: state: TBP>+≡

```

procedure :: await_request => request_state_await_request

```

<Request state: sub interfaces>+≡

```

module subroutine request_state_await_request (state)
  class(request_state_t), intent(inout) :: state
  end subroutine request_state_await_request

```

<Request state: procedures>+≡

```

module subroutine request_state_await_request (state)
  class(request_state_t), intent(inout) :: state
  integer :: error
  if (state%is_terminated ()) return
  !! We verify that we have active handles associated with request state.
  call MPI_TESTSOME (state%n_workers, state%request, state%n_workers_done, &
    state%indices, state%status, error)
  if (error /= 0) then
    write (ERROR_UNIT, "(A)") "Error occured during await (testing) request..."
    call state%write (ERROR_UNIT)
    call MPI_ABORT (state%comm, MPI_STATE_ERR)
  else if (state%n_workers_done == MPI_UNDEFINED) then
    write (ERROR_UNIT, "(A)") "TEST_WAITSOME returned with MPI_UNDEFINED."
    call state%write (ERROR_UNIT)
    call MPI_ABORT (state%comm, MPI_STATE_ERR)
  end if

```



```

!! Wait a little bit...
if (state%n_workers_done == 0) then
  !! Proof: REQUEST(i), i \in {1, N_workers}, i is equivalent to rank.
  !! Proof: INDICES(j), STATUS(j), j \in {1, N_workers_done}
  !! Proof: INDICES(j) -> i, injectiv.
  call MPI_WAIT_SOME (state%n_workers, state%request, state%n_workers_done, &
    state%indices, state%status, error)
  if (error /= 0) then
    write (ERROR_UNIT, "(A)") "Error occurred during await request..."
    call state%write (ERROR_UNIT)
    call MPI_ABORT (state%comm, MPI_STATE_ERR)
  end if
endif
call state%request_iterator%init (1, state%n_workers_done)
end subroutine request_state_await_request

```

```

<Request state: state: TBP>+≡
  procedure :: has_request => request_state_has_request

```

```

<Request state: sub interfaces>+≡
  pure module function request_state_has_request (state) result (flag)
    class(request_state_t), intent(in) :: state
    logical :: flag
  end function request_state_has_request

```

```

<Request state: procedures>+≡
  pure module function request_state_has_request (state) result (flag)
    class(request_state_t), intent(in) :: state
    logical :: flag
    flag = state%request_iterator%is_iterable ()
  end function request_state_has_request

```

```

<Request state: state: TBP>+≡
  procedure :: get_request => request_state_get_request

```

```

<Request state: sub interfaces>+≡
  module subroutine request_state_get_request (state, rank, tag, handler)
    class(request_state_t), intent(inout) :: state
    integer, intent(out) :: rank
    integer, intent(out) :: tag
    integer, intent(out) :: handler
  end subroutine request_state_get_request

```

```

<Request state: procedures>+≡
  module subroutine request_state_get_request (state, rank, tag, handler)
    class(request_state_t), intent(inout) :: state
    integer, intent(out) :: rank
    integer, intent(out) :: tag
    integer, intent(out) :: handler
    integer :: ndx
    if (.not. state%has_request ()) then
      call msg_bug ("Request: Cannot access missing request.")
    end if
    ndx = state%request_iterator%next ()
    rank = state%indices(ndx)

```

```

if (rank /= state%status(ndx)%MPI_SOURCE) then
  write (msg_buffer, "(A,2(1X,I3))") &
    "Request: RANK and SOURCE mismatch", rank, &
    state%status(ndx)%MPI_SOURCE
  call msg_bug ()
end if
tag = state%status(ndx)%MPI_TAG
handler = state%handler(rank)
end subroutine request_state_get_request

```

<Request state: state: TBP>+≡

```

  procedure :: update_request => request_state_update_request

```

<Request state: sub interfaces>+≡

```

  module subroutine request_state_update_request (state, rank, tag, handler)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
    integer, intent(in) :: tag
    integer, intent(in) :: handler
  end subroutine request_state_update_request

```

<Request state: procedures>+≡

```

  module subroutine request_state_update_request (state, rank, tag, handler)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
    integer, intent(in) :: tag
    integer, intent(in) :: handler
    integer :: error
    state%handler(rank) = handler
    call MPI_SEND (handler, 1, MPI_INTEGER, &
      rank, tag, state%comm, error)
    if (error /= 0) then
      write (msg_buffer, "(A,3(A,1X,I3))") "Request: Error occurred during update, &
        &RANK", rank, "TAG", tag, "HANDLER", handler
      call msg_bug ()
    end if
  end subroutine request_state_update_request

```

<Request state: state: TBP>+≡

```

  procedure :: free_request => request_state_free_request

```

<Request state: sub interfaces>+≡

```

  module subroutine request_state_free_request (state)
    class(request_state_t), intent(inout) :: state
  end subroutine request_state_free_request

```

<Request state: procedures>+≡

```

  module subroutine request_state_free_request (state)
    class(request_state_t), intent(inout) :: state
    integer :: rank
    do rank = 1, state%n_workers
      if (state%request(rank) == MPI_REQUEST_NULL) cycle
      call MPI_REQUEST_FREE (state%request(rank))
    end do
  end subroutine request_state_free_request

```

```

<Request state: state: TBP>+≡
    procedure :: provide_request_group => &
        request_state_provide_request_group

<Request state: sub interfaces>+≡
    module subroutine request_state_provide_request_group &
        (state, dest_rank, worker)
        class(request_state_t), intent(in) :: state
        integer, intent(in) :: dest_rank
        integer, dimension(:), intent(in) :: worker
    end subroutine request_state_provide_request_group

<Request state: procedures>+≡
    module subroutine request_state_provide_request_group &
        (state, dest_rank, worker)
        class(request_state_t), intent(in) :: state
        integer, intent(in) :: dest_rank
        integer, dimension(:), intent(in) :: worker
        call MPI_SEND (worker, size (worker), MPI_INTEGER, &
            dest_rank, MPI_TAG_COMMUNICATOR_GROUP, state%comm)
    end subroutine request_state_provide_request_group

<Request state: state: TBP>+≡
    procedure :: retrieve_request_group => &
        request_state_retrieve_request_group

<Request state: sub interfaces>+≡
    module subroutine request_state_retrieve_request_group (state, worker)
        class(request_state_t), intent(inout) :: state
        integer, dimension(:), allocatable, intent(out) :: worker
    end subroutine request_state_retrieve_request_group

<Request state: procedures>+≡
    module subroutine request_state_retrieve_request_group (state, worker)
        class(request_state_t), intent(inout) :: state
        integer, dimension(:), allocatable, intent(out) :: worker
        type(MPI_STATUS) :: status
        integer :: n_workers
        call MPI_PROBE (0, MPI_TAG_COMMUNICATOR_GROUP, state%comm, status)
        call MPI_GET_COUNT(status, MPI_INTEGER, n_workers)
        allocate (worker (n_workers), source = 0)
        call MPI_RECV (worker, n_workers, MPI_INTEGER, &
            0, MPI_TAG_COMMUNICATOR_GROUP, state%comm, status)
    end subroutine request_state_retrieve_request_group

```

Query for a request (send an request tag, then receive a handler).

```

<Request state: state: TBP>+≡
    procedure :: client_serve => request_state_client_serve

<Request state: sub interfaces>+≡
    module subroutine request_state_client_serve (state, handler_id, status)
        class(request_state_t), intent(in) :: state
        integer, intent(out) :: handler_id
        type(MPI_STATUS), intent(out) :: status
    end subroutine request_state_client_serve

```

```

<Request state: procedures>+≡
  module subroutine request_state_client_serve (state, handler_id, status)
    class(request_state_t), intent(in) :: state
    integer, intent(out) :: handler_id
    type(MPI_STATUS), intent(out) :: status
    call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
      0, MPI_TAG_REQUEST, state%comm)
    call MPI_RECV (handler_id, 1, MPI_INTEGER, &
      0, MPI_ANY_TAG, state%comm, status)
  end subroutine request_state_client_serve

```

Free handler from worker.

```

<Request state: state: TBP>+≡
  procedure :: client_free => request_state_client_free

```

```

<Request state: sub interfaces>+≡
  module subroutine request_state_client_free (state, handler_id, has_callback)
    class(request_state_t), intent(in) :: state
    integer, intent(in) :: handler_id
    logical, intent(in) :: has_callback
  end subroutine request_state_client_free

```

```

<Request state: procedures>+≡
  module subroutine request_state_client_free (state, handler_id, has_callback)
    class(request_state_t), intent(in) :: state
    integer, intent(in) :: handler_id
    logical, intent(in) :: has_callback
    integer :: tag
    tag = merge (MPI_TAG_HANDLER_AND_RELEASE, MPI_TAG_RELEASE, has_callback)
    call MPI_SEND (handler_id, 1, MPI_INTEGER, &
      0, tag, state%comm)
  end subroutine request_state_client_free

```

20.15.4 Balancer Base

Balancer Base Base type for usage for extensions of request_base.

```

<balancer_base.f90>≡
  module balancer_base

    use array_list

    <Standard module head>

    <Balancer base: public>

    <Balancer base: parameters>

    <Balancer base: types>

    <Balancer base: interfaces>

    interface

```

```

    <Balancer base: sub interfaces>
    end interface

end module balancer_base

<balancer_base_sub.f90>≡
<File header>

submodule (balancer_base) balancer_base_s

    use io_units
    use diagnostics

    implicit none

contains

    <Balancer base: procedures>

end submodule balancer_base_s

<Balancer base: parameters>≡
    integer, parameter, public :: STATE_SINGLE = 1, &
        STATE_ALL = 2

<Balancer base: types>≡
    type :: worker_t
    private
    integer :: resource = 0
    integer :: state = 0
    integer :: n_resources = 0
    logical :: assigned = .false.
    contains
    <Balancer base: worker: TBP>
end type worker_t

<Balancer base: types>+≡
    type :: resource_t
    private
    integer :: resource_id = 0
    logical :: active = .false.
    integer :: n_assigned_workers = 0
    contains
    <Balancer base: resource: TBP>
end type resource_t

<Balancer base: public>≡
    public :: resource_state_t

<Balancer base: types>+≡
    type :: resource_state_t
    integer :: n_workers = 0
    integer :: mode = 0

```

```

        type(array_list_t) :: resource_stack
        type(array_list_t) :: finished_stack
    contains
        <Balancer base: resource state: TBP>
    end type resource_state_t

```

Dynamic load balancer. We organize resources and workers in a transparent way using indices. These indices replace pointer magic. The balancer aggregates a dynamic state, however, we allow the state by the use of a pointer, to access the static fields of the balancer.

```

<Balancer base: public>+≡
    public :: balancer_base_t

```

```

<Balancer base: types>+≡
    type, abstract :: balancer_base_t
        integer :: n_workers = 0
        integer :: n_resources = 0
        integer :: n_states = 0
        type(worker_t), dimension(:), allocatable :: worker
        type(resource_t), dimension(:), allocatable :: resource
        type(resource_state_t), dimension(:), allocatable :: state
    contains
        <Balancer base: base: TBP>
    end type balancer_base_t

```

```

<Balancer base: interfaces>≡
    abstract interface
        subroutine balancer_base_deferred_write (balancer, unit)
            import :: balancer_base_t
            class(balancer_base_t), intent(in) :: balancer
            integer, intent(in), optional :: unit
        end subroutine balancer_base_deferred_write
    end interface

```

```

<Balancer base: interfaces>+≡
    !> Has resource an associated resource group.
    !!
    !! \note .true. only on an active resource, else .false.
    abstract interface
        pure logical function balancer_base_has_resource_group (balancer, resource_id) &
            result (flag)
            import :: balancer_base_t
            class(balancer_base_t), intent(in) :: balancer
            integer, intent(in) :: resource_id
        end function balancer_base_has_resource_group
    end interface

```

```

<Balancer base: interfaces>+≡
    !> Get resource group.
    !!
    !! \note Implementation must check against group existence.
    !! \return group (allocated|NOT allocated for (inactive|non-group) resource)

```

```

abstract interface
  pure subroutine balancer_base_get_resource_group (balancer, resource_id, group)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
  end subroutine balancer_base_get_resource_group
end interface

```

(Balancer base: interfaces)+≡

```

!> Get resource master (worker).
!!
!! Return worker as given, however, if extended type is used in a non-local
!! or in combination with a communicative request type, then check on activation status of as
!!
!! \return worker Valid worker index (\in {1, ..., N}) only on active resource*, else -1.
abstract interface
  pure integer function balancer_base_get_resource_master (balancer, resource_id) &
    result (worker)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
  end function balancer_base_get_resource_master
end interface

```

(Balancer base: interfaces)+≡

```

!> Assign resource to a given worker or retrieve current assigned resource.
!!
!! If worker has already a resource assigned, return resource.
!! If worker has not been assigned a resource, retrieve new resource from state.
!!
!! \note Each call must check if a worker is assignable, if not, the procedure must return re
abstract interface
  subroutine balancer_base_assign_worker (balancer, worker_id, resource_id)
    import :: balancer_base_t
    class(balancer_base_t), intent(inout) :: balancer
    integer, intent(in) :: worker_id
    integer, intent(out) :: resource_id
  end subroutine balancer_base_assign_worker
end interface

```

Free assignment of worker. If the worker is not assigned, this procedure is idempotent. If the worker is assigned, alter state correspondingly. In order to correctly free a worker from a resource, we have to explicitly keep track of the association status of a worker and a resource. This feature is mostly relevant for resources with a worker group. The resource may be disassociated from their worker by earlier calls or the former worker may be already assigned to a new resource. In the latter case, we are not allowed to free them (as the new resource is still active). Therefore, each call must check if a worker and resource are still associated and the resource is still active. Only, in this case, disassociating workers and resource is allowed.

(Balancer base: interfaces)+≡

```

abstract interface
  subroutine balancer_base_free_worker (balancer, worker_id, resource_id)
    import :: balancer_base_t
    class(balancer_base_t), intent(inout) :: balancer
    integer, intent(in) :: worker_id
    integer, intent(in) :: resource_id
  end subroutine balancer_base_free_worker
end interface

<Balancer base: public>+≡
  public :: shift_rank_to_worker

<Balancer base: sub interfaces>≡
  elemental module function shift_rank_to_worker (rank) result (worker)
    integer, intent(in) :: rank
    integer :: worker
  end function shift_rank_to_worker

<Balancer base: procedures>≡
  !> Shift rank index to worker index.
  !! Proof: rank \in {0, ..., N - 1}, worker \in {1, ..., N}
  elemental module function shift_rank_to_worker (rank) result (worker)
    integer, intent(in) :: rank
    integer :: worker
    worker = rank + 1
  end function shift_rank_to_worker

<Balancer base: public>+≡
  public :: shift_worker_to_rank

<Balancer base: sub interfaces>+≡
  elemental module function shift_worker_to_rank (worker) result (rank)
    integer, intent(in) :: worker
    integer :: rank
  end function shift_worker_to_rank

<Balancer base: procedures>+≡
  !> Shift worker index to rank index.
  !! Proof: rank \in {0, ..., N - 1}, worker \in {1, ..., N}
  elemental module function shift_worker_to_rank (worker) result (rank)
    integer, intent(in) :: worker
    integer :: rank
    rank = worker - 1
  end function shift_worker_to_rank

<Balancer base: worker: TBP>≡
  procedure :: write => worker_write

<Balancer base: sub interfaces>+≡
  module subroutine worker_write (worker, unit)
    class(worker_t), intent(in) :: worker
    integer, intent(in), optional :: unit
  end subroutine worker_write

```



```

<Balancer base: procedures>+≡
module subroutine worker_write (worker, unit)
  class(worker_t), intent(in) :: worker
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(3(A,1X,I3,1X),A,1X,L1)") "RESOURCE", worker%resource, &
    "STATE", worker%state, &
    "N_RESOURCES", worker%n_resources, &
    "ASSIGNED", worker%assigned
end subroutine worker_write

<Balancer base: worker: TBP>+≡
procedure :: is_assigned => worker_is_assigned

<Balancer base: sub interfaces>+≡
  elemental module function worker_is_assigned (worker) result (flag)
    class(worker_t), intent(in) :: worker
    logical :: flag
  end function worker_is_assigned

<Balancer base: procedures>+≡
  elemental module function worker_is_assigned (worker) result (flag)
    class(worker_t), intent(in) :: worker
    logical :: flag
    flag = worker%assigned
  end function worker_is_assigned

<Balancer base: worker: TBP>+≡
procedure :: get_resource => worker_get_resource

<Balancer base: sub interfaces>+≡
  elemental module function worker_get_resource (worker) result (resource_id)
    class(worker_t), intent(in) :: worker
    integer :: resource_id
  end function worker_get_resource

<Balancer base: procedures>+≡
  elemental module function worker_get_resource (worker) result (resource_id)
    class(worker_t), intent(in) :: worker
    integer :: resource_id
    resource_id = worker%resource
  end function worker_get_resource

<Balancer base: worker: TBP>+≡
procedure :: get_state => worker_get_state

<Balancer base: sub interfaces>+≡
  elemental module function worker_get_state (worker) result (i_state)
    class(worker_t), intent(in) :: worker
    integer :: i_state
  end function worker_get_state

```

```

<Balancer base: procedures>+≡
    elemental module function worker_get_state (worker) result (i_state)
        class(worker_t), intent(in) :: worker
        integer :: i_state
        i_state = worker%state
    end function worker_get_state

<Balancer base: worker: TBP>+≡
    procedure :: add_resource => worker_add_resource

<Balancer base: sub interfaces>+≡
    elemental module subroutine worker_add_resource (worker, resource_id)
        class(worker_t), intent(inout) :: worker
        integer, intent(in) :: resource_id
    end subroutine worker_add_resource

<Balancer base: procedures>+≡
    elemental module subroutine worker_add_resource (worker, resource_id)
        class(worker_t), intent(inout) :: worker
        integer, intent(in) :: resource_id
        worker%n_resources = worker%n_resources + 1
        worker%assigned = .true.
        worker%resource = resource_id
    end subroutine worker_add_resource

<Balancer base: worker: TBP>+≡
    procedure :: free => worker_free

<Balancer base: sub interfaces>+≡
    elemental module subroutine worker_free (worker)
        class(worker_t), intent(inout) :: worker
    end subroutine worker_free

<Balancer base: procedures>+≡
    elemental module subroutine worker_free (worker)
        class(worker_t), intent(inout) :: worker
        worker%assigned = .false.
        worker%resource = 0
    end subroutine worker_free

<Balancer base: resource: TBP>≡
    procedure :: write => resource_write

<Balancer base: sub interfaces>+≡
    module subroutine resource_write (resource, unit)
        class(resource_t), intent(in) :: resource
        integer, intent(in), optional :: unit
    end subroutine resource_write

<Balancer base: procedures>+≡
    module subroutine resource_write (resource, unit)
        class(resource_t), intent(in) :: resource
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A,1X,I3,1X,A,1X,L1,1X,A,1X,I3)") &

```

```

        "RESOURCE_ID", resource%resource_id, &
        "ACTIVE", resource%active, &
        "N_ASSIGNED_WORKERS", resource%n_assigned_workers
    end subroutine resource_write

<Balancer base: resource: TBP>+≡
    procedure :: is_active => resource_is_active

<Balancer base: sub interfaces>+≡
    elemental module function resource_is_active (resource) result (flag)
        class(resource_t), intent(in) :: resource
        logical :: flag
    end function resource_is_active

<Balancer base: procedures>+≡
    elemental module function resource_is_active (resource) result (flag)
        class(resource_t), intent(in) :: resource
        logical :: flag
        flag = resource%active
    end function resource_is_active

<Balancer base: resource: TBP>+≡
    procedure :: set_active => resource_set_active

<Balancer base: sub interfaces>+≡
    module subroutine resource_set_active (resource, n_workers)
        class(resource_t), intent(inout) :: resource
        integer, intent(in) :: n_workers
    end subroutine resource_set_active

<Balancer base: procedures>+≡
    module subroutine resource_set_active (resource, n_workers)
        class(resource_t), intent(inout) :: resource
        integer, intent(in) :: n_workers
        resource%active = .true.
        resource%n_assigned_workers = n_workers
    end subroutine resource_set_active

<Balancer base: resource: TBP>+≡
    procedure :: set_inactive => resource_set_inactive

<Balancer base: sub interfaces>+≡
    module subroutine resource_set_inactive (resource)
        class(resource_t), intent(inout) :: resource
    end subroutine resource_set_inactive

<Balancer base: procedures>+≡
    module subroutine resource_set_inactive (resource)
        class(resource_t), intent(inout) :: resource
        resource%active = .false.
    end subroutine resource_set_inactive

<Balancer base: resource state: TBP>≡
    procedure :: write => resource_state_write

```

<Balancer base: sub interfaces>+≡

```
module subroutine resource_state_write (state, unit)
  class(resource_state_t), intent(in) :: state
  integer, intent(in), optional :: unit
end subroutine resource_state_write
```

<Balancer base: procedures>+≡

```
module subroutine resource_state_write (state, unit)
  class(resource_state_t), intent(in) :: state
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(A,1X,10)") "N_STATE_WORKERS", state%n_workers
  select case (state%mode)
  case (STATE_SINGLE)
    write (u, "(A)") "MODE ONE-TO-ONE"
  case (STATE_ALL)
    write (u, "(A)") "MODE ALL-TO-ONE"
  case default
    write (u, "(A)") "UNSUPPORTED MODE"
  end select
  write (u, "(A)") "RESOURCE"
  call state%resource_stack%write (u)
  write (u, "(A)") "FINISHED"
  call state%finished_stack%write (u)
end subroutine resource_state_write
```

<Balancer base: resource state: TBP>+≡

```
procedure :: init => resource_state_init
```

<Balancer base: sub interfaces>+≡

```
module subroutine resource_state_init (state, mode, n_workers)
  class(resource_state_t), intent(out) :: state
  integer, intent(in) :: mode
  integer, intent(in) :: n_workers
end subroutine resource_state_init
```

<Balancer base: procedures>+≡

```
module subroutine resource_state_init (state, mode, n_workers)
  class(resource_state_t), intent(out) :: state
  integer, intent(in) :: mode
  integer, intent(in) :: n_workers
  state%mode = mode
  state%n_workers = n_workers
  call state%resource_stack%init ()
  call state%finished_stack%init ()
end subroutine resource_state_init
```

<Balancer base: resource state: TBP>+≡

```
procedure :: add_resource => resource_state_add_resource
```

<Balancer base: sub interfaces>+≡

```
module subroutine resource_state_add_resource (state, i_resource)
  class(resource_state_t), intent(inout) :: state
  integer, intent(in) :: i_resource
end subroutine resource_state_add_resource
```

```

<Balancer base: procedures>+≡
    module subroutine resource_state_add_resource (state, i_resource)
        class(resource_state_t), intent(inout) :: state
        integer, intent(in) :: i_resource
        call state%resource_stack%add (i_resource)
    end subroutine resource_state_add_resource

<Balancer base: resource state: TBP>+≡
    procedure :: freeze => resource_state_freeze

<Balancer base: sub interfaces>+≡
    module subroutine resource_state_freeze (state)
        class(resource_state_t), intent(inout) :: state
    end subroutine resource_state_freeze

<Balancer base: procedures>+≡
    module subroutine resource_state_freeze (state)
        class(resource_state_t), intent(inout) :: state
        call state%resource_stack%sort ()
        call state%resource_stack %reverse_order ()
    end subroutine resource_state_freeze

<Balancer base: resource state: TBP>+≡
    procedure :: clear => resource_state_clear

<Balancer base: sub interfaces>+≡
    module subroutine resource_state_clear (state)
        class(resource_state_t), intent(inout) :: state
    end subroutine resource_state_clear

<Balancer base: procedures>+≡
    module subroutine resource_state_clear (state)
        class(resource_state_t), intent(inout) :: state
        call state%resource_stack%clear ()
        call state%finished_stack%clear ()
    end subroutine resource_state_clear

<Balancer base: resource state: TBP>+≡
    procedure :: has_resource => resource_state_has_resource

<Balancer base: sub interfaces>+≡
    elemental module function resource_state_has_resource (state) result (flag)
        class(resource_state_t), intent(in) :: state
        logical :: flag
    end function resource_state_has_resource

<Balancer base: procedures>+≡
    elemental module function resource_state_has_resource (state) result (flag)
        class(resource_state_t), intent(in) :: state
        logical :: flag
        flag = .not. state%resource_stack%is_empty ()
    end function resource_state_has_resource

<Balancer base: resource state: TBP>+≡
    procedure :: assign_resource => resource_state_assign_resource

```

```

<Balancer base: sub interfaces>+≡
    module function resource_state_assign_resource (state) result (i_resource)
        class(resource_state_t), intent(inout) :: state
        integer :: i_resource
    end function resource_state_assign_resource

<Balancer base: procedures>+≡
    module function resource_state_assign_resource (state) result (i_resource)
        class(resource_state_t), intent(inout) :: state
        integer :: i_resource
        if (state%resource_stack%is_empty ()) then
            i_resource = 0
            call msg_bug ("Error: No leftover resource on stack.")
            return
        end if
        i_resource = state%resource_stack%remove () !! Pop last element from stack.
    end function resource_state_assign_resource

<Balancer base: resource state: TBP>+≡
    procedure :: free_resource => resource_state_free_resource

<Balancer base: sub interfaces>+≡
    module subroutine resource_state_free_resource (state, i_resource)
        class(resource_state_t), intent(inout) :: state
        integer, intent(in) :: i_resource
    end subroutine resource_state_free_resource

<Balancer base: procedures>+≡
    module subroutine resource_state_free_resource (state, i_resource)
        class(resource_state_t), intent(inout) :: state
        integer, intent(in) :: i_resource
        if (state%resource_stack%is_element (i_resource)) then
            call msg_bug &
                ("Error: Cannot free resource, still on resource stack.")
        end if
        call state%finished_stack%add (i_resource)
    end subroutine resource_state_free_resource

<Balancer base: base: TBP>≡
    procedure :: base_write => balancer_base_write
    procedure(balancer_base_deferred_write), deferred :: write

<Balancer base: sub interfaces>+≡
    module subroutine balancer_base_write (balancer, unit)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
    end subroutine balancer_base_write

<Balancer base: procedures>+≡
    module subroutine balancer_base_write (balancer, unit)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(A)") "[REQUEST BALANCER]"
        write (u, "(3(A,1X,I3,1X))") "N_WORKERS", balancer%n_workers, &

```

```

        "N_RESOURCES", balancer%n_resources, &
        "N_STATES", balancer%n_states
write (u, "(A)") "[WORKER]"
do i = 1, balancer%n_workers
    call balancer%worker(i)%write (u)
end do
write (u, "(A)") "[RESOURCE]"
do i = 1, balancer%n_resources
    call balancer%resource(i)%write (u)
end do
write (u, "(A)") "[STATES]"
do i = 1, balancer%n_states
    call balancer%state(i)%write (u)
end do
end subroutine balancer_base_write

```

<Balancer base: base: TBP>+≡

```

procedure :: base_init => balancer_base_base_init

```

<Balancer base: sub interfaces>+≡

```

module subroutine balancer_base_base_init (balancer, n_workers, n_resources)
    class(balancer_base_t), intent(out) :: balancer
    integer, intent(in) :: n_workers
    integer, intent(in) :: n_resources
end subroutine balancer_base_base_init

```

<Balancer base: procedures>+≡

```

module subroutine balancer_base_base_init (balancer, n_workers, n_resources)
    class(balancer_base_t), intent(out) :: balancer
    integer, intent(in) :: n_workers
    integer, intent(in) :: n_resources
    balancer%n_workers = n_workers
    balancer%n_resources = n_resources
    allocate (balancer%worker (n_workers))
    allocate (balancer%resource (n_resources))
    call init_resource ()
contains
    subroutine init_resource ()
        integer :: i
        do i = 1, balancer%n_resources
            balancer%resource(i)%resource_id = i
        end do
    end subroutine init_resource
end subroutine balancer_base_base_init

```

Add partition of workers and link with workers. We move the allocated partition object into the balancer. We then assign each partition its respective number of workers in a incrementing linear fashion. However, we postpone the linking of the resources to the partition, which can be either done dynamically with the balancer state or directly with the appropriate type-bound procedure.

<Balancer base: base: TBP>+≡

```

procedure :: add_state => balancer_base_add_state

```

```

<Balancer base: sub interfaces>+≡
    module subroutine balancer_base_add_state (balancer, state)
        class(balancer_base_t), intent(inout) :: balancer
        type(resource_state_t), dimension(:), allocatable, intent(inout) :: state
    end subroutine balancer_base_add_state

<Balancer base: procedures>+≡
    module subroutine balancer_base_add_state (balancer, state)
        class(balancer_base_t), intent(inout) :: balancer
        type(resource_state_t), dimension(:), allocatable, intent(inout) :: state
        balancer%n_states = size (state)
        call move_alloc (state, balancer%state)
        call balancer%link_worker_and_state ()
    end subroutine balancer_base_add_state

<Balancer base: base: TBP>+≡
    procedure, private :: link_worker_and_state => &
        balancer_base_link_worker_and_state

<Balancer base: sub interfaces>+≡
    module subroutine balancer_base_link_worker_and_state (balancer)
        class(balancer_base_t), intent(inout) :: balancer
    end subroutine balancer_base_link_worker_and_state

<Balancer base: procedures>+≡
    module subroutine balancer_base_link_worker_and_state (balancer)
        class(balancer_base_t), intent(inout) :: balancer
        integer :: i, j, i_worker
        if (.not. allocated (balancer%state)) &
            call msg_bug ("Error: resource state not allocated.")
        !! Link worker to a state.
        i_worker = 1
        do i = 1, balancer%n_states
            do j = 1, balancer%state(i)%n_workers
                if (i_worker > balancer%n_workers) then
                    call msg_bug ("Balancer: Number of state workers&
                        & exceeding global number of workers")
                end if
                associate (worker => balancer%worker(i_worker))
                    worker%state = i
                    !! Reset worker attributes.
                    worker%resource = 0
                    worker%n_resources = 0
                    worker%assigned = .false.
                end associate
                i_worker = i_worker + 1
            end do
        end do
    end subroutine balancer_base_link_worker_and_state

```

Is a worker unassigned, or is a worker assigned, but already assigned to an active resource? This is a fence for the `assign_worker` TBP. The `assign_worker` TBP must call `is_assignable` in order to retrieve the worker status. The input is the worker ID, the return flag tells: if the worker is NOT assigned, return `.true.` if

state has resources. If worker is assigned, return `.true.` if associated resource is active.

```

<Balancer base: base: TBP>+≡
    procedure :: is_assignable => balancer_base_is_assignable

<Balancer base: sub interfaces>+≡
    pure module function balancer_base_is_assignable &
        (balancer, worker_id) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in) :: worker_id
        integer :: i_state, resource_id
        logical :: flag
    end function balancer_base_is_assignable

<Balancer base: procedures>+≡
    pure module function balancer_base_is_assignable &
        (balancer, worker_id) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in) :: worker_id
        integer :: i_state, resource_id
        logical :: flag
        flag = .false.
        if (balancer%worker(worker_id)%assigned) then
            resource_id = balancer%worker(worker_id)%resource
            flag = balancer%resource(resource_id)%is_active ()
        else
            i_state = balancer%worker(worker_id)%get_state ()
            flag = balancer%state(i_state)%has_resource ()
        end if
    end function balancer_base_is_assignable

```

Is a worker still pending. Test worker assignment, and if there is a (valid) resource and if it is still active.

```

<Balancer base: base: TBP>+≡
    procedure :: is_worker_pending => balancer_base_is_worker_pending

<Balancer base: sub interfaces>+≡
    pure module function balancer_base_is_worker_pending &
        (balancer, worker_id) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in) :: worker_id
        integer :: resource_id
        logical :: flag
    end function balancer_base_is_worker_pending

<Balancer base: procedures>+≡
    pure module function balancer_base_is_worker_pending &
        (balancer, worker_id) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        integer, intent(in) :: worker_id
        integer :: resource_id
        logical :: flag
        flag = balancer%worker(worker_id)%assigned
        if (flag) then
            resource_id = balancer%worker(worker_id)%get_resource ()
        end if
    end function balancer_base_is_worker_pending

```

```

        flag = balancer%resource(resource_id)%is_active ()
    end if
end function balancer_base_is_worker_pending

<Balancer base: base: TBP>+≡
    procedure :: is_pending => balancer_base_is_pending
    procedure(balancer_base_has_resource_group), deferred :: has_resource_group
    procedure(balancer_base_get_resource_group), deferred :: get_resource_group
    procedure(balancer_base_get_resource_master), deferred :: get_resource_master
    procedure(balancer_base_assign_worker), deferred :: assign_worker
    procedure(balancer_base_free_worker), deferred :: free_worker

<Balancer base: sub interfaces>+≡
    module function balancer_base_is_pending (balancer) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        logical :: flag
    end function balancer_base_is_pending

<Balancer base: procedures>+≡
    module function balancer_base_is_pending (balancer) result (flag)
        class(balancer_base_t), intent(in) :: balancer
        logical :: flag
        flag = all (balancer%state%has_resource ())
    end function balancer_base_is_pending

```

20.15.5 Balancer Simple

This module is the simple balancer. The simple balancer distribute the channel among the N workers using a modulo prescription. However, it does assign all workers to a channel capable of grid with parallelizable structure. The balancer use local, non-communicative approach; each worker allocates an own instance of the balancer and fills it with the respecting resources. We defer possible checks (or sentinels) to the request module, e.g. such as checking whether all channels are computed globally.

```

(balancer_simple.f90)≡
    <File header>
    module balancer_simple

        use balancer_base

        <Standard module head>

        <Balancer simple: parameters>

        <Balancer simple: public>

        <Balancer simple: types>

        interface
        <Balancer simple: sub interfaces>
        end interface

    end module balancer_simple

```

```

<balancer_simple_sub.f90>≡
  <File header>

  submodule (balancer_simple) balancer_simple_s

    use io_units
    use diagnostics

    implicit none

  contains

    <Balancer simple: procedures>

  end submodule balancer_simple_s

<Balancer simple: parameters>≡
  integer, parameter :: N_BALANCER_SIMPLE_STATES = 1, &
    BALANCER_SIMPLE_CHANNEL = 1

<Balancer simple: public>≡
  public :: balancer_simple_t

<Balancer simple: types>≡
  type, extends (balancer_base_t) :: balancer_simple_t
    logical, dimension(:), allocatable :: parallel_grid
  contains
    <Balancer simple: simple: TBP>
  end type balancer_simple_t

<Balancer simple: simple: TBP>≡
  procedure :: init => balancer_simple_init

<Balancer simple: sub interfaces>≡
  module subroutine balancer_simple_init (balancer, n_workers, n_resources)
    class(balancer_simple_t), intent(out) :: balancer
    integer, intent(in) :: n_workers
    integer, intent(in) :: n_resources
  end subroutine balancer_simple_init

<Balancer simple: procedures>≡
  module subroutine balancer_simple_init (balancer, n_workers, n_resources)
    class(balancer_simple_t), intent(out) :: balancer
    integer, intent(in) :: n_workers
    integer, intent(in) :: n_resources
    type(resource_state_t), dimension(:), allocatable :: state
    call balancer%base_init (n_workers, n_resources)
    allocate (balancer%parallel_grid(n_resources), source = .false.)
    allocate (state (N_BALANCER_SIMPLE_STATES))
    call state(BALANCER_SIMPLE_CHANNEL)%init ( &
      mode = STATE_SINGLE, &
      n_workers = balancer%n_workers)
    call balancer%add_state (state)
  end subroutine balancer_simple_init

```

```

<Balancer simple: simple: TBP>+≡
    procedure :: write => balancer_simple_write

<Balancer simple: sub interfaces>+≡
    module subroutine balancer_simple_write (balancer, unit)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
    end subroutine balancer_simple_write

<Balancer simple: procedures>+≡
    module subroutine balancer_simple_write (balancer, unit)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
        integer :: u, n_size
        u = given_output_unit (unit)
        call balancer%base_write (u)
        n_size = min (25, size (balancer%parallel_grid))
        write (u, "(A,25(1X,L1))") "Parallel Grids:", balancer%parallel_grid(:n_size)
    end subroutine balancer_simple_write

```

Update balancer state. Each worker update its own balancer state requiring information about the `worker_id`.

```

<Balancer simple: simple: TBP>+≡
    procedure :: update_state => balancer_simple_update_state

<Balancer simple: sub interfaces>+≡
    module subroutine balancer_simple_update_state &
        (balancer, worker_id, parallel_grid)
        class(balancer_simple_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        logical, dimension(:), intent(in) :: parallel_grid
    end subroutine balancer_simple_update_state

<Balancer simple: procedures>+≡
    module subroutine balancer_simple_update_state &
        (balancer, worker_id, parallel_grid)
        class(balancer_simple_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        logical, dimension(:), intent(in) :: parallel_grid
        integer :: ch, worker
        balancer%parallel_grid = parallel_grid
        if (.not. allocated (balancer%state)) then
            call msg_bug ("Error: balancer state not allocated.")
        end if
        associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))
            call state%clear ()
            do ch = 1, balancer%n_resources
                if (parallel_grid(ch)) then
                    call state%add_resource (ch)
                else
                    worker = balancer%map_channel_to_worker (ch)
                    if (worker == worker_id) then
                        call state%add_resource (ch)
                    end if
                end if
            end do
        end associate
    end subroutine balancer_simple_update_state

```

```

        call state%freeze ()
    end associate
end subroutine balancer_simple_update_state

<Balancer simple: simple: TBP>+≡
    procedure :: has_resource_group => balancer_simple_has_resource_group

<Balancer simple: sub interfaces>+≡
    pure module function balancer_simple_has_resource_group &
        (balancer, resource_id) result (flag)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in) :: resource_id
        logical :: flag
    end function balancer_simple_has_resource_group

<Balancer simple: procedures>+≡
    pure module function balancer_simple_has_resource_group &
        (balancer, resource_id) result (flag)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in) :: resource_id
        logical :: flag
        if (.not. balancer%resource(resource_id)%is_active ()) then
            flag = .false.
            return
        end if
        flag = balancer%parallel_grid (resource_id)
    end function balancer_simple_has_resource_group

<Balancer simple: simple: TBP>+≡
    procedure :: get_resource_group => balancer_simple_get_resource_group

<Balancer simple: sub interfaces>+≡
    pure module subroutine balancer_simple_get_resource_group &
        (balancer, resource_id, group)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in) :: resource_id
        integer, dimension(:), allocatable, intent(out) :: group
    end subroutine balancer_simple_get_resource_group

<Balancer simple: procedures>+≡
    pure module subroutine balancer_simple_get_resource_group &
        (balancer, resource_id, group)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in) :: resource_id
        integer, dimension(:), allocatable, intent(out) :: group
        integer :: i
        if (.not. balancer%has_resource_group (resource_id)) return
        group = pack ([i, i=1,balancer%n_workers]), &
            mask = balancer%worker%get_resource () == resource_id
    end subroutine balancer_simple_get_resource_group

```

Retrieve resource master holding the results to be communicated. As the simple balancer operates locally on each worker, we do not need to check whether a

resource is currently active. All the resources (and their respective order) is fixed at each update of the balancer.

```

<Balancer simple: simple: TBP>+≡
    procedure :: get_resource_master => balancer_simple_get_resource_master

<Balancer simple: sub interfaces>+≡
    pure module function balancer_simple_get_resource_master &
        (balancer, resource_id) result (worker_id)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer :: worker_id
    end function balancer_simple_get_resource_master

<Balancer simple: procedures>+≡
    pure module function balancer_simple_get_resource_master &
        (balancer, resource_id) result (worker_id)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer :: worker_id
    !! \note Do NOT check on resource activation (see interface prescription).
    if (balancer%parallel_grid(resource_id)) then
        worker_id = 1
    else
        worker_id = balancer%map_channel_to_worker (resource_id)
    end if
    end function balancer_simple_get_resource_master

<Balancer simple: simple: TBP>+≡
    procedure, private :: map_channel_to_worker => &
        balancer_simple_map_channel_to_worker

<Balancer simple: sub interfaces>+≡
    pure module function balancer_simple_map_channel_to_worker &
        (balancer, channel) result (worker)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: channel
    integer :: worker
    end function balancer_simple_map_channel_to_worker

<Balancer simple: procedures>+≡
    pure module function balancer_simple_map_channel_to_worker &
        (balancer, channel) result (worker)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: channel
    integer :: worker
    !! Proof: channel \in {1, N_c}, number of workers N, rank \in {0, ..., N - 1}
    !! Proof: worker \in {1, ..., N}
    !! a = b mod c, then 0 <= a < c
    worker = mod (channel - 1, balancer%n_workers) + 1
    end function balancer_simple_map_channel_to_worker

<Balancer simple: simple: TBP>+≡
    procedure :: assign_worker => balancer_simple_assign_worker

```

<Balancer simple: sub interfaces>+≡

```

module subroutine balancer_simple_assign_worker (balancer, worker_id, resource_id)
  class(balancer_simple_t), intent(inout) :: balancer
  integer, intent(in) :: worker_id
  integer, intent(out) :: resource_id
end subroutine balancer_simple_assign_worker

```

<Balancer simple: procedures>+≡

```

module subroutine balancer_simple_assign_worker (balancer, worker_id, resource_id)
  class(balancer_simple_t), intent(inout) :: balancer
  integer, intent(in) :: worker_id
  integer, intent(out) :: resource_id
  integer :: i
  if (.not. balancer%is_assignable (worker_id)) then
    resource_id = -1
    RETURN
  end if
  if (balancer%worker(worker_id)%is_assigned ()) then
    resource_id = balancer%worker(worker_id)%get_resource ()
    RETURN
  end if
  associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))
    if (.not. state%has_resource ()) then
      resource_id = 0
      return
    end if
    resource_id = state%assign_resource ()
    if (balancer%parallel_grid(resource_id)) then
      do i = 1, balancer%n_workers
        if (balancer%is_worker_pending (i)) then
          write (msg_buffer, "(A,1X,I0,1X,A,1X,I0,1X,A)") &
            "WORKER", i, "ASSIGNED"
          call msg_bug ()
        end if
        call balancer%worker(i)%add_resource (resource_id)
      end do
      call balancer%resource(resource_id)%set_active &
        (n_workers = balancer%n_workers)
    else
      call balancer%worker(worker_id)%add_resource (resource_id)
      call balancer%resource(resource_id)%set_active (n_workers = 1)
    end if
  end associate
end subroutine balancer_simple_assign_worker

```

<Balancer simple: simple: TBP>+≡

```

procedure :: free_worker => balancer_simple_free_worker

```

<Balancer simple: sub interfaces>+≡

```

module subroutine balancer_simple_free_worker &
  (balancer, worker_id, resource_id)
  class(balancer_simple_t), intent(inout) :: balancer
  integer, intent(in) :: worker_id
  integer, intent(in) :: resource_id
end subroutine balancer_simple_free_worker

```

```

<Balancer simple: procedures>+≡
  module subroutine balancer_simple_free_worker &
    (balancer, worker_id, resource_id)
    class(balancer_simple_t), intent(inout) :: balancer
    integer, intent(in) :: worker_id
    integer, intent(in) :: resource_id
    integer :: i
    if (.not. balancer%worker(worker_id)%is_assigned ()) return
    if (.not. resource_id == &
        balancer%worker(worker_id)%get_resource ()) then
      call msg_bug ("Balancer simple: resource and " // &
        "associated resource do not match.")
    end if
    associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))
      call balancer%resource(resource_id)%set_inactive ()
      call state%free_resource (resource_id)
      if (balancer%parallel_grid(resource_id)) then
        do i = 1, balancer%n_workers
          call balancer%worker(i)%free ()
        end do
      else
        call balancer%worker(worker_id)%free ()
      end if
    end associate
  end subroutine balancer_simple_free_worker

```

20.15.6 Balancer Channel

```

<balancer_channel.f90>≡
  <File header>
  module balancer_channel

    <Use kinds>
    use balancer_base

    <Standard module head>

    <Balancer channel: public>

    <Balancer channel: parameters>

    <Balancer channel: types>

    interface
    <Balancer channel: sub interfaces>
    end interface

  end module balancer_channel

<balancer_channel_sub.f90>≡
  <File header>

  submodule (balancer_channel) balancer_channel_s

```



```

    use io_units
    use diagnostics

    implicit none

contains

    <Balancer channel: procedures>

end submodule balancer_channel_s

<Balancer channel: parameters>≡
    real(default), parameter :: BETA = 1.5_default

    integer, parameter :: N_BALANCER_CHANNEL_STATE = 2, &
        CHANNEL_STATE = 1, &
        GRID_STATE = 2

<Balancer channel: public>≡
    public :: balancer_channel_t

<Balancer channel: types>≡
    type, extends(balancer_base_t) :: balancer_channel_t
    private
    integer :: n_parallel_grids = 0
    integer :: n_parallel_channels = 0
    integer :: n_grid_workers = 0
    integer :: n_channel_workers = 0
    logical, dimension(:), allocatable :: parallel_grid
contains
    <Balancer channel: base: TBP>
end type balancer_channel_t

<Balancer channel: base: TBP>≡
    procedure :: init => balancer_channel_init

<Balancer channel: sub interfaces>≡
    module subroutine balancer_channel_init (balancer, n_workers, n_resources)
        class(balancer_channel_t), intent(out), target :: balancer
        integer, intent(in) :: n_workers
        integer, intent(in) :: n_resources
    end subroutine balancer_channel_init

<Balancer channel: procedures>≡
    module subroutine balancer_channel_init (balancer, n_workers, n_resources)
        class(balancer_channel_t), intent(out), target :: balancer
        integer, intent(in) :: n_workers
        integer, intent(in) :: n_resources
        call balancer%base_init (n_workers, n_resources)
        allocate (balancer%parallel_grid(n_resources), source = .false.)
    end subroutine balancer_channel_init

```

```

<Balancer channel: base: TBP>+≡
    procedure :: write => balancer_channel_write

<Balancer channel: sub interfaces>+≡
    module subroutine balancer_channel_write (balancer, unit)
        class(balancer_channel_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
    end subroutine balancer_channel_write

<Balancer channel: procedures>+≡
    module subroutine balancer_channel_write (balancer, unit)
        class(balancer_channel_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
        integer :: u, n_size
        u = given_output_unit (unit)
        write (u, "(A)") "Channel Balancer."
        write (u, "(A,1X,I3)") "Parallel grids: ", balancer%n_parallel_grids
        write (u, "(A,1X,I3)") "Parallel channels: ", balancer%n_parallel_channels
        write (u, "(A,1X,I3)") "Grid workers: ", balancer%n_grid_workers
        write (u, "(A,1X,I3)") "Channel workers: ", balancer%n_channel_workers
        n_size = min (25, size (balancer%parallel_grid))
        write (u, "(A,25(1X,L1))") "Parallel Grids:", balancer%parallel_grid(:n_size)
        call balancer%base_write (u)
    end subroutine balancer_channel_write

<Balancer channel: base: TBP>+≡
    procedure :: update_state => balancer_channel_update_state

<Balancer channel: sub interfaces>+≡
    module subroutine balancer_channel_update_state &
        (balancer, weight, parallel_grid)
        class(balancer_channel_t), intent(inout) :: balancer
        real(default), dimension(:), intent(in) :: weight
        logical, dimension(:), intent(in) :: parallel_grid
    end subroutine balancer_channel_update_state

<Balancer channel: procedures>+≡
    module subroutine balancer_channel_update_state &
        (balancer, weight, parallel_grid)
        class(balancer_channel_t), intent(inout) :: balancer
        real(default), dimension(:), intent(in) :: weight
        logical, dimension(:), intent(in) :: parallel_grid
        real(default) :: min_parallel_weight
        balancer%parallel_grid = parallel_grid
        min_parallel_weight = &
            balancer%n_resources**((1._default - 1_default / BETA) &
            / balancer%n_workers**BETA
        balancer%parallel_grid = &
            balancer%parallel_grid .and. (weight >= min_parallel_weight)
        if (balancer%n_resources >= balancer%n_workers) then
            !! Apply full multi-channel parallelization.
            balancer%n_parallel_grids = 0
            balancer%n_parallel_channels = balancer%n_resources
            balancer%parallel_grid = .false.
            balancer%n_grid_workers = 0
            balancer%n_channel_workers = balancer%n_workers

```

```

else
  if (count (balancer%parallel_grid) == balancer%n_resources) then
    !! Apply full VEGAS parallelization.
    balancer%n_parallel_grids = balancer%n_resources
    balancer%n_parallel_channels = 0
    balancer%n_grid_workers = balancer%n_workers
    balancer%n_channel_workers = 0
  else
    !! Apply mixed mode.
    balancer%n_parallel_grids = count (balancer%parallel_grid)
    balancer%n_parallel_channels = balancer%n_resources - &
      balancer%n_parallel_grids
    call compute_mixed_mode (weight)
  end if
end if
if(allocated (balancer%state)) then
  deallocate (balancer%state)
end if
call allocate_state ()
contains
subroutine compute_mixed_mode (weight)
  real(default), dimension(:), intent(in) :: weight
  real(default) :: weight_parallel_grids, &
    ratio_weight, &
    ratio_n_channels, &
    ratio
  !! Apply mixed mode.
  weight_parallel_grids = sum (weight, balancer%parallel_grid)
  !! Overall normalization of weight,  $\alpha_{\text{grids}} + \alpha_{\text{channels}} = 1$ .
  !!  $\alpha_{\text{channels}} = 1 - \alpha_{\text{grids}}$ 
  ratio_weight = weight_parallel_grids / (1 - weight_parallel_grids)
  ratio_n_channels = real (balancer%n_parallel_grids, default) &
    / (balancer%n_resources - balancer%n_parallel_grids)
  !! The average computation of channel is proportional to its weight.
  !! Reweight number of channels (per mode) by their summed weights.
  !!  $R = w * N / (w * N + w' * N')$ ; primed refer to parallel grid entities.
  !!  $= 1 / (1 + w' / w * N' / N)$ 
  ratio = 1 / (1 + ratio_weight * ratio_n_channels)
  ratio = min (max (ratio, 0.0_default), 1.0_default) !! Safe-guard ratio computation.
  !! In the case of small numbers of workers and a very small ratio,
  !! nint can assign no worker to channel/grid parallelization,
  !! which is still requested by n_parallel_channels/grids.
  !! In that case, we have to enforce: n_worker = n_channel_worker + n_grid_worker
  balancer%n_channel_workers = nint (ratio * balancer%n_workers)
  balancer%n_grid_workers = nint ((1 - ratio) * balancer%n_workers)
  !! In the case of small numbers of workers and a very small ratio,
  !! nint can assign no worker to channel/grid parallelization,
  !! which is still requested by n_parallel_channels/grids.
  !! In that case, we have to enforce: n_worker = n_channel_worker + n_grid_worker
  if (balancer%n_workers >= 2 &
    .AND. (balancer%n_parallel_channels > 0 .and. balancer%n_channel_workers < 1)) then
    balancer%n_channel_workers = 1
    balancer%n_grid_workers = balancer%n_grid_workers - 1
  end if
end subroutine

```

```

end if
!! The grid resources will only be increased to N = 2
!! if more than 3 workers are present.
if (balancer%n_workers >= 3 &
    .AND. (balancer%n_parallel_grids > 0 .and. balancer%n_grid_workers < 2)) then
    balancer%n_grid_workers = 2
    balancer%n_channel_workers = balancer%n_channel_workers - 2
end if
end subroutine compute_mixed_mode

subroutine allocate_state ()
type(resource_state_t), dimension(:), allocatable :: state
integer :: ch
allocate (state(N_BALANCER_CHANNEL_STATE))
call state(CHANNEL_STATE)%init ( &
    mode = STATE_SINGLE, &
    n_workers = balancer%n_channel_workers)
call state(GRID_STATE)%init ( &
    mode = STATE_ALL, &
    n_workers = balancer%n_grid_workers)
do ch = 1, balancer%n_resources
    if (balancer%parallel_grid(ch)) then
        call state(GRID_STATE)%add_resource (ch)
    else
        call state(CHANNEL_STATE)%add_resource (ch)
    end if
end do
call state(CHANNEL_STATE)%freeze ()
call state(GRID_STATE)%freeze ()
call balancer%add_state (state)
end subroutine allocate_state
end subroutine balancer_channel_update_state

```

<Balancer channel: base: TBP>+≡

```
procedure :: has_resource_group => balancer_channel_has_resource_group
```

<Balancer channel: sub interfaces>+≡

```

pure module function balancer_channel_has_resource_group &
    (balancer, resource_id) result (flag)
class(balancer_channel_t), intent(in) :: balancer
integer, intent(in) :: resource_id
logical :: flag
end function balancer_channel_has_resource_group

```

<Balancer channel: procedures>+≡

```

pure module function balancer_channel_has_resource_group &
    (balancer, resource_id) result (flag)
class(balancer_channel_t), intent(in) :: balancer
integer, intent(in) :: resource_id
logical :: flag
if (.not. balancer%resource(resource_id)%is_active ()) then
    flag = .false.
return
end if
flag = balancer%parallel_grid(resource_id)

```

```

end function balancer_channel_has_resource_group

<Balancer channel: base: TBP>+≡
  procedure :: get_resource_group => balancer_channel_get_resource_group

<Balancer channel: sub interfaces>+≡
  pure module subroutine balancer_channel_get_resource_group &
    (balancer, resource_id, group)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
  end subroutine balancer_channel_get_resource_group

<Balancer channel: procedures>+≡
  pure module subroutine balancer_channel_get_resource_group &
    (balancer, resource_id, group)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
    integer :: i
    if (.not. balancer%has_resource_group (resource_id)) return
    group = pack ([i, i = 1, balancer%n_workers]), &
      mask = balancer%worker%get_resource () == resource_id
  end subroutine balancer_channel_get_resource_group

<Balancer channel: base: TBP>+≡
  procedure :: get_resource_master => balancer_channel_get_resource_master

<Balancer channel: sub interfaces>+≡
  pure module function balancer_channel_get_resource_master &
    (balancer, resource_id) result (worker_id)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer :: worker_id
  end function balancer_channel_get_resource_master

<Balancer channel: procedures>+≡
  pure module function balancer_channel_get_resource_master &
    (balancer, resource_id) result (worker_id)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer :: worker_id
    integer :: i
    if (.not. balancer%resource(resource_id)%is_active ()) then
      worker_id = -1
      return
    end if
    !! Linear search.
    !! First element in worker group is defined as master.
    associate (worker => balancer%worker)
      do i = 1, balancer%n_workers
        if (worker(i)%get_resource () == resource_id) then
          worker_id = i
          exit
        end if
      end if
    end associate
  end function balancer_channel_get_resource_master

```

```

        end do
    end associate
end function balancer_channel_get_resource_master

```

(Balancer channel: base: TBP)+≡

```

    procedure :: assign_worker => balancer_channel_assign_worker

```

(Balancer channel: sub interfaces)+≡

```

    module subroutine balancer_channel_assign_worker &
        (balancer, worker_id, resource_id)
        class(balancer_channel_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        integer, intent(out) :: resource_id
    end subroutine balancer_channel_assign_worker

```

(Balancer channel: procedures)+≡

```

    module subroutine balancer_channel_assign_worker &
        (balancer, worker_id, resource_id)
        class(balancer_channel_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        integer, intent(out) :: resource_id
        integer :: i_state
        if (.not. balancer%is_assignable (worker_id)) then
            resource_id = -1
            return
        end if
        if (balancer%worker(worker_id)%is_assigned ()) then
            resource_id = balancer%worker(worker_id)%get_resource ()
            return
        end if
        associate (state => balancer%state)
            i_state = balancer%worker(worker_id)%get_state ()
            if (.not. state(i_state)%has_resource ()) then
                resource_id = 0
                return
            end if
            resource_id = state(i_state)%assign_resource ()
            select case (state(i_state)%mode)
            case (STATE_SINGLE)
                call balancer%worker(worker_id)%add_resource (resource_id)
                call balancer%resource(resource_id)%set_active (n_workers = 1)
            case (STATE_ALL)
                call fill_resource_group (i_state, resource_id)
            end select
        end associate
contains
        subroutine fill_resource_group (i_state, resource_id)
            integer, intent(in) :: i_state
            integer, intent(in) :: resource_id
            integer :: i, n_workers
            n_workers = 0
            do i = 1, balancer%n_workers
                if (.not. balancer%worker(i)%get_state () == i_state) cycle
                if (balancer%is_worker_pending (i)) then
                    write (msg_buffer, "(A,1X,I0,1X,A,1X,I0,1X,A)") &

```

```

        "WORKER", i, "STATE", i_state, "ASSIGNED"
        call msg_bug ()
    end if
    call balancer%worker(i)%add_resource (resource_id)
    n_workers = n_workers + 1
end do
if (n_workers /= balancer%state(i_state)%n_workers) then
    call msg_bug ("Number of assigned workers unequal to " // &
        "number of state workers.")
end if
call balancer%resource(resource_id)%set_active (n_workers = n_workers)
end subroutine fill_resource_group
end subroutine balancer_channel_assign_worker

```

Free worker from associated resource. Idempotent. Depending on state association, given resource must equal worker's resource (check) for single state. For all state, the *current* resource of the worker may differ (grouping behavior!), only in case, that the older resource is inactive, return as idempotent. Else, free all worker from resource group.

(Balancer channel: base: TBP)+≡

```

    procedure :: free_worker => balancer_channel_free_worker

```

(Balancer channel: sub interfaces)+≡

```

    module subroutine balancer_channel_free_worker &
        (balancer, worker_id, resource_id)
        class(balancer_channel_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        integer, intent(in) :: resource_id
    end subroutine balancer_channel_free_worker

```

(Balancer channel: procedures)+≡

```

    module subroutine balancer_channel_free_worker &
        (balancer, worker_id, resource_id)
        class(balancer_channel_t), intent(inout) :: balancer
        integer, intent(in) :: worker_id
        integer, intent(in) :: resource_id
        integer :: i, i_state
        if (.not. balancer%worker(worker_id)%is_assigned ()) return
        associate (state => balancer%state)
            i_state = balancer%worker(worker_id)%get_state ()
            select case (state(i_state)%mode)
            case (STATE_SINGLE)
                if (.not. resource_id == &
                    balancer%worker(worker_id)%get_resource ()) then
                    call msg_bug ("Channel balancer: resource and associated " // &
                        "resource do not match.")
                end if
                call balancer%resource(resource_id)%set_inactive ()
                call state(i_state)%free_resource (resource_id)
                call balancer%worker(worker_id)%free ()
            case (STATE_ALL)
                if (resource_id /= balancer%worker(worker_id)%get_resource ()) then
                    if (balancer%resource(resource_id)%is_active ()) then
                        msg_buffer = "Channel balancer: resource is still active,&

```

```

        & but worker is assigned to another resource."
    call msg_bug ()
else
    !! Special case: Worker was already freed from (now inactive)
    !! resource_id (by another call to free_worker),
    !! and in the mean time assigned to a new resource.
    !! So, nothing to do.
    return
end if
end if
call balancer%resource(resource_id)%set_inactive ()
call state(i_state)%free_resource (resource_id)
do i = 1, balancer%n_workers
    if (.not. balancer%worker(i)%get_state () == i_state) cycle
    call balancer%worker(i)%free ()
end do
end select
end associate
end subroutine balancer_channel_free_worker

```

20.15.7 Request Callback

request handler Base type and interface for providing two-sided communication in a callback fashion.

request handler manager Manages handler with a binary tree.

This module constitutes the request handler. A request handler allows to dispatch an object for communication a priori for a slave and a master. Typically, each slave register its own request handles, whereas the master requests all possible requests handles matching those of the slaves. The requests can then be used later on, e.g. during a computation, a slave may add a request to the master worker and starts sending an object. The master worker looks up the appropriate request handler, which then closes the communication, i.e. by a receive call. Most important: Only a pointer to the buffer object is stored, therefore, the calling function has to ensure, that the communication object (buffer) will not be changed during a request handle (receive or send).

Remark: The handler allows for a tag offset which allows to unify the the communication. The problem occurs when multiple callback need to handled simultaneously and MPI needs to connect the communication calls accordingly. Each message has a tuple of (source, tag, comm) associated, we can unify this tuple by a unique tag. $\text{tag} = \text{tag_offset} + \{1, \dots, \text{N_requests}\}$ where tag_offsets are multiple of N_requests . The latter condition should be checked by a modulo. What happens if the communication is out of order (is this a problem? check with standard)?

```

(request_callback.f90)≡
module request_callback

    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT
    use binary_tree

```



```

    use mpi_f08 !NODEP!

    <Standard module head>

    <Request callback: public>

    <Request callback: types>

    <Request callback: interfaces>

    interface
    <Request callback: sub interfaces>
    end interface

    end module request_callback

<request_callback_sub.f90>≡
    <File header>

    submodule (request_callback) request_callback_s

        use diagnostics

        implicit none

    contains

    <Request callback: procedures>

    end submodule request_callback_s

    <Request callback: public>≡
        public :: request_handler_t

    <Request callback: types>≡
        type, abstract :: request_handler_t
            integer :: n_requests = 0
            integer :: tag_offset = 0
            type(MPI_REQUEST), dimension(:), allocatable :: request
            type(MPI_STATUS), dimension(:), allocatable :: status
            logical :: activated = .false.
            logical :: finished = .false.
        contains
            procedure :: base_write => request_handler_base_write
            procedure(request_handler_write), deferred :: write
            !! \todo{sbrass} implement initialization procedure.
            procedure(request_handler_handle), deferred :: handle
            procedure(request_handler_client_handle), deferred :: client_handle
            procedure :: allocate => request_handler_allocate
            procedure :: get_status => request_handler_get_status
            procedure :: testall => request_handler_testall
            procedure :: waitall => request_handler_waitall
            procedure :: free => request_handler_free
        end type request_handler_t

```

```

<Request callback: public>+≡
    public :: request_handler_manager_t

<Request callback: types>+≡
    type :: request_handler_manager_t
    private
    type(MPI_COMM) :: comm
    type(binary_tree_t) :: tree
    contains
    <Request callback: handler manager: TBP>
    end type request_handler_manager_t

<Request callback: interfaces>≡
    abstract interface
    subroutine request_handler_write (handler, unit)
    import :: request_handler_t
    class(request_handler_t), intent(in) :: handler
    integer, intent(in), optional :: unit
    end subroutine request_handler_write
    end interface

<Request callback: interfaces>+≡
    abstract interface
    !> Handle a request from server side.
    !!
    !! The message tag can be used in order to unify the respective messages between master and slave.
    !! E.g. by explicitly setting it, or by using it in a computation  $i * N_R + j$ ,  $i \in \{1, \dots, N_R\}$ ,  $j \in \{1, \dots, N_S\}$ .
    !!
    !! Must set *activated* to .true. when called.
    !! \param[in] source Integer rank of the source in comm.
    !! \param[in] tag Specify the message tag.
    !! \param[in] comm MPI communicator.
    subroutine request_handler_handle (handler, source_rank, comm)
    import :: request_handler_t, MPI_COMM
    class(request_handler_t), intent(inout) :: handler
    integer, intent(in) :: source_rank
    type(MPI_COMM), intent(in) :: comm
    end subroutine request_handler_handle
    end interface

<Request callback: interfaces>+≡
    abstract interface
    !> Handle a request from client side.
    !!
    !! Must set *activated* to .true. when called.
    !! \param[in] rank Integer of the receiver in comm.
    !! \param[in] tag Specify the message tag.
    !! \param[in] comm MPI communicator.
    subroutine request_handler_client_handle (handler, dest_rank, comm)
    import :: request_handler_t, MPI_COMM
    class(request_handler_t), intent(inout) :: handler

```

```

        integer, intent(in) :: dest_rank
        type(MPI_COMM), intent(in) :: comm
    end subroutine request_handler_client_handle
end interface

```

Request handler. Write routine.

```

<Request callback: sub interfaces>≡
    module subroutine request_handler_base_write (handler, unit)
        class(request_handler_t), intent(in) :: handler
        integer, intent(in), optional :: unit
    end subroutine request_handler_base_write

```

```

<Request callback: procedures>≡
    module subroutine request_handler_base_write (handler, unit)
        class(request_handler_t), intent(in) :: handler
        integer, intent(in), optional :: unit
        integer :: u, i
        u = ERROR_UNIT; if (present (unit)) u = unit
        write (u, "(A,1X,I0)") "N_REQUESTS", handler%n_requests
        write (u, "(A,1X,I0)") "TAG_OFFSET", handler%tag_offset
        write (u, "(A,1X,L1)") "FINISHED", handler%finished
        write (u, "(A,1X,L1)") "ACTIVATED", handler%activated
        write (u, "(A)") "I | SOURCE | TAG | ERROR | REQUEST_NULL"
        do i = 1, handler%n_requests
            write (u, "(A,4(1X,I0),1X,L1)") "REQUEST", i, &
                handler%status(i)%MPI_SOURCE, &
                handler%status(i)%MPI_TAG, &
                handler%status(i)%MPI_ERROR, &
                (handler%request(i) == MPI_REQUEST_NULL)
        end do
    end subroutine request_handler_base_write

```

Allocate MPI request and status object. Must be called during or after object-initialization.

```

<Request callback: sub interfaces>+≡
    module subroutine request_handler_allocate (handler, n_requests, tag_offset)
        class(request_handler_t), intent(inout) :: handler
        integer, intent(in) :: n_requests
        integer, intent(in) :: tag_offset
    end subroutine request_handler_allocate

```

```

<Request callback: procedures>+≡
    !! \param[inout] handler Handler must be intent inout, as the calling function may already manip
    !! \param[in] n_requests Number of MPI requests the objects needs to be able to handle.
    !! \param[in] tag_offset First tag to be used, all other must follow in an increasing manner unt
    !! Proof: tag \in {tag_offset, tag_offset + n_requests}.
    module subroutine request_handler_allocate (handler, n_requests, tag_offset)
        class(request_handler_t), intent(inout) :: handler
        integer, intent(in) :: n_requests
        integer, intent(in) :: tag_offset
        allocate (handler%request(n_requests), source = MPI_REQUEST_NULL)
        allocate (handler%status(n_requests))
        handler%n_requests = n_requests
        if (mod (tag_offset, n_requests) /= 0) &

```

```

        call msg_bug ("Error during handler allocate, tag_offset " // &
            "is not a multiple of n_requests.")
    !! What is the max.-allowed MPI_TAG?
    handler%tag_offset = tag_offset
    handler%activated = .false.
    handler%finished = .false.
end subroutine request_handler_allocate

```

Get status from request objects in a non-destructive way.

```

<Request callback: sub interfaces>+≡
    module subroutine request_handler_get_status (handler)
        class(request_handler_t), intent(inout) :: handler
    end subroutine request_handler_get_status

<Request callback: procedures>+≡
    module subroutine request_handler_get_status (handler)
        class(request_handler_t), intent(inout) :: handler
        integer :: i
        logical :: flag
        if (.not. handler%activated) return
        handler%finished = .true.
        do i = 1, handler%n_requests
            call MPI_REQUEST_GET_STATUS (handler%request(i), flag, &
                handler%status(i))
            handler%finished = handler%finished .and. flag
        end do
    end subroutine request_handler_get_status

```

Call MPI_WAITALL and raise finished flag.

```

<Request callback: sub interfaces>+≡
    module subroutine request_handler_waitall (handler)
        class(request_handler_t), intent(inout) :: handler
    end subroutine request_handler_waitall

<Request callback: procedures>+≡
    module subroutine request_handler_waitall (handler)
        class(request_handler_t), intent(inout) :: handler
        integer :: error
        if (.not. handler%activated .or. handler%finished) return
        call MPI_WAITALL (handler%n_requests, handler%request, &
            handler%status, error)
        if (error /= 0) then
            call msg_bug ("Request: Error occurred during waitall on handler.")
        end if
        handler%finished = .true.
    end subroutine request_handler_waitall

```

```

<Request callback: sub interfaces>+≡
    module function request_handler_testall (handler) result (flag)
        class(request_handler_t), intent(inout) :: handler
        logical :: flag
    end function request_handler_testall

```

```

<Request callback: procedures>+≡
module function request_handler_testall (handler) result (flag)
  class(request_handler_t), intent(inout) :: handler
  logical :: flag
  integer :: error
  if (.not. handler%activated .or. .not. handler%finished) then
    call MPI_TESTALL (handler%n_requests, handler%request, &
      handler%finished, handler%status, error)
    ! call print_status ()
    if (error /= 0) then
      call msg_bug ("Request: Error occurred during testall on handler.")
    end if
  end if
  flag = handler%finished
contains
  subroutine print_status ()
    integer :: i
    do i = 1, handler%n_requests
      associate (status => handler%status(i))
        write (ERROR_UNIT, *) status%MPI_SOURCE, status%MPI_TAG, &
          status%MPI_ERROR
      end associate
    end do
  end subroutine print_status
end function request_handler_testall

```

```

<Request callback: sub interfaces>+≡
module subroutine request_handler_free (handler)
  class(request_handler_t), intent(inout) :: handler
end subroutine request_handler_free

```

```

<Request callback: procedures>+≡
module subroutine request_handler_free (handler)
  class(request_handler_t), intent(inout) :: handler
  integer :: i, error
  do i = 1, handler%n_requests
    if (handler%request(i) == MPI_REQUEST_NULL) cycle
    call MPI_REQUEST_FREE (handler%request(i), error)
    if (error /= 0) then
      call msg_bug ("Request: Error occurred during free " // &
        "request on handler.")
    end if
  end do
end subroutine request_handler_free

```

Request handler manager.

```

<Request callback: handler manager: TBP>≡
procedure :: init => request_handler_manager_init

```

```

<Request callback: sub interfaces>+≡
module subroutine request_handler_manager_init (rhman, comm)
  class(request_handler_manager_t), intent(out) :: rhman
  type(MPI_COMM), intent(in) :: comm
end subroutine request_handler_manager_init

```

```

<Request callback: procedures>+≡
  module subroutine request_handler_manager_init (rhm, comm)
    class(request_handler_manager_t), intent(out) :: rhm
    type(MPI_COMM), intent(in) :: comm
    call MPI_COMM_DUP (comm, rhm%comm)
  end subroutine request_handler_manager_init

<Request callback: handler manager: TBP>+≡
  procedure :: write => request_handler_manager_write

<Request callback: sub interfaces>+≡
  module subroutine request_handler_manager_write (rhm, unit)
    class(request_handler_manager_t), intent(in) :: rhm
    integer, intent(in), optional :: unit
  end subroutine request_handler_manager_write

<Request callback: procedures>+≡
  module subroutine request_handler_manager_write (rhm, unit)
    class(request_handler_manager_t), intent(in) :: rhm
    integer, intent(in), optional :: unit
    integer :: u
    u = ERROR_UNIT; if (present (unit)) u = unit
    write (u, "(A)") "[REQUEST_CALLBACK_MANAGER]"
    call rhm%tree%write (u)
  end subroutine request_handler_manager_write

<Request callback: handler manager: TBP>+≡
  procedure :: add => request_handler_manager_add

<Request callback: sub interfaces>+≡
  module subroutine request_handler_manager_add (rhm, handler_id, handler)
    class(request_handler_manager_t), intent(inout) :: rhm
    integer, intent(in) :: handler_id
    class(request_handler_t), pointer, intent(in) :: handler
  end subroutine request_handler_manager_add

<Request callback: procedures>+≡
  module subroutine request_handler_manager_add (rhm, handler_id, handler)
    class(request_handler_manager_t), intent(inout) :: rhm
    integer, intent(in) :: handler_id
    class(request_handler_t), pointer, intent(in) :: handler
    class(*), pointer :: obj
    obj => handler
    call rhm%tree%insert (handler_id, obj)
  end subroutine request_handler_manager_add

<Request callback: handler manager: TBP>+≡
  procedure :: clear => request_handler_manager_clear

<Request callback: sub interfaces>+≡
  module subroutine request_handler_manager_clear (rhm)
    class(request_handler_manager_t), intent(inout) :: rhm
  end subroutine request_handler_manager_clear

```

<Request callback: procedures>+≡

```
module subroutine request_handler_manager_clear (rhm)
  class(request_handler_manager_t), intent(inout) :: rhm
  call rhm%tree%clear ()
end subroutine request_handler_manager_clear
```

Get status (in a non-destructive way) for all associated handler.

<Request callback: handler manager: TBP>+≡

```
procedure, private :: fill_status => request_handler_manager_fill_status
```

<Request callback: sub interfaces>+≡

```
module subroutine request_handler_manager_fill_status (rhm)
  class(request_handler_manager_t), intent(inout) :: rhm
end subroutine request_handler_manager_fill_status
```

<Request callback: procedures>+≡

```
module subroutine request_handler_manager_fill_status (rhm)
  class(request_handler_manager_t), intent(inout) :: rhm
  type(binary_tree_iterator_t) :: iterator
  integer :: handler_id
  class(request_handler_t), pointer :: handler
  call iterator%init (rhm%tree)
  do while (iterator%is_iterable ())
    call iterator%next (handler_id)
    call rhm%handler_at (handler_id, handler)
    call handler%get_status ()
  end do
end subroutine request_handler_manager_fill_status
```

<Request callback: handler manager: TBP>+≡

```
procedure :: test => request_handler_manager_test
```

<Request callback: sub interfaces>+≡

```
module function request_handler_manager_test &
  (rhm, handler_id) result (flag)
  class(request_handler_manager_t), intent(inout) :: rhm
  integer, intent(in) :: handler_id
  logical :: flag
end function request_handler_manager_test
```

<Request callback: procedures>+≡

```
module function request_handler_manager_test &
  (rhm, handler_id) result (flag)
  class(request_handler_manager_t), intent(inout) :: rhm
  integer, intent(in) :: handler_id
  logical :: flag
  class(request_handler_t), pointer :: handler
  call rhm%handler_at (handler_id, handler)
  flag = handler%testall ()
end function request_handler_manager_test
```

<Request callback: handler manager: TBP>+≡

```
procedure :: wait => request_handler_manager_wait
```

```

<Request callback: sub interfaces>+≡
    module subroutine request_handler_manager_wait (rhbm, handler_id)
        class(request_handler_manager_t), intent(inout) :: rhbm
        integer, intent(in) :: handler_id
    end subroutine request_handler_manager_wait

<Request callback: procedures>+≡
    module subroutine request_handler_manager_wait (rhbm, handler_id)
        class(request_handler_manager_t), intent(inout) :: rhbm
        integer, intent(in) :: handler_id
        class(request_handler_t), pointer :: handler
        call rhbm%handler_at (handler_id, handler)
        call handler%waitall ()
    end subroutine request_handler_manager_wait

<Request callback: handler manager: TBP>+≡
    procedure :: waitall => request_handler_manager_waitall

<Request callback: sub interfaces>+≡
    module subroutine request_handler_manager_waitall (rhbm)
        class(request_handler_manager_t), intent(inout) :: rhbm
    end subroutine request_handler_manager_waitall

<Request callback: procedures>+≡
    module subroutine request_handler_manager_waitall (rhbm)
        class(request_handler_manager_t), intent(inout) :: rhbm
        type(binary_tree_iterator_t) :: iterator
        integer :: handler_id
        call iterator%init (rhbm%tree)
        do while (iterator%is_iterable ())
            call iterator%next (handler_id)
            !! Test handler (destructive test on request handler).
            if (.not. rhbm%test (handler_id)) &
                call rhbm%wait (handler_id)
        end do
    end subroutine request_handler_manager_waitall

<Request callback: handler manager: TBP>+≡
    procedure, private :: handler_at => request_handler_manager_handler_at

<Request callback: sub interfaces>+≡
    module subroutine request_handler_manager_handler_at &
        (rhbm, handler_id, handler)
        class(request_handler_manager_t), intent(in) :: rhbm
        integer, intent(in) :: handler_id
        class(request_handler_t), pointer, intent(out) :: handler
    end subroutine request_handler_manager_handler_at

<Request callback: procedures>+≡
    module subroutine request_handler_manager_handler_at &
        (rhbm, handler_id, handler)
        class(request_handler_manager_t), intent(in) :: rhbm
        integer, intent(in) :: handler_id
        class(request_handler_t), pointer, intent(out) :: handler
        class(*), pointer :: obj
        call rhbm%tree%search (handler_id, obj)

```



```

select type (obj)
class is (request_handler_t)
  handler => obj
class default
  call msg_bug ("Object is not derived from request_handler_t.")
end select
end subroutine request_handler_manager_handler_at

```

```

<Request callback: handler manager: TBP>+≡
  procedure :: has_handler => request_handler_manager_has_handler

```

```

<Request callback: sub interfaces>+≡
  module function request_handler_manager_has_handler &
    (rhmm, handler_id) result (flag)
    class(request_handler_manager_t), intent(inout) :: rhmm
    integer, intent(in) :: handler_id
    logical :: flag
  end function request_handler_manager_has_handler

```

```

<Request callback: procedures>+≡
  module function request_handler_manager_has_handler &
    (rhmm, handler_id) result (flag)
    class(request_handler_manager_t), intent(inout) :: rhmm
    integer, intent(in) :: handler_id
    logical :: flag
    flag = rhmm%tree%has_key (handler_id)
  end function request_handler_manager_has_handler

```

Call server-sided procedure of callback with handler_id. Ingoing variables are handler_id and source.

```

<Request callback: handler manager: TBP>+≡
  procedure :: callback => request_handler_manager_callback

```

```

<Request callback: sub interfaces>+≡
  module subroutine request_handler_manager_callback &
    (rhmm, handler_id, source_rank)
    class(request_handler_manager_t), intent(inout) :: rhmm
    integer, intent(in) :: handler_id
    integer, intent(in) :: source_rank
  end subroutine request_handler_manager_callback

```

```

<Request callback: procedures>+≡
  module subroutine request_handler_manager_callback &
    (rhmm, handler_id, source_rank)
    class(request_handler_manager_t), intent(inout) :: rhmm
    integer, intent(in) :: handler_id
    integer, intent(in) :: source_rank
    class(request_handler_t), pointer :: handler
    if (.not. rhmm%tree%has_key (handler_id)) return
    call rhmm%handler_at (handler_id, handler)
    call handler%handle (source_rank = source_rank, comm = rhmm%comm)
  end subroutine request_handler_manager_callback

```

Call client-sided procedure of callback with `handler_id`, which is the input, as well as the destination rank.

(Request callback: handler manager: TBP)+≡

```
procedure :: client_callback => request_handler_manager_client_callback
```

(Request callback: sub interfaces)+≡

```
module subroutine request_handler_manager_client_callback &
  (rhm, handler_id, dest_rank)
  class(request_handler_manager_t), intent(inout) :: rhm
  integer, intent(in) :: handler_id
  integer, intent(in) :: dest_rank
end subroutine request_handler_manager_client_callback
```

(Request callback: procedures)+≡

```
module subroutine request_handler_manager_client_callback &
  (rhm, handler_id, dest_rank)
  class(request_handler_manager_t), intent(inout) :: rhm
  integer, intent(in) :: handler_id
  integer, intent(in) :: dest_rank
  class(request_handler_t), pointer :: handler
  if (.not. rhm%tree%has_key (handler_id)) return
  call rhm%handler_at (handler_id, handler)
  call handler%client_handle (dest_rank = dest_rank, comm = rhm%comm)
end subroutine request_handler_manager_client_callback
```

Chapter 21

Multi-Channel Integration

The abstract representation of multi-channel Monte Carlo algorithms for integration and event generation.

Module `mci_base`: The abstract types and their methods. It provides a test integrator that is referenced in later unit tests.

`iterations` Container for defining integration call and pass settings.

`integration_results` This module handles results from integrating processes. It records passes and iterations, calculates statistical averages, and provides the user output of integration results.

These are the implementations:

Module `mci_midpoint`: A simple integrator that uses the midpoint rule to sample the integrand uniformly over the unit hypercube. There is only one integration channel, so this can be matched only to single-channel phase space.

Module `mci_vamp`: Interface for the VAMP package.

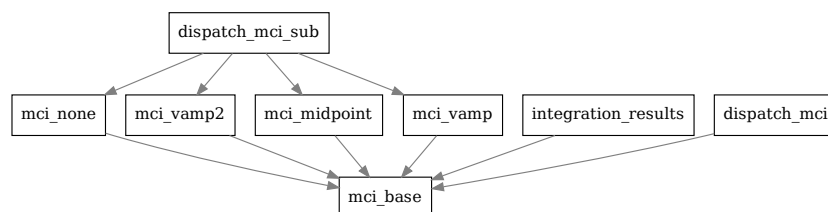


Figure 21.1: Module dependencies in `src/mci`.

21.1 Generic Integrator

This module provides a multi-channel integrator (MCI) base type, a corresponding configuration type, and methods for integration and event generation.

```
<mci_base.f90>≡  
  <File header>  
  
  module mci_base  
  
    use kinds  
    use cputime  
    use phs_base  
    use rng_base  
  
    <Standard module head>  
  
    <MCI base: public>  
  
    <MCI base: types>  
  
    <MCI base: interfaces>  
  
    interface  
    <MCI base: sub interfaces>  
    end interface  
  
  end module mci_base  
  
<mci_base_sub.f90>≡  
  <File header>  
  
  submodule (mci_base) mci_base_s  
  
    use io_units  
    use format_utils, only: pac_fmt  
    use format_defs, only: FMT_14, FMT_17  
    use diagnostics  
  
    implicit none  
  
    contains  
  
    <MCI base: procedures>  
  
  end submodule mci_base_s
```

21.1.1 MCI: integrator

The MCI object contains the methods for integration and event generation. For the actual work and data storage, it spawns an MCI instance object.

The base object contains the number of integration dimensions and the number of channels as configuration data. Further configuration data are stored in

the concrete extensions.

The MCI sum contains all relevant information about the integrand. It can be used for comparing the current configuration against a previous one. If they match, we can skip an actual integration. (Implemented only for the VAMP version.)

There is a random-number generator (its state with associated methods) available as `rng`. It may or may not be used for integration. It will be used for event generation.

```

<MCI base: public>≡
  public :: mci_t

<MCI base: types>≡
  type, abstract :: mci_t
    integer :: n_dim = 0
    integer :: n_channel = 0
    integer :: n_chain = 0
    integer, dimension(:), allocatable :: chain
    real(default), dimension(:), allocatable :: chain_weights
    character(32) :: md5sum = ""
    logical :: integral_known = .false.
    logical :: error_known = .false.
    logical :: efficiency_known = .false.
    real(default) :: integral = 0
    real(default) :: error = 0
    real(default) :: efficiency = 0
    logical :: use_timer = .false.
    type(timer_t) :: timer
    class(rng_t), allocatable :: rng
  contains
    <MCI base: mci: TBP>
  end type mci_t

```

Finalizer: the random-number generator may need one.

```

<MCI base: mci: TBP>≡
  procedure :: base_final => mci_final
  procedure (mci_final), deferred :: final

<MCI base: sub interfaces>≡
  module subroutine mci_final (object)
    class(mci_t), intent(inout) :: object
  end subroutine mci_final

<MCI base: procedures>≡
  module subroutine mci_final (object)
    class(mci_t), intent(inout) :: object
    if (allocated (object%rng)) call object%rng%final ()
  end subroutine mci_final

```

Output: basic and extended output.

```

<MCI base: mci: TBP>+≡
  procedure :: base_write => mci_write
  procedure (mci_write), deferred :: write

```

```

<MCI base: sub interfaces>+≡
  module subroutine mci_write (object, unit, pacify, md5sum_version)
    class(mci_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
  end subroutine mci_write

<MCI base: procedures>+≡
  module subroutine mci_write (object, unit, pacify, md5sum_version)
    class(mci_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
    logical :: md5sum_ver
    integer :: u, i, j
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    md5sum_ver = .false.
    if (present (md5sum_version)) md5sum_ver = md5sum_version
    if (object%use_timer .and. .not. md5sum_ver) then
      write (u, "(2x)", advance="no")
      call object%timer%write (u)
    end if
    if (object%integral_known) then
      write (u, "(3x,A," // fmt // ")") &
        "Integral" = ", object%integral
    end if
    if (object%error_known) then
      write (u, "(3x,A," // fmt // ")") &
        "Error" = ", object%error
    end if
    if (object%efficiency_known) then
      write (u, "(3x,A," // fmt // ")") &
        "Efficiency" = ", object%efficiency
    end if
    write (u, "(3x,A,I0)") "Number of channels" = ", object%n_channel
    write (u, "(3x,A,I0)") "Number of dimensions" = ", object%n_dim
    if (object%n_chain > 0) then
      write (u, "(3x,A,I0)") "Number of chains" = ", object%n_chain
      write (u, "(3x,A)") "Chains:"
      do i = 1, object%n_chain
        write (u, "(5x,I0,':')", advance = "no") i
        do j = 1, object%n_channel
          if (object%chain(j) == i) &
            write (u, "(1x,I0)", advance = "no") j
          end do
          write (u, "(A)")
        end do
      end if
    end subroutine mci_write

```

Print an informative message when starting integration.

```

<MCI base: mci: TBP>+≡
  procedure (mci_startup_message), deferred :: startup_message
  procedure :: base_startup_message => mci_startup_message

<MCI base: sub interfaces>+≡
  module subroutine mci_startup_message (mci, unit, n_calls)
    class(mci_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
  end subroutine mci_startup_message

<MCI base: procedures>+≡
  module subroutine mci_startup_message (mci, unit, n_calls)
    class(mci_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    if (mci%n_chain > 0) then
      write (msg_buffer, "(A,3(1x,I0,1x,A))") &
        "Integrator:", mci%n_chain, "chains,", &
        mci%n_channel, "channels,", &
        mci%n_dim, "dimensions"
    else
      write (msg_buffer, "(A,3(1x,I0,1x,A))") &
        "Integrator:", &
        mci%n_channel, "channels,", &
        mci%n_dim, "dimensions"
    end if
    call msg_message (unit = unit)
  end subroutine mci_startup_message

```

Dump type-specific info to a logfile.

```

<MCI base: mci: TBP>+≡
  procedure(mci_write_log_entry), deferred :: write_log_entry

<MCI base: interfaces>≡
  abstract interface
    subroutine mci_write_log_entry (mci, u)
      import
      class(mci_t), intent(in) :: mci
      integer, intent(in) :: u
    end subroutine mci_write_log_entry
  end interface

```

In order to avoid dependencies on definite MCI implementations, we introduce a MD5 sum calculator.

```

<MCI base: mci: TBP>+≡
  procedure(mci_compute_md5sum), deferred :: compute_md5sum

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_compute_md5sum (mci, pacify)
      import
      class(mci_t), intent(inout) :: mci
      logical, intent(in), optional :: pacify
    end subroutine mci_compute_md5sum
  end interface

```

Record the index of the MCI object within a process. For multi-component processes with more than one integrator, the integrator should know about its own index, so file names can be unique, etc. The default implementation does nothing, however.

```

<MCI base: mci: TBP>+≡
  procedure :: record_index => mci_record_index

<MCI base: sub interfaces>+≡
  module subroutine mci_record_index (mci, i_mci)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: i_mci
  end subroutine mci_record_index

<MCI base: procedures>+≡
  module subroutine mci_record_index (mci, i_mci)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: i_mci
  end subroutine mci_record_index

```

There is no Initializer for the abstract type, but a generic setter for the number of channels and dimensions. We make two aliases available, to be able to override it.

```

<MCI base: mci: TBP>+≡
  procedure :: set_dimensions => mci_set_dimensions
  procedure :: base_set_dimensions => mci_set_dimensions

<MCI base: sub interfaces>+≡
  module subroutine mci_set_dimensions (mci, n_dim, n_channel)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
  end subroutine mci_set_dimensions

<MCI base: procedures>+≡
  module subroutine mci_set_dimensions (mci, n_dim, n_channel)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    mci%n_dim = n_dim
    mci%n_channel = n_channel
  end subroutine mci_set_dimensions

```

Declare particular dimensions as flat. This information can be used to simplify integration. When generating events, the flat dimensions should be sampled with uniform and uncorrelated distribution. It depends on the integrator what to do with that information.

```

<MCI base: mci: TBP>+≡
  procedure (mci_declare_flat_dimensions), deferred :: declare_flat_dimensions

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_declare_flat_dimensions (mci, dim_flat)
      import
      class(mci_t), intent(inout) :: mci

```



```

        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_declare_flat_dimensions
end interface

```

Declare particular channels as equivalent, possibly allowing for permutations or reflections of dimensions. We use the information stored in the `phs_channel_t` object array that the phase-space module provides.

(We do not test this here, deferring the unit test to the `mci_vamp` implementation where we actually use this feature.)

```

<MCI base: mci: TBP>+≡
    procedure (mci_declare_equivalences), deferred :: declare_equivalences

<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_declare_equivalences (mci, channel, dim_offset)
            import
            class(mci_t), intent(inout) :: mci
            type(phs_channel_t), dimension(:), intent(in) :: channel
            integer, intent(in) :: dim_offset
        end subroutine mci_declare_equivalences
    end interface

```

Declare particular channels as chained together. The implementation may use this array for keeping their weights equal to each other, etc.

The chain array is an array sized by the number of channels. For each channel, there is an integer entry that indicates the corresponding chains. The total number of chains is the maximum value of this entry.

```

<MCI base: mci: TBP>+≡
    procedure :: declare_chains => mci_declare_chains

<MCI base: sub interfaces>+≡
    module subroutine mci_declare_chains (mci, chain)
        class(mci_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: chain
    end subroutine mci_declare_chains

<MCI base: procedures>+≡
    module subroutine mci_declare_chains (mci, chain)
        class(mci_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: chain
        allocate (mci%chain (size (chain)))
        mci%n_chain = maxval (chain)
        allocate (mci%chain_weights (mci%n_chain), source = 0._default)
        mci%chain = chain
    end subroutine mci_declare_chains

```

Collect channel weights according to chains and store them in the `chain_weights` for output. We sum up the weights for all channels that share the same `chain` index and store the results in the `chain_weights` array.

```

<MCI base: mci: TBP>+≡
    procedure :: collect_chain_weights => mci_collect_chain_weights

```

```

<MCI base: sub interfaces>+≡
    module subroutine mci_collect_chain_weights (mci, weight)
        class(mci_t), intent(inout) :: mci
        real(default), dimension(:), intent(in) :: weight
    end subroutine mci_collect_chain_weights

<MCI base: procedures>+≡
    module subroutine mci_collect_chain_weights (mci, weight)
        class(mci_t), intent(inout) :: mci
        real(default), dimension(:), intent(in) :: weight
        integer :: i, c
        if (allocated (mci%chain)) then
            mci%chain_weights = 0
            do i = 1, size (mci%chain)
                c = mci%chain(i)
                mci%chain_weights(c) = mci%chain_weights(c) + weight(i)
            end do
        end if
    end subroutine mci_collect_chain_weights

```

Check if there are chains.

```

<MCI base: mci: TBP>+≡
    procedure :: has_chains => mci_has_chains

<MCI base: sub interfaces>+≡
    module function mci_has_chains (mci) result (flag)
        class(mci_t), intent(in) :: mci
        logical :: flag
    end function mci_has_chains

<MCI base: procedures>+≡
    module function mci_has_chains (mci) result (flag)
        class(mci_t), intent(in) :: mci
        logical :: flag
        flag = allocated (mci%chain)
    end function mci_has_chains

```

Output of the chain weights, kept separate from the main `write` method.

[The formatting will work as long as the number of chains is less than 10^{10} ...]

```

<MCI base: mci: TBP>+≡
    procedure :: write_chain_weights => mci_write_chain_weights

<MCI base: sub interfaces>+≡
    module subroutine mci_write_chain_weights (mci, unit)
        class(mci_t), intent(in) :: mci
        integer, intent(in), optional :: unit
    end subroutine mci_write_chain_weights

<MCI base: procedures>+≡
    module subroutine mci_write_chain_weights (mci, unit)
        class(mci_t), intent(in) :: mci
        integer, intent(in), optional :: unit
        integer :: u, i, n, n_digits
        character(4) :: ifmt
        u = given_output_unit (unit)

```

```

if (allocated (mci%chain_weights)) then
  write (u, "(1x,A)") "Weights of channel chains (groves):"
  n_digits = 0
  n = size (mci%chain_weights)
  do while (n > 0)
    n = n / 10
    n_digits = n_digits + 1
  end do
  write (ifmt, "(A1,I1)") "I", n_digits
  do i = 1, size (mci%chain_weights)
    write (u, "(3x," // ifmt // ",F13.10)") i, mci%chain_weights(i)
  end do
end if
end subroutine mci_write_chain_weights

```

Set the MD5 sum, independent of initialization.

```

<MCI base: mci: TBP>+≡
  procedure :: set_md5sum => mci_set_md5sum

<MCI base: sub interfaces>+≡
  module subroutine mci_set_md5sum (mci, md5sum)
    class(mci_t), intent(inout) :: mci
    character(32), intent(in) :: md5sum
  end subroutine mci_set_md5sum

<MCI base: procedures>+≡
  module subroutine mci_set_md5sum (mci, md5sum)
    class(mci_t), intent(inout) :: mci
    character(32), intent(in) :: md5sum
    mci%md5sum = md5sum
  end subroutine mci_set_md5sum

```

Initialize a new integration pass. This is not necessarily meaningful, so we provide an empty base method. The `mci_vamp` implementation overrides this.

```

<MCI base: mci: TBP>+≡
  procedure :: add_pass => mci_add_pass

<MCI base: sub interfaces>+≡
  module subroutine mci_add_pass (mci, adapt_grids, adapt_weights, final_pass)
    class(mci_t), intent(inout) :: mci
    logical, intent(in), optional :: adapt_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: final_pass
  end subroutine mci_add_pass

<MCI base: procedures>+≡
  module subroutine mci_add_pass (mci, adapt_grids, adapt_weights, final_pass)
    class(mci_t), intent(inout) :: mci
    logical, intent(in), optional :: adapt_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: final_pass
  end subroutine mci_add_pass

```

Allocate an instance with matching type. This must be deferred.

```

<MCI base: mci: TBP>+≡
  procedure (mci_allocate_instance), deferred :: allocate_instance

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_allocate_instance (mci, mci_instance)
      import
      class(mci_t), intent(in) :: mci
      class(mci_instance_t), intent(out), pointer :: mci_instance
    end subroutine mci_allocate_instance
  end interface

```

Import a random-number generator. We transfer the allocation of an existing generator state into the object. The generator state may already be initialized, or we can reset it by its `init` method.

```

<MCI base: mci: TBP>+≡
  procedure :: import_rng => mci_import_rng

<MCI base: sub interfaces>+≡
  module subroutine mci_import_rng (mci, rng)
    class(mci_t), intent(inout) :: mci
    class(rng_t), intent(inout), allocatable :: rng
  end subroutine mci_import_rng

<MCI base: procedures>+≡
  module subroutine mci_import_rng (mci, rng)
    class(mci_t), intent(inout) :: mci
    class(rng_t), intent(inout), allocatable :: rng
    call move_alloc (rng, mci%rng)
  end subroutine mci_import_rng

```

Activate or deactivate the timer.

```

<MCI base: mci: TBP>+≡
  procedure :: set_timer => mci_set_timer

<MCI base: sub interfaces>+≡
  module subroutine mci_set_timer (mci, active)
    class(mci_t), intent(inout) :: mci
    logical, intent(in) :: active
  end subroutine mci_set_timer

<MCI base: procedures>+≡
  module subroutine mci_set_timer (mci, active)
    class(mci_t), intent(inout) :: mci
    logical, intent(in) :: active
    mci%use_timer = active
  end subroutine mci_set_timer

```

Start and stop signal for the timer, if active. The elapsed time can then be retrieved from the MCI record.

```

<MCI base: mci: TBP>+≡
  procedure :: start_timer => mci_start_timer
  procedure :: stop_timer => mci_stop_timer

```

```

<MCI base: sub interfaces>+≡
  module subroutine mci_start_timer (mci)
    class(mci_t), intent(inout) :: mci
  end subroutine mci_start_timer
  module subroutine mci_stop_timer (mci)
    class(mci_t), intent(inout) :: mci
  end subroutine mci_stop_timer
<MCI base: procedures>+≡
  module subroutine mci_start_timer (mci)
    class(mci_t), intent(inout) :: mci
    if (mci%use_timer) call mci%timer%start ()
  end subroutine mci_start_timer

  module subroutine mci_stop_timer (mci)
    class(mci_t), intent(inout) :: mci
    if (mci%use_timer) call mci%timer%stop ()
  end subroutine mci_stop_timer

```

Sampler test. Evaluate the sampler a given number of times. Results are discarded, so we don't need the MCI instance which would record them.

The evaluation channel is iterated, and the x parameters are randomly chosen.

```

<MCI base: mci: TBP>+≡
  procedure :: sampler_test => mci_sampler_test
<MCI base: sub interfaces>+≡
  module subroutine mci_sampler_test (mci, sampler, n_calls)
    class(mci_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_calls
  end subroutine mci_sampler_test
<MCI base: procedures>+≡
  module subroutine mci_sampler_test (mci, sampler, n_calls)
    class(mci_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_calls
    real(default), dimension(:), allocatable :: x_in, f
    real(default), dimension(:,:), allocatable :: x_out
    real(default) :: val
    integer :: i, c
    allocate (x_in (mci%n_dim))
    allocate (f (mci%n_channel))
    allocate (x_out (mci%n_dim, mci%n_channel))
    do i = 1, n_calls
      c = mod (i, mci%n_channel) + 1
      call mci%rng%generate_array (x_in)
      call sampler%evaluate (c, x_in, val, x_out, f)
    end do
  end subroutine mci_sampler_test

```

Integrate: this depends on the implementation. We foresee a pacify flag to take care of small numerical noise on different platforms.

```

<MCI base: mci: TBP>+≡

```

```

    procedure (mci_integrate), deferred :: integrate
  <MCI base: interfaces>+≡
  abstract interface
    subroutine mci_integrate (mci, instance, sampler, &
      n_it, n_calls, results, pacify)
    import
    class(mci_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
  end subroutine mci_integrate
end interface

```

Event generation. Depending on the implementation, event generation may or may not require a previous integration pass.

Instead of a black-box **simulate** method, we require an initializer, a finalizer, and procedures for generating a single event. This allows us to interface simulation event by event from the outside, and it facilitates the further processing of an event after successful generation. For integration, this is not necessary.

The initializer has **intent(inout)** for the **mci** passed object. The reason is that the initializer can read integration results and grids from file, where the results can modify the **mci** record.

```

  <MCI base: mci: TBP>+≡
  procedure (mci_prepare_simulation), deferred :: prepare_simulation
  <MCI base: interfaces>+≡
  abstract interface
    subroutine mci_prepare_simulation (mci)
    import
    class(mci_t), intent(inout) :: mci
  end subroutine mci_prepare_simulation
end interface

```

The generated event will reside in in the **instance** object (overall results and weight) and in the **sampler** object (detailed data). In the real application, we can subsequently call methods of the **sampler** in order to further process the generated event.

The **target** attributes are required by the VAMP implementation, which uses pointers to refer to the instance and sampler objects from within the integration function.

```

  <MCI base: mci: TBP>+≡
  procedure (mci_generate), deferred :: generate_weighted_event
  procedure (mci_generate), deferred :: generate_unweighted_event
  <MCI base: interfaces>+≡
  abstract interface
    subroutine mci_generate (mci, instance, sampler)
    import
    class(mci_t), intent(inout) :: mci

```

```

        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_generate
end interface

```

This is analogous, but we rebuild the event from the information stored in `state` instead of generating it.

Note: currently unused outside of tests, might be deleted later.

```

<MCI base: mci: TBP>+≡
    procedure (mci_rebuild), deferred :: rebuild_event

<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_rebuild (mci, instance, sampler, state)
            import
            class(mci_t), intent(inout) :: mci
            class(mci_instance_t), intent(inout) :: instance
            class(mci_sampler_t), intent(inout) :: sampler
            class(mci_state_t), intent(in) :: state
        end subroutine mci_rebuild
    end interface

```

Pacify: reduce numerical noise. The base implementation does nothing.

```

<MCI base: mci: TBP>+≡
    procedure :: pacify => mci_pacify

<MCI base: sub interfaces>+≡
    module subroutine mci_pacify (object, efficiency_reset, error_reset)
        class(mci_t), intent(inout) :: object
        logical, intent(in), optional :: efficiency_reset, error_reset
    end subroutine mci_pacify

<MCI base: procedures>+≡
    module subroutine mci_pacify (object, efficiency_reset, error_reset)
        class(mci_t), intent(inout) :: object
        logical, intent(in), optional :: efficiency_reset, error_reset
    end subroutine mci_pacify

```

Return the value of the integral, error, efficiency, and time per call.

```

<MCI base: mci: TBP>+≡
    procedure :: get_integral => mci_get_integral
    procedure :: get_error => mci_get_error
    procedure :: get_efficiency => mci_get_efficiency
    procedure :: get_time => mci_get_time

<MCI base: sub interfaces>+≡
    module function mci_get_integral (mci) result (integral)
        class(mci_t), intent(in) :: mci
        real(default) :: integral
    end function mci_get_integral
    module function mci_get_error (mci) result (error)
        class(mci_t), intent(in) :: mci
        real(default) :: error
    end function mci_get_error

```

```

module function mci_get_efficiency (mci) result (efficiency)
  class(mci_t), intent(in) :: mci
  real(default) :: efficiency
end function mci_get_efficiency
module function mci_get_time (mci) result (time)
  class(mci_t), intent(in) :: mci
  real(default) :: time
end function mci_get_time
<MCI base: procedures>+≡
module function mci_get_integral (mci) result (integral)
  class(mci_t), intent(in) :: mci
  real(default) :: integral
  if (mci%integral_known) then
    integral = mci%integral
  else
    call msg_bug ("The integral is unknown. This is presumably a" // &
      "WHIZARD bug.")
  end if
end function mci_get_integral

module function mci_get_error (mci) result (error)
  class(mci_t), intent(in) :: mci
  real(default) :: error
  if (mci%error_known) then
    error = mci%error
  else
    error = 0
  end if
end function mci_get_error

module function mci_get_efficiency (mci) result (efficiency)
  class(mci_t), intent(in) :: mci
  real(default) :: efficiency
  if (mci%efficiency_known) then
    efficiency = mci%efficiency
  else
    efficiency = 0
  end if
end function mci_get_efficiency

module function mci_get_time (mci) result (time)
  class(mci_t), intent(in) :: mci
  real(default) :: time
  if (mci%use_timer) then
    time = mci%timer
  else
    time = 0
  end if
end function mci_get_time

```

Return the MD5 sum of the configuration. This may be overridden in an extension, to return a different MD5 sum.

<MCI base: mci: TBP>+≡


```

    procedure :: get_md5sum => mci_get_md5sum
<MCI base: sub interfaces>+≡
    pure module function mci_get_md5sum (mci) result (md5sum)
        class(mci_t), intent(in) :: mci
        character(32) :: md5sum
    end function mci_get_md5sum
<MCI base: procedures>+≡
    pure module function mci_get_md5sum (mci) result (md5sum)
        class(mci_t), intent(in) :: mci
        character(32) :: md5sum
        md5sum = mci%md5sum
    end function mci_get_md5sum

```

21.1.2 MCI instance

The base type contains an array of channel weights. The value `mci_weight` is the combined MCI weight that corresponds to a particular sampling point.

For convenience, we also store the `x` and Jacobian values for this sampling point.

```

<MCI base: public>+≡
    public :: mci_instance_t
<MCI base: types>+≡
    type, abstract :: mci_instance_t
        logical :: valid = .false.
        real(default), dimension(:), allocatable :: w
        real(default), dimension(:), allocatable :: f
        real(default), dimension(:,:), allocatable :: x
        integer :: selected_channel = 0
        real(default) :: mci_weight = 0
        real(default) :: integrand = 0
        logical :: negative_weights = .false.
        integer :: n_dropped = 0
    contains
        <MCI base: mci instance: TBP>
    end type mci_instance_t

```

Output: deferred

```

<MCI base: mci instance: TBP>≡
    procedure (mci_instance_write), deferred :: write
<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_instance_write (object, unit, pacify)
            import
            class(mci_instance_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: pacify
        end subroutine mci_instance_write
    end interface

```

A finalizer, just in case.

```

<MCI base: mci_instance: TBP>+≡
  procedure (mci_instance_final), deferred :: final

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_instance_final (object)
      import
      class(mci_instance_t), intent(inout) :: object
    end subroutine mci_instance_final
  end interface

```

Init: basic initializer for the arrays, otherwise deferred. Assigning the mci object is also deferred, because it depends on the concrete type.

The weights are initialized with a uniform normalized value.

```

<MCI base: mci_instance: TBP>+≡
  procedure (mci_instance_base_init), deferred :: init
  procedure :: base_init => mci_instance_base_init

<MCI base: sub interfaces>+≡
  module subroutine mci_instance_base_init (mci_instance, mci)
    class(mci_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
  end subroutine mci_instance_base_init

<MCI base: procedures>+≡
  module subroutine mci_instance_base_init (mci_instance, mci)
    class(mci_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
    allocate (mci_instance%w (mci%n_channel))
    allocate (mci_instance%f (mci%n_channel))
    allocate (mci_instance%x (mci%n_dim, mci%n_channel))
    if (mci%n_channel > 0) then
      call mci_instance%set_channel_weights &
        (spread (1._default, dim=1, ncopies=mci%n_channel))
    end if
    mci_instance%f = 0
    mci_instance%x = 0
  end subroutine mci_instance_base_init

```

Explicitly set the array of channel weights.

```

<MCI base: mci_instance: TBP>+≡
  procedure :: set_channel_weights => mci_instance_set_channel_weights

<MCI base: sub interfaces>+≡
  module subroutine mci_instance_set_channel_weights &
    (mci_instance, weights, sum_non_zero)
    class(mci_instance_t), intent(inout) :: mci_instance
    real(default), dimension(:), intent(in) :: weights
    logical, intent(out), optional :: sum_non_zero
  end subroutine mci_instance_set_channel_weights

<MCI base: procedures>+≡
  module subroutine mci_instance_set_channel_weights &
    (mci_instance, weights, sum_non_zero)

```

```

class(mci_instance_t), intent(inout) :: mci_instance
real(default), dimension(:), intent(in) :: weights
logical, intent(out), optional :: sum_non_zero
real(default) :: wsum
wsum = sum (weights)
if (wsum /= 0) then
    mci_instance%w = weights / wsum
    if (present (sum_non_zero)) sum_non_zero = .true.
else
    if (present (sum_non_zero)) sum_non_zero = .false.
    call msg_warning ("MC sampler initialization:&
    & sum of channel weights is zero")
end if
end subroutine mci_instance_set_channel_weights

```

Compute the overall weight factor for a configuration of x values and Jacobians f . The x values come in `n_channel` rows with `n_dim` entries each. The f factors constitute an array with `n_channel` entries.

We assume that the x and f arrays are already stored inside the MC instance. The result is also stored there.

(MCI base: mci_instance: TBP)+≡

```

procedure (mci_instance_compute_weight), deferred :: compute_weight

```

(MCI base: interfaces)+≡

```

abstract interface
    subroutine mci_instance_compute_weight (mci, c)
    import
    class(mci_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
    end subroutine mci_instance_compute_weight
end interface

```

Record the integrand as returned by the sampler. Depending on the implementation, this may merely copy the value, or do more complicated things.

We may need the MCI weight for the actual computations, so this should be called after the previous routine.

(MCI base: mci_instance: TBP)+≡

```

procedure (mci_instance_record_integrand), deferred :: record_integrand

```

(MCI base: interfaces)+≡

```

abstract interface
    subroutine mci_instance_record_integrand (mci, integrand)
    import
    class(mci_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    end subroutine mci_instance_record_integrand
end interface

```

Sample a point directly: evaluate the sampler, then compute the weight and the weighted integrand. Finally, record the integrand within the MCI instance.

If a signal (interrupt) was raised recently, we abort the calculation before entering the sampler. Thus, a previous calculation will have completed and any

data are already recorded, but any new point can be discarded. If the `abort` flag is present, we may delay the interrupt, so we can do some cleanup.

```

(MCI base: mci instance: TBP)+≡
  procedure :: evaluate => mci_instance_evaluate

(MCI base: sub interfaces)+≡
  module subroutine mci_instance_evaluate (mci, sampler, c, x)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x
  end subroutine mci_instance_evaluate

(MCI base: procedures)+≡
  module subroutine mci_instance_evaluate (mci, sampler, c, x)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x
    real(default) :: val
    call sampler%evaluate (c, x, val, mci%x, mci%f)
    mci%valid = sampler%is_valid ()
    if (mci%valid) then
      call mci%compute_weight (c)
      call mci%record_integrand (val)
    end if
  end subroutine mci_instance_evaluate

```

Initiate and terminate simulation. In contrast to integration, we implement these as methods of the process instance, since the `mci` configuration object is unchanged.

The safety factor reduces the acceptance probability for unweighted events. The implementation of this feature depends on the concrete type.

```

(MCI base: mci instance: TBP)+≡
  procedure (mci_instance_init_simulation), deferred :: init_simulation
  procedure (mci_instance_final_simulation), deferred :: final_simulation

(MCI base: interfaces)+≡
  abstract interface
    subroutine mci_instance_init_simulation (instance, safety_factor)
      import
      class(mci_instance_t), intent(inout) :: instance
      real(default), intent(in), optional :: safety_factor
    end subroutine mci_instance_init_simulation
  end interface

  abstract interface
    subroutine mci_instance_final_simulation (instance)
      import
      class(mci_instance_t), intent(inout) :: instance
    end subroutine mci_instance_final_simulation
  end interface

```

Assuming that the sampler is in a completely defined state, just extract the data that `evaluate` would compute. Also record the integrand.

```

(MCI base: mci instance: TBP)+≡
  procedure :: fetch => mci_instance_fetch

(MCI base: sub interfaces)+≡
  module subroutine mci_instance_fetch (mci, sampler, c)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(in) :: sampler
    integer, intent(in) :: c
  end subroutine mci_instance_fetch

(MCI base: procedures)+≡
  module subroutine mci_instance_fetch (mci, sampler, c)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(in) :: sampler
    integer, intent(in) :: c
    real(default) :: val
    mci%valid = sampler%is_valid ()
    if (mci%valid) then
      call sampler%fetch (val, mci%x, mci%f)
      call mci%compute_weight (c)
      call mci%record_integrand (val)
    end if
  end subroutine mci_instance_fetch

```

The value, i.e., the weighted integrand, is the integrand (which should be taken as-is from the sampler) multiplied by the MCI weight.

```

(MCI base: mci instance: TBP)+≡
  procedure :: get_value => mci_instance_get_value

(MCI base: sub interfaces)+≡
  module function mci_instance_get_value (mci) result (value)
    class(mci_instance_t), intent(in) :: mci
    real(default) :: value
  end function mci_instance_get_value

(MCI base: procedures)+≡
  module function mci_instance_get_value (mci) result (value)
    class(mci_instance_t), intent(in) :: mci
    real(default) :: value
    if (mci%valid) then
      value = mci%integrand * mci%mci_weight
    else
      value = 0
    end if
  end function mci_instance_get_value

```

This is an extra routine. By default, the event weight is equal to the value returned by the previous routine. However, if we select a channel for event generation not just based on the channel weights, the event weight has to account for this bias, so the event weight that applies to event generation is different. In that case, we should override the default routine.

```

(MCI base: mci instance: TBP)+≡
  procedure :: get_event_weight => mci_instance_get_value

```

Excess weight can occur during unweighted event generation, if the assumed maximum value of the integrand is too small. This excess should be normalized in the same way as the event weight above (which for unweighted events becomes unity).

```

(MCI base: mci instance: TBP)+≡
  procedure (mci_instance_get_event_excess), deferred :: get_event_excess

(MCI base: interfaces)+≡
  abstract interface
    function mci_instance_get_event_excess (mci) result (excess)
      import
      class(mci_instance_t), intent(in) :: mci
      real(default) :: excess
    end function mci_instance_get_event_excess
  end interface

```

Dropped events (i.e., events with zero weight that are not retained) are counted within the `mci_instance` object.

```

(MCI base: mci instance: TBP)+≡
  procedure :: get_n_event_dropped => mci_instance_get_n_event_dropped
  procedure :: reset_n_event_dropped => mci_instance_reset_n_event_dropped
  procedure :: record_event_dropped => mci_instance_record_event_dropped

(MCI base: sub interfaces)+≡
  module function mci_instance_get_n_event_dropped (mci) result (n_dropped)
    class(mci_instance_t), intent(in) :: mci
    integer :: n_dropped
  end function mci_instance_get_n_event_dropped
  module subroutine mci_instance_reset_n_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
  end subroutine mci_instance_reset_n_event_dropped
  module subroutine mci_instance_record_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
  end subroutine mci_instance_record_event_dropped

(MCI base: procedures)+≡
  module function mci_instance_get_n_event_dropped (mci) result (n_dropped)
    class(mci_instance_t), intent(in) :: mci
    integer :: n_dropped
    n_dropped = mci%n_dropped
  end function mci_instance_get_n_event_dropped

  module subroutine mci_instance_reset_n_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
    mci%n_dropped = 0
  end subroutine mci_instance_reset_n_event_dropped

  module subroutine mci_instance_record_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
    mci%n_dropped = mci%n_dropped + 1
  end subroutine mci_instance_record_event_dropped

```

21.1.3 MCI state

This object can hold the relevant information that allows us to reconstruct the MCI instance without re-evaluating the sampler completely.

We store the `x_in` MC input parameter set, which coincides with the section of the complete `x` array that belongs to a particular channel. We also store the MC function value. When we want to reconstruct the state, we can use the input array to recover the complete `x` and `f` arrays (i.e., the kinematics), but do not need to recompute the MC function value (the dynamics).

The `mci_state_t` may be extended, to allow storing/recalling more information. In that case, we would override the type-bound procedures. However, the base type is also a concrete type and self-contained.

```

<MCI base: public>+≡
    public :: mci_state_t

<MCI base: types>+≡
    type :: mci_state_t
        integer :: selected_channel = 0
        real(default), dimension(:), allocatable :: x_in
        real(default) :: val
    contains
        <MCI base: mci state: TBP>
    end type mci_state_t

```

Output:

```

<MCI base: mci state: TBP>≡
    procedure :: write => mci_state_write

<MCI base: sub interfaces>+≡
    module subroutine mci_state_write (object, unit)
        class(mci_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine mci_state_write

<MCI base: procedures>+≡
    module subroutine mci_state_write (object, unit)
        class(mci_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "MCI state:"
        write (u, "(3x,A,I0)") "Channel   = ", object%selected_channel
        write (u, "(3x,A,999(1x,F12.10))") "x (in)    = ", object%x_in
        write (u, "(3x,A,ES19.12)") "Integrand = ", object%val
    end subroutine mci_state_write

```

To store the object, we take the relevant section of the `x` array. The channel used for storing data is taken from the `instance` object, but it could be arbitrary in principle.

```

<MCI base: mci instance: TBP>+≡
    procedure :: store => mci_instance_store

```

```

<MCI base: sub interfaces>+≡
  module subroutine mci_instance_store (mci, state)
    class(mci_instance_t), intent(in) :: mci
    class(mci_state_t), intent(out) :: state
  end subroutine mci_instance_store

```

```

<MCI base: procedures>+≡
  module subroutine mci_instance_store (mci, state)
    class(mci_instance_t), intent(in) :: mci
    class(mci_state_t), intent(out) :: state
    state%selected_channel = mci%selected_channel
    allocate (state%x_in (size (mci%x, 1)))
    state%x_in = mci%x(:,mci%selected_channel)
    state%val = mci%integrand
  end subroutine mci_instance_store

```

Recalling the state, we must consult the sampler in order to fully reconstruct the x and f arrays. The integrand value is known, and we also give it to the sampler, bypassing evaluation.

The final steps are equivalent to the `evaluate` method above.

```

<MCI base: mci instance: TBP>+≡
  procedure :: recall => mci_instance_recall

```

```

<MCI base: sub interfaces>+≡
  module subroutine mci_instance_recall (mci, sampler, state)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
  end subroutine mci_instance_recall

```

```

<MCI base: procedures>+≡
  module subroutine mci_instance_recall (mci, sampler, state)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    if (size (state%x_in) == size (mci%x, 1) &
        .and. state%selected_channel <= size (mci%x, 2)) then
      call sampler%rebuild (state%selected_channel, &
        state%x_in, state%val, mci%x, mci%f)
      call mci%compute_weight (state%selected_channel)
      call mci%record_integrand (state%val)
    else
      call msg_fatal ("Recalling event: mismatch in channel or dimension")
    end if
  end subroutine mci_instance_recall

```

21.1.4 MCI sampler

A sampler is an object that implements a multi-channel parameterization of the unit hypercube. Specifically, it is able to compute, given a channel and a set of x MC parameter values, the complete set of x values and associated Jacobian factors f for all channels.

Furthermore, the sampler should return a single real value, the integrand, for the given point in the hypercube.

It must implement a method `evaluate` for performing the above computations.

```

<MCI base: public>+≡
  public :: mci_sampler_t
<MCI base: types>+≡
  type, abstract :: mci_sampler_t
  contains
    <MCI base: mci_sampler: TBP>
  end type mci_sampler_t

```

Output, deferred to the implementation.

```

<MCI base: mci_sampler: TBP>≡
  procedure (mci_sampler_write), deferred :: write
<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_sampler_write (object, unit, testflag)
      import
      class(mci_sampler_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: testflag
    end subroutine mci_sampler_write
  end interface

```

The evaluation routine. Input is the channel index `c` and the one-dimensional parameter array `x_in`. Output are the integrand value `val`, the two-dimensional parameter array `x` and the Jacobian array `f`.

```

<MCI base: mci_sampler: TBP>+≡
  procedure (mci_sampler_evaluate), deferred :: evaluate
<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_sampler_evaluate (sampler, c, x_in, val, x, f)
      import
      class(mci_sampler_t), intent(inout) :: sampler
      integer, intent(in) :: c
      real(default), dimension(:), intent(in) :: x_in
      real(default), intent(out) :: val
      real(default), dimension(:,:), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_evaluate
  end interface

```

Query the validity of the sampling point. Can be called after `evaluate`.

```

<MCI base: mci_sampler: TBP>+≡
  procedure (mci_sampler_is_valid), deferred :: is_valid
<MCI base: interfaces>+≡
  abstract interface
    function mci_sampler_is_valid (sampler) result (valid)

```

```

import
class(mci_sampler_t), intent(in) :: sampler
logical :: valid
end function mci_sampler_is_valid
end interface

```

The shortcut. Again, the channel index `c` and the parameter array `x_in` are input. However, we also provide the integrand value `val`, and we just require that the complete parameter array `x` and Jacobian array `f` are recovered.

```

⟨MCI base: mci_sampler: TBP⟩+≡
  procedure (mci_sampler_rebuild), deferred :: rebuild
⟨MCI base: interfaces⟩+≡
  abstract interface
    subroutine mci_sampler_rebuild (sampler, c, x_in, val, x, f)
      import
      class(mci_sampler_t), intent(inout) :: sampler
      integer, intent(in) :: c
      real(default), dimension(:), intent(in) :: x_in
      real(default), intent(in) :: val
      real(default), dimension(:, :), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_rebuild
  end interface

```

This routine should extract the important data from a sampler that has been filled by other means. We fetch the integrand value `val`, the two-dimensional parameter array `x` and the Jacobian array `f`.

```

⟨MCI base: mci_sampler: TBP⟩+≡
  procedure (mci_sampler_fetch), deferred :: fetch
⟨MCI base: interfaces⟩+≡
  abstract interface
    subroutine mci_sampler_fetch (sampler, val, x, f)
      import
      class(mci_sampler_t), intent(in) :: sampler
      real(default), intent(out) :: val
      real(default), dimension(:, :), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_fetch
  end interface

```

21.1.5 Results record

This is an abstract type which allows us to implement callback: each integration results can optionally be recorded to an instance of this object. The actual object may store a new result, average results, etc. It may also display a result on-line or otherwise, whenever the `record` method is called.

```

⟨MCI base: public⟩+≡
  public :: mci_results_t

```

```

<MCI base: types>+≡
  type, abstract :: mci_results_t
  contains
    <MCI base: mci results: TBP>
  end type mci_results_t

```

The output routine is deferred. We provide an extra `verbose` flag, which could serve any purpose.

```

<MCI base: mci results: TBP>≡
  procedure (mci_results_write), deferred :: write
  procedure (mci_results_write_verbose), deferred :: write_verbose
<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_results_write (object, unit, suppress)
      import
        class(mci_results_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: suppress
    end subroutine mci_results_write

    subroutine mci_results_write_verbose (object, unit)
      import
        class(mci_results_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine mci_results_write_verbose
  end interface

```

This is the generic `record` method, which can be called directly from the integrator. The `record_extended` procedure store additionally the valid calls, positive and negative efficiency.

```

<MCI base: mci results: TBP>+≡
  generic :: record => record_simple, record_extended
  procedure (mci_results_record_simple), deferred :: record_simple
  procedure (mci_results_record_extended), deferred :: record_extended
<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_results_record_simple (object, n_it, &
      n_calls, integral, error, efficiency, chain_weights, suppress)
      import
        class(mci_results_t), intent(inout) :: object
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        real(default), intent(in) :: integral
        real(default), intent(in) :: error
        real(default), intent(in) :: efficiency
        real(default), dimension(:), intent(in), optional :: chain_weights
        logical, intent(in), optional :: suppress
    end subroutine mci_results_record_simple

    subroutine mci_results_record_extended (object, n_it, n_calls,&
      & n_calls_valid, integral, error, efficiency_pos,&
      & efficiency_neg, chain_weights, suppress)

```

```

import
class(mci_results_t), intent(inout) :: object
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
integer, intent(in) :: n_calls_valid
real(default), intent(in) :: integral
real(default), intent(in) :: error
real(default), intent(in) :: efficiency
real(default), intent(in) :: efficiency_pos
real(default), intent(in) :: efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
end subroutine mci_results_record_extended
end interface

```

21.1.6 Unit tests

Test module, followed by the corresponding implementation module.

<mci_base_ut.f90>≡

<File header>

```

module mci_base_ut
  use unit_tests
  use mci_base_uti

```

<Standard module head>

<MCI base: public test>

<MCI base: public test auxiliary>

contains

<MCI base: test driver>

```

end module mci_base_ut

```

<mci_base_uti.f90>≡

<File header>

```

module mci_base_uti

```

<Use kinds>

```

  use io_units
  use diagnostics
  use phs_base
  use rng_base

```

```

  use mci_base

```

```

  use rng_base_ut, only: rng_test_t

```

<Standard module head>

```

    <MCI base: public test auxiliary>

    <MCI base: test declarations>

    <MCI base: test types>

contains

    <MCI base: tests>

end module mci_base_util

API: driver for the unit tests below.
<MCI base: public test>≡
    public :: mci_base_test

<MCI base: test driver>≡
    subroutine mci_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <MCI base: execute tests>
    end subroutine mci_base_test

```

Test implementation of the configuration type

The concrete type contains the number of requested calls and the integral result, to be determined.

The `max_factor` entry is set for the actual test integration, where the integrand is not unity but some other constant value. This value should be set here, such that the actual maximum of the integrand is known when vetoing unweighted events.

```

<MCI base: public test auxiliary>≡
    public :: mci_test_t

<MCI base: test types>≡
    type, extends (mci_t) :: mci_test_t
        integer :: divisions = 0
        integer :: tries = 0
        real(default) :: max_factor = 1
    contains
        procedure :: final => mci_test_final
        procedure :: write => mci_test_write
        procedure :: startup_message => mci_test_startup_message
        procedure :: write_log_entry => mci_test_write_log_entry
        procedure :: compute_md5sum => mci_test_compute_md5sum
        procedure :: declare_flat_dimensions => mci_test_ignore_flat_dimensions
        procedure :: declare_equivalences => mci_test_ignore_equivalences
        procedure :: set_divisions => mci_test_set_divisions
        procedure :: set_max_factor => mci_test_set_max_factor
        procedure :: allocate_instance => mci_test_allocate_instance
        procedure :: integrate => mci_test_integrate
        procedure :: prepare_simulation => mci_test_ignore_prepare_simulation

```

```

        procedure :: generate_weighted_event => mci_test_generate_weighted_event
        procedure :: generate_unweighted_event => &
            mci_test_generate_unweighted_event
        procedure :: rebuild_event => mci_test_rebuild_event
    end type mci_test_t

```

Finalizer: base version is sufficient

```

<MCI base: tests>+≡
    subroutine mci_test_final (object)
        class(mci_test_t), intent(inout) :: object
        call object%base_final ()
    end subroutine mci_test_final

```

Output: trivial

```

<MCI base: tests>+≡
    subroutine mci_test_write (object, unit, pacify, md5sum_version)
        class(mci_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Test integrator:"
        call object%base_write (u, pacify, md5sum_version)
        if (object%divisions /= 0) then
            write (u, "(3x,A,I0)") "Number of divisions = ", object%divisions
        end if
        if (allocated (object%rng)) call object%rng%write (u)
    end subroutine mci_test_write

```

Short version.

```

<MCI base: tests>+≡
    subroutine mci_test_startup_message (mci, unit, n_calls)
        class(mci_test_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
        call mci%base_startup_message (unit = unit, n_calls = n_calls)
        write (msg_buffer, "(A,1x,I0,1x,A)") &
            "Integrator: Test:", mci%divisions, "divisions"
        call msg_message (unit = unit)
    end subroutine mci_test_startup_message

```

Log entry: nothing.

```

<MCI base: tests>+≡
    subroutine mci_test_write_log_entry (mci, u)
        class(mci_test_t), intent(in) :: mci
        integer, intent(in) :: u
    end subroutine mci_test_write_log_entry

```

Compute MD5 sum: nothing.

```

<MCI base: tests>+≡
    subroutine mci_test_compute_md5sum (mci, pacify)

```

```

        class(mci_test_t), intent(inout) :: mci
        logical, intent(in), optional :: pacify
    end subroutine mci_test_compute_md5sum

```

This is a no-op for the test integrator.

```

<MCI base: tests>+≡
    subroutine mci_test_ignore_flat_dimensions (mci, dim_flat)
        class(mci_test_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_test_ignore_flat_dimensions

```

Ditto.

```

<MCI base: tests>+≡
    subroutine mci_test_ignore_equivalences (mci, channel, dim_offset)
        class(mci_test_t), intent(inout) :: mci
        type(phs_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_test_ignore_equivalences

```

Set the number of divisions to a nonzero value.

```

<MCI base: tests>+≡
    subroutine mci_test_set_divisions (object, divisions)
        class(mci_test_t), intent(inout) :: object
        integer, intent(in) :: divisions
        object%divisions = divisions
    end subroutine mci_test_set_divisions

```

Set the maximum factor (default is 1).

```

<MCI base: tests>+≡
    subroutine mci_test_set_max_factor (object, max_factor)
        class(mci_test_t), intent(inout) :: object
        real(default), intent(in) :: max_factor
        object%max_factor = max_factor
    end subroutine mci_test_set_max_factor

```

Allocate instance with matching type.

```

<MCI base: tests>+≡
    subroutine mci_test_allocate_instance (mci, mci_instance)
        class(mci_test_t), intent(in) :: mci
        class(mci_instance_t), intent(out), pointer :: mci_instance
        allocate (mci_test_instance_t :: mci_instance)
    end subroutine mci_test_allocate_instance

```

Integrate: sample at the midpoints of uniform bits and add the results. We implement this for one and for two dimensions. In the latter case, we scan over two channels and multiply with the channel weights.

The arguments `n_it` and `n_calls` are ignored in this implementations.

The test integrator does not set error or efficiency, so those will remain undefined.

```

<MCI base: tests>+≡

```

```

subroutine mci_test_integrate (mci, instance, sampler, &
    n_it, n_calls, results, pacify)
    class(mci_test_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
    real(default), dimension(:), allocatable :: integral
    real(default), dimension(:), allocatable :: x
    integer :: i, j, c
    select type (instance)
    type is (mci_test_instance_t)
        allocate (integral (mci%n_channel))
        integral = 0
        allocate (x (mci%n_dim))
        select case (mci%n_dim)
        case (1)
            do c = 1, mci%n_channel
                do i = 1, mci%divisions
                    x(1) = (i - 0.5_default) / mci%divisions
                    call instance%evaluate (sampler, c, x)
                    integral(c) = integral(c) + instance%get_value ()
                end do
            end do
            mci%integral = dot_product (instance%w, integral) &
                / mci%divisions
            mci%integral_known = .true.
        case (2)
            do c = 1, mci%n_channel
                do i = 1, mci%divisions
                    x(1) = (i - 0.5_default) / mci%divisions
                do j = 1, mci%divisions
                    x(2) = (j - 0.5_default) / mci%divisions
                    call instance%evaluate (sampler, c, x)
                    integral(c) = integral(c) + instance%get_value ()
                end do
            end do
            mci%integral = dot_product (instance%w, integral) &
                / mci%divisions / mci%divisions
            mci%integral_known = .true.
        end select
        if (present (results)) then
            call results%record (n_it, n_calls, &
                mci%integral, mci%error, &
                efficiency = 0._default)
        end if
    end select
end subroutine mci_test_integrate

```

Simulation initializer and finalizer: nothing to do here.

(MCI base: tests)+≡


```

subroutine mci_test_ignore_prepare_simulation (mci)
  class(mci_test_t), intent(inout) :: mci
end subroutine mci_test_ignore_prepare_simulation

```

Event generator. We use mock random numbers for first selecting the channel and then setting the x values. The results reside in the state of `instance` and `sampler`.

```

<MCI base: tests>+≡
subroutine mci_test_generate_weighted_event (mci, instance, sampler)
  class(mci_test_t), intent(inout) :: mci
  class(mci_instance_t), intent(inout), target :: instance
  class(mci_sampler_t), intent(inout), target :: sampler
  real(default) :: r
  real(default), dimension(:), allocatable :: x
  integer :: c
  select type (instance)
  type is (mci_test_instance_t)
    allocate (x (mci%n_dim))
    select case (mci%n_channel)
    case (1)
      c = 1
      call mci%rng%generate (x(1))
    case (2)
      call mci%rng%generate (r)
      if (r < instance%w(1)) then
        c = 1
      else
        c = 2
      end if
      call mci%rng%generate (x)
    end select
    call instance%evaluate (sampler, c, x)
  end select
end subroutine mci_test_generate_weighted_event

```

For unweighted events, we generate weighted events and apply a simple rejection step to the relative event weight, until an event passes.

(This might result in an endless loop if we happen to be in sync with the mock random generator cycle. Therefore, limit the number of tries.)

```

<MCI base: tests>+≡
subroutine mci_test_generate_unweighted_event (mci, instance, sampler)
  class(mci_test_t), intent(inout) :: mci
  class(mci_instance_t), intent(inout), target :: instance
  class(mci_sampler_t), intent(inout), target :: sampler
  real(default) :: r
  integer :: i
  select type (instance)
  type is (mci_test_instance_t)
    mci%tries = 0
    do i = 1, 10
      call mci%generate_weighted_event (instance, sampler)
      mci%tries = mci%tries + 1
      call mci%rng%generate (r)
    end do
  end select
end subroutine mci_test_generate_unweighted_event

```

```

        if (r < instance%rel_value) exit
      end do
    end select
  end subroutine mci_test_generate_unweighted_event

```

Here, we rebuild the event from the state without consulting the rng.

```

<MCI base: tests>+≡
  subroutine mci_test_rebuild_event (mci, instance, sampler, state)
    class(mci_test_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    select type (instance)
    type is (mci_test_instance_t)
      call instance%recall (sampler, state)
    end select
  end subroutine mci_test_rebuild_event

```

Instance of the test MCI type

This instance type simulates the VAMP approach. We implement the VAMP multi-channel formula, but keep the channel-specific probability functions g_i smooth and fixed. We also keep the weights fixed.

The setup is as follows: we have n mappings of the unit hypercube

$$x = x(x^{(k)}) \quad \text{where } x = (x_1, \dots). \quad (21.1)$$

The Jacobian factors are the determinants

$$f^{(k)}(x^{(k)}) = \left| \frac{\partial x}{\partial x^{(k)}} \right| \quad (21.2)$$

We introduce arbitrary probability functions

$$g^{(k)}(x^{(k)}) \quad \text{with} \quad \int dx^{(k)} g^{(k)}(x^{(k)}) = 1 \quad (21.3)$$

and weights

$$w_k \quad \text{with} \quad \sum_k w_k = 1 \quad (21.4)$$

and construct the joint probability function

$$g(x) = \sum_k w_k \frac{g^{(k)}(x^{(k)}(x))}{f^{(k)}(x^{(k)}(x))} \quad (21.5)$$

which also satisfies

$$\int g(x) dx = 1. \quad (21.6)$$

The algorithm implements a resolution of unity as follows

$$\begin{aligned}
1 &= \int dx = \int \frac{g(x)}{g(x)} dx \\
&= \sum w_k \int \frac{g^{(k)}(x^{(k)}(x))}{f^{(k)}(x^{(k)}(x))} \frac{dx}{g(x)} \\
&= \sum w_k \int g^{(k)}(x^{(k)}) \frac{dx^{(k)}}{g(x(x^{(k)}))}
\end{aligned} \tag{21.7}$$

where each of the integrals in the sum is evaluated using the channel-specific variables $x^{(k)}$.

We provide two examples: (1) trivial with one channel, one dimension, and all functions unity and (2) two channels and two dimensions with

$$\begin{aligned}
x(x^{(1)}) &= (x_1^{(1)}, x_2^{(1)}) \\
x(x^{(2)}) &= (x_1^{(2)2}, x_2^{(2)})
\end{aligned} \tag{21.8}$$

hence

$$f^{(1)} \equiv 1, \quad f^{(2)}(x^{(2)}) = 2x_1^{(2)} \tag{21.9}$$

The probability functions are

$$g^{(1)} \equiv 1, \quad g^{(2)}(x^{(2)}) = 2x_2^{(2)} \tag{21.10}$$

In the concrete implementation of the integrator instance we store values for the channel probabilities g_i and the accumulated probability g .

We also store the result (product of integrand and MCI weight), the expected maximum for the result in each channel.

```

<XXX MCI base: public>≡
  public :: mci_test_instance_t

<MCI base: test types>+≡
  type, extends (mci_instance_t) :: mci_test_instance_t
    type(mci_test_t), pointer :: mci => null ()
    real(default) :: g = 0
    real(default), dimension(:), allocatable :: gi
    real(default) :: value = 0
    real(default) :: rel_value = 0
    real(default), dimension(:), allocatable :: max
  contains
    procedure :: write => mci_test_instance_write
    procedure :: final => mci_test_instance_final
    procedure :: init => mci_test_instance_init
    procedure :: compute_weight => mci_test_instance_compute_weight
    procedure :: record_integrand => mci_test_instance_record_integrand
    procedure :: init_simulation => mci_test_instance_init_simulation
    procedure :: final_simulation => mci_test_instance_final_simulation
    procedure :: get_event_excess => mci_test_instance_get_event_excess
  end type mci_test_instance_t

```

Output: trivial

<MCI base: tests>+≡

```

subroutine mci_test_instance_write (object, unit, pacify)
  class(mci_test_instance_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  integer :: u, c
  u = given_output_unit (unit)
  write (u, "(1x,A,ES13.7)") "Result value = ", object%value
  write (u, "(1x,A,ES13.7)") "Rel. weight = ", object%rel_value
  write (u, "(1x,A,ES13.7)") "Integrand = ", object%integrand
  write (u, "(1x,A,ES13.7)") "MCI weight = ", object%pci_weight
  write (u, "(3x,A,IO)") "c = ", object%selected_channel
  write (u, "(3x,A,ES13.7)") "g = ", object%g
  write (u, "(1x,A)") "Channel parameters:"
  do c = 1, object%pci_n_channel
    write (u, "(1x,IO,A,4(1x,ES13.7))") c, ": w/f/g/m =", &
      object%w(c), object%f(c), object%gi(c), object%max(c)
    write (u, "(4x,A,9(1x,F9.7))") "x =", object%x(:,c)
  end do
end subroutine mci_test_instance_write

```

The finalizer is empty.

<MCI base: tests>+≡

```

subroutine mci_test_instance_final (object)
  class(mci_test_instance_t), intent(inout) :: object
end subroutine mci_test_instance_final

```

Initializer. We make use of the analytical result that the maximum of the weighted integrand, in each channel, is equal to 1 (one-dimensional case) and 2 (two-dimensional case), respectively.

<MCI base: tests>+≡

```

subroutine mci_test_instance_init (mci_instance, mci)
  class(mci_test_instance_t), intent(out) :: mci_instance
  class(mci_t), intent(in), target :: mci
  call mci_instance%base_init (mci)
  select type (mci)
  type is (mci_test_t)
    mci_instance%pci => mci
  end select
  allocate (mci_instance%gi (mci%n_channel))
  mci_instance%gi = 0
  allocate (mci_instance%max (mci%n_channel))
  select case (mci%n_channel)
  case (1)
    mci_instance%max = 1._default
  case (2)
    mci_instance%max = 2._default
  end select
end subroutine mci_test_instance_init

```

Compute weight: we implement the VAMP multi-channel formula. The channel probabilities `gi` are predefined functions.

```

(MCI base: tests)+≡
subroutine mci_test_instance_compute_weight (mci, c)
  class(mci_test_instance_t), intent(inout) :: mci
  integer, intent(in) :: c
  integer :: i
  mci%selected_channel = c
  select case (mci%mci%n_dim)
  case (1)
    mci%gi(1) = 1
  case (2)
    mci%gi(1) = 1
    mci%gi(2) = 2 * mci%x(2,2)
  end select
  mci%g = 0
  do i = 1, mci%mci%n_channel
    mci%g = mci%g + mci%w(i) * mci%gi(i) / mci%f(i)
  end do
  mci%mci_weight = mci%gi(c) / mci%g
end subroutine mci_test_instance_compute_weight

```

Record the integrand. Apply the Jacobian weight to get the absolute value. Divide by the channel maximum and by any overall factor to get the value relative to the maximum.

```

(MCI base: tests)+≡
subroutine mci_test_instance_record_integrand (mci, integrand)
  class(mci_test_instance_t), intent(inout) :: mci
  real(default), intent(in) :: integrand
  mci%integrand = integrand
  mci%value = mci%integrand * mci%mci_weight
  mci%rel_value = mci%value / mci%max(mci%selected_channel) &
    / mci%mci%max_factor
end subroutine mci_test_instance_record_integrand

```

Nothing to do here.

```

(MCI base: tests)+≡
subroutine mci_test_instance_init_simulation (instance, safety_factor)
  class(mci_test_instance_t), intent(inout) :: instance
  real(default), intent(in), optional :: safety_factor
end subroutine mci_test_instance_init_simulation

subroutine mci_test_instance_final_simulation (instance)
  class(mci_test_instance_t), intent(inout) :: instance
end subroutine mci_test_instance_final_simulation

```

Return always zero.

```

(MCI base: tests)+≡
function mci_test_instance_get_event_excess (mci) result (excess)
  class(mci_test_instance_t), intent(in) :: mci
  real(default) :: excess
  excess = 0
end function mci_test_instance_get_event_excess

```

```
end function mci_test_instance_get_event_excess
```

Test sampler

The test sampler implements a fixed configuration, either trivial (one-channel, one-dimension), or slightly nontrivial (two-channel, two-dimension). In the second channel, the first parameter is mapped according to $x_1 = x_1^{(2)2}$, so we have $f^{(2)}(x^{(2)}) = 2x_1^{(2)}$.

For display purposes, we store the return values inside the object. This is not strictly necessary.

```
<MCI base: test types>+≡
type, extends (mci_sampler_t) :: test_sampler_t
  real(default) :: integrand = 0
  integer :: selected_channel = 0
  real(default), dimension(:,:), allocatable :: x
  real(default), dimension(:), allocatable :: f
contains
  procedure :: init => test_sampler_init
  procedure :: write => test_sampler_write
  procedure :: compute => test_sampler_compute
  procedure :: is_valid => test_sampler_is_valid
  procedure :: evaluate => test_sampler_evaluate
  procedure :: rebuild => test_sampler_rebuild
  procedure :: fetch => test_sampler_fetch
end type test_sampler_t
```

```
<MCI base: tests>+≡
subroutine test_sampler_init (sampler, n)
  class(test_sampler_t), intent(out) :: sampler
  integer, intent(in) :: n
  allocate (sampler%x (n, n))
  allocate (sampler%f (n))
end subroutine test_sampler_init
```

Output

```
<MCI base: tests>+≡
subroutine test_sampler_write (object, unit, testflag)
  class(test_sampler_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u, c
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Test sampler:"
  write (u, "(3x,A,ES13.7)") "Integrand = ", object%integrand
  write (u, "(3x,A,I0)") "Channel = ", object%selected_channel
  do c = 1, size (object%f)
    write (u, "(1x,I0,':',1x,A,ES13.7)") c, "f = ", object%f(c)
    write (u, "(4x,A,9(1x,F9.7))") "x =", object%x(:,c)
  end do
end subroutine test_sampler_write
```

Compute x and Jacobians, given the input parameter array. This is called both by `evaluate` and `rebuild`.

```

(MCI base: tests)+≡
subroutine test_sampler_compute (sampler, c, x_in)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  sampler%selected_channel = c
  select case (size (sampler%f))
  case (1)
    sampler%x(:,1) = x_in
    sampler%f = 1
  case (2)
    select case (c)
    case (1)
      sampler%x(:,1) = x_in
      sampler%x(1,2) = sqrt (x_in(1))
      sampler%x(2,2) = x_in(2)
    case (2)
      sampler%x(1,1) = x_in(1) ** 2
      sampler%x(2,1) = x_in(2)
      sampler%x(:,2) = x_in
    end select
    sampler%f(1) = 1
    sampler%f(2) = 2 * sampler%x(1,2)
  end select
end subroutine test_sampler_compute

```

The point is always valid.

```

(MCI base: tests)+≡
function test_sampler_is_valid (sampler) result (valid)
  class(test_sampler_t), intent(in) :: sampler
  logical :: valid
  valid = .true.
end function test_sampler_is_valid

```

The integrand is always equal to 1.

```

(MCI base: tests)+≡
subroutine test_sampler_evaluate (sampler, c, x_in, val, x, f)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call sampler%compute (c, x_in)
  sampler%integrand = 1
  val = sampler%integrand
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_evaluate

```

Construct kinematics from the input x array. Set the integrand instead of evaluating it.

```

<MCI base: tests>+≡
subroutine test_sampler_rebuild (sampler, c, x_in, val, x, f)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(in) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call sampler%compute (c, x_in)
  sampler%integrand = val
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_rebuild

```

Recall contents.

```

<MCI base: tests>+≡
subroutine test_sampler_fetch (sampler, val, x, f)
  class(test_sampler_t), intent(in) :: sampler
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  val = sampler%integrand
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_fetch

```

Test results object

This mock object just stores and displays the current result.

```

<MCI base: test types>+≡
type, extends (mci_results_t) :: mci_test_results_t
  integer :: n_it = 0
  integer :: n_calls = 0
  real(default) :: integral = 0
  real(default) :: error = 0
  real(default) :: efficiency = 0
contains
  <MCI base: mci test results: TBP>
end type mci_test_results_t

```

Output.

```

<MCI base: mci test results: TBP>≡
  procedure :: write => mci_test_results_write
  procedure :: write_verbose => mci_test_results_write_verbose
<MCI base: tests>+≡
subroutine mci_test_results_write (object, unit, suppress)
  class(mci_test_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: suppress

```



```

integer :: u
u = given_output_unit (unit)
write (u, "(3x,A,1x,I0)") "Iterations = ", object%n_it
write (u, "(3x,A,1x,I0)") "Calls      = ", object%n_calls
write (u, "(3x,A,1x,F12.10)") "Integral  = ", object%integral
write (u, "(3x,A,1x,F12.10)") "Error     = ", object%error
write (u, "(3x,A,1x,F12.10)") "Efficiency = ", object%efficiency
end subroutine mci_test_results_write

subroutine mci_test_results_write_verbose (object, unit)
class(mci_test_results_t), intent(in) :: object
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
write (u, "(3x,A,1x,I0)") "Iterations = ", object%n_it
write (u, "(3x,A,1x,I0)") "Calls      = ", object%n_calls
write (u, "(3x,A,1x,F12.10)") "Integral  = ", object%integral
write (u, "(3x,A,1x,F12.10)") "Error     = ", object%error
write (u, "(3x,A,1x,F12.10)") "Efficiency = ", object%efficiency
end subroutine mci_test_results_write_verbose

```

Record result.

(MCI base: mci test results: TBP)+=

```

procedure :: record_simple => mci_test_results_record_simple
procedure :: record_extended => mci_test_results_record_extended

```

(MCI base: tests)+=

```

subroutine mci_test_results_record_simple (object, n_it, n_calls, &
      integral, error, efficiency, chain_weights, suppress)
class(mci_test_results_t), intent(inout) :: object
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
real(default), intent(in) :: integral
real(default), intent(in) :: error
real(default), intent(in) :: efficiency
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
object%n_it = n_it
object%n_calls = n_calls
object%integral = integral
object%error = error
object%efficiency = efficiency
end subroutine mci_test_results_record_simple

subroutine mci_test_results_record_extended (object, n_it, n_calls, &
      & n_calls_valid, integral, error, efficiency, efficiency_pos, &
      & efficiency_neg, chain_weights, suppress)
class(mci_test_results_t), intent(inout) :: object
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
integer, intent(in) :: n_calls_valid
real(default), intent(in) :: integral
real(default), intent(in) :: error
real(default), intent(in) :: efficiency

```

```

real(default), intent(in) :: efficiency_pos
real(default), intent(in) :: efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
object%n_it = n_it
object%n_calls = n_calls
object%integral = integral
object%error = error
object%efficiency = efficiency
end subroutine mci_test_results_record_extended

```

Integrator configuration data

Construct and display a test integrator configuration object.

```

<MCI base: execute tests>≡
  call test (mci_base_1, "mci_base_1", &
    "integrator configuration", &
    u, results)

<MCI base: test declarations>≡
  public :: mci_base_1

<MCI base: tests>+≡
  subroutine mci_base_1 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    real(default) :: integrand

    write (u, "(A)")  "* Test output: mci_base_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test integrator"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_test_t :: mci)
    call mci%set_dimensions (2, 2)

    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    write (u, "(A)")  "* Initialize test sampler"
    write (u, "(A)")

```

```

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

write (u, "(A)")  "* Evaluate sampler for given point and channel"
write (u, "(A)")

call sampler%evaluate (1, [0.25_default, 0.8_default], &
    integrand, mci_instance%x, mci_instance%f)

call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute MCI weight"
write (u, "(A)")

call mci_instance%compute_weight (1)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get integrand and compute weight for another point"
write (u, "(A)")

call mci_instance%evaluate (sampler, 2, [0.5_default, 0.6_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recall results, again"
write (u, "(A)")

call mci_instance%final ()
deallocate (mci_instance)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

call mci_instance%fetch (sampler, 2)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Retrieve value"
write (u, "(A)")

write (u, "(1x,A,ES13.7)")  "Weighted integrand = ", &
    mci_instance%get_value ()

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_1"

```

```
end subroutine mci_base_1
```

Trivial integral

Use the MCI approach to compute a trivial one-dimensional integral.

```
<MCI base: execute tests>+≡
  call test (mci_base_2, "mci_base_2", &
    "integration", &
    u, results)

<MCI base: test declarations>+≡
  public :: mci_base_2

<MCI base: tests>+≡
  subroutine mci_base_2 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_base_2"
    write (u, "(A)")  "* Purpose: perform a test integral"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_test_t :: mci)
    call mci%set_dimensions (1, 1)
    select type (mci)
    type is (mci_test_t)
      call mci%set_divisions (10)
    end select

    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    write (u, "(A)")  "* Initialize test sampler"
    write (u, "(A)")

    allocate (test_sampler_t :: sampler)
    select type (sampler)
    type is (test_sampler_t)
      call sampler%init (1)
    end select

    write (u, "(A)")  "* Integrate"
    write (u, "(A)")
```

```

call mci%integrate (mci_instance, sampler, 0, 0)

call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_2"

end subroutine mci_base_2

```

Nontrivial integral

Use the MCI approach to compute a simple two-dimensional integral with two channels.

```

<MCI base: execute tests>+≡
call test (mci_base_3, "mci_base_3", &
  "integration (two channels)", &
  u, results)

<MCI base: test declarations>+≡
public :: mci_base_3

<MCI base: tests>+≡
subroutine mci_base_3 (u)
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler

  write (u, "(A)")  "* Test output: mci_base_3"
  write (u, "(A)")  "* Purpose: perform a nontrivial test integral"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize integrator"
  write (u, "(A)")

  allocate (mci_test_t :: mci)
  call mci%set_dimensions (2, 2)
  select type (mci)
  type is (mci_test_t)
    call mci%set_divisions (10)
  end select

  write (u, "(A)")  "* Initialize instance"
  write (u, "(A)")

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  write (u, "(A)")  "* Initialize test sampler"

```

```

write (u, "(A)")

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
  call sampler%init (2)
end select

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 0, 0)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with higher resolution"
write (u, "(A)")

select type (mci)
type is (mci_test_t)
  call mci%set_divisions (100)
end select

call mci%integrate (mci_instance, sampler, 0, 0)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_3"

end subroutine mci_base_3

```

Event generation

We generate “random” events, one weighted and one unweighted. The test implementation does not require an integration pass, we can generate events immediately.

```

<MCI base: execute tests>+≡
  call test (mci_base_4, "mci_base_4", &
    "event generation (two channels)", &
    u, results)

<MCI base: test declarations>+≡
  public :: mci_base_4

<MCI base: tests>+≡
  subroutine mci_base_4 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

```

```

class(rng_t), allocatable :: rng

write (u, "(A)")  "* Test output: mci_base_4"
write (u, "(A)")  "* Purpose: generate events"
write (u, "(A)")

write (u, "(A)")  "* Initialize integrator, instance, sampler"
write (u, "(A)")

allocate (mci_test_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_test_t)
    call mci%set_divisions (10)
end select

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

allocate (rng_test_t :: rng)
call mci%import_rng (rng)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call mci%generate_weighted_event (mci_instance, sampler)

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)

select type (mci)
type is (mci_test_t)
    write (u, "(A,I0)")  " Success in try ", mci%tries
    write (u, "(A)")
end select

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

call mci_instance%final ()

```

```

call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_4"

end subroutine mci_base_4

```

Store and recall data

We generate an event and store the relevant data, i.e., the input parameters and the result value for a particular channel. Then we use those data to recover the event, as far as the MCI record is concerned.

```

<MCI base: execute tests>+≡
  call test (mci_base_5, "mci_base_5", &
    "store and recall", &
    u, results)

<MCI base: test declarations>+≡
  public :: mci_base_5

<MCI base: tests>+≡
  subroutine mci_base_5 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng
    class(mci_state_t), allocatable :: state

    write (u, "(A)")  "* Test output: mci_base_5"
    write (u, "(A)")  "* Purpose: store and recall an event"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator, instance, sampler"
    write (u, "(A)")

    allocate (mci_test_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_test_t)
      call mci%set_divisions (10)
    end select

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_t :: sampler)
    select type (sampler)
    type is (test_sampler_t)
      call sampler%init (2)
    end select

    allocate (rng_test_t :: rng)

```



```

call mci%import_rng (rng)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call mci%generate_weighted_event (mci_instance, sampler)

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Store data"
write (u, "(A)")

allocate (state)
call mci_instance%store (state)
call mci_instance%final ()
deallocate (mci_instance)

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recall data and rebuild event"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)
call mci%rebuild_event (mci_instance, sampler, state)

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_5"

end subroutine mci_base_5

```

Chained channels

Chain channels together. In the base configuration, this just fills entries in an extra array (each channel may belong to a chain). In type implementations, this will be used for grouping equivalent channels by keeping their weights equal.

```

(MCI base: execute tests) +=
  call test (mci_base_6, "mci_base_6", &
    "chained channels", &
    u, results)

```

```

<MCI base: test declarations>+≡
    public :: mci_base_6

<MCI base: tests>+≡
    subroutine mci_base_6 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci

        write (u, "(A)")  "* Test output: mci_base_6"
        write (u, "(A)")  "*   Purpose: initialize and display &
            &test integrator with chains"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_test_t :: mci)
        call mci%set_dimensions (1, 5)

        write (u, "(A)")  "* Introduce chains"
        write (u, "(A)")

        call mci%declare_chains ([1, 2, 2, 1, 2])

        call mci%write (u)

        call mci%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: mci_base_6"

    end subroutine mci_base_6

```

Recording results

Compute a simple two-dimensional integral and record the result.

```

<MCI base: execute tests>+≡
    call test (mci_base_7, "mci_base_7", &
        "recording results", &
        u, results)

<MCI base: test declarations>+≡
    public :: mci_base_7

<MCI base: tests>+≡
    subroutine mci_base_7 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(mci_results_t), allocatable :: results

        write (u, "(A)")  "* Test output: mci_base_7"
        write (u, "(A)")  "*   Purpose: perform a nontrivial test integral &

```

```

        &and record results"
write (u, "(A)")

write (u, "(A)")  "* Initialize integrator"
write (u, "(A)")

allocate (mci_test_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_test_t)
    call mci%set_divisions (10)
end select

write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

allocate (mci_test_results_t :: results)

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000, results)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Display results"
write (u, "(A)")

call results%write(u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_7"

end subroutine mci_base_7

```

Timer

Simple checks for the embedded timer.

```

<MCI base: execute tests>+≡
    call test (mci_base_8, "mci_base_8", &
               "timer", &
               u, results)
<MCI base: test declarations>+≡
    public :: mci_base_8
<MCI base: tests>+≡
    subroutine mci_base_8 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci

        real(default) :: dummy

        write (u, "(A)")  "* Test output: mci_base_8"
        write (u, "(A)")  "* Purpose: check timer availability"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator with timer"
        write (u, "(A)")

        allocate (mci_test_t :: mci)
        call mci%set_dimensions (2, 2)
        select type (mci)
        type is (mci_test_t)
            call mci%set_divisions (10)
        end select

        call mci%set_timer (active = .true.)
        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Start timer"
        write (u, "(A)")

        call mci%start_timer ()
        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Stop timer"
        write (u, "(A)")

        call mci%stop_timer ()
        write (u, "(A)")  " (ok)"

        write (u, "(A)")
        write (u, "(A)")  "* Readout"
        write (u, "(A)")

        dummy = mci%get_time ()
        write (u, "(A)")  " (ok)"

        write (u, "(A)")
        write (u, "(A)")  "* Deactivate timer"

```

```

write (u, "(A)")

call mci%set_timer (active = .false.)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_8"

end subroutine mci_base_8

```

21.2 Iterations

This module defines a container for the list of iterations and calls, to be submitted to integration.

```

<iterations.f90>≡
  <File header>

  module iterations

    <Use kinds>
    <Use strings>

    <Standard module head>

    <Iterations: public>

    <Iterations: types>

    interface
    <Iterations: sub interfaces>
    end interface

  end module iterations

<iterations_sub.f90>≡
  <File header>

  submodule (iterations) iterations_s

    use io_units
    use diagnostics

    implicit none

  contains

    <Iterations: procedures>

```

```
end submodule iterations_s
```

21.2.1 The iterations list

Each integration pass has a number of iterations and a number of calls per iteration. The last pass produces the end result; the previous passes are used for adaptation.

The flags `adapt_grid` and `adapt_weight` are used only if `custom_adaptation` is set. Otherwise, default settings are used that depend on the integration pass.

```
<Iterations: types>≡
  type :: iterations_spec_t
    private
    integer :: n_it = 0
    integer :: n_calls = 0
    logical :: custom_adaptation = .false.
    logical :: adapt_grids = .false.
    logical :: adapt_weights = .false.
  end type iterations_spec_t
```

We build up a list of iterations.

```
<Iterations: public>≡
  public :: iterations_list_t

<Iterations: types>+≡
  type :: iterations_list_t
    private
    integer :: n_pass = 0
    type(iterations_spec_t), dimension(:), allocatable :: pass
  contains
    <Iterations: iterations list: TBP>
  end type iterations_list_t
```

Initialize an iterations list. For each pass, we have to specify the number of iterations and calls. We may provide the adaptation conventions explicitly, either as character codes or as logicals.

For passes where the adaptation conventions are not specified, we use the following default setting: adapt weights and grids for all passes except the last one.

```
<Iterations: iterations list: TBP>≡
  procedure :: init => iterations_list_init

<Iterations: sub interfaces>≡
  module subroutine iterations_list_init &
    (it_list, n_it, n_calls, adapt, adapt_code, adapt_grids, adapt_weights)
    class(iterations_list_t), intent(inout) :: it_list
    integer, dimension(:), intent(in) :: n_it, n_calls
    logical, dimension(:), intent(in), optional :: adapt
    type(string_t), dimension(:), intent(in), optional :: adapt_code
    logical, dimension(:), intent(in), optional :: adapt_grids, adapt_weights
  end subroutine iterations_list_init
```

<Iterations: procedures>+≡

```

module subroutine iterations_list_init &
  (it_list, n_it, n_calls, adapt, adapt_code, adapt_grids, adapt_weights)
  class(iterations_list_t), intent(inout) :: it_list
  integer, dimension(:), intent(in) :: n_it, n_calls
  logical, dimension(:), intent(in), optional :: adapt
  type(string_t), dimension(:), intent(in), optional :: adapt_code
  logical, dimension(:), intent(in), optional :: adapt_grids, adapt_weights
  integer :: i
  it_list%n_pass = size (n_it)
  if (allocated (it_list%pass)) deallocate (it_list%pass)
  allocate (it_list%pass (it_list%n_pass))
  it_list%pass%n_it = n_it
  it_list%pass%n_calls = n_calls
  if (present (adapt)) then
    it_list%pass%custom_adaptation = adapt
    do i = 1, it_list%n_pass
      if (adapt(i)) then
        if (verify (adapt_code(i), "wg") /= 0) then
          call msg_error ("iteration specification: " &
            // "adaptation code letters must be 'w' or 'g'")
        end if
        it_list%pass(i)%adapt_grids = scan (adapt_code(i), "g") /= 0
        it_list%pass(i)%adapt_weights = scan (adapt_code(i), "w") /= 0
      end if
    end do
  else if (present (adapt_grids) .and. present (adapt_weights)) then
    it_list%pass%custom_adaptation = .true.
    it_list%pass%adapt_grids = adapt_grids
    it_list%pass%adapt_weights = adapt_weights
  end if
  do i = 1, it_list%n_pass - 1
    if (.not. it_list%pass(i)%custom_adaptation) then
      it_list%pass(i)%adapt_grids = .true.
      it_list%pass(i)%adapt_weights = .true.
    end if
  end do
end subroutine iterations_list_init

```

<Iterations: iterations list: TBP>+≡

```

procedure :: clear => iterations_list_clear

```

<Iterations: sub interfaces>+≡

```

module subroutine iterations_list_clear (it_list)
  class(iterations_list_t), intent(inout) :: it_list
end subroutine iterations_list_clear

```

<Iterations: procedures>+≡

```

module subroutine iterations_list_clear (it_list)
  class(iterations_list_t), intent(inout) :: it_list
  it_list%n_pass = 0
  deallocate (it_list%pass)
end subroutine iterations_list_clear

```

Write the list of iterations.

```

<Iterations: iterations list: TBP>+≡
    procedure :: write => iterations_list_write

<Iterations: sub interfaces>+≡
    module subroutine iterations_list_write (it_list, unit)
        class(iterations_list_t), intent(in) :: it_list
        integer, intent(in), optional :: unit
    end subroutine iterations_list_write

<Iterations: procedures>+≡
    module subroutine iterations_list_write (it_list, unit)
        class(iterations_list_t), intent(in) :: it_list
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A)") char (it_list%to_string ())
    end subroutine iterations_list_write

```

The output as a single-line string.

```

<Iterations: iterations list: TBP>+≡
    procedure :: to_string => iterations_list_to_string

<Iterations: sub interfaces>+≡
    module function iterations_list_to_string (it_list) result (buffer)
        class(iterations_list_t), intent(in) :: it_list
        type(string_t) :: buffer
    end function iterations_list_to_string

<Iterations: procedures>+≡
    module function iterations_list_to_string (it_list) result (buffer)
        class(iterations_list_t), intent(in) :: it_list
        type(string_t) :: buffer
        character(30) :: ibuf
        integer :: i
        buffer = "iterations = "
        if (it_list%n_pass > 0) then
            do i = 1, it_list%n_pass
                if (i > 1) buffer = buffer // ", "
                write (ibuf, "(I0,':',I0)") &
                    it_list%pass(i)%n_it, it_list%pass(i)%n_calls
                buffer = buffer // trim (ibuf)
                if (it_list%pass(i)%custom_adaptation &
                    .or. it_list%pass(i)%adapt_grids &
                    .or. it_list%pass(i)%adapt_weights) then
                    buffer = buffer // ':'
                    if (it_list%pass(i)%adapt_grids) buffer = buffer // "g"
                    if (it_list%pass(i)%adapt_weights) buffer = buffer // "w"
                    buffer = buffer // '"'
                end if
            end do
        else
            buffer = buffer // "[undefined]"
        end if
    end function iterations_list_to_string

```


21.2.2 Tools

Return the total number of passes.

```
<Iterations: iterations list: TBP>+≡
    procedure :: get_n_pass => iterations_list_get_n_pass

<Iterations: sub interfaces>+≡
    module function iterations_list_get_n_pass (it_list) result (n_pass)
        class(iterations_list_t), intent(in) :: it_list
        integer :: n_pass
    end function iterations_list_get_n_pass

<Iterations: procedures>+≡
    module function iterations_list_get_n_pass (it_list) result (n_pass)
        class(iterations_list_t), intent(in) :: it_list
        integer :: n_pass
        n_pass = it_list%n_pass
    end function iterations_list_get_n_pass
```

Return the number of calls for a specific pass.

```
<Iterations: iterations list: TBP>+≡
    procedure :: get_n_calls => iterations_list_get_n_calls

<Iterations: sub interfaces>+≡
    module function iterations_list_get_n_calls (it_list, pass) result (n_calls)
        class(iterations_list_t), intent(in) :: it_list
        integer :: n_calls
        integer, intent(in) :: pass
    end function iterations_list_get_n_calls

<Iterations: procedures>+≡
    module function iterations_list_get_n_calls (it_list, pass) result (n_calls)
        class(iterations_list_t), intent(in) :: it_list
        integer :: n_calls
        integer, intent(in) :: pass
        if (pass <= it_list%n_pass) then
            n_calls = it_list%pass(pass)%n_calls
        else
            n_calls = 0
        end if
    end function iterations_list_get_n_calls

<Iterations: iterations list: TBP>+≡
    procedure :: set_n_calls => iterations_list_set_n_calls

<Iterations: sub interfaces>+≡
    module subroutine iterations_list_set_n_calls (it_list, pass, n_calls)
        class(iterations_list_t), intent(inout) :: it_list
        integer, intent(in) :: pass, n_calls
    end subroutine iterations_list_set_n_calls

<Iterations: procedures>+≡
    module subroutine iterations_list_set_n_calls (it_list, pass, n_calls)
        class(iterations_list_t), intent(inout) :: it_list
        integer, intent(in) :: pass, n_calls
        it_list%pass(pass)%n_calls = n_calls
```

```
end subroutine iterations_list_set_n_calls
```

Get the adaptation mode (automatic/custom) and, for custom adaptation, the flags for a specific pass.

(Iterations: iterations list: TBP)+≡

```
procedure :: adapt_grids => iterations_list_adapt_grids
procedure :: adapt_weights => iterations_list_adapt_weights
```

(Iterations: sub interfaces)+≡

```
module function iterations_list_adapt_grids (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
end function iterations_list_adapt_grids
module function iterations_list_adapt_weights (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
end function iterations_list_adapt_weights
```

(Iterations: procedures)+≡

```
module function iterations_list_adapt_grids (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    flag = it_list%pass(pass)%adapt_grids
  else
    flag = .false.
  end if
end function iterations_list_adapt_grids

module function iterations_list_adapt_weights (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    flag = it_list%pass(pass)%adapt_weights
  else
    flag = .false.
  end if
end function iterations_list_adapt_weights
```

Return the total number of iterations / the iterations for a specific pass.

(Iterations: iterations list: TBP)+≡

```
procedure :: get_n_it => iterations_list_get_n_it
```

(Iterations: sub interfaces)+≡

```
module function iterations_list_get_n_it (it_list, pass) result (n_it)
  class(iterations_list_t), intent(in) :: it_list
  integer :: n_it
  integer, intent(in) :: pass
end function iterations_list_get_n_it
```

```

<Iterations: procedures>+≡
  module function iterations_list_get_n_it (it_list, pass) result (n_it)
    class(iterations_list_t), intent(in) :: it_list
    integer :: n_it
    integer, intent(in) :: pass
    if (pass <= it_list%n_pass) then
      n_it = it_list%pass(pass)%n_it
    else
      n_it = 0
    end if
  end function iterations_list_get_n_it

```

21.2.3 Iteration Multipliers

```

<Iterations: public>+≡
  public :: iteration_multipliers_t

<Iterations: types>+≡
  type :: iteration_multipliers_t
    real(default) :: mult_real = 1._default
    real(default) :: mult_virt = 1._default
    real(default) :: mult_dglap = 1._default
    real(default) :: mult_threshold = 1._default
    integer, dimension(:), allocatable :: n_calls0
  end type iteration_multipliers_t

```

21.2.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<iterations_ut.f90>≡
  <File header>

  module iterations_ut
    use unit_tests
    use iterations_uti

    <Standard module head>

    <Iterations: public test>

    contains

    <Iterations: test driver>

  end module iterations_ut

<iterations_uti.f90>≡
  <File header>

  module iterations_uti

    <Use strings>

```

```

        use iterations

        <Standard module head>

        <Iterations: test declarations>

contains

        <Iterations: tests>

    end module iterations_util

API: driver for the unit tests below.
<Iterations: public test>≡
    public :: iterations_test
<Iterations: test driver>≡
    subroutine iterations_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        <Iterations: execute tests>
    end subroutine iterations_test

```

Empty list

```

<Iterations: execute tests>≡
    call test (iterations_1, "iterations_1", &
        "empty iterations list", &
        u, results)
<Iterations: test declarations>≡
    public :: iterations_1
<Iterations: tests>≡
    subroutine iterations_1 (u)
        integer, intent(in) :: u
        type(iterations_list_t) :: it_list

        write (u, "(A)")  "* Test output: iterations_1"
        write (u, "(A)")  "*   Purpose: display empty iterations list"
        write (u, "(A)")

        call it_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: iterations_1"

    end subroutine iterations_1

```

Fill list

```

<Iterations: execute tests>+≡

```

```

    call test (iterations_2, "iterations_2", &
               "create iterations list", &
               u, results)
<Iterations: test declarations>+≡
    public :: iterations_2
<Iterations: tests>+≡
    subroutine iterations_2 (u)
        integer, intent(in) :: u
        type(iterations_list_t) :: it_list

        write (u, "(A)")  "* Test output: iterations_2"
        write (u, "(A)")  "* Purpose: fill and display iterations list"
        write (u, "(A)")

        write (u, "(A)")  "* Minimal setup (2 passes)"
        write (u, "(A)")

        call it_list%init ([2, 4], [5000, 20000])

        call it_list%write (u)
        call it_list%clear ()

        write (u, "(A)")
        write (u, "(A)")  "* Setup with flags (3 passes)"
        write (u, "(A)")

        call it_list%init ([2, 4, 5], [5000, 20000, 400], &
                           [.false., .true., .true.], &
                           [var_str (""), var_str ("g"), var_str ("wg")])

        call it_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Extract data"
        write (u, "(A)")

        write (u, "(A,I0)") "n_pass = ", it_list%get_n_pass ()
        write (u, "(A)")
        write (u, "(A,I0)") "n_calls(2) = ", it_list%get_n_calls (2)
        write (u, "(A)")
        write (u, "(A,I0)") "n_it(3) = ", it_list%get_n_it (3)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: iterations_2"

    end subroutine iterations_2

```

21.3 Integration results

We record integration results and errors in a dedicated type. This allows us to do further statistics such as weighted average, chi-squared, grouping by integration

passes, etc.

```
<integration_results.f90>≡
  module integration_results

    <Use kinds>
    <Use strings>
    use os_interface
    use mci_base

    <Standard module head>

    <Integration results: public>

    <Integration results: parameters>

    <Integration results: types>

    <Integration results: interfaces>

    interface
    <Integration results: sub interfaces>
    end interface

  end module integration_results
<integration_results_sub.f90>≡
  <File header>

  submodule (integration_results) integration_results_s

    use io_units
    use format_utils, only: mp_format, pac_fmt
    use format_defs, only: FMT_10, FMT_14
    use numeric_utils, only: pacify
    use diagnostics
    use md5

    implicit none

  contains

    <Integration results: procedures>

  end submodule integration_results_s
```

21.3.1 Integration results entry

This object collects the results of an integration pass and makes them available to the outside.

The results object has to distinguish the process type:

We store the process type, the index of the integration pass and the absolute iteration index, the number of iterations contained in this result (for averages), and the integral (cross section or partial width), error estimate, efficiency.

For intermediate results, we set a flag if this result is an improvement w.r.t. previous ones.

The process type indicates decay or scattering. Dummy entries (skipped iterations) have a process type of PRC_UNKNOWN.

The additional information `n_calls_valid`, `efficiency_pos` and `efficiency_neg` are stored, but only used in verbose mode.

```

<Integration results: public>≡
    public :: integration_entry_t

<Integration results: types>≡
    type :: integration_entry_t
        private
        integer :: process_type = PRC_UNKNOWN
        integer :: pass = 0
        integer :: it = 0
        integer :: n_it = 0
        integer :: n_calls = 0
        integer :: n_calls_valid = 0
        logical :: improved = .false.
        real(default) :: integral = 0
        real(default) :: error = 0
        real(default) :: efficiency = 0
        real(default) :: efficiency_pos = 0
        real(default) :: efficiency_neg = 0
        real(default) :: chi2 = 0
        real(default), dimension(:), allocatable :: chain_weights
    contains
    <Integration results: integration entry: TBP>
end type integration_entry_t

```

The possible values of the type indicator:

```

<Integration results: parameters>≡
    integer, parameter, public :: PRC_UNKNOWN = 0
    integer, parameter, public :: PRC_DECAY = 1
    integer, parameter, public :: PRC_SCATTERING = 2

```

Initialize with all relevant data.

```

<Integration results: interfaces>≡
    interface integration_entry_t
        module procedure integration_entry_init
    end interface integration_entry_t

<Integration results: sub interfaces>≡
    module function integration_entry_init (process_type, pass,&
        & it, n_it, n_calls, n_calls_valid, improved, integral, error,&
        & efficiency, efficiency_pos, efficiency_neg, chi2, chain_weights)&
        & result (entry)
    type(integration_entry_t) :: entry
    integer, intent(in) :: process_type, pass, it, n_it, &
        n_calls, n_calls_valid
    logical, intent(in) :: improved
    real(default), intent(in) :: integral, error, efficiency, &

```

```

        efficiency_pos, efficiency_neg
    real(default), intent(in), optional :: chi2
    real(default), dimension(:), intent(in), optional :: chain_weights
end function integration_entry_init

```

(Integration results: procedures)≡

```

module function integration_entry_init (process_type, pass,&
    & it, n_it, n_calls, n_calls_valid, improved, integral, error,&
    & efficiency, efficiency_pos, efficiency_neg, chi2, chain_weights)&
    & result (entry)
type(integration_entry_t) :: entry
integer, intent(in) :: process_type, pass, it, n_it, n_calls, n_calls_valid
logical, intent(in) :: improved
real(default), intent(in) :: integral, error, efficiency, &
    efficiency_pos, efficiency_neg
real(default), intent(in), optional :: chi2
real(default), dimension(:), intent(in), optional :: chain_weights
entry%process_type = process_type
entry%pass = pass
entry%it = it
entry%n_it = n_it
entry%n_calls = n_calls
entry%n_calls_valid = n_calls_valid
entry%improved = improved
entry%integral = integral
entry%error = error
entry%efficiency = efficiency
entry%efficiency_pos = efficiency_pos
entry%efficiency_neg = efficiency_neg
if (present (chi2)) entry%chi2 = chi2
if (present (chain_weights)) then
    allocate (entry%chain_weights (size (chain_weights)))
    entry%chain_weights = chain_weights
end if
end function integration_entry_init

```

Access values, some of them computed on demand:

(Integration results: integration entry: TBP)≡

```

procedure :: get_pass => integration_entry_get_pass
procedure :: get_n_calls => integration_entry_get_n_calls
procedure :: get_n_calls_valid => integration_entry_get_n_calls_valid
procedure :: get_integral => integration_entry_get_integral
procedure :: get_error => integration_entry_get_error
procedure :: get_rel_error => integration_entry_get_relative_error
procedure :: get_accuracy => integration_entry_get_accuracy
procedure :: get_efficiency => integration_entry_get_efficiency
procedure :: get_efficiency_pos => integration_entry_get_efficiency_pos
procedure :: get_efficiency_neg => integration_entry_get_efficiency_neg
procedure :: get_chi2 => integration_entry_get_chi2
procedure :: has_improved => integration_entry_has_improved
procedure :: get_n_groves => integration_entry_get_n_groves

```

(Integration results: sub interfaces)+≡

```

elemental module function integration_entry_get_pass (entry) result (n)
    integer :: n

```



```

    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_pass
elemental module function integration_entry_get_n_calls (entry) result (n)
    integer :: n
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_n_calls
elemental module function integration_entry_get_n_calls_valid &
    (entry) result (n)
    integer :: n
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_n_calls_valid
elemental module function integration_entry_get_integral (entry) result (int)
    real(default) :: int
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_integral
elemental module function integration_entry_get_error (entry) result (err)
    real(default) :: err
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_error
elemental module function integration_entry_get_relative_error &
    (entry) result (err)
    real(default) :: err
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_relative_error
elemental module function integration_entry_get_accuracy &
    (entry) result (acc)
    real(default) :: acc
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_accuracy
elemental module function accuracy (integral, error, n_calls) result (acc)
    real(default) :: acc
    real(default), intent(in) :: integral, error
    integer, intent(in) :: n_calls
end function accuracy
elemental module function integration_entry_get_efficiency &
    (entry) result (eff)
    real(default) :: eff
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_efficiency
elemental module function integration_entry_get_efficiency_pos &
    (entry) result (eff)
    real(default) :: eff
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_efficiency_pos
elemental module function integration_entry_get_efficiency_neg &
    (entry) result (eff)
    real(default) :: eff
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_efficiency_neg
elemental module function integration_entry_get_chi2 (entry) result (chi2)
    real(default) :: chi2
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_chi2
elemental module function integration_entry_has_improved &

```

```

        (entry) result (flag)
    logical :: flag
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_has_improved
elemental module function integration_entry_get_n_groves &
    (entry) result (n_groves)
    integer :: n_groves
    class(integration_entry_t), intent(in) :: entry
end function integration_entry_get_n_groves

<Integration results: procedures>+=
elemental module function integration_entry_get_pass (entry) result (n)
    integer :: n
    class(integration_entry_t), intent(in) :: entry
    n = entry%pass
end function integration_entry_get_pass

elemental module function integration_entry_get_n_calls (entry) result (n)
    integer :: n
    class(integration_entry_t), intent(in) :: entry
    n = entry%n_calls
end function integration_entry_get_n_calls

elemental module function integration_entry_get_n_calls_valid &
    (entry) result (n)
    integer :: n
    class(integration_entry_t), intent(in) :: entry
    n = entry%n_calls_valid
end function integration_entry_get_n_calls_valid

elemental module function integration_entry_get_integral (entry) result (int)
    real(default) :: int
    class(integration_entry_t), intent(in) :: entry
    int = entry%integral
end function integration_entry_get_integral

elemental module function integration_entry_get_error (entry) result (err)
    real(default) :: err
    class(integration_entry_t), intent(in) :: entry
    err = entry%error
end function integration_entry_get_error

elemental module function integration_entry_get_relative_error &
    (entry) result (err)
    real(default) :: err
    class(integration_entry_t), intent(in) :: entry
    err = 0
    if (entry%integral /= 0) then
        err = entry%error / entry%integral
    end if
end function integration_entry_get_relative_error

elemental module function integration_entry_get_accuracy &
    (entry) result (acc)
    real(default) :: acc

```

```

class(integration_entry_t), intent(in) :: entry
acc = accuracy (entry%integral, entry%error, entry%n_calls)
end function integration_entry_get_accuracy

elemental module function accuracy (integral, error, n_calls) result (acc)
real(default) :: acc
real(default), intent(in) :: integral, error
integer, intent(in) :: n_calls
acc = 0
if (integral /= 0) then
acc = error / integral * sqrt (real (n_calls, default))
end if
end function accuracy

elemental module function integration_entry_get_efficiency &
(entry) result (eff)
real(default) :: eff
class(integration_entry_t), intent(in) :: entry
eff = entry%efficiency
end function integration_entry_get_efficiency

elemental module function integration_entry_get_efficiency_pos &
(entry) result (eff)
real(default) :: eff
class(integration_entry_t), intent(in) :: entry
eff = entry%efficiency_pos
end function integration_entry_get_efficiency_pos

elemental module function integration_entry_get_efficiency_neg &
(entry) result (eff)
real(default) :: eff
class(integration_entry_t), intent(in) :: entry
eff = entry%efficiency_neg
end function integration_entry_get_efficiency_neg

elemental module function integration_entry_get_chi2 (entry) result (chi2)
real(default) :: chi2
class(integration_entry_t), intent(in) :: entry
chi2 = entry%chi2
end function integration_entry_get_chi2

elemental module function integration_entry_has_improved &
(entry) result (flag)
logical :: flag
class(integration_entry_t), intent(in) :: entry
flag = entry%improved
end function integration_entry_has_improved

elemental module function integration_entry_get_n_groves &
(entry) result (n_groves)
integer :: n_groves
class(integration_entry_t), intent(in) :: entry
n_groves = 0
if (allocated (entry%chain_weights)) then

```

```

        n_groves = size (entry%chain_weights, 1)
    end if
end function integration_entry_get_n_groves

```

This writes the standard result account into one screen line. The verbose version uses multiple lines and prints the unabridged values. Dummy entries are not written.

```

<Integration results: integration entry: TBP>+≡
    procedure :: write => integration_entry_write
    procedure :: write_verbose => integration_entry_write_verbose

<Integration results: sub interfaces>+≡
    module subroutine integration_entry_write (entry, unit, verbosity, suppress)
        class(integration_entry_t), intent(in) :: entry
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: verbosity
        logical, intent(in), optional :: suppress
    end subroutine integration_entry_write
    module subroutine integration_entry_write_verbose (entry, unit)
        class(integration_entry_t), intent(in) :: entry
        integer, intent(in) :: unit
    end subroutine integration_entry_write_verbose

<Integration results: procedures>+≡
    module subroutine integration_entry_write (entry, unit, verbosity, suppress)
        class(integration_entry_t), intent(in) :: entry
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: verbosity
        logical, intent(in), optional :: suppress
        integer :: u
        character(1) :: star
        character(12) :: fmt
        character(7) :: fmt2
        character(120) :: buffer
        integer :: verb
        logical :: supp
        u = given_output_unit (unit); if (u < 0) return
        verb = 0; if (present (verbosity)) verb = verbosity
        supp = .false.; if (present (suppress)) supp = suppress
        if (entry%process_type /= PRC_UNKNOWN) then
            if (entry%improved .and. .not. supp) then
                star = "*"
            else
                star = " "
            end if
            call pac_fmt (fmt, FMT_14, "3x," // FMT_10 // ",1x", suppress)
            call pac_fmt (fmt2, "1x,F6.2", "2x,F5.1", suppress)
            write (buffer, "(1x,I3,1x,I10)") entry%it, entry%n_calls
            if (verb > 1) then
                write (buffer, "(A,1x,I10)") trim (buffer), entry%n_calls_valid
            end if
            write (buffer, "(A,1x," // fmt // ",1x,ES9.2,1x,F7.2," // &
                "1x,F7.2,A1," // fmt2 // ")") &
                trim (buffer), &

```

```

        entry%integral, &
        abs(entry%error), &
        abs(integration_entry_get_relative_error (entry)) * 100, &
        abs(integration_entry_get_accuracy (entry)), &
        star, &
        entry%efficiency * 100
    if (verb > 2) then
        write (buffer, "(A,1X," // fmt2 // ",1X," // fmt2 // ")") &
            trim (buffer), &
            entry%efficiency_pos * 100, &
            entry%efficiency_neg * 100
    end if
    if (entry%n_it /= 1) then
        write (buffer, "(A,1x,F7.2,1x,I3)") &
            trim (buffer), &
            entry%chi2, &
            entry%n_it
    end if
    write (u, "(A)") trim (buffer)
end if
flush (u)
end subroutine integration_entry_write

module subroutine integration_entry_write_verbose (entry, unit)
    class(integration_entry_t), intent(in) :: entry
    integer, intent(in) :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, *) " process_type = ", entry%process_type
    write (u, *) "          pass = ", entry%pass
    write (u, *) "          it = ", entry%it
    write (u, *) "          n_it = ", entry%n_it
    write (u, *) "          n_calls = ", entry%n_calls
    write (u, *) " n_calls_valid = ", entry%n_calls_valid
    write (u, *) "          improved = ", entry%improved
    write (u, *) "          integral = ", entry%integral
    write (u, *) "          error = ", entry%error
    write (u, *) "          efficiency = ", entry%efficiency
    write (u, *) "efficiency_pos = ", entry%efficiency_pos
    write (u, *) "efficiency_neg = ", entry%efficiency_neg
    write (u, *) "          chi2 = ", entry%chi2
    if (allocated (entry%chain_weights)) then
        write (u, *) "          n_groves = ", size (entry%chain_weights)
        write (u, *) "chain_weights = ", entry%chain_weights
    else
        write (u, *) "          n_groves = 0"
    end if
    flush (u)
end subroutine integration_entry_write_verbose

```

Read the entry, assuming it has been written in verbose format.

```

<Integration results: integration entry: TBP>+≡
procedure :: read => integration_entry_read

```

```

<Integration results: sub interfaces>+≡
  module subroutine integration_entry_read (entry, unit)
    class(integration_entry_t), intent(out) :: entry
    integer, intent(in) :: unit
  end subroutine integration_entry_read

```

```

<Integration results: procedures>+≡
  module subroutine integration_entry_read (entry, unit)
    class(integration_entry_t), intent(out) :: entry
    integer, intent(in) :: unit
    character(30) :: dummy
    character :: equals
    integer :: n_groves
    read (unit, *) dummy, equals, entry%process_type
    read (unit, *) dummy, equals, entry%pass
    read (unit, *) dummy, equals, entry%it
    read (unit, *) dummy, equals, entry%n_it
    read (unit, *) dummy, equals, entry%n_calls
    read (unit, *) dummy, equals, entry%n_calls_valid
    read (unit, *) dummy, equals, entry%improved
    read (unit, *) dummy, equals, entry%integral
    read (unit, *) dummy, equals, entry%error
    read (unit, *) dummy, equals, entry%efficiency
    read (unit, *) dummy, equals, entry%efficiency_pos
    read (unit, *) dummy, equals, entry%efficiency_neg
    read (unit, *) dummy, equals, entry%chi2
    read (unit, *) dummy, equals, n_groves
    if (n_groves /= 0) then
      allocate (entry%chain_weights (n_groves))
      read (unit, *) dummy, equals, entry%chain_weights
    end if
  end subroutine integration_entry_read

```

Write an account of the channel weights, accumulated by groves.

```

<Integration results: integration entry: TBP>+≡
  procedure :: write_chain_weights => integration_entry_write_chain_weights

```

```

<Integration results: sub interfaces>+≡
  module subroutine integration_entry_write_chain_weights (entry, unit)
    class(integration_entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
  end subroutine integration_entry_write_chain_weights

```

```

<Integration results: procedures>+≡
  module subroutine integration_entry_write_chain_weights (entry, unit)
    class(integration_entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    if (allocated (entry%chain_weights)) then
      do i = 1, size (entry%chain_weights)
        write (u, "(1x,I3)", advance="no") &
          nint (entry%chain_weights(i) * 100)
      end do
      write (u, *)
    end if
  end subroutine integration_entry_write_chain_weights

```

```

        end if
    end subroutine integration_entry_write_chain_weights

```

21.3.2 Combined integration results

We collect a list of results which grows during the execution of the program. This is implemented as an array which grows if necessary; so we can easily compute averages.

We implement this as an extension of the `mci_results_t` which is defined in `mci_base` as an abstract type. We thus decouple the implementation of the integrator from the implementation of the results display, but nevertheless can record intermediate results during integration. This implies that the present extension implements a `record` method.

```

<Integration results: public>+≡
    public :: integration_results_t

<Integration results: types>+≡
    type, extends (mci_results_t) :: integration_results_t
    private
        integer :: process_type = PRC_UNKNOWN
        integer :: current_pass = 0
        integer :: n_pass = 0
        integer :: n_it = 0
        logical :: screen = .false.
        integer :: unit = 0
        integer :: verbosity = 0
        real(default) :: error_threshold = 0
        type(integration_entry_t), dimension(:), allocatable :: entry
        type(integration_entry_t), dimension(:), allocatable :: average
    contains
        <Integration results: integration results: TBP>
    end type integration_results_t

```

The array is extended in chunks of 10 entries.

```

<Integration results: parameters>+≡
    integer, parameter :: RESULTS_CHUNK_SIZE = 10

<Integration results: integration results: TBP>≡
    procedure :: init => integration_results_init

<Integration results: sub interfaces>+≡
    module subroutine integration_results_init (results, process_type)
        class(integration_results_t), intent(out) :: results
        integer, intent(in) :: process_type
    end subroutine integration_results_init

<Integration results: procedures>+≡
    module subroutine integration_results_init (results, process_type)
        class(integration_results_t), intent(out) :: results
        integer, intent(in) :: process_type
        results%process_type = process_type
        results%n_pass = 0
    end subroutine integration_results_init

```

```

    results%n_it = 0
    allocate (results%entry (RESULTS_CHUNK_SIZE))
    allocate (results%average (RESULTS_CHUNK_SIZE))
end subroutine integration_results_init

```

Set verbose output of the integration results. In verbose mode, valid calls, negative as positive efficiency will be printed.

```

<Integration results: integration results: TBP>+≡
    procedure :: set_verbosity => integration_results_set_verbosity

<Integration results: sub interfaces>+≡
    module subroutine integration_results_set_verbosity (results, verbosity)
        class(integration_results_t), intent(inout) :: results
        integer, intent(in) :: verbosity
    end subroutine integration_results_set_verbosity

<Integration results: procedures>+≡
    module subroutine integration_results_set_verbosity (results, verbosity)
        class(integration_results_t), intent(inout) :: results
        integer, intent(in) :: verbosity
        results%verbosity = verbosity
    end subroutine integration_results_set_verbosity

```

Set additional parameters: the `error_threshold` declares that any error value (in absolute numbers) smaller than this is to be considered zero.

```

<Integration results: integration results: TBP>+≡
    procedure :: set_error_threshold => integration_results_set_error_threshold

<Integration results: sub interfaces>+≡
    module subroutine integration_results_set_error_threshold &
        (results, error_threshold)
        class(integration_results_t), intent(inout) :: results
        real(default), intent(in) :: error_threshold
    end subroutine integration_results_set_error_threshold

<Integration results: procedures>+≡
    module subroutine integration_results_set_error_threshold &
        (results, error_threshold)
        class(integration_results_t), intent(inout) :: results
        real(default), intent(in) :: error_threshold
        results%error_threshold = error_threshold
    end subroutine integration_results_set_error_threshold

```

Output (ASCII format). The `verbose` format is used for writing the header in grid files.

```

<Integration results: integration results: TBP>+≡
    procedure :: write => integration_results_write
    procedure :: write_verbose => integration_results_write_verbose

<Integration results: sub interfaces>+≡
    module subroutine integration_results_write (object, unit, suppress)
        class(integration_results_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: suppress

```



```

end subroutine integration_results_write
module subroutine integration_results_write_verbose (object, unit)
  class(integration_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine integration_results_write_verbose

<Integration results: procedures>+≡
module subroutine integration_results_write (object, unit, suppress)
  class(integration_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: suppress
  logical :: verb
  integer :: u, n
  u = given_output_unit (unit); if (u < 0) return
  call object%write_dline (unit)
  if (object%n_it /= 0) then
    call object%write_header (unit, logfile = .false.)
    call object%write_dline (unit)
    do n = 1, object%n_it
      if (n > 1) then
        if (object%entry(n)%pass /= object%entry(n-1)%pass) then
          call object%write_hline (unit)
          call object%average(object%entry(n-1)%pass)%write ( &
            & unit, suppress = suppress)
          call object%write_hline (unit)
        end if
      end if
      call object%entry(n)%write (unit, &
        suppress = suppress)
    end do
    call object%write_hline(unit)
    call object%average(object%n_pass)%write (unit, suppress = suppress)
  else
    call msg_message ("[WHIZARD integration results: empty]", unit)
  end if
  call object%write_dline (unit)
  flush (u)
end subroutine integration_results_write

module subroutine integration_results_write_verbose (object, unit)
  class(integration_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, n
  u = given_output_unit (unit); if (u < 0) return
  write (u, *) "begin(integration_results)"
  write (u, *) "  n_pass = ", object%n_pass
  write (u, *) "    n_it = ", object%n_it
  if (object%n_it > 0) then
    write (u, *) "begin(integration_pass)"
    do n = 1, object%n_it
      if (n > 1) then
        if (object%entry(n)%pass /= object%entry(n-1)%pass) then
          write (u, *) "end(integration_pass)"
          write (u, *) "begin(integration_pass)"
        end if
      end if
    end do
  end if

```

```

        end if
        write (u, *) "begin(iteration)"
        call object%entry(n)%write_verbose (unit)
        write (u, *) "end(iteration)"
    end do
    write (u, *) "end(integration_pass)"
end if
write (u, *) "end(integration_results)"
flush (u)
end subroutine integration_results_write_verbose

```

Write a concise table of chain weights, i.e., the channel history where channels are collected by chains.

(Integration results: integration results: TBP)+≡

```

    procedure :: write_chain_weights => &
        integration_results_write_chain_weights

```

(Integration results: sub interfaces)+≡

```

    module subroutine integration_results_write_chain_weights (results, unit)
        class(integration_results_t), intent(in) :: results
        integer, intent(in), optional :: unit
    end subroutine integration_results_write_chain_weights

```

(Integration results: procedures)+≡

```

    module subroutine integration_results_write_chain_weights (results, unit)
        class(integration_results_t), intent(in) :: results
        integer, intent(in), optional :: unit
        integer :: u, i, n
        u = given_output_unit (unit); if (u < 0) return
        if (allocated (results%entry(1)%chain_weights) .and. results%n_it /= 0) then
            call msg_message ("Phase-space chain (grove) weight history: " &
                // "(numbers in %)", unit)
            write (u, "(A9)", advance="no") "| chain |"
            do i = 1, integration_entry_get_n_groves (results%entry(1))
                write (u, "(1x,I3)", advance="no") i
            end do
            write (u, *)
            call results%write_dline (unit)
            do n = 1, results%n_it
                if (n > 1) then
                    if (results%entry(n)%pass /= results%entry(n-1)%pass) then
                        call results%write_hline (unit)
                    end if
                end if
                write (u, "(1x,I6,1x,A1)", advance="no") n, "|"
                call results%entry(n)%write_chain_weights (unit)
            end do
            flush (u)
            call results%write_dline(unit)
        end if
    end subroutine integration_results_write_chain_weights

```

Read the list from file. The file must be written using the `verbose` option of the writing routine.

```

<Integration results: integration results: TBP>+≡
    procedure :: read => integration_results_read

<Integration results: sub interfaces>+≡
    module subroutine integration_results_read (results, unit)
        class(integration_results_t), intent(out) :: results
        integer, intent(in) :: unit
    end subroutine integration_results_read

<Integration results: procedures>+≡
    module subroutine integration_results_read (results, unit)
        class(integration_results_t), intent(out) :: results
        integer, intent(in) :: unit
        character(80) :: buffer
        character :: equals
        integer :: pass, it
        read (unit, *) buffer
        if (trim (adjustl (buffer)) /= "begin(integration_results)") then
            call read_err (); return
        end if
        read (unit, *) buffer, equals, results%n_pass
        read (unit, *) buffer, equals, results%n_it
        allocate (results%entry (results%n_it + RESULTS_CHUNK_SIZE))
        allocate (results%average (results%n_it + RESULTS_CHUNK_SIZE))
        it = 0
        do pass = 1, results%n_pass
            read (unit, *) buffer
            if (trim (adjustl (buffer)) /= "begin(integration_pass)") then
                call read_err (); return
            end if
            READ_ENTRIES: do
                read (unit, *) buffer
                if (trim (adjustl (buffer)) /= "begin(iteration)") then
                    exit READ_ENTRIES
                end if
                it = it + 1
                call results%entry(it)%read (unit)
                read (unit, *) buffer
                if (trim (adjustl (buffer)) /= "end(iteration)") then
                    call read_err (); return
                end if
            end do READ_ENTRIES
            if (trim (adjustl (buffer)) /= "end(integration_pass)") then
                call read_err (); return
            end if
            results%average(pass) = compute_average (results%entry, pass)
        end do
        read (unit, *) buffer
        if (trim (adjustl (buffer)) /= "end(integration_results)") then
            call read_err (); return
        end if
contains
    subroutine read_err ()
        call msg_fatal ("Reading integration results from file: syntax error")
    end subroutine read_err

```

```
end subroutine integration_results_read
```

Auxiliary output.

<Integration results: integration results: TBP>+≡

```
procedure, private :: write_header
procedure, private :: write_hline
procedure, private :: write_dline
```

<Integration results: sub interfaces>+≡

```
module subroutine write_header (results, unit, logfile)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: logfile
end subroutine write_header
module subroutine write_hline (results, unit)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
end subroutine write_hline
module subroutine write_dline (results, unit)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
end subroutine write_dline
```

<Integration results: procedures>+≡

```
module subroutine write_header (results, unit, logfile)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: logfile
  character(5) :: phys_unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  select case (results%process_type)
  case (PRC_DECAY);      phys_unit = "[GeV]"
  case (PRC_SCATTERING); phys_unit = "[fb]"
  case default
    phys_unit = " "
  end select
  write (msg_buffer, "(A, A)") &
    "It      Calls"
  if (results%verbosity > 1) then
    write (msg_buffer, "(A, A)") trim (msg_buffer), &
      "      Valid"
  end if
  write (msg_buffer, "(A, A)") trim (msg_buffer), &
    "  Integral" // phys_unit // &
    "  Error" // phys_unit // &
    "  Err[%]   Acc  Eff[%]"
  if (results%verbosity > 2) then
    write (msg_buffer, "(A, A)") trim (msg_buffer), &
      "  (+) [%]  (-) [%]"
  end if
  write (msg_buffer, "(A, A)") trim (msg_buffer), &
    "  Chi2 N[It] |"
  call msg_message (unit=u, logfile=logfile)
end subroutine write_header
```

```

module subroutine write_hline (results, unit)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
  integer :: u, len
  u = given_output_unit (unit); if (u < 0) return
  len = 77
  if (results%verbosity > 1) len = len + 11
  if (results%verbosity > 2) len = len + 16
  write (u, "(A)"  "| " // (repeat("-", len)) // "|")
  flush (u)
end subroutine write_hline

module subroutine write_dline (results, unit)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
  integer :: u, len
  u = given_output_unit (unit); if (u < 0) return
  len = 77
  if (results%verbosity > 1) len = len + 11
  if (results%verbosity > 2) len = len + 16
  write (u, "(A)"  "| " // (repeat("=", len)) // "|")
  flush (u)
end subroutine write_dline

```

During integration, we do not want to print all results at once, but each intermediate result as soon as we get it. Thus, the previous procedure is chopped in pieces. First piece: store the output unit and a flag whether we want to print to standard output as well. Then write the header if the results are still empty, i.e., before integration has started. The second piece writes a single result to the saved output channels. We call this from the `record` method, which can be called from the integrator directly. The third piece writes the average result, once a pass has been completed. The fourth piece writes a footer (if any), assuming that this is the final result.

(Integration results: integration results: TBP)+≡

```

procedure :: display_init => integration_results_display_init
procedure :: display_current => integration_results_display_current
procedure :: display_pass => integration_results_display_pass
procedure :: display_final => integration_results_display_final

```

(Integration results: sub interfaces)+≡

```

module subroutine integration_results_display_init &
  (results, screen, unit)
  class(integration_results_t), intent(inout) :: results
  logical, intent(in) :: screen
  integer, intent(in), optional :: unit
end subroutine integration_results_display_init
module subroutine integration_results_display_current (results, pacify)
  class(integration_results_t), intent(in) :: results
  logical, intent(in), optional :: pacify
end subroutine integration_results_display_current
module subroutine integration_results_display_pass (results, pacify)
  class(integration_results_t), intent(in) :: results

```

```

        logical, intent(in), optional :: pacify
    end subroutine integration_results_display_pass
    module subroutine integration_results_display_final (results)
        class(integration_results_t), intent(inout) :: results
    end subroutine integration_results_display_final

    <Integration results: procedures>+≡
    module subroutine integration_results_display_init &
        (results, screen, unit)
        class(integration_results_t), intent(inout) :: results
        logical, intent(in) :: screen
        integer, intent(in), optional :: unit
        integer :: u
        if (present (unit)) results%unit = unit
        u = given_output_unit ()
        results%screen = screen
        if (results%n_it == 0) then
            if (results%screen) then
                call results%write_dline (u)
                call results%write_header (u, &
                    logfile=.false.)
                call results%write_dline (u)
            end if
            if (results%unit /= 0) then
                call results%write_dline (results%unit)
                call results%write_header (results%unit, &
                    logfile=.false.)
                call results%write_dline (results%unit)
            end if
        else
            if (results%screen) then
                call results%write_hline (u)
            end if
            if (results%unit /= 0) then
                call results%write_hline (results%unit)
            end if
        end if
    end subroutine integration_results_display_init

    module subroutine integration_results_display_current (results, pacify)
        class(integration_results_t), intent(in) :: results
        integer :: u
        logical, intent(in), optional :: pacify
        u = given_output_unit ()
        if (results%screen) then
            call results%entry(results%n_it)%write (u, &
                verbosity = results%verbosity, suppress = pacify)
        end if
        if (results%unit /= 0) then
            call results%entry(results%n_it)%write ( &
                results%unit, verbosity = results%verbosity, suppress = pacify)
        end if
    end subroutine integration_results_display_current

    module subroutine integration_results_display_pass (results, pacify)

```

```

class(integration_results_t), intent(in) :: results
logical, intent(in), optional :: pacify
integer :: u
u = given_output_unit ()
if (results%screen) then
    call results%write_hline (u)
    call results%average(results%entry(results%n_it)%pass)%write ( &
        u, verbosity = results%verbosity, suppress = pacify)
end if
if (results%unit /= 0) then
    call results%write_hline (results%unit)
    call results%average(results%entry(results%n_it)%pass)%write ( &
        results%unit, verbosity = results%verbosity, suppress = pacify)
end if
end subroutine integration_results_display_pass

module subroutine integration_results_display_final (results)
    class(integration_results_t), intent(inout) :: results
    integer :: u
    u = given_output_unit ()
    if (results%screen) then
        call results%write_dline (u)
    end if
    if (results%unit /= 0) then
        call results%write_dline (results%unit)
    end if
    results%screen = .false.
    results%unit = 0
end subroutine integration_results_display_final

```

Expand the list of entries if the limit has been reached:

```

<Integration results: integration results: TBP>+≡
    procedure :: expand => integration_results_expand

<Integration results: sub interfaces>+≡
    module subroutine integration_results_expand (results)
        class(integration_results_t), intent(inout) :: results
        end subroutine integration_results_expand

<Integration results: procedures>+≡
    module subroutine integration_results_expand (results)
        class(integration_results_t), intent(inout) :: results
        type(integration_entry_t), dimension(:), allocatable :: entry_tmp
        if (results%n_it == size (results%entry)) then
            allocate (entry_tmp (results%n_it))
            entry_tmp = results%entry
            deallocate (results%entry)
            allocate (results%entry (results%n_it + RESULTS_CHUNK_SIZE))
            results%entry(:results%n_it) = entry_tmp
            deallocate (entry_tmp)
        end if
        if (results%n_pass == size (results%average)) then
            allocate (entry_tmp (results%n_pass))
            entry_tmp = results%average
            deallocate (results%average)

```

```

        allocate (results%average (results%n_it + RESULTS_CHUNK_SIZE))
        results%average(:results%n_pass) = entry_tmp
        deallocate (entry_tmp)
    end if
end subroutine integration_results_expand

```

Increment the `current_pass` counter. Must be done before each new integration pass; after integration, the recording method may use the value of this counter to define the entry.

```

<Integration results: integration results: TBP>+≡
    procedure :: new_pass => integration_results_new_pass

<Integration results: sub interfaces>+≡
    module subroutine integration_results_new_pass (results)
        class(integration_results_t), intent(inout) :: results
    end subroutine integration_results_new_pass

<Integration results: procedures>+≡
    module subroutine integration_results_new_pass (results)
        class(integration_results_t), intent(inout) :: results
        results%current_pass = results%current_pass + 1
    end subroutine integration_results_new_pass

```

Enter results into the results list. For the error value, we may compare them with a given threshold. This guards against numerical noise, if the exact error would be zero.

```

<Integration results: integration results: TBP>+≡
    procedure :: append => integration_results_append

<Integration results: sub interfaces>+≡
    module subroutine integration_results_append (results, &
        n_it, n_calls, n_calls_valid, &
        integral, error, efficiency, efficiency_pos, efficiency_neg, &
        chain_weights)
        class(integration_results_t), intent(inout) :: results
        integer, intent(in) :: n_it, n_calls, n_calls_valid
        real(default), intent(in) :: integral, error, efficiency, &
            efficiency_pos, efficiency_neg
        real(default), dimension(:), intent(in), optional :: chain_weights
    end subroutine integration_results_append

<Integration results: procedures>+≡
    module subroutine integration_results_append (results, &
        n_it, n_calls, n_calls_valid, &
        integral, error, efficiency, efficiency_pos, efficiency_neg, &
        chain_weights)
        class(integration_results_t), intent(inout) :: results
        integer, intent(in) :: n_it, n_calls, n_calls_valid
        real(default), intent(in) :: integral, error, efficiency, &
            efficiency_pos, efficiency_neg
        real(default), dimension(:), intent(in), optional :: chain_weights
        logical :: improved
        type(integration_entry_t) :: entry
        real(default) :: err_checked
        improved = .true.

```



```

if (results%n_it /= 0) improved = abs(accuracy (integral, error, n_calls)) &
    < abs(results%entry(results%n_it)%get_accuracy ())
err_checked = 0
if (abs (error) >= results%error_threshold) err_checked = error
entry = integration_entry_t ( &
    results%process_type, results%current_pass, &
    results%n_it+1, n_it, n_calls, n_calls_valid, improved, &
    integral, err_checked, efficiency, efficiency_pos, efficiency_neg, &
    chain_weights=chain_weights)
if (results%n_it == 0) then
    results%n_it = 1
    results%n_pass = 1
else
    call results%expand ()
    if (entry%pass /= results%entry(results%n_it)%pass) &
        results%n_pass = results%n_pass + 1
    results%n_it = results%n_it + 1
end if
results%entry(results%n_it) = entry
results%average(results%n_pass) = &
    compute_average (results%entry, entry%pass)
end subroutine integration_results_append

```

Record an integration pass executed by an mci integrator object.

There is a tolerance below we treat an error (relative to the integral) as zero.

<Integration results: parameters>+≡

```
real(default), parameter, public :: INTEGRATION_ERROR_TOLERANCE = 1e-10
```

<Integration results: integration results: TBP>+≡

```
procedure :: record_simple => integration_results_record_simple
```

<Integration results: sub interfaces>+≡

```

module subroutine integration_results_record_simple &
    (object, n_it, n_calls, integral, error, efficiency, &
    chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls
real(default), intent(in) :: integral, error, efficiency
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
end subroutine integration_results_record_simple

```

<Integration results: procedures>+≡

```

module subroutine integration_results_record_simple &
    (object, n_it, n_calls, integral, error, efficiency, &
    chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls
real(default), intent(in) :: integral, error, efficiency
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
real(default) :: err
err = 0._default
if (abs (error) >= abs (integral) * INTEGRATION_ERROR_TOLERANCE) then
    err = error

```

```

end if
call object%append (n_it, n_calls, 0, integral, err, efficiency, &
    0._default, 0._default, chain_weights)
call object%display_current (suppress)
end subroutine integration_results_record_simple

```

Record extended results from integration pass.

(Integration results: integration results: TBP)+≡

```

procedure :: record_extended => integration_results_record_extended

```

(Integration results: sub interfaces)+≡

```

module subroutine integration_results_record_extended (object, n_it, &
    n_calls, n_calls_valid, integral, error, efficiency, efficiency_pos, &
    efficiency_neg, chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls, n_calls_valid
real(default), intent(in) :: integral, error, efficiency, &
    efficiency_pos, efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
end subroutine integration_results_record_extended

```

(Integration results: procedures)+≡

```

module subroutine integration_results_record_extended (object, n_it, &
    n_calls, n_calls_valid, integral, error, efficiency, efficiency_pos, &
    efficiency_neg, chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls, n_calls_valid
real(default), intent(in) :: integral, error, efficiency, &
    efficiency_pos, efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
real(default) :: err
err = 0._default
if (abs (error) >= abs (integral) * INTEGRATION_ERROR_TOLERANCE) then
    err = error
end if
call object%append (n_it, n_calls, n_calls_valid, integral, err, &
    efficiency, efficiency_pos, efficiency_neg, chain_weights)
call object%display_current (suppress)
end subroutine integration_results_record_extended

```

Compute the average for all entries in the specified integration pass. The integrals are weighted w.r.t. their individual errors.

The quoted error of the result is the expected error, computed from the weighted average of the given individual errors.

This should be compared to the actual distribution of the results, from which we also can compute an error estimate if there is more than one iteration. The ratio of the distribution error and the averaged error, is the χ^2 value.

All error distributions are assumed Gaussian, of course. The χ^2 value is a partial check for this assumption. If it is significantly greater than unity, there is something wrong with the individual errors.

The efficiency returned is the one of the last entry in the integration pass.

If any error vanishes, averaging by this algorithm would fail. In this case, we simply average the entries and use the deviations from this average (if any) to estimate the error.

```

(Integration results: procedures)+≡
type(integration_entry_t) function compute_average (entry, pass) &
    & result (result)
type(integration_entry_t), dimension(:), intent(in) :: entry
integer, intent(in) :: pass
integer :: i
logical, dimension(size(entry)) :: mask
real(default), dimension(size(entry)) :: ivar
real(default) :: sum_ivar, variance
result%process_type = entry(1)%process_type
result%pass = pass
mask = entry%pass == pass .and. entry%process_type /= PRC_UNKNOWN
result%it = maxval (entry%it, mask)
result%n_it = count (mask)
result%n_calls = sum (entry%n_calls, mask)
result%n_calls_valid = sum (entry%n_calls_valid, mask)
if (.not. any (mask .and. entry%error == 0)) then
    where (mask)
        ivar = 1 / entry%error ** 2
    elsewhere
        ivar = 0
    end where
    sum_ivar = sum (ivar, mask)
    variance = 0
    if (sum_ivar /= 0) then
        variance = 1 / sum_ivar
    end if
    result%integral = sum (entry%integral * ivar, mask) * variance
    if (result%n_it > 1) then
        result%chi2 = &
            sum ((entry%integral - result%integral)**2 * ivar, mask) &
            / (result%n_it - 1)
    end if
else if (result%n_it /= 0) then
    result%integral = sum (entry%integral, mask) / result%n_it
    variance = 0
    if (result%n_it > 1) then
        variance = &
            sum ((entry%integral - result%integral)**2, mask) &
            / (result%n_it - 1)
    if (result%integral /= 0) then
        if (abs (variance / result%integral) &
            < 100 * epsilon (1._default)) then
            variance = 0
        end if
    end if
    end if
    result%chi2 = variance / result%n_it
end if
result%error = sqrt (variance)
result%efficiency = entry(last_index (mask))%efficiency

```

```

    result%efficiency_pos = entry(last_index (mask))%efficiency_pos
    result%efficiency_neg = entry(last_index (mask))%efficiency_neg
contains
    integer function last_index (mask) result (index)
        logical, dimension(:), intent(in) :: mask
        integer :: i
        do i = size (mask), 1, -1
            if (mask(i)) exit
        end do
        index = i
    end function last_index
end function compute_average

```

21.3.3 Access results

Return true if the results object has entries.

```

<Integration results: integration results: TBP>+≡
    procedure :: exist => integration_results_exist

<Integration results: sub interfaces>+≡
    module function integration_results_exist (results) result (flag)
        logical :: flag
        class(integration_results_t), intent(in) :: results
    end function integration_results_exist

<Integration results: procedures>+≡
    module function integration_results_exist (results) result (flag)
        logical :: flag
        class(integration_results_t), intent(in) :: results
        flag = results%n_pass > 0
    end function integration_results_exist

```

Retrieve information from the results record. If `last` is set and true, take the last iteration. If it is set instead, take this iteration. If `pass` is set, take this average. If none is set, take the final average.

If the result would be invalid, the entry is not assigned. Due to default initialization, this returns a null entry.

```

<Integration results: integration results: TBP>+≡
    procedure :: get_entry => results_get_entry

<Integration results: sub interfaces>+≡
    module function results_get_entry (results, last, it, pass) result (entry)
        class(integration_results_t), intent(in) :: results
        type(integration_entry_t) :: entry
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function results_get_entry

<Integration results: procedures>+≡
    module function results_get_entry (results, last, it, pass) result (entry)
        class(integration_results_t), intent(in) :: results
        type(integration_entry_t) :: entry
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function results_get_entry

```

```

if (present (last)) then
  if (allocated (results%entry) .and. results%n_it > 0) then
    entry = results%entry(results%n_it)
  else
    call error ()
  end if
else if (present (it)) then
  if (allocated (results%entry) .and. it > 0 .and. it <= results%n_it) then
    entry = results%entry(it)
  else
    call error ()
  end if
else if (present (pass)) then
  if (allocated (results%average) &
    .and. pass > 0 .and. pass <= results%n_pass) then
    entry = results%average (pass)
  else
    call error ()
  end if
else
  if (allocated (results%average) .and. results%n_pass > 0) then
    entry = results%average (results%n_pass)
  else
    call error ()
  end if
end if
contains
subroutine error ()
  call msg_fatal ("Requested integration result is not available")
end subroutine error
end function results_get_entry

```

The individual procedures. The `results` record should have the `target` attribute, but only locally within the function.

<Integration results: integration results: TBP>+≡

```

procedure :: get_n_calls => integration_results_get_n_calls
procedure :: get_integral => integration_results_get_integral
procedure :: get_error => integration_results_get_error
procedure :: get_accuracy => integration_results_get_accuracy
procedure :: get_chi2 => integration_results_get_chi2
procedure :: get_efficiency => integration_results_get_efficiency

```

<Integration results: sub interfaces>+≡

```

module function integration_results_get_n_calls (results, last, it, pass) &
  result (n_calls)
  class(integration_results_t), intent(in), target :: results
  integer :: n_calls
  logical, intent(in), optional :: last
  integer, intent(in), optional :: it, pass
end function integration_results_get_n_calls
module function integration_results_get_integral (results, last, it, pass) &
  result (integral)
  class(integration_results_t), intent(in), target :: results
  real(default) :: integral

```

```

        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function integration_results_get_integral
    module function integration_results_get_error (results, last, it, pass) &
        result (error)
        class(integration_results_t), intent(in), target :: results
        real(default) :: error
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function integration_results_get_error
    module function integration_results_get_accuracy (results, last, it, pass) &
        result (accuracy)
        class(integration_results_t), intent(in), target :: results
        real(default) :: accuracy
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function integration_results_get_accuracy
    module function integration_results_get_chi2 (results, last, it, pass) &
        result (chi2)
        class(integration_results_t), intent(in), target :: results
        real(default) :: chi2
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function integration_results_get_chi2
    module function integration_results_get_efficiency &
        (results, last, it, pass) result (efficiency)
        class(integration_results_t), intent(in), target :: results
        real(default) :: efficiency
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
    end function integration_results_get_efficiency

    (Integration results: procedures)+≡
    module function integration_results_get_n_calls (results, last, it, pass) &
        result (n_calls)
        class(integration_results_t), intent(in), target :: results
        integer :: n_calls
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
        type(integration_entry_t) :: entry
        entry = results%get_entry (last, it, pass)
        n_calls = entry%get_n_calls ()
    end function integration_results_get_n_calls

    module function integration_results_get_integral (results, last, it, pass) &
        result (integral)
        class(integration_results_t), intent(in), target :: results
        real(default) :: integral
        logical, intent(in), optional :: last
        integer, intent(in), optional :: it, pass
        type(integration_entry_t) :: entry
        entry = results%get_entry (last, it, pass)
        integral = entry%get_integral ()
    end function integration_results_get_integral

```

```

module function integration_results_get_error (results, last, it, pass) &
    result (error)
    class(integration_results_t), intent(in), target :: results
    real(default) :: error
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    error = entry%get_error ()
end function integration_results_get_error

module function integration_results_get_accuracy (results, last, it, pass) &
    result (accuracy)
    class(integration_results_t), intent(in), target :: results
    real(default) :: accuracy
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    accuracy = entry%get_accuracy ()
end function integration_results_get_accuracy

module function integration_results_get_chi2 (results, last, it, pass) &
    result (chi2)
    class(integration_results_t), intent(in), target :: results
    real(default) :: chi2
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    chi2 = entry%get_chi2 ()
end function integration_results_get_chi2

module function integration_results_get_efficiency (results, last, it, pass) &
    result (efficiency)
    class(integration_results_t), intent(in), target :: results
    real(default) :: efficiency
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    efficiency = entry%get_efficiency ()
end function integration_results_get_efficiency

```

Return the last pass index and the index of the last iteration *within* the last pass. The third routine returns the absolute index of the last iteration.

(*Integration results: procedures*) +=

```

function integration_results_get_current_pass (results) result (pass)
    integer :: pass
    type(integration_results_t), intent(in) :: results
    pass = results%n_pass
end function integration_results_get_current_pass

```

```

function integration_results_get_current_it (results) result (it)
  integer :: it
  type(integration_results_t), intent(in) :: results
  it = 0
  if (allocated (results%entry)) then
    it = count (results%entry(1:results%n_it)%pass == results%n_pass)
  end if
end function integration_results_get_current_it

function integration_results_get_last_it (results) result (it)
  integer :: it
  type(integration_results_t), intent(in) :: results
  it = results%n_it
end function integration_results_get_last_it

```

Return the index of the best iteration (lowest accuracy value) within the current pass. If none qualifies, return zero.

(Integration results: procedures)+≡

```

function integration_results_get_best_it (results) result (it)
  integer :: it
  type(integration_results_t), intent(in) :: results
  integer :: i
  real(default) :: acc, acc_best
  acc_best = -1
  it = 0
  do i = 1, results%n_it
    if (results%entry(i)%pass == results%n_pass) then
      acc = integration_entry_get_accuracy (results%entry(i))
      if (acc_best < 0 .or. acc <= acc_best) then
        acc_best = acc
        it = i
      end if
    end if
  end do
end function integration_results_get_best_it

```

Compute the MD5 sum by printing everything and checksumming the resulting file.

(Integration results: procedures)+≡

```

function integration_results_get_md5sum (results) result (md5sum_results)
  character(32) :: md5sum_results
  type(integration_results_t), intent(in) :: results
  integer :: u
  u = free_unit ()
  open (unit = u, status = "scratch", action = "readwrite")
  call results%write_verbose (u)
  rewind (u)
  md5sum_results = md5sum (u)
  close (u)
end function integration_results_get_md5sum

```

This is (ab)used to suppress numerical noise when integrating constant matrix

elements.

<Integration results: integration results: TBP>+≡

```
procedure :: pacify => integration_results_pacify
```

<Integration results: sub interfaces>+≡

```
module subroutine integration_results_pacify (results, efficiency_reset)
  class(integration_results_t), intent(inout) :: results
  logical, intent(in), optional :: efficiency_reset
end subroutine integration_results_pacify
```

<Integration results: procedures>+≡

```
module subroutine integration_results_pacify (results, efficiency_reset)
  class(integration_results_t), intent(inout) :: results
  logical, intent(in), optional :: efficiency_reset
  integer :: i
  logical :: reset
  reset = .false.
  if (present (efficiency_reset)) reset = efficiency_reset
  if (allocated (results%entry)) then
    do i = 1, size (results%entry)
      call pacify (results%entry(i)%error, &
        results%entry(i)%integral * 1.E-9_default)
      if (reset) results%entry(i)%efficiency = 1
    end do
  end if
  if (allocated (results%average)) then
    do i = 1, size (results%average)
      call pacify (results%average(i)%error, &
        results%average(i)%integral * 1.E-9_default)
      if (reset) results%average(i)%efficiency = 1
    end do
  end if
end subroutine integration_results_pacify
```

<Integration results: integration results: TBP>+≡

```
procedure :: record_correction => integration_results_record_correction
```

<Integration results: sub interfaces>+≡

```
module subroutine integration_results_record_correction (object, corr, err)
  class(integration_results_t), intent(inout) :: object
  real(default), intent(in) :: corr, err
end subroutine integration_results_record_correction
```

<Integration results: procedures>+≡

```
module subroutine integration_results_record_correction (object, corr, err)
  class(integration_results_t), intent(inout) :: object
  real(default), intent(in) :: corr, err
  integer :: u
  u = given_output_unit ()
  if (object%screen) then
    call object%write_hline (u)
    call msg_message ("NLO Correction: [O(alpha_s+1)/O(alpha_s)]")
    write(msg_buffer,'(1X,A1,F7.2,A4,F6.2,1X,A3)') '(', corr, ' +- ', err, ')'
    call msg_message ()
  end if
end subroutine integration_results_record_correction
```

21.3.4 Results display

Write a driver file for history visualization.

The ratio of y range over y value must not become too small, otherwise we run into an arithmetic overflow in GAMELAN. 2% appears to be safe.

```
<Integration results: parameters>+=  
    real, parameter, public :: GML_MIN_RANGE_RATIO = 0.02  
  
<Integration results: public>+=  
    public :: integration_results_write_driver  
  
<Integration results: sub interfaces>+=  
    module subroutine integration_results_write_driver &  
        (results, filename, eff_reset)  
        type(integration_results_t), intent(inout) :: results  
        type(string_t), intent(in) :: filename  
        logical, intent(in), optional :: eff_reset  
    end subroutine integration_results_write_driver  
  
<Integration results: procedures>+=  
    module subroutine integration_results_write_driver &  
        (results, filename, eff_reset)  
        type(integration_results_t), intent(inout) :: results  
        type(string_t), intent(in) :: filename  
        logical, intent(in), optional :: eff_reset  
        type(string_t) :: file_tex  
        integer :: unit  
        integer :: n, i, n_pass, pass  
        integer, dimension(:), allocatable :: ipass  
        real(default) :: ymin, ymax, yavg, ydif, y0, y1  
        real(default), dimension(results%n_it) :: ymin_arr, ymax_arr  
        logical :: reset  
        file_tex = filename // ".tex"  
        unit = free_unit ()  
        open (unit=unit, file=char(file_tex), action="write", status="replace")  
        reset = .false.; if (present (eff_reset)) reset = eff_reset  
        n = results%n_it  
        n_pass = results%n_pass  
        allocate (ipass (results%n_pass))  
        ipass(1) = 0  
        pass = 2  
        do i = 1, n-1  
            if (integration_entry_get_pass (results%entry(i)) &  
                /= integration_entry_get_pass (results%entry(i+1))) then  
                ipass(pass) = i  
                pass = pass + 1  
            end if  
        end do  
        ymin_arr = integration_entry_get_integral (results%entry(:n)) &  
            - integration_entry_get_error (results%entry(:n))  
        ymin = minval (ymin_arr)  
        ymax_arr = integration_entry_get_integral (results%entry(:n)) &  
            + integration_entry_get_error (results%entry(:n))
```

```

ymax = maxval (ymax_arr)
yavg = (ymax + ymin) / 2
ydif = (ymax - ymin)
if (ydif * 1.5 > GML_MIN_RANGE_RATIO * yavg) then
    y0 = yavg - ydif * 0.75
    y1 = yavg + ydif * 0.75
else
    y0 = yavg * (1 - GML_MIN_RANGE_RATIO / 2)
    y1 = yavg * (1 + GML_MIN_RANGE_RATIO / 2)
end if
write (unit, "(A)") "\documentclass{article}"
write (unit, "(A)") "\usepackage{a4wide}"
write (unit, "(A)") "\usepackage{gamelan}"
write (unit, "(A)") "\usepackage{amsmath}"
write (unit, "(A)") ""
write (unit, "(A)") "\begin{document}"
write (unit, "(A)") "\begin{gmlfile}"
write (unit, "(A)") "\section*{Integration Results Display}"
write (unit, "(A)") ""
write (unit, "(A)") "Process: \verb|" // char (filename) // "|"
write (unit, "(A)") ""
write (unit, "(A)") "\vspace*{2\baselineskip}"
write (unit, "(A)") "\unitlength 1mm"
write (unit, "(A)") "\begin{gmlcode}"
write (unit, "(A)") " picture sym; sym = fshape (circle scaled 1mm());"
write (unit, "(A)") " color col.band; col.band = 0.9white;"
write (unit, "(A)") " color col.eband; col.eband = 0.98white;"
write (unit, "(A)") "\end{gmlcode}"
write (unit, "(A)") "\begin{gmlgraph*}(130,180)[history]"
write (unit, "(A)") " setup (linear, linear);"
write (unit, "(A,I0,A)") " history.n_pass = ", n_pass, ";"
write (unit, "(A,I0,A,A)") " history.n_it = ", n, ";"
write (unit, "(A,A,A)") " history.y0 = #""", char (mp_format (y0)), """;"
write (unit, "(A,A,A)") " history.y1 = #""", char (mp_format (y1)), """;"
write (unit, "(A)") &
    " graphrange (#0.5, history.y0), (#(n+0.5), history.y1);"
do pass = 1, n_pass
    write (unit, "(A,I0,A,I0,A)") &
        " history.pass[" , pass, "] = ", ipass(pass), ";"
    write (unit, "(A,I0,A,A,A)") &
        " history.avg[" , pass, "] = #""", &
        char (mp_format &
            (integration_entry_get_integral (results%average(pass)))) , &
        """;"
    write (unit, "(A,I0,A,A,A)") &
        " history.err[" , pass, "] = #""", &
        char (mp_format &
            (integration_entry_get_error (results%average(pass)))) , &
        """;"
    write (unit, "(A,I0,A,A,A)") &
        " history.chi[" , pass, "] = #""", &
        char (mp_format &
            (integration_entry_get_chi2 (results%average(pass)))) , &
        """;"

```

```

end do
write (unit, "(A,I0,A,I0,A)") &
" history.pass[" , n_pass + 1, "] = " , n, ";"
write (unit, "(A)") " for i = 1 upto history.n_pass:"
write (unit, "(A)") " if history.chi[i] greater one:"
write (unit, "(A)") " fill plot ("
write (unit, "(A)") &
" (#(history.pass[i] +.5), " &
// "history.avg[i] minus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
" (#(history.pass[i+1]+.5), " &
// "history.avg[i] minus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
" (#(history.pass[i+1]+.5), " &
// "history.avg[i] plus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
" (#(history.pass[i] +.5), " &
// "history.avg[i] plus history.err[i] times history.chi[i])"
write (unit, "(A)") " ) withcolor col.eband fi;"
write (unit, "(A)") " fill plot ("
write (unit, "(A)") &
" (#(history.pass[i] +.5), history.avg[i] minus history.err[i]),"
write (unit, "(A)") &
" (#(history.pass[i+1]+.5), history.avg[i] minus history.err[i]),"
write (unit, "(A)") &
" (#(history.pass[i+1]+.5), history.avg[i] plus history.err[i]),"
write (unit, "(A)") &
" (#(history.pass[i] +.5), history.avg[i] plus history.err[i])"
write (unit, "(A)") " ) withcolor col.band;"
write (unit, "(A)") " draw plot ("
write (unit, "(A)") &
" (#(history.pass[i] +.5), history.avg[i]),"
write (unit, "(A)") &
" (#(history.pass[i+1]+.5), history.avg[i])"
write (unit, "(A)") " ) dashed evenly;"
write (unit, "(A)") " endfor"
write (unit, "(A)") " for i = 1 upto history.n_pass + 1:"
write (unit, "(A)") " draw plot ("
write (unit, "(A)") &
" (#(history.pass[i]+.5), history.y0),"
write (unit, "(A)") &
" (#(history.pass[i]+.5), history.y1)"
write (unit, "(A)") " ) dashed withdots;"
write (unit, "(A)") " endfor"
do i = 1, n
write (unit, "(A,I0,A,A,A,A)") " plot (history) (#", &
i, ", #""", &
char (mp_format (integration_entry_get_integral (results%entry(i))),&
""") vbar #""", &
char (mp_format (integration_entry_get_error (results%entry(i))), &
""";"
end do
write (unit, "(A)") " draw piecewise from (history) " &
// "withsymbol sym;"

```

```

write (unit, "(A)") " fullgrid.lr (5,20);"
write (unit, "(A)") " standardgrid.bt (n);"
write (unit, "(A)") " begingmleps ""Whizard-Logo.eps"";"
write (unit, "(A)") " base := (120*unitlength,170*unitlength);"
write (unit, "(A)") " height := 9.6*unitlength;"
write (unit, "(A)") " width := 11.2*unitlength;"
write (unit, "(A)") " endgmleps;"
write (unit, "(A)") "\end{gmlgraph*}"
write (unit, "(A)") "\end{gmlfile}"
write (unit, "(A)") "\clearpage"
write (unit, "(A)") "\begin{verbatim}"
if (reset) then
    call results%pacify (reset)
end if
call integration_results_write (results, unit)
write (unit, "(A)") "\end{verbatim}"
write (unit, "(A)") "\end{document}"
close (unit)
end subroutine integration_results_write_driver

```

Call L^AT_EX and Metapost for the history driver file, and convert to PS and PDF.

```

<Integration results: public>+=
    public :: integration_results_compile_driver

<Integration results: sub interfaces>+=
    module subroutine integration_results_compile_driver &
        (results, filename, os_data)
        type(integration_results_t), intent(in) :: results
        type(string_t), intent(in) :: filename
        type(os_data_t), intent(in) :: os_data
    end subroutine integration_results_compile_driver

<Integration results: procedures>+=
    module subroutine integration_results_compile_driver &
        (results, filename, os_data)
        type(integration_results_t), intent(in) :: results
        type(string_t), intent(in) :: filename
        type(os_data_t), intent(in) :: os_data
        integer :: unit_dev, status
        type(string_t) :: file_tex, file_dvi, file_ps, file_pdf, file_mp
        type(string_t) :: setenv_tex, setenv_mp, pipe, pipe_dvi
        if (.not. os_data%event_analysis) then
            call msg_warning ("Skipping integration history display " &
                // "because latex or mpost is not available")
            return
        end if
        file_tex = filename // ".tex"
        file_dvi = filename // ".dvi"
        file_ps = filename // ".ps"
        file_pdf = filename // ".pdf"
        file_mp = filename // ".mp"
        call msg_message ("Creating integration history display "&
            // char (file_ps) // " and " // char (file_pdf))
        BLOCK: do
            unit_dev = free_unit ()

```

```

open (file = "/dev/null", unit = unit_dev, &
      action = "write", iostat = status)
if (status /= 0) then
  pipe = ""
  pipe_dvi = ""
else
  pipe = " > /dev/null"
  pipe_dvi = " 2>/dev/null 1>/dev/null"
end if
close (unit_dev)
if (os_data%whizard_texpath /= "") then
  setenv_tex = &
    "TEXINPUTS=" // os_data%whizard_texpath // " :$TEXINPUTS "
  setenv_mp = &
    "MPINPUTS=" // os_data%whizard_texpath // " :$MPINPUTS "
else
  setenv_tex = ""
  setenv_mp = ""
end if
call os_system_call (setenv_tex // os_data%latex // " " // &
  file_tex // pipe, status)
if (status /= 0) exit BLOCK
if (os_data%gml /= "") then
  call os_system_call (setenv_mp // os_data%gml // " " // &
    file_mp // pipe, status)
else
  call msg_error ("Could not use GAMELAN/MetaPOST.")
  exit BLOCK
end if
if (status /= 0) exit BLOCK
call os_system_call (setenv_tex // os_data%latex // " " // &
  file_tex // pipe, status)
if (status /= 0) exit BLOCK
if (os_data%event_analysis_ps) then
  call os_system_call (os_data%dvips // " " // &
    file_dvi // pipe_dvi, status)
  if (status /= 0) exit BLOCK
else
  call msg_warning ("Skipping PostScript generation because dvips " &
    // "is not available")
  exit BLOCK
end if
if (os_data%event_analysis_pdf) then
  call os_system_call (os_data%ps2pdf // " " // &
    file_ps, status)
  if (status /= 0) exit BLOCK
else
  call msg_warning ("Skipping PDF generation because ps2pdf " &
    // "is not available")
  exit BLOCK
end if
exit BLOCK
end do BLOCK
if (status /= 0) then

```

```

        call msg_error ("Unable to compile integration history display")
    end if
end subroutine integration_results_compile_driver

```

21.3.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<integration_results_ut.f90>≡
  <File header>

```

```

module integration_results_ut
  use unit_tests
  use integration_results_util

```

```

  <Standard module head>

```

```

  <integration results: public test>

```

```

contains

```

```

  <integration results: test driver>

```

```

end module integration_results_ut

```

```

<integration_results_util.f90>≡
  <File header>

```

```

module integration_results_util

```

```

  <Use kinds>

```

```

  use integration_results

```

```

  <Standard module head>

```

```

  <integration results: test declarations>

```

```

contains

```

```

  <integration results: tests>

```

```

end module integration_results_util

```

API: driver for the unit tests below.

```

<integration results: public test>≡
  public :: integration_results_test

```

```

<integration results: test driver>≡
  subroutine integration_results_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <integration results: execute tests>
  end subroutine integration_results_test

```

Integration entry

```
<integration results: execute tests>≡
  call test (integration_results_1, "integration_results_1", &
    "record single line and write to log", &
    u, results)

<integration results: test declarations>≡
  public :: integration_results_1

<integration results: tests>≡
  subroutine integration_results_1 (u)
    integer, intent(in) :: u
    type(integration_entry_t) :: entry

    write (u, "(A)")  "* Test output: integration_results_1"
    write (u, "(A)")  "* Purpose: record single entry and write to log"
    write (u, "(A)")

    write (u, "(A)")  "* Write single line output"
    write (u, "(A)")

    entry = integration_entry_t ( &
      & process_type = 1, &
      & pass = 1, &
      & it = 1, &
      & n_it = 10, &
      & n_calls = 1000, &
      & n_calls_valid = 500, &
      & improved = .true., &
      & integral = 1.0_default, &
      & error = 0.5_default, &
      & efficiency = 0.25_default, &
      & efficiency_pos = 0.22_default, &
      & efficiency_neg = 0.03_default)
    call entry%write (u, 3)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: integration_results_1"

  end subroutine integration_results_1

<integration results: execute tests>+≡
  call test (integration_results_2, "integration_results_2", &
    "record single result and write to log", &
    u, results)

<integration results: test declarations>+≡
  public :: integration_results_2

<integration results: tests>+≡
  subroutine integration_results_2 (u)
    integer, intent(in) :: u
    type(integration_results_t) :: results

    write (u, "(A)")  "* Test output: integration_results_2"
```



```

write (u, "(A)")  "*" Purpose: record single result and write to log"
write (u, "(A)")

write (u, "(A)")  "*" Write single line output"
write (u, "(A)")

call results%init (PRC_DECAY)
call results%append (1, 250, 0, 1.0_default, 0.5_default, 0.25_default,&
    & 0._default, 0._default)

call results%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Test output end: integration_results_2"

end subroutine integration_results_2

<integration results: execute tests>+≡
call test (integration_results_3, "integration_results_3", &
    "initialize display and add/display each entry", &
    u, results)

<integration results: test declarations>+≡
public :: integration_results_3

<integration results: tests>+≡
subroutine integration_results_3 (u)
    integer, intent(in) :: u
    type(integration_results_t) :: results

    write (u, "(A)")  "*" Test output: integration_results_2"
    write (u, "(A)")  "*" Purpose: intialize display, record three entries,&
        & display pass average and finalize display"
    write (u, "(A)")

    write (u, "(A)")  "*" Initialize display and add entry"
    write (u, "(A)")

    call results%init (PRC_DECAY)
    call results%set_verbosity (1)
    call results%display_init (screen = .false., unit = u)
    call results%new_pass ()

    call results%record (1, 250, 1.0_default, 0.5_default, 0.25_default)
    call results%record (1, 250, 1.1_default, 0.5_default, 0.25_default)
    call results%record (1, 250, 0.9_default, 0.5_default, 0.25_default)

    write (u, "(A)")
    write (u, "(A)")  "*" Display pass"
    write (u, "(A)")

    call results%display_pass ()

    write (u, "(A)")
    write (u, "(A)")  "*" Finalize displays"

```

```

write (u, "(A)")

call results%display_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integration_results_3"

end subroutine integration_results_3

<integration results: execute tests>+≡
call test (integration_results_4, "integration_results_4", &
  "record extended results and display", &
  u, results)

<integration results: test declarations>+≡
public :: integration_results_4

<integration results: tests>+≡
subroutine integration_results_4 (u)
  integer, intent(in) :: u
  type(integration_results_t) :: results

  write (u, "(A)")  "* Test output: integration_results_4"
  write (u, "(A)")  "* Purpose: record extended results and display with verbosity = 2"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize display and record extended result"
  write (u, "(A)")

  call results%init (PRC_DECAY)
  call results%set_verbosity (2)
  call results%display_init (screen = .false., unit = u)
  call results%new_pass ()

  call results%record (1, 250, 150, 1.0_default, 0.5_default, 0.25_default,&
    & 0.22_default, 0.03_default)
  call results%record (1, 250, 180, 1.1_default, 0.5_default, 0.25_default,&
    & 0.23_default, 0.02_default)
  call results%record (1, 250, 130, 0.9_default, 0.5_default, 0.25_default,&
    & 0.25_default, 0.00_default)

  write (u, "(A)")
  write (u, "(A)")  "* Display pass"
  write (u, "(A)")

  call results%display_pass ()

  write (u, "(A)")
  write (u, "(A)")  "* Finalize displays"
  write (u, "(A)")

  call results%display_final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: integration_results_4"

```

```

end subroutine integration_results_4

<integration results: execute tests>+≡
  call test (integration_results_5, "integration_results_5", &
    "record extended results and display", &
    u, results)

<integration results: test declarations>+≡
  public :: integration_results_5

<integration results: tests>+≡
  subroutine integration_results_5 (u)
    integer, intent(in) :: u
    type(integration_results_t) :: results

    write (u, "(A)")  "* Test output: integration_results_5"
    write (u, "(A)")  "* Purpose: record extended results and display with verbosity = 3"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize display and record extended result"
    write (u, "(A)")

    call results%init (PRC_DECAY)
    call results%set_verbosity (3)
    call results%display_init (screen = .false., unit = u)
    call results%new_pass ()

    call results%record (1, 250, 150, 1.0_default, 0.5_default, 0.25_default,&
      & 0.22_default, 0.03_default)
    call results%record (1, 250, 180, 1.1_default, 0.5_default, 0.25_default,&
      & 0.23_default, 0.02_default)
    call results%record (1, 250, 130, 0.9_default, 0.5_default, 0.25_default,&
      & 0.25_default, 0.00_default)
    call results%display_pass ()
    call results%display_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: integration_results_5"

  end subroutine integration_results_5

```

21.4 Dummy integrator

This implementation acts as a placeholder for cases where no integration or event generation is required at all.

```
<mci_none.f90>≡  
<File header>  
  
module mci_none  
  
  <Use kinds>  
  use io_units, only: given_output_unit  
  use phs_base, only: phs_channel_t  
  
  use mci_base  
  
  <Standard module head>  
  
  <MCI none: public>  
  
  <MCI none: types>  
  
  interface  
  <MCI none: sub interfaces>  
  end interface  
  
contains  
  
  <MCI none: main procedures>  
  
end module mci_none  
  
<mci_none_sub.f90>≡  
<File header>  
  
submodule (mci_none) mci_none_s  
  
  use diagnostics, only: msg_message, msg_fatal  
  
  implicit none  
  
contains  
  
  <MCI none: procedures>  
  
end submodule mci_none_s
```

21.4.1 Integrator

The object contains the methods for integration and event generation. For the actual work and data storage, it spawns an instance object.

After an integration pass, we update the `max` parameter to indicate the maximum absolute value of the integrand that the integrator encountered. This

is required for event generation.

```
<MCI none: public>≡
    public :: mci_none_t
<MCI none: types>≡
    type, extends (mci_t) :: mci_none_t
    contains
    <MCI none: mci none: TBP>
    end type mci_none_t
```

Finalizer: no-op.

```
<MCI none: mci none: TBP>≡
    procedure :: final => mci_none_final
<MCI none: sub interfaces>≡
    module subroutine mci_none_final (object)
        class(mci_none_t), intent(inout) :: object
    end subroutine mci_none_final
<MCI none: procedures>≡
    module subroutine mci_none_final (object)
        class(mci_none_t), intent(inout) :: object
    end subroutine mci_none_final
```

Output.

```
<MCI none: mci none: TBP>+≡
    procedure :: write => mci_none_write
<MCI none: sub interfaces>+≡
    module subroutine mci_none_write (object, unit, pacify, md5sum_version)
        class(mci_none_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
    end subroutine mci_none_write
<MCI none: procedures>+≡
    module subroutine mci_none_write (object, unit, pacify, md5sum_version)
        class(mci_none_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Integrator: non-functional dummy"
    end subroutine mci_none_write
```

Startup message: short version.

```
<MCI none: mci none: TBP>+≡
    procedure :: startup_message => mci_none_startup_message
<MCI none: sub interfaces>+≡
    module subroutine mci_none_startup_message (mci, unit, n_calls)
        class(mci_none_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
    end subroutine mci_none_startup_message
```

```

<MCI none: procedures>+≡
  module subroutine mci_none_startup_message (mci, unit, n_calls)
    class(mci_none_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    call msg_message ("Integrator: none")
  end subroutine mci_none_startup_message

```

Log entry: just headline.

```

<MCI none: mci none: TBP>+≡
  procedure :: write_log_entry => mci_none_write_log_entry

<MCI none: sub interfaces>+≡
  module subroutine mci_none_write_log_entry (mci, u)
    class(mci_none_t), intent(in) :: mci
    integer, intent(in) :: u
  end subroutine mci_none_write_log_entry

<MCI none: procedures>+≡
  module subroutine mci_none_write_log_entry (mci, u)
    class(mci_none_t), intent(in) :: mci
    integer, intent(in) :: u
    write (u, "(1x,A)") "MC Integrator is none (no-op)"
  end subroutine mci_none_write_log_entry

```

MD5 sum: nothing.

```

<MCI none: mci none: TBP>+≡
  procedure :: compute_md5sum => mci_none_compute_md5sum

<MCI none: sub interfaces>+≡
  module subroutine mci_none_compute_md5sum (mci, pacify)
    class(mci_none_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
  end subroutine mci_none_compute_md5sum

<MCI none: procedures>+≡
  module subroutine mci_none_compute_md5sum (mci, pacify)
    class(mci_none_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
  end subroutine mci_none_compute_md5sum

```

The number of channels must be one.

```

<CCC MCI none: mci none: TBP>≡
  procedure :: set_dimensions => mci_none_set_dimensions

<CCC MCI none: procedures>≡
  subroutine mci_none_set_dimensions (mci, n_dim, n_channel)
    class(mci_none_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    if (n_channel == 1) then
      mci%n_channel = n_channel
      mci%n_dim = n_dim
      allocate (mci%dim_is_binned (mci%n_dim))
      mci%dim_is_binned = .true.
      mci%n_dim_binned = count (mci%dim_is_binned)
    end if
  end subroutine mci_none_set_dimensions

```

```

        allocate (mci%n_bin (mci%n_dim))
        mci%n_bin = 0
    else
        call msg_fatal ("Attempt to initialize single-channel integrator &
            &for multiple channels")
    end if
end subroutine mci_none_set_dimensions

```

Required by API.

```

<MCI none: mci none: TBP>+≡
    procedure :: declare_flat_dimensions => mci_none_ignore_flat_dimensions

<MCI none: sub interfaces>+≡
    module subroutine mci_none_ignore_flat_dimensions (mci, dim_flat)
        class(mci_none_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_none_ignore_flat_dimensions

<MCI none: procedures>+≡
    module subroutine mci_none_ignore_flat_dimensions (mci, dim_flat)
        class(mci_none_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_none_ignore_flat_dimensions

```

Required by API.

```

<MCI none: mci none: TBP>+≡
    procedure :: declare_equivalences => mci_none_ignore_equivalences

<MCI none: sub interfaces>+≡
    module subroutine mci_none_ignore_equivalences (mci, channel, dim_offset)
        class(mci_none_t), intent(inout) :: mci
        type(phs_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_none_ignore_equivalences

<MCI none: procedures>+≡
    module subroutine mci_none_ignore_equivalences (mci, channel, dim_offset)
        class(mci_none_t), intent(inout) :: mci
        type(phs_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_none_ignore_equivalences

```

Allocate instance with matching type. Gfortran 7/8/9 bug: has to remain in the main module.

```

<MCI none: mci none: TBP>+≡
    procedure :: allocate_instance => mci_none_allocate_instance

<MCI none: main procedures>≡
    subroutine mci_none_allocate_instance (mci, mci_instance)
        class(mci_none_t), intent(in) :: mci
        class(mci_instance_t), intent(out), pointer :: mci_instance
        allocate (mci_none_instance_t :: mci_instance)
    end subroutine mci_none_allocate_instance

```

Integrate. This must not be called at all.

```

<MCI none: mci none: TBP>+≡
  procedure :: integrate => mci_none_integrate

<MCI none: sub interfaces>+≡
  module subroutine mci_none_integrate (mci, instance, sampler, n_it, &
    n_calls, results, pacify)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
  end subroutine mci_none_integrate

<MCI none: procedures>+≡
  module subroutine mci_none_integrate (mci, instance, sampler, n_it, &
    n_calls, results, pacify)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
    call msg_fatal &
      ("Integration: attempt to integrate with the 'mci_none' method")
  end subroutine mci_none_integrate

```

Simulation initializer and finalizer: nothing to do here.

```

<MCI none: mci none: TBP>+≡
  procedure :: prepare_simulation => mci_none_ignore_prepare_simulation

<MCI none: sub interfaces>+≡
  module subroutine mci_none_ignore_prepare_simulation (mci)
    class(mci_none_t), intent(inout) :: mci
  end subroutine mci_none_ignore_prepare_simulation

<MCI none: procedures>+≡
  module subroutine mci_none_ignore_prepare_simulation (mci)
    class(mci_none_t), intent(inout) :: mci
  end subroutine mci_none_ignore_prepare_simulation

```

Generate events, must not be called.

```

<MCI none: mci none: TBP>+≡
  procedure :: generate_weighted_event => mci_none_generate_no_event
  procedure :: generate_unweighted_event => mci_none_generate_no_event

<MCI none: sub interfaces>+≡
  module subroutine mci_none_generate_no_event (mci, instance, sampler)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
  end subroutine mci_none_generate_no_event

```



```

<MCI none: procedures>+≡
  module subroutine mci_none_generate_no_event (mci, instance, sampler)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    call msg_fatal ("Integration: attempt to generate event " // &
      "with the 'mci_none' method")
  end subroutine mci_none_generate_no_event

```

Rebuild an event, no-op.

```

<MCI none: mci none: TBP>+≡
  procedure :: rebuild_event => mci_none_rebuild_event

<MCI none: sub interfaces>+≡
  module subroutine mci_none_rebuild_event (mci, instance, sampler, state)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
  end subroutine mci_none_rebuild_event

<MCI none: procedures>+≡
  module subroutine mci_none_rebuild_event (mci, instance, sampler, state)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
  end subroutine mci_none_rebuild_event

```

21.4.2 Integrator instance

Covering the case of flat dimensions, we store a complete x array. This is filled when generating events.

```

<MCI none: public>+≡
  public :: mci_none_instance_t

<MCI none: types>+≡
  type, extends (mci_instance_t) :: mci_none_instance_t
    contains
    <MCI none: mci none instance: TBP>
  end type mci_none_instance_t

```

Output.

```

<MCI none: mci none instance: TBP>≡
  procedure :: write => mci_none_instance_write

<MCI none: sub interfaces>+≡
  module subroutine mci_none_instance_write (object, unit, pacify)
    class(mci_none_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
  end subroutine mci_none_instance_write

```

```

<MCI none: procedures>+≡
module subroutine mci_none_instance_write (object, unit, pacify)
  class(mci_none_instance_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Integrator instance: non-functional dummy"
end subroutine mci_none_instance_write

```

The finalizer is empty.

```

<MCI none: mci none instance: TBP>+≡
  procedure :: final => mci_none_instance_final

<MCI none: sub interfaces>+≡
  module subroutine mci_none_instance_final (object)
    class(mci_none_instance_t), intent(inout) :: object
  end subroutine mci_none_instance_final

<MCI none: procedures>+≡
module subroutine mci_none_instance_final (object)
  class(mci_none_instance_t), intent(inout) :: object
end subroutine mci_none_instance_final

```

Initializer, empty.

```

<MCI none: mci none instance: TBP>+≡
  procedure :: init => mci_none_instance_init

<MCI none: sub interfaces>+≡
  module subroutine mci_none_instance_init (mci_instance, mci)
    class(mci_none_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
  end subroutine mci_none_instance_init

<MCI none: procedures>+≡
module subroutine mci_none_instance_init (mci_instance, mci)
  class(mci_none_instance_t), intent(out) :: mci_instance
  class(mci_t), intent(in), target :: mci
end subroutine mci_none_instance_init

```

Copy the stored extrema of the integrand in the instance record.

```

<CCC MCI none: mci none instance: TBP>≡
  procedure :: get_max => mci_none_instance_get_max

<CCC MCI none: procedures>+≡
  subroutine mci_none_instance_get_max (instance)
    class(mci_none_instance_t), intent(inout) :: instance
    associate (mci => instance%mci)
      if (mci%max_known) then
        instance%max_known = .true.
        instance%max = mci%max
        instance%min = mci%min
        instance%max_abs = mci%max_abs
        instance%min_abs = mci%min_abs
      end if
    end associate
  end subroutine

```

```

end associate
end subroutine mci_none_instance_get_max

```

Reverse operations: recall the extrema, but only if they are wider than the extrema already stored in the configuration. Also recalculate the efficiency value.

```

<CCC MCI none: mci none instance: TBP>+≡
  procedure :: set_max => mci_none_instance_set_max

<CCC MCI none: procedures>+≡
  subroutine mci_none_instance_set_max (instance)
    class(mci_none_instance_t), intent(inout) :: instance
    associate (mci => instance%mci)
      if (instance%max_known) then
        if (mci%max_known) then
          mci%max = max (mci%max, instance%max)
          mci%min = min (mci%min, instance%min)
          mci%max_abs = max (mci%max_abs, instance%max_abs)
          mci%min_abs = min (mci%min_abs, instance%min_abs)
        else
          mci%max = instance%max
          mci%min = instance%min
          mci%max_abs = instance%max_abs
          mci%min_abs = instance%min_abs
          mci%max_known = .true.
        end if
        if (mci%max_abs /= 0) then
          if (mci%integral_neg == 0) then
            mci%efficiency = mci%integral / mci%max_abs
            mci%efficiency_known = .true.
          else if (mci%n_calls /= 0) then
            mci%efficiency = &
              (mci%integral_pos - mci%integral_neg) / mci%max_abs
            mci%efficiency_known = .true.
          end if
        end if
      end if
    end associate
  end subroutine mci_none_instance_set_max

```

The weight cannot be computed.

```

<MCI none: mci none instance: TBP>+≡
  procedure :: compute_weight => mci_none_instance_compute_weight

<MCI none: sub interfaces>+≡
  module subroutine mci_none_instance_compute_weight (mci, c)
    class(mci_none_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
  end subroutine mci_none_instance_compute_weight

<MCI none: procedures>+≡
  module subroutine mci_none_instance_compute_weight (mci, c)
    class(mci_none_instance_t), intent(inout) :: mci
    integer, intent(in) :: c

```

```

        call msg_fatal ("Integration: attempt to compute weight " // &
            "with the 'mci_none' method")
    end subroutine mci_none_instance_compute_weight

```

Record the integrand, no-op.

```

<MCI none: mci none instance: TBP>+≡
    procedure :: record_integrand => mci_none_instance_record_integrand

<MCI none: sub interfaces>+≡
    module subroutine mci_none_instance_record_integrand (mci, integrand)
        class(mci_none_instance_t), intent(inout) :: mci
        real(default), intent(in) :: integrand
    end subroutine mci_none_instance_record_integrand

<MCI none: procedures>+≡
    module subroutine mci_none_instance_record_integrand (mci, integrand)
        class(mci_none_instance_t), intent(inout) :: mci
        real(default), intent(in) :: integrand
    end subroutine mci_none_instance_record_integrand

```

No-op.

```

<MCI none: mci none instance: TBP>+≡
    procedure :: init_simulation => mci_none_instance_init_simulation
    procedure :: final_simulation => mci_none_instance_final_simulation

<MCI none: sub interfaces>+≡
    module subroutine mci_none_instance_init_simulation &
        (instance, safety_factor)
        class(mci_none_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: safety_factor
    end subroutine mci_none_instance_init_simulation
    module subroutine mci_none_instance_final_simulation (instance)
        class(mci_none_instance_t), intent(inout) :: instance
    end subroutine mci_none_instance_final_simulation

<MCI none: procedures>+≡
    module subroutine mci_none_instance_init_simulation (instance, safety_factor)
        class(mci_none_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: safety_factor
    end subroutine mci_none_instance_init_simulation

    module subroutine mci_none_instance_final_simulation (instance)
        class(mci_none_instance_t), intent(inout) :: instance
    end subroutine mci_none_instance_final_simulation

```

Return excess weight for the current event: return zero, just in case.

```

<MCI none: mci none instance: TBP>+≡
    procedure :: get_event_excess => mci_none_instance_get_event_excess

<MCI none: sub interfaces>+≡
    module function mci_none_instance_get_event_excess (mci) result (excess)
        class(mci_none_instance_t), intent(in) :: mci
        real(default) :: excess
    end function mci_none_instance_get_event_excess

```

```

<MCI none: procedures>+≡
  module function mci_none_instance_get_event_excess (mci) result (excess)
    class(mci_none_instance_t), intent(in) :: mci
    real(default) :: excess
    excess = 0
  end function mci_none_instance_get_event_excess

```

21.4.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<mci_none_ut.f90>≡
  <File header>

  module mci_none_ut
    use unit_tests
    use mci_none_util

    <Standard module head>

    <MCI none: public test>

    contains

    <MCI none: test driver>

  end module mci_none_ut

<mci_none_util.f90>≡
  <File header>

  module mci_none_util

    use mci_base

    use mci_none

    <Standard module head>

    <MCI none: test declarations>

    <MCI none: test types>

    contains

    <MCI none: tests>

  end module mci_none_util

```

API: driver for the unit tests below.

```

<MCI none: public test>≡
  public :: mci_none_test

```

```

<MCI none: test driver>≡
  subroutine mci_none_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <MCI none: execute tests>
  end subroutine mci_none_test

```

Trivial sanity check

Construct an integrator and display it.

```

<MCI none: execute tests>≡
  call test (mci_none_1, "mci_none_1", &
    "dummy integrator", &
    u, results)

<MCI none: test declarations>≡
  public :: mci_none_1

<MCI none: tests>≡
  subroutine mci_none_1 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_none_1"
    write (u, "(A)")  "* Purpose: display mci configuration"
    write (u, "(A)")

    write (u, "(A)")  "* Allocate integrator"
    write (u, "(A)")

    allocate (mci_none_t :: mci)
    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    call mci_instance%write (u)

    call mci_instance%final ()
    call mci%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: mci_none_1"

  end subroutine mci_none_1

```

21.5 Simple midpoint integration

This is a most simple implementation of an integrator. The algorithm is the straightforward multi-dimensional midpoint rule, i.e., the integration hypercube is binned uniformly, the integrand is evaluated at the midpoints of each bin, and the result is the average. The binning is equivalent for all integration dimensions.

This rule is accurate to the order h^2 , where h is the bin width. Given that $h = N^{-1/d}$, where d is the integration dimension and N is the total number of sampling points, we get a relative error of order $N^{-2/d}$. This is superior to MC integration if $d < 4$, and equivalent if $d = 4$. It is not worse than higher-order formulas (such as Gauss integration) if the integrand is not smooth, e.g., if it contains cuts.

The integrator is specifically single-channel. However, we do not limit the dimension.

```
<mci_midpoint.f90>≡
  <File header>

  module mci_midpoint

    <Use kinds>
    use phs_base

    use mci_base

    <Standard module head>

    <MCI midpoint: public>

    <MCI midpoint: types>

    interface
    <MCI midpoint: sub interfaces>
    end interface

    contains

    <MCI midpoint: main procedures>

  end module mci_midpoint
<mci_midpoint_sub.f90>≡
  <File header>

  submodule (mci_midpoint) mci_midpoint_s

    use io_units
    use diagnostics

    implicit none

    contains

    <MCI midpoint: procedures>
```

```
end submodule mci_midpoint_s
```

21.5.1 Integrator

The object contains the methods for integration and event generation. For the actual work and data storage, it spawns an instance object.

After an integration pass, we update the `max` parameter to indicate the maximum absolute value of the integrand that the integrator encountered. This is required for event generation.

```
<MCI midpoint: public>≡
  public :: mci_midpoint_t

<MCI midpoint: types>≡
  type, extends (mci_t) :: mci_midpoint_t
    integer :: n_dim_binned = 0
    logical, dimension(:), allocatable :: dim_is_binned
    logical :: calls_known = .false.
    integer :: n_calls = 0
    integer :: n_calls_pos = 0
    integer :: n_calls_nul = 0
    integer :: n_calls_neg = 0
    real(default) :: integral_pos = 0
    real(default) :: integral_neg = 0
    integer, dimension(:), allocatable :: n_bin
    logical :: max_known = .false.
    real(default) :: max = 0
    real(default) :: min = 0
    real(default) :: max_abs = 0
    real(default) :: min_abs = 0
  contains
    <MCI midpoint: mci midpoint: TBP>
  end type mci_midpoint_t
```

Finalizer: base version is sufficient

```
<MCI midpoint: mci midpoint: TBP>≡
  procedure :: final => mci_midpoint_final

<MCI midpoint: sub interfaces>≡
  module subroutine mci_midpoint_final (object)
    class(mci_midpoint_t), intent(inout) :: object
  end subroutine mci_midpoint_final

<MCI midpoint: procedures>≡
  module subroutine mci_midpoint_final (object)
    class(mci_midpoint_t), intent(inout) :: object
    call object%base_final ()
  end subroutine mci_midpoint_final
```

Output.

```
<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: write => mci_midpoint_write
```


<MCI midpoint: sub interfaces>+≡

```
module subroutine mci_midpoint_write (object, unit, pacify, md5sum_version)
  class(mci_midpoint_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  logical, intent(in), optional :: md5sum_version
end subroutine mci_midpoint_write
```

<MCI midpoint: procedures>+≡

```
module subroutine mci_midpoint_write (object, unit, pacify, md5sum_version)
  class(mci_midpoint_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  logical, intent(in), optional :: md5sum_version
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Single-channel midpoint rule integrator:"
  call object%base_write (u, pacify, md5sum_version)
  if (object%n_dim_binned < object%n_dim) then
    write (u, "(3x,A,99(1x,I0))") "Flat dimensions      =", &
      pack ([i, i = 1, object%n_dim], mask = .not. object%dim_is_binned)
    write (u, "(3x,A,I0)") "Number of binned dim = ", object%n_dim_binned
  end if
  if (object%calls_known) then
    write (u, "(3x,A,99(1x,I0))") "Number of bins      =", object%n_bin
    write (u, "(3x,A,I0)") "Number of calls      = ", object%n_calls
    if (object%n_calls_pos /= object%n_calls) then
      write (u, "(3x,A,I0)") "  positive value      = ", object%n_calls_pos
      write (u, "(3x,A,I0)") "  zero value          = ", object%n_calls_nul
      write (u, "(3x,A,I0)") "  negative value       = ", object%n_calls_neg
      write (u, "(3x,A,ES17.10)") &
        "Integral (pos. part) = ", object%integral_pos
      write (u, "(3x,A,ES17.10)") &
        "Integral (neg. part) = ", object%integral_neg
    end if
  end if
  if (object%max_known) then
    write (u, "(3x,A,ES17.10)") "Maximum of integrand = ", object%max
    write (u, "(3x,A,ES17.10)") "Minimum of integrand = ", object%min
    if (object%min /= object%min_abs) then
      write (u, "(3x,A,ES17.10)") "Maximum (abs. value) = ", object%max_abs
      write (u, "(3x,A,ES17.10)") "Minimum (abs. value) = ", object%min_abs
    end if
  end if
  if (allocated (object%rng)) call object%rng%write (u)
end subroutine mci_midpoint_write
```

Startup message: short version.

<MCI midpoint: mci midpoint: TBP>+≡

```
procedure :: startup_message => mci_midpoint_startup_message
```

<MCI midpoint: sub interfaces>+≡

```
module subroutine mci_midpoint_startup_message (mci, unit, n_calls)
  class(mci_midpoint_t), intent(in) :: mci
  integer, intent(in), optional :: unit, n_calls
```

```

        end subroutine mci_midpoint_startup_message
<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_startup_message (mci, unit, n_calls)
    class(mci_midpoint_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    call mci%base_startup_message (unit = unit, n_calls = n_calls)
    if (mci%n_dim_binned < mci%n_dim) then
        write (msg_buffer, "(A,2(1x,I0,1x,A))" ) &
            "Integrator: Midpoint rule:", &
            mci%n_dim_binned, "binned dimensions"
    else
        write (msg_buffer, "(A,2(1x,I0,1x,A))" ) &
            "Integrator: Midpoint rule"
    end if
    call msg_message (unit = unit)
end subroutine mci_midpoint_startup_message

```

Log entry: just headline.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: write_log_entry => mci_midpoint_write_log_entry
<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_write_log_entry (mci, u)
        class(mci_midpoint_t), intent(in) :: mci
        integer, intent(in) :: u
    end subroutine mci_midpoint_write_log_entry
<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_write_log_entry (mci, u)
    class(mci_midpoint_t), intent(in) :: mci
    integer, intent(in) :: u
    write (u, "(1x,A)") "MC Integrator is Midpoint rule"
end subroutine mci_midpoint_write_log_entry

```

MD5 sum: nothing.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: compute_md5sum => mci_midpoint_compute_md5sum
<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_compute_md5sum (mci, pacify)
        class(mci_midpoint_t), intent(inout) :: mci
        logical, intent(in), optional :: pacify
    end subroutine mci_midpoint_compute_md5sum
<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_compute_md5sum (mci, pacify)
    class(mci_midpoint_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
end subroutine mci_midpoint_compute_md5sum

```

The number of channels must be one.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: set_dimensions => mci_midpoint_set_dimensions

```

```

<MCI midpoint: sub interfaces>+≡
  module subroutine mci_midpoint_set_dimensions (mci, n_dim, n_channel)
    class(mci_midpoint_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
  end subroutine mci_midpoint_set_dimensions

<MCI midpoint: procedures>+≡
  module subroutine mci_midpoint_set_dimensions (mci, n_dim, n_channel)
    class(mci_midpoint_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    if (n_channel == 1) then
      mci%n_channel = n_channel
      mci%n_dim = n_dim
      allocate (mci%dim_is_binned (mci%n_dim))
      mci%dim_is_binned = .true.
      mci%n_dim_binned = count (mci%dim_is_binned)
      allocate (mci%n_bin (mci%n_dim))
      mci%n_bin = 0
    else
      call msg_fatal ("Attempt to initialize single-channel integrator &
        &for multiple channels")
    end if
  end subroutine mci_midpoint_set_dimensions

```

Declare particular dimensions as flat. These dimensions will not be binned.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: declare_flat_dimensions => mci_midpoint_declare_flat_dimensions

<MCI midpoint: sub interfaces>+≡
  module subroutine mci_midpoint_declare_flat_dimensions (mci, dim_flat)
    class(mci_midpoint_t), intent(inout) :: mci
    integer, dimension(:), intent(in) :: dim_flat
  end subroutine mci_midpoint_declare_flat_dimensions

<MCI midpoint: procedures>+≡
  module subroutine mci_midpoint_declare_flat_dimensions (mci, dim_flat)
    class(mci_midpoint_t), intent(inout) :: mci
    integer, dimension(:), intent(in) :: dim_flat
    integer :: d
    mci%n_dim_binned = mci%n_dim - size (dim_flat)
    do d = 1, size (dim_flat)
      mci%dim_is_binned(dim_flat(d)) = .false.
    end do
    mci%n_dim_binned = count (mci%dim_is_binned)
  end subroutine mci_midpoint_declare_flat_dimensions

```

Declare particular channels as equivalent. This has no effect.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: declare_equivalences => mci_midpoint_ignore_equivalences

<MCI midpoint: sub interfaces>+≡
  module subroutine mci_midpoint_ignore_equivalences &
    (mci, channel, dim_offset)

```

```

        class(mci_midpoint_t), intent(inout) :: mci
        type(phs_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_midpoint_ignore_equivalences
<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_ignore_equivalences (mci, channel, dim_offset)
    class(mci_midpoint_t), intent(inout) :: mci
    type(phs_channel_t), dimension(:), intent(in) :: channel
    integer, intent(in) :: dim_offset
end subroutine mci_midpoint_ignore_equivalences

```

Allocate instance with matching type. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: allocate_instance => mci_midpoint_allocate_instance
<MCI midpoint: main procedures>≡
subroutine mci_midpoint_allocate_instance (mci, mci_instance)
    class(mci_midpoint_t), intent(in) :: mci
    class(mci_instance_t), intent(out), pointer :: mci_instance
    allocate (mci_midpoint_instance_t :: mci_instance)
end subroutine mci_midpoint_allocate_instance

```

Integrate. The number of dimensions is arbitrary. We make sure that the number of calls is evenly distributed among the dimensions. The actual number of calls will typically be smaller than the requested number, but never smaller than 1.

The sampling over a variable number of dimensions implies a variable number of nested loops. We implement this by a recursive subroutine, one loop in each recursion level.

The number of iterations `n_it` is ignored. Also, the error is set to zero in the current implementation.

With this integrator, we allow the calculation to abort immediately when forced by a signal. There is no state that we can save, hence we do not catch an interrupt.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: integrate => mci_midpoint_integrate
<MCI midpoint: sub interfaces>+≡
module subroutine mci_midpoint_integrate (mci, instance, sampler, n_it, &
    n_calls, results, pacify)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
end subroutine mci_midpoint_integrate
<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_integrate (mci, instance, sampler, n_it, &
    n_calls, results, pacify)

```

```

class(mci_midpoint_t), intent(inout) :: mci
class(mci_instance_t), intent(inout), target :: instance
class(mci_sampler_t), intent(inout), target :: sampler
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
logical, intent(in), optional :: pacify
class(mci_results_t), intent(inout), optional :: results
real(default), dimension(:), allocatable :: x
real(default) :: integral, integral_pos, integral_neg
integer :: n_bin
select type (instance)
type is (mci_midpoint_instance_t)
    allocate (x (mci%n_dim))
    integral = 0
    integral_pos = 0
    integral_neg = 0
    select case (mci%n_dim_binned)
    case (1)
        n_bin = n_calls
    case (2:)
        n_bin = max (int (n_calls ** (1. / mci%n_dim_binned)), 1)
    end select
    where (mci%dim_is_binned)
        mci%n_bin = n_bin
    elsewhere
        mci%n_bin = 1
    end where
    mci%n_calls = product (mci%n_bin)
    mci%n_calls_pos = 0
    mci%n_calls_nul = 0
    mci%n_calls_neg = 0
    mci%calls_known = .true.
    call sample_dim (mci%n_dim)
    mci%integral = integral / mci%n_calls
    mci%integral_pos = integral_pos / mci%n_calls
    mci%integral_neg = integral_neg / mci%n_calls
    mci%integral_known = .true.
    call instance%set_max ()
    if (present (results)) then
        call results%record (1, mci%n_calls, &
            mci%integral, mci%error, mci%efficiency)
    end if
end select
contains
recursive subroutine sample_dim (d)
    integer, intent(in) :: d
    integer :: i
    real(default) :: value
    do i = 1, mci%n_bin(d)
        x(d) = (i - 0.5_default) / mci%n_bin(d)
        if (d > 1) then
            call sample_dim (d - 1)
        else
            if (signal_is_pending ()) return
        end if
    end do
end subroutine sample_dim

```

```

        call instance%evaluate (sampler, 1, x)
        value = instance%get_value ()
        if (value > 0) then
            mci%n_calls_pos = mci%n_calls_pos + 1
            integral = integral + value
            integral_pos = integral_pos + value
        else if (value == 0) then
            mci%n_calls_nul = mci%n_calls_nul + 1
        else
            mci%n_calls_neg = mci%n_calls_neg + 1
            integral = integral + value
            integral_neg = integral_neg + value
        end if
    end if
end do
end subroutine sample_dim
end subroutine mci_midpoint_integrate

```

Simulation initializer and finalizer: nothing to do here.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: prepare_simulation => mci_midpoint_ignore_prepare_simulation

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_ignore_prepare_simulation (mci)
        class(mci_midpoint_t), intent(inout) :: mci
    end subroutine mci_midpoint_ignore_prepare_simulation

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_ignore_prepare_simulation (mci)
        class(mci_midpoint_t), intent(inout) :: mci
    end subroutine mci_midpoint_ignore_prepare_simulation

```

Generate weighted event.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: generate_weighted_event => mci_midpoint_generate_weighted_event

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_generate_weighted_event &
        (mci, instance, sampler)
        class(mci_midpoint_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_midpoint_generate_weighted_event

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_generate_weighted_event &
        (mci, instance, sampler)
        class(mci_midpoint_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        real(default), dimension(mci%n_dim) :: x
        select type (instance)
        type is (mci_midpoint_instance_t)
            call mci%rng%generate (x)
            call instance%evaluate (sampler, 1, x)

```

```

        instance%excess_weight = 0
    end select
end subroutine mci_midpoint_generate_weighted_event

```

For unweighted events, we generate weighted events and apply a simple rejection step to the relative event weight, until an event passes.

Note that we use the `max_abs` value stored in the configuration record, not the one stored in the instance. The latter may change during event generation. After an event generation pass is over, we may update the value for a subsequent pass.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: generate_unweighted_event => &
        mci_midpoint_generate_unweighted_event

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_generate_unweighted_event &
        (mci, instance, sampler)
        class(mci_midpoint_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_midpoint_generate_unweighted_event

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_generate_unweighted_event &
        (mci, instance, sampler)
        class(mci_midpoint_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        real(default) :: x, norm, int
        select type (instance)
        type is (mci_midpoint_instance_t)
            if (mci%max_known .and. mci%max_abs > 0) then
                norm = abs (mci%max_abs * instance%safety_factor)
                REJECTION: do
                    call mci%generate_weighted_event (instance, sampler)
                    if (sampler%is_valid ()) then
                        call mci%rng%generate (x)
                        int = abs (instance%integrand)
                        if (x * norm <= int) then
                            if (norm > 0 .and. norm < int) then
                                instance%excess_weight = int / norm - 1
                            end if
                            exit REJECTION
                        end if
                    end if
                end do REJECTION
            else
                call msg_fatal ("Unweighted event generation: &
                    &maximum of integrand is zero or unknown")
            end if
        end select
    end subroutine mci_midpoint_generate_unweighted_event

```

Rebuild an event, using the `state` input.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: rebuild_event => mci_midpoint_rebuild_event

<MCI midpoint: sub interfaces>+≡
  module subroutine mci_midpoint_rebuild_event (mci, instance, sampler, state)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
  end subroutine mci_midpoint_rebuild_event

<MCI midpoint: procedures>+≡
  module subroutine mci_midpoint_rebuild_event (mci, instance, sampler, state)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    select type (instance)
    type is (mci_midpoint_instance_t)
      call instance%recall (sampler, state)
    end select
  end subroutine mci_midpoint_rebuild_event

```

21.5.2 Integrator instance

Covering the case of flat dimensions, we store a complete `x` array. This is filled when generating events.

```

<MCI midpoint: public>+≡
  public :: mci_midpoint_instance_t

<MCI midpoint: types>+≡
  type, extends (mci_instance_t) :: mci_midpoint_instance_t
    type(mci_midpoint_t), pointer :: mci => null ()
    logical :: max_known = .false.
    real(default) :: max = 0
    real(default) :: min = 0
    real(default) :: max_abs = 0
    real(default) :: min_abs = 0
    real(default) :: safety_factor = 1
    real(default) :: excess_weight = 0
  contains
    <MCI midpoint: mci midpoint instance: TBP>
  end type mci_midpoint_instance_t

```

Output.

```

<MCI midpoint: mci midpoint instance: TBP>≡
  procedure :: write => mci_midpoint_instance_write

<MCI midpoint: sub interfaces>+≡
  module subroutine mci_midpoint_instance_write (object, unit, pacify)
    class(mci_midpoint_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit

```



```

        logical, intent(in), optional :: pacify
    end subroutine mci_midpoint_instance_write

<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_instance_write (object, unit, pacify)
    class(mci_midpoint_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,9(1x,F12.10))") "x =", object%x(:,1)
    write (u, "(1x,A,ES19.12)") "Integrand = ", object%integrand
    write (u, "(1x,A,ES19.12)") "Weight      = ", object%mci_weight
    if (object%safety_factor /= 1) then
        write (u, "(1x,A,ES19.12)") "Safety f  = ", object%safety_factor
    end if
    if (object%excess_weight /= 0) then
        write (u, "(1x,A,ES19.12)") "Excess    = ", object%excess_weight
    end if
    if (object%max_known) then
        write (u, "(1x,A,ES19.12)") "Maximum   = ", object%max
        write (u, "(1x,A,ES19.12)") "Minimum   = ", object%min
        if (object%min /= object%min_abs) then
            write (u, "(1x,A,ES19.12)") "Max.(abs) = ", object%max_abs
            write (u, "(1x,A,ES19.12)") "Min.(abs) = ", object%min_abs
        end if
    end if
end if
end subroutine mci_midpoint_instance_write

```

The finalizer is empty.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: final => mci_midpoint_instance_final

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_final (object)
        class(mci_midpoint_instance_t), intent(inout) :: object
    end subroutine mci_midpoint_instance_final

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_instance_final (object)
        class(mci_midpoint_instance_t), intent(inout) :: object
    end subroutine mci_midpoint_instance_final

```

Initializer.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: init => mci_midpoint_instance_init

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_init (mci_instance, mci)
        class(mci_midpoint_instance_t), intent(out) :: mci_instance
        class(mci_t), intent(in), target :: mci
    end subroutine mci_midpoint_instance_init

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_instance_init (mci_instance, mci)

```

```

class(mci_midpoint_instance_t), intent(out) :: mci_instance
class(mci_t), intent(in), target :: mci
call mci_instance%base_init (mci)
select type (mci)
type is (mci_midpoint_t)
    mci_instance%mci => mci
    call mci_instance%get_max ()
    mci_instance%selected_channel = 1
end select
end subroutine mci_midpoint_instance_init

```

Copy the stored extrema of the integrand in the instance record.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: get_max => mci_midpoint_instance_get_max

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_get_max (instance)
        class(mci_midpoint_instance_t), intent(inout) :: instance
    end subroutine mci_midpoint_instance_get_max

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_instance_get_max (instance)
        class(mci_midpoint_instance_t), intent(inout) :: instance
        associate (mci => instance%mci)
            if (mci%max_known) then
                instance%max_known = .true.
                instance%max = mci%max
                instance%min = mci%min
                instance%max_abs = mci%max_abs
                instance%min_abs = mci%min_abs
            end if
        end associate
    end subroutine mci_midpoint_instance_get_max

```

Reverse operations: recall the extrema, but only if they are wider than the extrema already stored in the configuration. Also recalculate the efficiency value.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: set_max => mci_midpoint_instance_set_max

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_set_max (instance)
        class(mci_midpoint_instance_t), intent(inout) :: instance
    end subroutine mci_midpoint_instance_set_max

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_instance_set_max (instance)
        class(mci_midpoint_instance_t), intent(inout) :: instance
        associate (mci => instance%mci)
            if (instance%max_known) then
                if (mci%max_known) then
                    mci%max = max (mci%max, instance%max)
                    mci%min = min (mci%min, instance%min)
                    mci%max_abs = max (mci%max_abs, instance%max_abs)
                    mci%min_abs = min (mci%min_abs, instance%min_abs)
                end if
            end if
        end associate
    end subroutine mci_midpoint_instance_set_max

```

```

else
    mci%max = instance%max
    mci%min = instance%min
    mci%max_abs = instance%max_abs
    mci%min_abs = instance%min_abs
    mci%max_known = .true.
end if
if (mci%max_abs /= 0) then
    if (mci%integral_neg == 0) then
        mci%efficiency = mci%integral / mci%max_abs
        mci%efficiency_known = .true.
    else if (mci%n_calls /= 0) then
        mci%efficiency = &
            (mci%integral_pos - mci%integral_neg) / mci%max_abs
        mci%efficiency_known = .true.
    end if
end if
end if
end associate
end subroutine mci_midpoint_instance_set_max

```

The weight is the Jacobian of the mapping for the only channel.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: compute_weight => mci_midpoint_instance_compute_weight

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_compute_weight (mci, c)
        class(mci_midpoint_instance_t), intent(inout) :: mci
        integer, intent(in) :: c
        end subroutine mci_midpoint_instance_compute_weight

<MCI midpoint: procedures>+≡
    module subroutine mci_midpoint_instance_compute_weight (mci, c)
        class(mci_midpoint_instance_t), intent(inout) :: mci
        integer, intent(in) :: c
        select case (c)
        case (1)
            mci%mci_weight = mci%f(1)
        case default
            call msg_fatal ("MCI midpoint integrator: only single channel supported")
        end select
    end subroutine mci_midpoint_instance_compute_weight

```

Record the integrand. Update stored values for maximum and minimum.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: record_integrand => mci_midpoint_instance_record_integrand

<MCI midpoint: sub interfaces>+≡
    module subroutine mci_midpoint_instance_record_integrand (mci, integrand)
        class(mci_midpoint_instance_t), intent(inout) :: mci
        real(default), intent(in) :: integrand
    end subroutine mci_midpoint_instance_record_integrand

```

```

<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_instance_record_integrand (mci, integrand)
  class(mci_midpoint_instance_t), intent(inout) :: mci
  real(default), intent(in) :: integrand
  mci%integrand = integrand
  if (mci%max_known) then
    mci%max = max (mci%max, integrand)
    mci%min = min (mci%min, integrand)
    mci%max_abs = max (mci%max_abs, abs (integrand))
    mci%min_abs = min (mci%min_abs, abs (integrand))
  else
    mci%max = integrand
    mci%min = integrand
    mci%max_abs = abs (integrand)
    mci%min_abs = abs (integrand)
    mci%max_known = .true.
  end if
end subroutine mci_midpoint_instance_record_integrand

```

We store the safety factor, otherwise nothing to do here.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
procedure :: init_simulation => mci_midpoint_instance_init_simulation
procedure :: final_simulation => mci_midpoint_instance_final_simulation

```

```

<MCI midpoint: sub interfaces>+≡
module subroutine mci_midpoint_instance_init_simulation &
  (instance, safety_factor)
  class(mci_midpoint_instance_t), intent(inout) :: instance
  real(default), intent(in), optional :: safety_factor
end subroutine mci_midpoint_instance_init_simulation
module subroutine mci_midpoint_instance_final_simulation (instance)
  class(mci_midpoint_instance_t), intent(inout) :: instance
end subroutine mci_midpoint_instance_final_simulation

```

```

<MCI midpoint: procedures>+≡
module subroutine mci_midpoint_instance_init_simulation &
  (instance, safety_factor)
  class(mci_midpoint_instance_t), intent(inout) :: instance
  real(default), intent(in), optional :: safety_factor
  if (present (safety_factor)) instance%safety_factor = safety_factor
end subroutine mci_midpoint_instance_init_simulation

module subroutine mci_midpoint_instance_final_simulation (instance)
  class(mci_midpoint_instance_t), intent(inout) :: instance
end subroutine mci_midpoint_instance_final_simulation

```

Return excess weight for the current event.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
procedure :: get_event_excess => mci_midpoint_instance_get_event_excess

<MCI midpoint: sub interfaces>+≡
module function mci_midpoint_instance_get_event_excess (mci) result (excess)
  class(mci_midpoint_instance_t), intent(in) :: mci
  real(default) :: excess
end function mci_midpoint_instance_get_event_excess

```

```

<MCI midpoint: procedures>+≡
  module function mci_midpoint_instance_get_event_excess (mci) result (excess)
    class(mci_midpoint_instance_t), intent(in) :: mci
    real(default) :: excess
    excess = mci%excess_weight
  end function mci_midpoint_instance_get_event_excess

```

21.5.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<mci_midpoint_ut.f90>≡
  <File header>

  module mci_midpoint_ut
    use unit_tests
    use mci_midpoint_utl

    <Standard module head>

    <MCI midpoint: public test>

    contains

    <MCI midpoint: test driver>

  end module mci_midpoint_ut

<mci_midpoint_uti.f90>≡
  <File header>

  module mci_midpoint_uti

    <Use kinds>
    use io_units
    use rng_base
    use mci_base

    use mci_midpoint

    use rng_base_ut, only: rng_test_t

    <Standard module head>

    <MCI midpoint: test declarations>

    <MCI midpoint: test types>

    contains

    <MCI midpoint: tests>

  end module mci_midpoint_uti

```

API: driver for the unit tests below.

```

<MCI midpoint: public test>≡
    public :: mci_midpoint_test

<MCI midpoint: test driver>≡
    subroutine mci_midpoint_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <MCI midpoint: execute tests>
    end subroutine mci_midpoint_test

```

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

This is the function $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

Mimicking the behavior of a process object, we store the argument and result inside the sampler, so we can `fetch` results.

```

<MCI midpoint: test types>≡
    type, extends (mci_sampler_t) :: test_sampler_1_t
        real(default), dimension(:), allocatable :: x
        real(default) :: val
    contains
    <MCI midpoint: test sampler 1: TBP>
    end type test_sampler_1_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI midpoint: test sampler 1: TBP>≡
    procedure :: write => test_sampler_1_write

<MCI midpoint: tests>≡
    subroutine test_sampler_1_write (object, unit, testflag)
        class(test_sampler_1_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"
    end subroutine test_sampler_1_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI midpoint: test sampler 1: TBP>+≡
    procedure :: evaluate => test_sampler_1_evaluate

<MCI midpoint: tests>+≡
    subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in

```

```

    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    sampler%val = 3 * x_in(1) ** 2
    call sampler%fetch (val, x, f)
end subroutine test_sampler_1_evaluate

```

The point is always valid.

```

⟨MCI midpoint: test sampler 1: TBP⟩+≡
    procedure :: is_valid => test_sampler_1_is_valid

⟨MCI midpoint: tests⟩+≡
    function test_sampler_1_is_valid (sampler) result (valid)
        class(test_sampler_1_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

⟨MCI midpoint: test sampler 1: TBP⟩+≡
    procedure :: rebuild => test_sampler_1_rebuild

⟨MCI midpoint: tests⟩+≡
    subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        if (allocated (sampler%x)) deallocate (sampler%x)
        allocate (sampler%x (size (x_in)))
        sampler%x = x_in
        sampler%val = val
        x(:,1) = sampler%x
        f = 1
    end subroutine test_sampler_1_rebuild

```

Extract the results.

```

⟨MCI midpoint: test sampler 1: TBP⟩+≡
    procedure :: fetch => test_sampler_1_fetch

⟨MCI midpoint: tests⟩+≡
    subroutine test_sampler_1_fetch (sampler, val, x, f)
        class(test_sampler_1_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x(:,1) = sampler%x
        f = 1
    end subroutine test_sampler_1_fetch

```

```
end subroutine test_sampler_1_fetch
```

This is the function $f(x) = 3x^2 + 2y$ with integral $\int_0^1 f(x,y) dx dy = 2$ and maximum $f(1) = 5$.

```
<MCI midpoint: test types>+≡
  type, extends (mci_sampler_t) :: test_sampler_2_t
    real(default) :: val
    real(default), dimension(2) :: x
  contains
    <MCI midpoint: test sampler 2: TBP>
  end type test_sampler_2_t
```

Output: There is nothing stored inside, so just print an informative line.

```
<MCI midpoint: test sampler 2: TBP>≡
  procedure :: write => test_sampler_2_write

<MCI midpoint: tests>+≡
  subroutine test_sampler_2_write (object, unit, testflag)
    class(test_sampler_2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2 + 2 y"
  end subroutine test_sampler_2_write
```

Evaluate: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```
<MCI midpoint: test sampler 2: TBP>+≡
  procedure :: evaluate => test_sampler_2_evaluate

<MCI midpoint: tests>+≡
  subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    sampler%x = x_in
    sampler%val = 3 * x_in(1) ** 2 + 2 * x_in(2)
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_2_evaluate
```

The point is always valid.

```
<MCI midpoint: test sampler 2: TBP>+≡
  procedure :: is_valid => test_sampler_2_is_valid

<MCI midpoint: tests>+≡
  function test_sampler_2_is_valid (sampler) result (valid)
    class(test_sampler_2_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
```



```
end function test_sampler_2_is_valid
```

Rebuild: compute all but the function value.

```
<MCI midpoint: test sampler 2: TBP>+≡
  procedure :: rebuild => test_sampler_2_rebuild

<MCI midpoint: tests>+≡
  subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_2_rebuild
```

```
<MCI midpoint: test sampler 2: TBP>+≡
  procedure :: fetch => test_sampler_2_fetch

<MCI midpoint: tests>+≡
  subroutine test_sampler_2_fetch (sampler, val, x, f)
    class(test_sampler_2_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_2_fetch
```

This is the function $f(x) = (1 - 3x^2)\theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

```
<MCI midpoint: test types>+≡
  type, extends (mci_sampler_t) :: test_sampler_4_t
    real(default) :: val
    real(default), dimension(:), allocatable :: x
  contains
    <MCI midpoint: test sampler 4: TBP>
  end type test_sampler_4_t
```

Output: There is nothing stored inside, so just print an informative line.

```
<MCI midpoint: test sampler 4: TBP>≡
  procedure :: write => test_sampler_4_write

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_write (object, unit, testflag)
    class(test_sampler_4_t), intent(in) :: object
```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
integer :: u
u = given_output_unit (unit)
write (u, "(1x,A)") "Test sampler: f(x) = 1 - 3 x^2"
end subroutine test_sampler_4_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: evaluate => test_sampler_4_evaluate

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_4_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (x_in(1) >= .5_default) then
      sampler%val = 1 - 3 * x_in(1) ** 2
    else
      sampler%val = 0
    end if
    if (.not. allocated (sampler%x)) allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_4_evaluate

```

The point is always valid.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: is_valid => test_sampler_4_is_valid

<MCI midpoint: tests>+≡
  function test_sampler_4_is_valid (sampler) result (valid)
    class(test_sampler_4_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_4_is_valid

```

Rebuild: compute all but the function value.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: rebuild => test_sampler_4_rebuild

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_4_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f

```

```

    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
end subroutine test_sampler_4_rebuild

```

```

<MCI midpoint: test sampler 4: TBP>+≡
    procedure :: fetch => test_sampler_4_fetch

```

```

<MCI midpoint: tests>+≡
    subroutine test_sampler_4_fetch (sampler, val, x, f)
        class(test_sampler_4_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x(:,1) = sampler%x
        f = 1
    end subroutine test_sampler_4_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

```

<MCI midpoint: execute tests>≡
    call test (mci_midpoint_1, "mci_midpoint_1", &
        "one-dimensional integral", &
        u, results)

<MCI midpoint: test declarations>≡
    public :: mci_midpoint_1

<MCI midpoint: tests>+≡
    subroutine mci_midpoint_1 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler

        write (u, "(A)")  "* Test output: mci_midpoint_1"
        write (u, "(A)")  "* Purpose: integrate function in one dimension"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_midpoint_t :: mci)
        call mci%set_dimensions (1, 1)

        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

```

```

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_1_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.8"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.8_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.7"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.7_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.9"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.9_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_1"

end subroutine mci_midpoint_1

```

Two-dimensional integration

Construct an integrator and use it for a two-dimensional sampler.

(MCI midpoint: execute tests) +=

```

call test (mci_midpoint_2, "mci_midpoint_2", &
  "two-dimensional integral", &
  u, results)

```

```

<MCI midpoint: test declarations>+≡
    public :: mci_midpoint_2

<MCI midpoint: tests>+≡
    subroutine mci_midpoint_2 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler

        write (u, "(A)")  "* Test output: mci_midpoint_2"
        write (u, "(A)")  "* Purpose: integrate function in two dimensions"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_midpoint_t :: mci)
        call mci%set_dimensions (2, 1)

        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")  "* Initialize test sampler"
        write (u, "(A)")

        allocate (test_sampler_2_t :: sampler)
        call sampler%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Evaluate for x = 0.8, y = 0.2"
        write (u, "(A)")

        call mci_instance%evaluate (sampler, 1, [0.8_default, 0.2_default])
        call mci_instance%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Integrate with n_calls = 1000"
        write (u, "(A)")

        call mci%integrate (mci_instance, sampler, 1, 1000)
        call mci%write (u)

        call mci_instance%final ()
        call mci%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: mci_midpoint_2"

```

```
end subroutine mci_midpoint_2
```

Two-dimensional integration with flat dimension

Construct an integrator and use it for a two-dimensional sampler, where the function is constant in the second dimension.

```
<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_3, "mci_midpoint_3", &
    "two-dimensional integral with flat dimension", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_3

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_3 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_midpoint_3"
    write (u, "(A)")  "* Purpose: integrate function with one flat dimension"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_midpoint_t :: mci)
    select type (mci)
    type is (mci_midpoint_t)
      call mci%set_dimensions (2, 1)
      call mci%declare_flat_dimensions ([2])
    end select

    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    write (u, "(A)")  "* Initialize test sampler"
    write (u, "(A)")

    allocate (test_sampler_1_t :: sampler)
    call sampler%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Evaluate for x = 0.8, y = 0.2"
    write (u, "(A)")
```

```

call mci_instance%evaluate (sampler, 1, [0.8_default, 0.2_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_3"

end subroutine mci_midpoint_3

```

Integrand with sign flip

Construct an integrator and use it for a one-dimensional sampler.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_4, "mci_midpoint_4", &
    "integrand with sign flip", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_4

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_4 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_midpoint_4"
    write (u, "(A)")  "* Purpose: integrate function with sign flip &
      &in one dimension"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_midpoint_t :: mci)
    call mci%set_dimensions (1, 1)

    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

```

```

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_4_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.8"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.8_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_4"

end subroutine mci_midpoint_4

```

Weighted events

Generate weighted events. Without rejection, we do not need to know maxima and minima, so we can start generating events immediately. We have two dimensions.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_5, "mci_midpoint_5", &
    "weighted events", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_5

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_5 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng
    class(mci_state_t), allocatable :: state

```



```

write (u, "(A)")  "* Test output: mci_midpoint_5"
write (u, "(A)")  "* Purpose: generate weighted events"
write (u, "(A)")

write (u, "(A)")  "* Initialize integrator"
write (u, "(A)")

allocate (mci_midpoint_t :: mci)
call mci%set_dimensions (2, 1)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_2_t :: sampler)

write (u, "(A)")  "* Initialize random-number generator"
write (u, "(A)")

allocate (rng_test_t :: rng)
call rng%init ()
call mci%import_rng (rng)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call mci%generate_weighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call mci%generate_weighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Store data"
write (u, "(A)")

allocate (state)
call mci_instance%store (state)
call mci_instance%final ()
deallocate (mci_instance)

call state%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Recall data and rebuild event"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)
call mci%rebuild_event (mci_instance, sampler, state)

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_5"

end subroutine mci_midpoint_5

```

Unweighted events

Generate unweighted events. The integrand has a sign flip in it.

```

<MCI midpoint: execute tests>+≡
call test (mci_midpoint_6, "mci_midpoint_6", &
  "unweighted events", &
  u, results)

<MCI midpoint: test declarations>+≡
public :: mci_midpoint_6

<MCI midpoint: tests>+≡
subroutine mci_midpoint_6 (u)
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng

  write (u, "(A)")  "* Test output: mci_midpoint_6"
  write (u, "(A)")  "* Purpose: generate unweighted events"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize integrator"
  write (u, "(A)")

  allocate (mci_midpoint_t :: mci)
  call mci%set_dimensions (1, 1)

  write (u, "(A)")  "* Initialize instance"
  write (u, "(A)")

```

```

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_4_t :: sampler)

write (u, "(A)")  "* Initialize random-number generator"
write (u, "(A)")

allocate (rng_test_t :: rng)
call rng%init ()
call mci%import_rng (rng)

write (u, "(A)")  "* Integrate (determine maximum of integrand"
write (u, "(A)")
call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_6"

end subroutine mci_midpoint_6

```

Excess weight

Generate unweighted events. With only 2 points for integration, the maximum of the integrand is too low, and we produce excess weight.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_7, "mci_midpoint_7", &
    "excess weight", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_7

<MCI midpoint: tests>+≡

```

```

subroutine mci_midpoint_7 (u)
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng

  write (u, "(A)")  "* Test output: mci_midpoint_7"
  write (u, "(A)")  "* Purpose: generate unweighted event &
    &with excess weight"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize integrator"
  write (u, "(A)")

  allocate (mci_midpoint_t :: mci)
  call mci%set_dimensions (1, 1)

  write (u, "(A)")  "* Initialize instance"
  write (u, "(A)")

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  write (u, "(A)")  "* Initialize test sampler"
  write (u, "(A)")

  allocate (test_sampler_4_t :: sampler)

  write (u, "(A)")  "* Initialize random-number generator"
  write (u, "(A)")

  allocate (rng_test_t :: rng)
  call rng%init ()
  call mci%import_rng (rng)

  write (u, "(A)")  "* Integrate (determine maximum of integrand"
  write (u, "(A)")
  call mci%integrate (mci_instance, sampler, 1, 2)
  call mci%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Generate unweighted event"
  write (u, "(A)")

  call mci_instance%init_simulation ()
  call mci%generate_unweighted_event (mci_instance, sampler)
  call mci_instance%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Use getter methods"
  write (u, "(A)")

  write (u, "(1x,A,1x,ES19.12)")  "weight =", mci_instance%get_event_weight ()

```

```

write (u, "(1x,A,1x,ES19.12)") "excess =", mci_instance%get_event_excess ()

write (u, "(A)")
write (u, "(A)")  "* Apply safety factor"
write (u, "(A)")

call mci_instance%init_simulation (safety_factor = 2.1_default)

write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Use getter methods"
write (u, "(A)")

write (u, "(1x,A,1x,ES19.12)") "weight =", mci_instance%get_event_weight ()
write (u, "(1x,A,1x,ES19.12)") "excess =", mci_instance%get_event_excess ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_7"

end subroutine mci_midpoint_7

```

21.6 VAMP interface

The standard method for integration is **VAMP**: the multi-channel version of the VEGAS algorithm. Each parameterization (channel) of the hypercube is binned in each dimension. The binning is equally equidistant, but an iteration of the integration procedure, the binning is updated for each dimension, according to the variance distribution of the integrand, summed over all other dimension. In the next iteration, the binning approximates (hopefully) follows the integrand more closely, and the accuracy of the result is increased. Furthermore, the relative weight of the individual channels is also updated after an iteration.

The bin distribution is denoted as the grid for a channel, which we can write to file and reuse later.

In our implementation we specify the generic **VAMP** algorithm more tightly: the number of bins is equal for all dimensions, the initial weights are all equal. The user controls whether to update bins and/or weights after each iteration. The integration is organized in passes, each one consisting of several iterations with a common number of calls to the integrand. The first passes are intended as warmup, so the results are displayed but otherwise discarded. In the final pass, the integration estimates for the individual iterations are averaged for the final result.

```
<mci_vamp.f90>≡  
  <File header>  
  
  module mci_vamp  
  
    <Use kinds>  
    <Use strings>  
    use diagnostics  
    use phs_base  
    use rng_base  
    use rng_tao  
    use vamp !NODEP!  
    use exceptions !NODEP!  
  
    use mci_base  
  
    <Standard module head>  
  
    <MCI vamp: public>  
  
    <MCI vamp: types>  
  
    <MCI vamp: interfaces>  
  
    interface  
    <MCI vamp: sub interfaces>  
    end interface  
  
  contains  
  
    <MCI vamp: main procedures>
```

```

    end module mci_vamp

    <mci_vamp_sub.f90>≡
    <File header>

    submodule (mci_vamp) mci_vamp_s

        use io_units
        use constants, only: zero
        use format_utils, only: pac_fmt
        use format_utils, only: write_separator
        use format_defs, only: FMT_12, FMT_14, FMT_17, FMT_19
        use md5

        implicit none

    contains

    <MCI vamp: procedures>

    end submodule mci_vamp_s

```

21.6.1 Grid parameters

This is a transparent container. It holds the parameters that are stored in grid files, and are checked when grid files are read.

```

<MCI vamp: public>≡
    public :: grid_parameters_t

<MCI vamp: types>≡
    type :: grid_parameters_t
        integer :: threshold_calls = 0
        integer :: min_calls_per_channel = 10
        integer :: min_calls_per_bin = 10
        integer :: min_bins = 3
        integer :: max_bins = 20
        logical :: stratified = .true.
        logical :: use_vamp_equivalences = .true.
        real(default) :: channel_weights_power = 0.25_default
        real(default) :: accuracy_goal = 0
        real(default) :: error_goal = 0
        real(default) :: rel_error_goal = 0
    contains
    <MCI vamp: grid parameters: TBP>
    end type grid_parameters_t

```

I/O:

```

<MCI vamp: grid parameters: TBP>≡
    procedure :: write => grid_parameters_write

<MCI vamp: sub interfaces>≡
    module subroutine grid_parameters_write (object, unit)
        class(grid_parameters_t), intent(in) :: object

```

```

        integer, intent(in), optional :: unit
    end subroutine grid_parameters_write

<MCI vamp: procedures>≡
module subroutine grid_parameters_write (object, unit)
    class(grid_parameters_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,I0)") "threshold_calls      = ", &
        object%threshold_calls
    write (u, "(3x,A,I0)") "min_calls_per_channel = ", &
        object%min_calls_per_channel
    write (u, "(3x,A,I0)") "min_calls_per_bin    = ", &
        object%min_calls_per_bin
    write (u, "(3x,A,I0)") "min_bins          = ", &
        object%min_bins
    write (u, "(3x,A,I0)") "max_bins          = ", &
        object%max_bins
    write (u, "(3x,A,L1)") "stratified        = ", &
        object%stratified
    write (u, "(3x,A,L1)") "use_vamp_equivalences = ", &
        object%use_vamp_equivalences
    write (u, "(3x,A,F10.7)") "channel_weights_power = ", &
        object%channel_weights_power
    if (object%accuracy_goal > 0) then
        write (u, "(3x,A,F10.7)") "accuracy_goal      = ", &
            object%accuracy_goal
    end if
    if (object%error_goal > 0) then
        write (u, "(3x,A,F10.7)") "error_goal        = ", &
            object%error_goal
    end if
    if (object%rel_error_goal > 0) then
        write (u, "(3x,A,F10.7)") "rel_error_goal     = ", &
            object%rel_error_goal
    end if
end subroutine grid_parameters_write

```

21.6.2 History parameters

The history parameters are also stored in a transparent container. This is not a part of the grid definition, and should not be included in the MD5 sum.

```

<MCI vamp: public>+≡
    public :: history_parameters_t

<MCI vamp: types>+≡
    type :: history_parameters_t
        logical :: global = .true.
        logical :: global_verbose = .false.
        logical :: channel = .false.
        logical :: channel_verbose = .false.
    contains

```



```

    <MCI vamp: history parameters: TBP>
end type history_parameters_t

```

I/O:

```

<MCI vamp: history parameters: TBP>≡
    procedure :: write => history_parameters_write

<MCI vamp: sub interfaces>+≡
    module subroutine history_parameters_write (object, unit)
        class(history_parameters_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine history_parameters_write

<MCI vamp: procedures>+≡
    module subroutine history_parameters_write (object, unit)
        class(history_parameters_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A,L1)") "history(global)          = ", object%global
        write (u, "(3x,A,L1)") "history(global) verb. = ", object%global_verbose
        write (u, "(3x,A,L1)") "history(channels)       = ", object%channel
        write (u, "(3x,A,L1)") "history(chann.) verb. = ", object%channel_verbose
    end subroutine history_parameters_write

```

21.6.3 Integration pass

We store the parameters for each integration pass in a linked list.

```

<MCI vamp: types>+≡
    type :: pass_t
        integer :: i_pass = 0
        integer :: i_first_it = 0
        integer :: n_it = 0
        integer :: n_calls = 0
        integer :: n_bins = 0
        logical :: adapt_grids = .false.
        logical :: adapt_weights = .false.
        logical :: is_final_pass = .false.
        logical :: integral_defined = .false.
        integer, dimension(:), allocatable :: calls
        integer, dimension(:), allocatable :: calls_valid
        real(default), dimension(:), allocatable :: integral
        real(default), dimension(:), allocatable :: error
        real(default), dimension(:), allocatable :: efficiency
        type(vamp_history), dimension(:), allocatable :: v_history
        type(vamp_history), dimension(:, :), allocatable :: v_histories
        type(pass_t), pointer :: next => null ()
    contains
        <MCI vamp: pass: TBP>
    end type pass_t

```

Finalizer. The VAMP histories contain a pointer array.

```

<MCI vamp: pass: TBP>≡
  procedure :: final => pass_final

<MCI vamp: sub interfaces>+≡
  module subroutine pass_final (object)
    class(pass_t), intent(inout) :: object
  end subroutine pass_final

<MCI vamp: procedures>+≡
  module subroutine pass_final (object)
    class(pass_t), intent(inout) :: object
    if (allocated (object%v_history)) then
      call vamp_delete_history (object%v_history)
    end if
    if (allocated (object%v_histories)) then
      call vamp_delete_history (object%v_histories)
    end if
  end subroutine pass_final

```

Output. Note that the precision of the numerical values should match the precision for comparing output from file with data.

```

<MCI vamp: pass: TBP>+≡
  procedure :: write => pass_write

<MCI vamp: sub interfaces>+≡
  module subroutine pass_write (object, unit, pacify)
    class(pass_t), intent(in) :: object
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
  end subroutine pass_write

<MCI vamp: procedures>+≡
  module subroutine pass_write (object, unit, pacify)
    class(pass_t), intent(in) :: object
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3x,A,I0)") "n_it          = ", object%n_it
    write (u, "(3x,A,I0)") "n_calls       = ", object%n_calls
    write (u, "(3x,A,I0)") "n_bins        = ", object%n_bins
    write (u, "(3x,A,L1)") "adapt grids   = ", object%adapt_grids
    write (u, "(3x,A,L1)") "adapt weights = ", object%adapt_weights
    if (object%integral_defined) then
      write (u, "(3x,A)") "Results: [it, calls, valid, integral, error, efficiency]"
      do i = 1, object%n_it
        write (u, "(5x,I0,2(1x,I0),3(1x," // fmt // "))" &
              i, object%calls(i), object%calls_valid(i), object%integral(i), object%error(i), &
              object%efficiency(i)
      end do
    else
      write (u, "(3x,A)") "Results: [undefined]"
    end if
  end subroutine pass_write

```

```

        end if
    end subroutine pass_write

```

Read and reconstruct the pass.

(MCI vamp: pass: TBP)+≡

```

    procedure :: read => pass_read

```

(MCI vamp: sub interfaces)+≡

```

    module subroutine pass_read (object, u, n_pass, n_it)
        class(pass_t), intent(out) :: object
        integer, intent(in) :: u, n_pass, n_it
    end subroutine pass_read

```

(MCI vamp: procedures)+≡

```

    module subroutine pass_read (object, u, n_pass, n_it)
        class(pass_t), intent(out) :: object
        integer, intent(in) :: u, n_pass, n_it
        integer :: i, j
        character(80) :: buffer
        object%i_pass = n_pass + 1
        object%i_first_it = n_it + 1
        call read_ival (u, object%n_it)
        call read_ival (u, object%n_calls)
        call read_ival (u, object%n_bins)
        call read_lval (u, object%adapt_grids)
        call read_lval (u, object%adapt_weights)
        allocate (object%calls (object%n_it), source = 0)
        allocate (object%calls_valid (object%n_it), source = 0)
        allocate (object%integral (object%n_it), source = 0._default)
        allocate (object%error (object%n_it), source = 0._default)
        allocate (object%efficiency (object%n_it), source = 0._default)
        read (u, "(A)") buffer
        select case (trim (adjustl (buffer)))
        case ("Results: [it, calls, valid, integral, error, efficiency]")
            do i = 1, object%n_it
                read (u, *) &
                    j, object%calls(i), object%calls_valid(i), object%integral(i), object%error(i), &
                    object%efficiency(i)
            end do
            object%integral_defined = .true.
        case ("Results: [undefined]")
            object%integral_defined = .false.
        case default
            call msg_fatal ("Reading integration pass: corrupted file")
        end select
    end subroutine pass_read

```

Write the VAMP history for this pass. (The subroutine writes the whole array at once.)

(MCI vamp: pass: TBP)+≡

```

    procedure :: write_history => pass_write_history

```

(MCI vamp: sub interfaces)+≡

```

    module subroutine pass_write_history (pass, unit)

```

```

        class(pass_t), intent(in) :: pass
        integer, intent(in), optional :: unit
    end subroutine pass_write_history
<MCI vamp: procedures>+≡
module subroutine pass_write_history (pass, unit)
    class(pass_t), intent(in) :: pass
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (allocated (pass%v_history)) then
        call vamp_write_history (u, pass%v_history)
    else
        write (u, "(1x,A)") "Global history: [undefined]"
    end if
    if (allocated (pass%v_histories)) then
        write (u, "(1x,A)") "Channel histories:"
        call vamp_write_history (u, pass%v_histories)
    else
        write (u, "(1x,A)") "Channel histories: [undefined]"
    end if
end subroutine pass_write_history

Given a number of calls and iterations, compute remaining data.
<MCI vamp: pass: TBP>+≡
    procedure :: configure => pass_configure
<MCI vamp: sub interfaces>+≡
    module subroutine pass_configure (pass, n_it, n_calls, min_calls, &
        min_bins, max_bins, min_channel_calls)
        class(pass_t), intent(inout) :: pass
        integer, intent(in) :: n_it, n_calls, min_channel_calls
        integer, intent(in) :: min_calls, min_bins, max_bins
    end subroutine pass_configure
<MCI vamp: procedures>+≡
module subroutine pass_configure (pass, n_it, n_calls, min_calls, &
    min_bins, max_bins, min_channel_calls)
    class(pass_t), intent(inout) :: pass
    integer, intent(in) :: n_it, n_calls, min_channel_calls
    integer, intent(in) :: min_calls, min_bins, max_bins
    pass%n_it = n_it
    if (min_calls /= 0) then
        pass%n_bins = max (min_bins, &
            min (n_calls / min_calls, max_bins))
    else
        pass%n_bins = max_bins
    end if
    pass%n_calls = max (n_calls, max (min_calls, min_channel_calls))
    if (pass%n_calls /= n_calls) then
        write (msg_buffer, "(A,I0)") "VAMP: too few calls, resetting " &
            // "n_calls to ", pass%n_calls
        call msg_warning ()
    end if
    allocate (pass%calls (n_it), source = 0)

```

```

        allocate (pass%calls_valid (n_it), source = 0)
        allocate (pass%integral (n_it), source = 0._default)
        allocate (pass%error (n_it), source = 0._default)
        allocate (pass%efficiency (n_it), source = 0._default)
    end subroutine pass_configure

```

Allocate the VAMP history and give options. We assume that the `configure` routine above has been executed, so the number of iterations is known.

```

<MCI vamp: pass: TBP>+≡
    procedure :: configure_history => pass_configure_history

<MCI vamp: sub interfaces>+≡
    module subroutine pass_configure_history (pass, n_channels, par)
        class(pass_t), intent(inout) :: pass
        integer, intent(in) :: n_channels
        type(history_parameters_t), intent(in) :: par
    end subroutine pass_configure_history

<MCI vamp: procedures>+≡
    module subroutine pass_configure_history (pass, n_channels, par)
        class(pass_t), intent(inout) :: pass
        integer, intent(in) :: n_channels
        type(history_parameters_t), intent(in) :: par
        if (par%global) then
            allocate (pass%v_history (pass%n_it))
            call vamp_create_history (pass%v_history, &
                verbose = par%global_verbose)
        end if
        if (par%channel) then
            allocate (pass%v_histories (pass%n_it, n_channels))
            call vamp_create_history (pass%v_histories, &
                verbose = par%channel_verbose)
        end if
    end subroutine pass_configure_history

```

Given two pass objects, compare them. All parameters must match. Where integrations are done in both (number of calls nonzero), the results must be equal (up to numerical noise).

The allocated array sizes might be different, but should match up to the common `n_it` value.

```

<MCI vamp: interfaces>≡
    interface operator (.matches.)
        module procedure pass_matches
    end interface operator (.matches.)

<MCI vamp: sub interfaces>+≡
    module function pass_matches (pass, ref) result (ok)
        type(pass_t), intent(in) :: pass, ref
        integer :: n
        logical :: ok
    end function pass_matches

<MCI vamp: procedures>+≡
    module function pass_matches (pass, ref) result (ok)

```

```

type(pass_t), intent(in) :: pass, ref
integer :: n
logical :: ok
ok = .true.
if (ok) ok = pass%i_pass == ref%i_pass
if (ok) ok = pass%i_first_it == ref%i_first_it
if (ok) ok = pass%n_it == ref%n_it
if (ok) ok = pass%n_calls == ref%n_calls
if (ok) ok = pass%n_bins == ref%n_bins
if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
if (ok) ok = pass%integral_defined .eqv. ref%integral_defined
if (pass%integral_defined) then
  n = pass%n_it
  if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
  if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid (:n))
  if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
  if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
  if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
end if
end function pass_matches

```

Update a pass object, given a reference. The parameters must match, except for the `n_it` entry. The number of complete iterations must be less or equal to the reference, and the number of complete iterations in the reference must be no larger than `n_it`. Where results are present in both passes, they must match. Where results are present in the reference only, the pass is updated accordingly.

(MCI vamp: pass: TBP)+≡

```

procedure :: update => pass_update

```

(MCI vamp: sub interfaces)+≡

```

module subroutine pass_update (pass, ref, ok)
  class(pass_t), intent(inout) :: pass
  type(pass_t), intent(in) :: ref
  logical, intent(out) :: ok
end subroutine pass_update

```

(MCI vamp: procedures)+≡

```

module subroutine pass_update (pass, ref, ok)
  class(pass_t), intent(inout) :: pass
  type(pass_t), intent(in) :: ref
  logical, intent(out) :: ok
  integer :: n, n_ref
  ok = .true.
  if (ok) ok = pass%i_pass == ref%i_pass
  if (ok) ok = pass%i_first_it == ref%i_first_it
  if (ok) ok = pass%n_calls == ref%n_calls
  if (ok) ok = pass%n_bins == ref%n_bins
  if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
  if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
  if (ok) then
    if (ref%integral_defined) then
      if (.not. allocated (pass%calls)) then
        allocate (pass%calls (pass%n_it), source = 0)

```

```

        allocate (pass%calls_valid (pass%n_it), source = 0)
        allocate (pass%integral (pass%n_it), source = 0._default)
        allocate (pass%error (pass%n_it), source = 0._default)
        allocate (pass%efficiency (pass%n_it), source = 0._default)
    end if
    n = count (pass%calls /= 0)
    n_ref = count (ref%calls /= 0)
    ok = n <= n_ref .and. n_ref <= pass%n_it
    if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
    if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
    if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
    if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
    if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
    if (ok) then
        pass%calls(n+1:n_ref) = ref%calls(n+1:n_ref)
        pass%calls_valid(n+1:n_ref) = ref%calls_valid(n+1:n_ref)
        pass%integral(n+1:n_ref) = ref%integral(n+1:n_ref)
        pass%error(n+1:n_ref) = ref%error(n+1:n_ref)
        pass%efficiency(n+1:n_ref) = ref%efficiency(n+1:n_ref)
        pass%integral_defined = any (pass%calls /= 0)
    end if
end if
end if
end subroutine pass_update

```

Match two real numbers: they are equal up to a tolerance, which is 10^{-8} , matching the number of digits that are output by `pass_write`. In particular, if one number is exactly zero, the other one must also be zero.

```

<MCI vamp: interfaces>+≡
    interface operator (.matches.)
        module procedure real_matches
    end interface operator (.matches.)

<MCI vamp: sub interfaces>+≡
    elemental module function real_matches (x, y) result (ok)
        real(default), intent(in) :: x, y
        logical :: ok
    end function real_matches

<MCI vamp: procedures>+≡
    elemental module function real_matches (x, y) result (ok)
        real(default), intent(in) :: x, y
        logical :: ok
        real(default), parameter :: tolerance = 1.e-8_default
        ok = abs (x - y) <= tolerance * max (abs (x), abs (y))
    end function real_matches

```

Return the index of the most recent complete integration. If there is none, return zero.

```

<MCI vamp: pass: TBP>+≡
    procedure :: get_integration_index => pass_get_integration_index

<MCI vamp: sub interfaces>+≡
    module function pass_get_integration_index (pass) result (n)

```

```

        class (pass_t), intent(in) :: pass
        integer :: n
    end function pass_get_integration_index
<MCI vamp: procedures>+≡
module function pass_get_integration_index (pass) result (n)
    class (pass_t), intent(in) :: pass
    integer :: n
    integer :: i
    n = 0
    if (allocated (pass%calls)) then
        do i = 1, pass%n_it
            if (pass%calls(i) == 0) exit
            n = i
        end do
    end if
end function pass_get_integration_index

Return the most recent integral and error, if available.
<MCI vamp: pass: TBP>+≡
procedure :: get_calls => pass_get_calls
procedure :: get_calls_valid => pass_get_calls_valid
procedure :: get_integral => pass_get_integral
procedure :: get_error => pass_get_error
procedure :: get_efficiency => pass_get_efficiency
<MCI vamp: sub interfaces>+≡
module function pass_get_calls (pass) result (calls)
    class(pass_t), intent(in) :: pass
    integer :: calls
end function pass_get_calls
module function pass_get_calls_valid (pass) result (calls_valid)
    class(pass_t), intent(in) :: pass
    integer :: calls_valid
end function pass_get_calls_valid
module function pass_get_integral (pass) result (integral)
    class(pass_t), intent(in) :: pass
    real(default) :: integral
end function pass_get_integral
module function pass_get_error (pass) result (error)
    class(pass_t), intent(in) :: pass
    real(default) :: error
end function pass_get_error
module function pass_get_efficiency (pass) result (efficiency)
    class(pass_t), intent(in) :: pass
    real(default) :: efficiency
end function pass_get_efficiency
<MCI vamp: procedures>+≡
module function pass_get_calls (pass) result (calls)
    class(pass_t), intent(in) :: pass
    integer :: calls
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then

```



```

        calls = pass%calls(n)
    else
        calls = 0
    end if
end function pass_get_calls

module function pass_get_calls_valid (pass) result (calls_valid)
    class(pass_t), intent(in) :: pass
    integer :: calls_valid
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then
        calls_valid = pass%calls_valid(n)
    else
        calls_valid = 0
    end if
end function pass_get_calls_valid

module function pass_get_integral (pass) result (integral)
    class(pass_t), intent(in) :: pass
    real(default) :: integral
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then
        integral = pass%integral(n)
    else
        integral = 0
    end if
end function pass_get_integral

module function pass_get_error (pass) result (error)
    class(pass_t), intent(in) :: pass
    real(default) :: error
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then
        error = pass%error(n)
    else
        error = 0
    end if
end function pass_get_error

module function pass_get_efficiency (pass) result (efficiency)
    class(pass_t), intent(in) :: pass
    real(default) :: efficiency
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then
        efficiency = pass%efficiency(n)
    else
        efficiency = 0
    end if
end function pass_get_efficiency

```

21.6.4 Integrator

```

<MCI vamp: public>+≡
    public :: mci_vamp_t

<MCI vamp: types>+≡
    type, extends (mci_t) :: mci_vamp_t
        logical, dimension(:), allocatable :: dim_is_flat
        type(grid_parameters_t) :: grid_par
        type(history_parameters_t) :: history_par
        integer :: min_calls = 0
        type(pass_t), pointer :: first_pass => null ()
        type(pass_t), pointer :: current_pass => null ()
        type(vamp_equivalences_t) :: equivalences
        logical :: rebuild = .true.
        logical :: check_grid_file = .true.
        logical :: grid_filename_set = .false.
        logical :: negative_weights = .false.
        logical :: verbose = .false.
        type(string_t) :: grid_filename
        character(32) :: md5sum_adapted = ""
    contains
        <MCI vamp: mci vamp: TBP>
    end type mci_vamp_t

```

Reset: delete integration-pass entries.

```

<MCI vamp: mci vamp: TBP>≡
    procedure :: reset => mci_vamp_reset

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_reset (object)
        class(mci_vamp_t), intent(inout) :: object
    end subroutine mci_vamp_reset

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_reset (object)
        class(mci_vamp_t), intent(inout) :: object
        type(pass_t), pointer :: current_pass
        do while (associated (object%first_pass))
            current_pass => object%first_pass
            object%first_pass => current_pass%next
            call current_pass%final ()
            deallocate (current_pass)
        end do
        object%current_pass => null ()
    end subroutine mci_vamp_reset

```

Finalizer: reset and finalize the equivalences list.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: final => mci_vamp_final

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_final (object)
        class(mci_vamp_t), intent(inout) :: object
    end subroutine mci_vamp_final

```

```

<MCI vamp: procedures>+=
module subroutine mci_vamp_final (object)
  class(mci_vamp_t), intent(inout) :: object
  call object%reset ()
  call vamp_equivalences_final (object%equivalences)
  call object%base_final ()
end subroutine mci_vamp_final

```

Output. Do not output the grids themselves, this may result in tons of data.

```

<MCI vamp: mci vamp: TBP>+=
  procedure :: write => mci_vamp_write

<MCI vamp: sub interfaces>+=
  module subroutine mci_vamp_write (object, unit, pacify, md5sum_version)
    class(mci_vamp_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
  end subroutine mci_vamp_write

<MCI vamp: procedures>+=
module subroutine mci_vamp_write (object, unit, pacify, md5sum_version)
  class(mci_vamp_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  logical, intent(in), optional :: md5sum_version
  type(pass_t), pointer :: current_pass
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "VAMP integrator:"
  call object%base_write (u, pacify, md5sum_version)
  if (allocated (object%dim_is_flat)) then
    write (u, "(3x,A,999(1x,I0))") "Flat dimensions      =", &
      pack ([ (i, i = 1, object%n_dim)], object%dim_is_flat)
  end if
  write (u, "(1x,A)") "Grid parameters:"
  call object%grid_par%write (u)
  write (u, "(3x,A,I0)") "min_calls              =", object%min_calls
  write (u, "(3x,A,L1)") "negative weights      =", &
    object%negative_weights
  write (u, "(3x,A,L1)") "verbose                =", &
    object%verbose
  if (object%grid_par%use_vamp_equivalences) then
    call vamp_equivalences_write (object%equivalences, u)
  end if
  current_pass => object%first_pass
  do while (associated (current_pass))
    write (u, "(1x,A,I0,A)") "Integration pass:"
    call current_pass%write (u, pacify)
    current_pass => current_pass%next
  end do
  if (object%md5sum_adapted /= "") then
    write (u, "(1x,A,A,A)") "MD5 sum (including results) = '", &
      object%md5sum_adapted, "'"
  end if
end if

```

```
end subroutine mci_vamp_write
```

Write the history parameters.

```
<MCI vamp: mci vamp: TBP>+≡
  procedure :: write_history_parameters => mci_vamp_write_history_parameters

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_write_history_parameters (mci, unit)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit
  end subroutine mci_vamp_write_history_parameters

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_write_history_parameters (mci, unit)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "VAMP history parameters:"
    call mci%history_par%write (unit)
  end subroutine mci_vamp_write_history_parameters
```

Write the history, iterating over passes. We keep this separate from the generic write routine.

```
<MCI vamp: mci vamp: TBP>+≡
  procedure :: write_history => mci_vamp_write_history

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_write_history (mci, unit)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit
  end subroutine mci_vamp_write_history

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_write_history (mci, unit)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit
    type(pass_t), pointer :: current_pass
    integer :: i_pass
    integer :: u
    u = given_output_unit (unit)
    if (associated (mci%first_pass)) then
      write (u, "(1x,A)") "VAMP history (global):"
      i_pass = 0
      current_pass => mci%first_pass
      do while (associated (current_pass))
        i_pass = i_pass + 1
        write (u, "(1x,A,IO,':')") "Pass #", i_pass
        call current_pass%write_history (u)
        current_pass => current_pass%next
      end do
    end if
  end subroutine mci_vamp_write_history
```

Compute the MD5 sum, including the configuration MD5 sum and the printout, which incorporates the current results.

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: compute_md5sum => mci_vamp_compute_md5sum

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_compute_md5sum (mci, pacify)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
  end subroutine mci_vamp_compute_md5sum

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_compute_md5sum (mci, pacify)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
    integer :: u
    mci%md5sum_adapted = ""
    u = free_unit ()
    open (u, status = "scratch", action = "readwrite")
    write (u, "(A)") mci%md5sum
    call mci%write (u, pacify, md5sum_version = .true.)
    rewind (u)
    mci%md5sum_adapted = md5sum (u)
    close (u)
  end subroutine mci_vamp_compute_md5sum

```

Return the MD5 sum: If available, return the adapted one.

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: get_md5sum => mci_vamp_get_md5sum

<MCI vamp: sub interfaces>+≡
  pure module function mci_vamp_get_md5sum (mci) result (md5sum)
    class(mci_vamp_t), intent(in) :: mci
    character(32) :: md5sum
  end function mci_vamp_get_md5sum

<MCI vamp: procedures>+≡
  pure module function mci_vamp_get_md5sum (mci) result (md5sum)
    class(mci_vamp_t), intent(in) :: mci
    character(32) :: md5sum
    if (mci%md5sum_adapted /= "") then
      md5sum = mci%md5sum_adapted
    else
      md5sum = mci%md5sum
    end if
  end function mci_vamp_get_md5sum

```

Startup message: short version.

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: startup_message => mci_vamp_startup_message

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_startup_message (mci, unit, n_calls)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
  end subroutine mci_vamp_startup_message

```

```

<MCI vamp: procedures>+=
module subroutine mci_vamp_startup_message (mci, unit, n_calls)
  class(mci_vamp_t), intent(in) :: mci
  integer, intent(in), optional :: unit, n_calls
  integer :: num_calls, n_bins
  if (present (n_calls)) then
    num_calls = n_calls
  else
    num_calls = 0
  end if
  if (mci%min_calls /= 0) then
    n_bins = max (mci%grid_par%min_bins, &
      min (num_calls / mci%min_calls, &
        mci%grid_par%max_bins))
  else
    n_bins = mci%grid_par%max_bins
  end if
  call mci%base_startup_message (unit = unit, n_calls = n_calls)
  if (mci%grid_par%use_vamp_equivalences) then
    write (msg_buffer, "(A,2(1x,I0,1x,A))" &
      "Integrator: Using VAMP channel equivalences"
    call msg_message (unit = unit)
  end if
  write (msg_buffer, "(A,2(1x,I0,1x,A),L1)" &
    "Integrator:", num_calls, &
    "initial calls,", n_bins, &
    "bins, stratified = ", &
    mci%grid_par%stratified
  call msg_message (unit = unit)
  write (msg_buffer, "(A,2(1x,I0,1x,A))" &
    "Integrator: VAMP"
  call msg_message (unit = unit)
end subroutine mci_vamp_startup_message

```

Log entry: just headline.

```

<MCI vamp: mci vamp: TBP>+=
  procedure :: write_log_entry => mci_vamp_write_log_entry

<MCI vamp: sub interfaces>+=
  module subroutine mci_vamp_write_log_entry (mci, u)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in) :: u
  end subroutine mci_vamp_write_log_entry

<MCI vamp: procedures>+=
module subroutine mci_vamp_write_log_entry (mci, u)
  class(mci_vamp_t), intent(in) :: mci
  integer, intent(in) :: u
  write (u, "(1x,A)") "MC Integrator is VAMP"
  call write_separator (u)
  call mci%write_history (u)
  call write_separator (u)
  if (mci%grid_par%use_vamp_equivalences) then
    call vamp_equivalences_write (mci%equivalences, u)
  else

```

```

        write (u, "(3x,A)") "No VAMP equivalences have been used"
    end if
    call write_separator (u)
    call mci%write_chain_weights (u)
end subroutine mci_vamp_write_log_entry

```

Set the MCI index (necessary for processes with multiple components). We append the index to the grid filename, just before the final dotted suffix.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: record_index => mci_vamp_record_index

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_record_index (mci, i_mci)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: i_mci
    end subroutine mci_vamp_record_index

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_record_index (mci, i_mci)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: i_mci
        type(string_t) :: basename, suffix
        character(32) :: buffer
        if (mci%grid_filename_set) then
            basename = mci%grid_filename
            call split (basename, suffix, ".", back=.true.)
            write (buffer, "(I0)") i_mci
            if (basename /= "") then
                mci%grid_filename = basename // ".m" // trim (buffer) // "." // suffix
            else
                mci%grid_filename = suffix // ".m" // trim (buffer) // ".vg"
            end if
        end if
    end subroutine mci_vamp_record_index

```

Set the grid parameters.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: set_grid_parameters => mci_vamp_set_grid_parameters

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_set_grid_parameters (mci, grid_par)
        class(mci_vamp_t), intent(inout) :: mci
        type(grid_parameters_t), intent(in) :: grid_par
    end subroutine mci_vamp_set_grid_parameters

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_set_grid_parameters (mci, grid_par)
        class(mci_vamp_t), intent(inout) :: mci
        type(grid_parameters_t), intent(in) :: grid_par
        mci%grid_par = grid_par
        mci%min_calls = grid_par%min_calls_per_bin * mci%n_channel
    end subroutine mci_vamp_set_grid_parameters

```

Set the history parameters.

```
<MCI vamp: mci vamp: TBP>+≡  
  procedure :: set_history_parameters => mci_vamp_set_history_parameters  
  
<MCI vamp: sub interfaces>+≡  
  module subroutine mci_vamp_set_history_parameters (mci, history_par)  
    class(mci_vamp_t), intent(inout) :: mci  
    type(history_parameters_t), intent(in) :: history_par  
  end subroutine mci_vamp_set_history_parameters  
  
<MCI vamp: procedures>+≡  
  module subroutine mci_vamp_set_history_parameters (mci, history_par)  
    class(mci_vamp_t), intent(inout) :: mci  
    type(history_parameters_t), intent(in) :: history_par  
    mci%history_par = history_par  
  end subroutine mci_vamp_set_history_parameters
```

Set the rebuild flag, also the flag for checking the grid file.

```
<MCI vamp: mci vamp: TBP>+≡  
  procedure :: set_rebuild_flag => mci_vamp_set_rebuild_flag  
  
<MCI vamp: sub interfaces>+≡  
  module subroutine mci_vamp_set_rebuild_flag (mci, rebuild, check_grid_file)  
    class(mci_vamp_t), intent(inout) :: mci  
    logical, intent(in) :: rebuild  
    logical, intent(in) :: check_grid_file  
  end subroutine mci_vamp_set_rebuild_flag  
  
<MCI vamp: procedures>+≡  
  module subroutine mci_vamp_set_rebuild_flag (mci, rebuild, check_grid_file)  
    class(mci_vamp_t), intent(inout) :: mci  
    logical, intent(in) :: rebuild  
    logical, intent(in) :: check_grid_file  
    mci%rebuild = rebuild  
    mci%check_grid_file = check_grid_file  
  end subroutine mci_vamp_set_rebuild_flag
```

Set the filename.

```
<MCI vamp: mci vamp: TBP>+≡  
  procedure :: set_grid_filename => mci_vamp_set_grid_filename  
  
<MCI vamp: sub interfaces>+≡  
  module subroutine mci_vamp_set_grid_filename (mci, name, run_id)  
    class(mci_vamp_t), intent(inout) :: mci  
    type(string_t), intent(in) :: name  
    type(string_t), intent(in), optional :: run_id  
  end subroutine mci_vamp_set_grid_filename  
  
<MCI vamp: procedures>+≡  
  module subroutine mci_vamp_set_grid_filename (mci, name, run_id)  
    class(mci_vamp_t), intent(inout) :: mci  
    type(string_t), intent(in) :: name  
    type(string_t), intent(in), optional :: run_id  
    if (present (run_id)) then  
      mci%grid_filename = name // "." // run_id // ".vg"  
    else
```



```

        mci%grid_filename = name // ".vg"
    end if
    mci%grid_filename_set = .true.
end subroutine mci_vamp_set_grid_filename

```

To simplify the interface, we prepend a grid path in a separate subroutine.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: prepend_grid_path => mci_vamp_prepend_grid_path

<MCI vamp: sub interfaces>+=
    module subroutine mci_vamp_prepend_grid_path (mci, prefix)
        class(mci_vamp_t), intent(inout) :: mci
        type(string_t), intent(in) :: prefix
    end subroutine mci_vamp_prepend_grid_path

<MCI vamp: procedures>+=
    module subroutine mci_vamp_prepend_grid_path (mci, prefix)
        class(mci_vamp_t), intent(inout) :: mci
        type(string_t), intent(in) :: prefix
        if (mci%grid_filename_set) then
            mci%grid_filename = prefix // "/" // mci%grid_filename
        else
            call msg_warning ("Cannot add prefix to invalid grid filename!")
        end if
    end subroutine mci_vamp_prepend_grid_path

```

Declare particular dimensions as flat.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: declare_flat_dimensions => mci_vamp_declare_flat_dimensions

<MCI vamp: sub interfaces>+=
    module subroutine mci_vamp_declare_flat_dimensions (mci, dim_flat)
        class(mci_vamp_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_vamp_declare_flat_dimensions

<MCI vamp: procedures>+=
    module subroutine mci_vamp_declare_flat_dimensions (mci, dim_flat)
        class(mci_vamp_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
        integer :: d
        allocate (mci%dim_is_flat (mci%n_dim), source = .false.)
        do d = 1, size (dim_flat)
            mci%dim_is_flat(dim_flat(d)) = .true.
        end do
    end subroutine mci_vamp_declare_flat_dimensions

```

Declare equivalences. We have an array of channel equivalences, provided by the phase-space module. Here, we translate this into the `vamp_equivalences` array.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: declare_equivalences => mci_vamp_declare_equivalences

```

```

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_declare_equivalences (mci, channel, dim_offset)
    class(mci_vamp_t), intent(inout) :: mci
    type(phys_channel_t), dimension(:), intent(in) :: channel
    integer, intent(in) :: dim_offset
  end subroutine mci_vamp_declare_equivalences

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_declare_equivalences (mci, channel, dim_offset)
    class(mci_vamp_t), intent(inout) :: mci
    type(phys_channel_t), dimension(:), intent(in) :: channel
    integer, intent(in) :: dim_offset
    integer, dimension(:), allocatable :: perm, mode
    integer :: n_channels, n_dim, n_equivalences
    integer :: c, i, j, left, right
    integer :: n_dim_perm
    n_channels = mci%n_channel
    n_dim = mci%n_dim
    n_equivalences = 0
    do c = 1, n_channels
      n_equivalences = n_equivalences + size (channel(c)%eq)
    end do
    call vamp_equivalences_init (mci%equivalences, &
      n_equivalences, n_channels, n_dim)
    allocate (perm (n_dim))
    allocate (mode (n_dim))
    perm = [(i, i = 1, n_dim)]
    mode = VEQ_IDENTITY
    c = 1
    j = 0
    do i = 1, n_equivalences
      if (j < size (channel(c)%eq)) then
        j = j + 1
      else
        c = c + 1
        j = 1
      end if
      associate (eq => channel(c)%eq(j))
        left = c
        right = eq%c
        n_dim_perm = size (eq%perm)
        perm(dim_offset + 1:dim_offset + n_dim_perm) = eq%perm + dim_offset
        mode(dim_offset + 1:dim_offset + n_dim_perm) = eq%mode
        call vamp_equivalence_set (mci%equivalences, &
          i, left, right, perm, mode)
      end associate
    end do
    call vamp_equivalences_complete (mci%equivalences)
  end subroutine mci_vamp_declare_equivalences

```

Allocate instance with matching type. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: allocate_instance => mci_vamp_allocate_instance

```

```

<MCI vamp: main procedures>+=
subroutine mci_vamp_allocate_instance (mci, mci_instance)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(out), pointer :: mci_instance
  allocate (mci_vamp_instance_t :: mci_instance)
end subroutine mci_vamp_allocate_instance

```

Allocate a new integration pass. We can preset everything that does not depend on the number of iterations and calls. This is postponed to the `integrate` method.

In the final pass, we do not check accuracy goal etc., since we can assume that the user wants to perform and average all iterations in this pass.

```

<MCI vamp: mci vamp: TBP>+=
  procedure :: add_pass => mci_vamp_add_pass

<MCI vamp: sub interfaces>+=
  module subroutine mci_vamp_add_pass &
    (mci, adapt_grids, adapt_weights, final_pass)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
  end subroutine mci_vamp_add_pass

<MCI vamp: procedures>+=
  module subroutine mci_vamp_add_pass &
    (mci, adapt_grids, adapt_weights, final_pass)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
    integer :: i_pass, i_it
    type(pass_t), pointer :: new
    allocate (new)
    if (associated (mci%current_pass)) then
      i_pass = mci%current_pass%i_pass + 1
      i_it   = mci%current_pass%i_first_it + mci%current_pass%n_it
      mci%current_pass%next => new
    else
      i_pass = 1
      i_it   = 1
      mci%first_pass => new
    end if
    mci%current_pass => new
    new%i_pass = i_pass
    new%i_first_it = i_it
    if (present (adapt_grids)) then
      new%adapt_grids = adapt_grids
    else
      new%adapt_grids = .false.
    end if
    if (present (adapt_weights)) then
      new%adapt_weights = adapt_weights
    else
      new%adapt_weights = .false.
    end if
    if (present (final_pass)) then
      new%is_final_pass = final_pass
    end if
  end module

```

```

else
    new%is_final_pass = .false.
end if
end subroutine mci_vamp_add_pass

```

Update the list of integration passes. All passes except for the last one must match exactly. For the last one, integration results are updated. The reference output may contain extra passes, these are ignored.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: update_from_ref => mci_vamp_update_from_ref

<MCI vamp: sub interfaces>+=
    module subroutine mci_vamp_update_from_ref (mci, mci_ref, success)
        class(mci_vamp_t), intent(inout) :: mci
        class(mci_t), intent(in) :: mci_ref
        logical, intent(out) :: success
    end subroutine mci_vamp_update_from_ref

<MCI vamp: procedures>+=
    module subroutine mci_vamp_update_from_ref (mci, mci_ref, success)
        class(mci_vamp_t), intent(inout) :: mci
        class(mci_t), intent(in) :: mci_ref
        logical, intent(out) :: success
        type(pass_t), pointer :: current_pass, ref_pass
        select type (mci_ref)
        type is (mci_vamp_t)
            current_pass => mci%first_pass
            ref_pass => mci_ref%first_pass
            success = .true.
            do while (success .and. associated (current_pass))
                if (associated (ref_pass)) then
                    if (associated (current_pass%next)) then
                        success = current_pass .matches. ref_pass
                    else
                        call current_pass%update (ref_pass, success)
                        if (current_pass%integral_defined) then
                            mci%integral = current_pass%get_integral ()
                            mci%error = current_pass%get_error ()
                            mci%efficiency = current_pass%get_efficiency ()
                            mci%integral_known = .true.
                            mci%error_known = .true.
                            mci%efficiency_known = .true.
                        end if
                    end if
                    current_pass => current_pass%next
                    ref_pass => ref_pass%next
                else
                    success = .false.
                end if
            end do
        end select
    end subroutine mci_vamp_update_from_ref

```

Update the MCI record (i.e., the integration passes) by reading from input stream. The stream should contain a `write` output from a previous run. We first check the MD5 sum of the configuration parameters. If that matches, we proceed directly to the stored integration passes. If successful, we may continue to read the file; the position will be after a blank line that must follow the MCI record.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: update => mci_vamp_update

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_update (mci, u, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: u
        logical, intent(out) :: success
    end subroutine mci_vamp_update

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_update (mci, u, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: u
        logical, intent(out) :: success
        character(80) :: buffer
        character(32) :: md5sum_file
        type(mci_vamp_t) :: mci_file
        integer :: n_pass, n_it
        call read_sval (u, md5sum_file)
        if (mci%check_grid_file) then
            success = md5sum_file == mci%md5sum
        else
            success = .true.
        end if
        if (success) then
            read (u, *)
            read (u, "(A)") buffer
            if (trim (adjustl (buffer)) == "VAMP integrator:") then
                n_pass = 0
                n_it = 0
                do
                    read (u, "(A)") buffer
                    select case (trim (adjustl (buffer)))
                        case ("")
                            exit
                        case ("Integration pass:")
                            call mci_file%add_pass ()
                            call mci_file%current_pass%read (u, n_pass, n_it)
                            n_pass = n_pass + 1
                            n_it = n_it + mci_file%current_pass%n_it
                        end select
                end do
                call mci%update_from_ref (mci_file, success)
                call mci_file%final ()
            else
                call msg_fatal ("VAMP: reading grid file: corrupted data")
            end if
        end if
    end if
end if

```

```
end subroutine mci_vamp_update
```

Read / write grids from / to file.

Bug fix for 2.2.5: after reading grids from file, channel weights must be copied back to the mci_instance record.

(MCI vamp: mci vamp: TBP)+≡

```
procedure :: write_grids => mci_vamp_write_grids
procedure :: read_grids_header => mci_vamp_read_grids_header
procedure :: read_grids_data => mci_vamp_read_grids_data
procedure :: read_grids => mci_vamp_read_grids
```

(MCI vamp: sub interfaces)+≡

```
module subroutine mci_vamp_write_grids (mci, instance)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(inout) :: instance
end subroutine mci_vamp_write_grids
module subroutine mci_vamp_read_grids_header (mci, success)
  class(mci_vamp_t), intent(inout) :: mci
  logical, intent(out) :: success
end subroutine mci_vamp_read_grids_header
module subroutine mci_vamp_read_grids_data (mci, instance, read_integrals)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(inout) :: instance
  logical, intent(in), optional :: read_integrals
end subroutine mci_vamp_read_grids_data
module subroutine mci_vamp_read_grids (mci, instance, success)
  class(mci_vamp_t), intent(inout) :: mci
  class(mci_instance_t), intent(inout) :: instance
  logical, intent(out) :: success
end subroutine mci_vamp_read_grids
```

(MCI vamp: procedures)+≡

```
module subroutine mci_vamp_write_grids (mci, instance)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(inout) :: instance
  integer :: u
  select type (instance)
  type is (mci_vamp_instance_t)
    if (mci%grid_filename_set) then
      if (instance%grids_defined) then
        u = free_unit ()
        open (u, file = char (mci%grid_filename), &
              action = "write", status = "replace")
        write (u, "(1x,A,A,A)") "MD5sum = '", mci%md5sum, "'"
        write (u, *)
        call mci%write (u)
        write (u, *)
        write (u, "(1x,A)") "VAMP grids:"
        call vamp_write_grids (instance%grids, u, &
                              write_integrals = .true.)
        close (u)
      else
        call msg_bug ("VAMP: write grids: grids undefined")
      end if
    end if
  end select
end subroutine mci_vamp_write_grids
```

```

        else
            call msg_bug ("VAMP: write grids: filename undefined")
        end if
    end select
end subroutine mci_vamp_write_grids

module subroutine mci_vamp_read_grids_header (mci, success)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(out) :: success
    logical :: exist
    integer :: u
    success = .false.
    if (mci%grid_filename_set) then
        inquire (file = char (mci%grid_filename), exist = exist)
        if (exist) then
            u = free_unit ()
            open (u, file = char (mci%grid_filename), &
                action = "read", status = "old")
            call mci%update (u, success)
            close (u)
            if (.not. success) then
                write (msg_buffer, "(A,A,A)") &
                    "VAMP: parameter mismatch, discarding grid file '", &
                    char (mci%grid_filename), "'"
                call msg_message ()
            end if
        end if
    else
        call msg_bug ("VAMP: read grids: filename undefined")
    end if
end subroutine mci_vamp_read_grids_header

module subroutine mci_vamp_read_grids_data (mci, instance, read_integrals)
    class(mci_vamp_t), intent(in) :: mci
    class(mci_instance_t), intent(inout) :: instance
    logical, intent(in), optional :: read_integrals
    integer :: u
    character(80) :: buffer
    select type (instance)
    type is (mci_vamp_instance_t)
        if (.not. instance%grids_defined) then
            u = free_unit ()
            open (u, file = char (mci%grid_filename), &
                action = "read", status = "old")
            do
                read (u, "(A)") buffer
                if (trim (adjustl (buffer)) == "VAMP grids:") exit
            end do
            call vamp_read_grids (instance%grids, u, read_integrals)
            close (u)
            call instance%set_channel_weights (instance%grids%weights)
            instance%grids_defined = .true.
        else
            call msg_bug ("VAMP: read grids: grids already defined")
        end if
    end select
end subroutine mci_vamp_read_grids_data

```

```

        end if
    end select
end subroutine mci_vamp_read_grids_data

module subroutine mci_vamp_read_grids (mci, instance, success)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    logical, intent(out) :: success
    logical :: exist
    integer :: u
    character(80) :: buffer
    select type (instance)
    type is (mci_vamp_instance_t)
        success = .false.
        if (mci%grid_filename_set) then
            if (.not. instance%grids_defined) then
                inquire (file = char (mci%grid_filename), exist = exist)
                if (exist) then
                    u = free_unit ()
                    open (u, file = char (mci%grid_filename), &
                        action = "read", status = "old")
                    call mci%update (u, success)
                    if (success) then
                        read (u, "(A)") buffer
                        if (trim (adjustl (buffer)) == "VAMP grids:") then
                            call vamp_read_grids (instance%grids, u)
                        else
                            call msg_fatal ("VAMP: reading grid file: &
                                &corrupted grid data")
                        end if
                    else
                        write (msg_buffer, "(A,A,A)") &
                            "VAMP: parameter mismatch, discarding grid file '", &
                                char (mci%grid_filename), "'"
                        call msg_message ()
                    end if
                    close (u)
                    instance%grids_defined = success
                end if
            else
                call msg_bug ("VAMP: read grids: grids already defined")
            end if
        else
            call msg_bug ("VAMP: read grids: filename undefined")
        end if
    end select
end subroutine mci_vamp_read_grids

```

Auxiliary: Read real, integer, string value. We search for an equals sign, the value must follow.

```

(MCI vamp: procedures)+≡
subroutine read_rval (u, rval)
    integer, intent(in) :: u

```



```

    real(default), intent(out) :: rval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) rval
end subroutine read_rval

subroutine read_ival (u, ival)
    integer, intent(in) :: u
    integer, intent(out) :: ival
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) ival
end subroutine read_ival

subroutine read_sval (u, sval)
    integer, intent(in) :: u
    character(*), intent(out) :: sval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) sval
end subroutine read_sval

subroutine read_lval (u, lval)
    integer, intent(in) :: u
    logical, intent(out) :: lval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) lval
end subroutine read_lval

```

Integrate. Perform a new integration pass (possibly reusing previous results), which may consist of several iterations.

Note: we record the integral once per iteration. The integral stored in the `mci` record itself is the last integral of the current iteration, no averaging done. The `results` record may average results.

In case we read the integration from file and we added new iterations to the pass preserving number of calls, we need to reshape the grids in order to incorporate the correct number of calls. Else the grids would be sampled with the number of calls from the grids file, which does not need to coincide with the number of calls from the pass.

Note: recording the efficiency is not supported yet.

<MCI vamp: mci vamp: TBP>+≡

```
procedure :: integrate => mci_vamp_integrate
```

<MCI vamp: sub interfaces>+≡

```

module subroutine mci_vamp_integrate (mci, instance, sampler, &
    n_it, n_calls, results, pacify)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance

```

```

class(mci_sampler_t), intent(inout), target :: sampler
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
class(mci_results_t), intent(inout), optional :: results
logical, intent(in), optional :: pacify
end subroutine mci_vamp_integrate

(MCI vamp: procedures)+≡
module subroutine mci_vamp_integrate (mci, instance, sampler, &
    n_it, n_calls, results, pacify)
class(mci_vamp_t), intent(inout) :: mci
class(mci_instance_t), intent(inout), target :: instance
class(mci_sampler_t), intent(inout), target :: sampler
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
class(mci_results_t), intent(inout), optional :: results
logical, intent(in), optional :: pacify
integer :: it
logical :: reshape, from_file, success
select type (instance)
type is (mci_vamp_instance_t)
    if (associated (mci%current_pass)) then
        mci%current_pass%integral_defined = .false.
        call mci%current_pass%configure (n_it, n_calls, &
            mci%min_calls, mci%grid_par%min_bins, &
            mci%grid_par%max_bins, &
            mci%grid_par%min_calls_per_channel * mci%n_channel)
        call mci%current_pass%configure_history &
            (mci%n_channel, mci%history_par)
        instance%pass_complete = .false.
        instance%it_complete = .false.
        call instance%new_pass (reshape)
        if (.not. instance%grids_defined .or. instance%grids_from_file) then
            if (mci%grid_filename_set .and. .not. mci%rebuild) then
                call mci%read_grids_header (success)
                from_file = success
                if (.not. instance%grids_defined .and. success) then
                    call mci%read_grids_data (instance)
                end if
            else
                from_file = .false.
            end if
        else
            from_file = .false.
        end if
    end if
    if (from_file) then
        if (.not. mci%check_grid_file) &
            call msg_warning ("Reading grid file: MD5 sum check disabled")
        call msg_message ("VAMP: " &
            // "using grids and results from file '" &
            // char (mci%grid_filename) // "'")
    else if (.not. instance%grids_defined) then
        call instance%create_grids ()
    end if
    do it = 1, instance%n_it

```

```

if (signal_is_pending ()) return
reshape = reshape .or. &
    (instance%grids_from_file .and. n_it > mci%current_pass%get_integration_index ())
instance%grids_from_file = from_file .and. &
    it <= mci%current_pass%get_integration_index ()
if (.not. instance%grids_from_file) then
    instance%it_complete = .false.
    call instance%adapt_grids ()
    if (signal_is_pending ()) return
    call instance%adapt_weights ()
    if (signal_is_pending ()) return
    call instance%discard_integrals (reshape)
    if (mci%grid_par%use_vamp_equivalences) then
        call instance%sample_grids (mci%rng, sampler, &
            mci%equivalences)
    else
        call instance%sample_grids (mci%rng, sampler)
    end if
    if (signal_is_pending ()) return
    instance%it_complete = .true.
    if (instance%integral /= 0) then
        mci%current_pass%calls(it) = instance%calls
        mci%current_pass%calls_valid(it) = instance%calls_valid
        mci%current_pass%integral(it) = instance%integral
        if (abs (instance%error / instance%integral) &
            > epsilon (1._default)) then
            mci%current_pass%error(it) = instance%error
        end if
        mci%current_pass%efficiency(it) = instance%efficiency
    end if
    mci%current_pass%integral_defined = .true.
end if
if (present (results)) then
    if (mci%has_chains ()) then
        call mci%collect_chain_weights (instance%w)
        call results%record (1, &
            n_calls      = mci%current_pass%calls(it), &
            n_calls_valid = mci%current_pass%calls_valid(it), &
            integral      = mci%current_pass%integral(it), &
            error         = mci%current_pass%error(it), &
            efficiency    = mci%current_pass%efficiency(it), &
            ! TODO Insert pos. and neg. Efficiency from VAMP.
            efficiency_pos = 0._default, &
            efficiency_neg = 0._default, &
            chain_weights = mci%chain_weights, &
            suppress      = pacify)
    else
        call results%record (1, &
            n_calls      = mci%current_pass%calls(it), &
            n_calls_valid = mci%current_pass%calls_valid(it), &
            integral      = mci%current_pass%integral(it), &
            error         = mci%current_pass%error(it), &
            efficiency    = mci%current_pass%efficiency(it), &
            ! TODO Insert pos. and neg. Efficiency from VAMP.

```

```

        efficiency_pos = 0._default, &
        efficiency_neg = 0._default, &
        suppress = pacify)
    end if
end if
if (.not. instance%grids_from_file &
    .and. mci%grid_filename_set) then
    call mci%write_grids (instance)
end if
call instance%allow_adaptation ()
reshape = .false.
if (.not. mci%current_pass%is_final_pass) then
    call mci%check_goals (it, success)
    if (success) exit
end if
end do
if (signal_is_pending ()) return
instance%pass_complete = .true.
mci%integral = mci%current_pass%get_integral()
mci%error = mci%current_pass%get_error()
mci%efficiency = mci%current_pass%get_efficiency()
mci%integral_known = .true.
mci%error_known = .true.
mci%efficiency_known = .true.
call mci%compute_md5sum (pacify)
else
    call msg_bug ("MCI integrate: current_pass object not allocated")
end if
end select
end subroutine mci_vamp_integrate

```

Check whether we are already finished with this pass.

(MCI vamp: mci vamp: TBP)+≡

```

    procedure :: check_goals => mci_vamp_check_goals

```

(MCI vamp: sub interfaces)+≡

```

    module subroutine mci_vamp_check_goals (mci, it, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: it
        logical, intent(out) :: success
    end subroutine mci_vamp_check_goals

```

(MCI vamp: procedures)+≡

```

    module subroutine mci_vamp_check_goals (mci, it, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: it
        logical, intent(out) :: success
        success = .false.
        if (mci%error_reached (it)) then
            mci%current_pass%n_it = it
            call msg_message ("VAMP: error goal reached; &
                &skipping iterations")
            success = .true.
            return
        end if
    end subroutine mci_vamp_check_goals

```

```

    if (mci%rel_error_reached (it)) then
        mci%current_pass%n_it = it
        call msg_message ("VAMP: relative error goal reached; &
            &skipping iterations")
        success = .true.
        return
    end if
    if (mci%accuracy_reached (it)) then
        mci%current_pass%n_it = it
        call msg_message ("VAMP: accuracy goal reached; &
            &skipping iterations")
        success = .true.
        return
    end if
end subroutine mci_vamp_check_goals

```

Return true if the error, relative error, or accuracy goal has been reached, if any.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: error_reached => mci_vamp_error_reached
    procedure :: rel_error_reached => mci_vamp_rel_error_reached
    procedure :: accuracy_reached => mci_vamp_accuracy_reached

<MCI vamp: sub interfaces>+≡
    module function mci_vamp_error_reached (mci, it) result (flag)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in) :: it
        logical :: flag
    end function mci_vamp_error_reached
    module function mci_vamp_rel_error_reached (mci, it) result (flag)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in) :: it
        logical :: flag
    end function mci_vamp_rel_error_reached
    module function mci_vamp_accuracy_reached (mci, it) result (flag)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in) :: it
        logical :: flag
    end function mci_vamp_accuracy_reached

<MCI vamp: procedures>+≡
    module function mci_vamp_error_reached (mci, it) result (flag)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in) :: it
        logical :: flag
        real(default) :: error_goal, error
        error_goal = mci%grid_par%error_goal
        if (error_goal > 0) then
            associate (pass => mci%current_pass)
                if (pass%integral_defined) then
                    error = abs (pass%error(it))
                    flag = error < error_goal
                else
                    flag = .false.
                end if
            end associate
        end if
    end function mci_vamp_error_reached

```

```

        end associate
    else
        flag = .false.
    end if
end function mci_vamp_error_reached

module function mci_vamp_rel_error_reached (mci, it) result (flag)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in) :: it
    logical :: flag
    real(default) :: rel_error_goal, rel_error
    rel_error_goal = mci%grid_par%rel_error_goal
    if (rel_error_goal > 0) then
        associate (pass => mci%current_pass)
            if (pass%integral_defined) then
                if (pass%integral(it) /= 0) then
                    rel_error = abs (pass%error(it) / pass%integral(it))
                    flag = rel_error < rel_error_goal
                else
                    flag = .true.
                end if
            else
                flag = .false.
            end if
        end associate
    else
        flag = .false.
    end if
end function mci_vamp_rel_error_reached

module function mci_vamp_accuracy_reached (mci, it) result (flag)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in) :: it
    logical :: flag
    real(default) :: accuracy_goal, accuracy
    accuracy_goal = mci%grid_par%accuracy_goal
    if (accuracy_goal > 0) then
        associate (pass => mci%current_pass)
            if (pass%integral_defined) then
                if (pass%integral(it) /= 0) then
                    accuracy = abs (pass%error(it) / pass%integral(it)) &
                        * sqrt (real (pass%calls(it), default))
                    flag = accuracy < accuracy_goal
                else
                    flag = .true.
                end if
            else
                flag = .false.
            end if
        end associate
    else
        flag = .false.
    end if
end function mci_vamp_accuracy_reached

```

Prepare an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

The pass-specific data of the previous integration pass are retained, but we reset the number of iterations and calls to zero. The latter now counts the number of events (calls to the sampling function, actually).

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: prepare_simulation => mci_vamp_prepare_simulation

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_prepare_simulation (mci)
    class(mci_vamp_t), intent(inout) :: mci
  end subroutine mci_vamp_prepare_simulation

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_prepare_simulation (mci)
    class(mci_vamp_t), intent(inout) :: mci
    logical :: success
    if (mci%grid_filename_set) then
      call mci%read_grids_header (success)
      call mci%compute_md5sum ()
      if (.not. success) then
        call msg_fatal ("Simulate: " &
          // "reading integration grids from file '" &
          // char (mci%grid_filename) // "' failed")
      end if
    else
      call msg_bug ("VAMP: simulation: no grids, no grid filename")
    end if
  end subroutine mci_vamp_prepare_simulation

```

21.6.5 Sampling function

The VAMP sampling function has a well-defined interface which we have to implement. The `data` argument allows us to pass pointers to the `sampler` and `instance` objects, so we can access configuration data and fill point-dependent contents within these objects.

The `weights` and `channel` argument must be present in the call.

Note: this is the place where we must look for external signals, i.e., interrupt from the OS. We would like to raise a VAMP exception which is then caught by `vamp_sample_grids` as the caller, so it dumps its current state and returns (with the signal still pending). WHIZARD will then terminate gracefully. Of course, VAMP should be able to resume from the dump.

In the current implementation, we handle the exception in place and terminate immediately. The incomplete current integration pass is lost.

```

<MCI vamp: main procedures>+≡
  function vamp_sampling_function &
    (xi, data, weights, channel, grids) result (f)
    real(default) :: f
    real(default), dimension(:), intent(in) :: xi
    class(vamp_data_t), intent(in) :: data

```

```

real(default), dimension(:), intent(in), optional :: weights
integer, intent(in), optional :: channel
type(vamp_grid), dimension(:), intent(in), optional :: grids
type(exception) :: exc
logical :: verbose
character(*), parameter :: FN = "WHIZARD sampling function"
class(mci_instance_t), pointer :: instance
select type (data)
type is (mci_workspace_t)
  instance => data%instance
  select type (instance)
  class is (mci_vamp_instance_t)
    verbose = instance%mci%verbose
    call instance%evaluate (data%sampler, channel, xi)
    if (signal_is_pending ()) then
      call raise_exception (exc, EXC_FATAL, FN, "signal received")
      call handle_vamp_exception (exc, verbose)
      call terminate_now_if_signal ()
    end if
    instance%calls = instance%calls + 1
    if (data%sampler%is_valid ()) &
      & instance%calls_valid = instance%calls_valid + 1
    f = instance%get_value ()
    call terminate_now_if_single_event ()
  class default
    call msg_bug("VAMP: " // FN // ": unknown MCI instance type")
  end select
end select
end function vamp_sampling_function

```

This is supposed to be the mapping between integration channels. The VAMP event generating procedures technically require it, but it is meaningless in our setup where all transformations happen inside the sampler object. So, this implementation is trivial: Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: main procedures>+=
pure function phi_trivial (xi, channel_dummy) result (x)
  real(default), dimension(:), intent(in) :: xi
  integer, intent(in) :: channel_dummy
  real(default), dimension(size(xi)) :: x
  x = xi
end function phi_trivial

```

Generate weighted event. Note that the event weight (`vamp_weight`) is not just the MCI weight. `vamp_next_event` selects a channel based on the channel weights multiplied by the (previously recorded) maximum integrand value of the channel. The MCI weight is renormalized accordingly, to cancel this effect on the result. Gfortran 7/8/9/ bug, has to remain in the main module:

```

<MCI vamp: mci vamp: TBP>+=
procedure :: generate_weighted_event => mci_vamp_generate_weighted_event
<MCI vamp: main procedures>+=
subroutine mci_vamp_generate_weighted_event (mci, instance, sampler)
  class(mci_vamp_t), intent(inout) :: mci

```



```

class(mci_instance_t), intent(inout), target :: instance
class(mci_sampler_t), intent(inout), target :: sampler
class(vamp_data_t), allocatable :: data
type(exception) :: vamp_exception
select type (instance)
type is (mci_vamp_instance_t)
  instance%vamp_weight_set = .false.
  allocate (mci_workspace_t :: data)
  select type (data)
  type is (mci_workspace_t)
    data%sampler => sampler
    data%instance => instance
  end select
  select type (rng => mci%rng)
  type is (rng_tao_t)
    if (instance%grids_defined) then
      call vamp_next_event ( &
        instance%vamp_x, &
        rng%state, &
        instance%grids, &
        vamp_sampling_function, &
        data, &
        phi = phi_trivial, &
        weight = instance%vamp_weight, &
        exc = vamp_exception)
      call handle_vamp_exception (vamp_exception, mci%verbose)
      instance%vamp_excess = 0
      instance%vamp_weight_set = .true.
    else
      call msg_bug ("VAMP: generate event: grids undefined")
    end if
  class default
    call msg_fatal ("VAMP event generation: &
      &random-number generator must be TAO")
  end select
end select
end subroutine mci_vamp_generate_weighted_event

```

Generate unweighted event. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: generate_unweighted_event => &
    mci_vamp_generate_unweighted_event

<MCI vamp: main procedures>+≡
  subroutine mci_vamp_generate_unweighted_event &
    (mci, instance, sampler)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    class(vamp_data_t), allocatable :: data
    logical :: positive
    type(exception) :: vamp_exception
    select type (instance)

```

```

type is (mci_vamp_instance_t)
  instance%vamp_weight_set = .false.
  allocate (mci_workspace_t :: data)
  select type (data)
  type is (mci_workspace_t)
    data%sampler => sampler
    data%instance => instance
  end select
  select type (rng => mci%rng)
  type is (rng_tao_t)
    if (instance%grids_defined) then
      REJECTION: do
        call vamp_next_event ( &
          instance%vamp_x, &
          rng%state, &
          instance%grids, &
          vamp_sampling_function, &
          data, &
          phi = phi_trivial, &
          excess = instance%vamp_excess, &
          positive = positive, &
          exc = vamp_exception)
        if (signal_is_pending ()) return
        if (sampler%is_valid ()) exit REJECTION
      end do REJECTION
      call handle_vamp_exception (vamp_exception, mci%verbose)
      if (positive) then
        instance%vamp_weight = 1
      else if (instance%negative_weights) then
        instance%vamp_weight = -1
      else
        call msg_fatal ("VAMP: event with negative weight generated")
        instance%vamp_weight = 0
      end if
      instance%vamp_weight_set = .true.
    else
      call msg_bug ("VAMP: generate event: grids undefined")
    end if
  class default
    call msg_fatal ("VAMP event generation: &
      &random-number generator must be TAO")
  end select
end select
end subroutine mci_vamp_generate_unweighted_event

```

Rebuild an event, using the state input.

Note: This feature is currently unused.

(MCI vamp: mci vamp: TBP)+≡

```
procedure :: rebuild_event => mci_vamp_rebuild_event
```

(MCI vamp: sub interfaces)+≡

```

module subroutine mci_vamp_rebuild_event (mci, instance, sampler, state)
  class(mci_vamp_t), intent(inout) :: mci
  class(mci_instance_t), intent(inout) :: instance

```

```

        class(mci_sampler_t), intent(inout) :: sampler
        class(mci_state_t), intent(in) :: state
    end subroutine mci_vamp_rebuild_event
<MCI vamp: procedures>+=
module subroutine mci_vamp_rebuild_event (mci, instance, sampler, state)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    call msg_bug ("MCI vamp rebuild event not implemented yet")
end subroutine mci_vamp_rebuild_event

Pacify: override the default no-op, since VAMP numerics might need some
message.
<MCI vamp: mci vamp: TBP>+=
    procedure :: pacify => mci_vamp_pacify
<MCI vamp: sub interfaces>+=
    module subroutine mci_vamp_pacify (object, efficiency_reset, error_reset)
        class(mci_vamp_t), intent(inout) :: object
        logical, intent(in), optional :: efficiency_reset, error_reset
    end subroutine mci_vamp_pacify
<MCI vamp: procedures>+=
module subroutine mci_vamp_pacify (object, efficiency_reset, error_reset)
    class(mci_vamp_t), intent(inout) :: object
    logical, intent(in), optional :: efficiency_reset, error_reset
    logical :: err_reset
    type(pass_t), pointer :: current_pass
    err_reset = .false.
    if (present (error_reset)) err_reset = error_reset
    current_pass => object%first_pass
    do while (associated (current_pass))
        if (allocated (current_pass%error) .and. err_reset) then
            current_pass%error = 0
        end if
        if (allocated (current_pass%efficiency) .and. err_reset) then
            current_pass%efficiency = 1
        end if
        current_pass => current_pass%next
    end do
end subroutine mci_vamp_pacify

```

21.6.6 Sampler as Workspace

In the full setup, the sampling function requires the process instance object as workspace. We implement this by (i) implementing the process instance as a type extension of the abstract `sampler_t` object used by the MCI implementation and (ii) providing such an object as an extra argument to the sampling function that VAMP can call. To minimize cross-package dependencies, we use an abstract type `vamp_workspace` that VAMP declares and extend this by including a pointer to the `sampler` and `instance` objects. In the body of the

sampling function, we dereference this pointer and can then work with the contents.

```

<MCI vamp: types>+≡
  type, extends (vamp_data_t) :: mci_workspace_t
    class(mci_sampler_t), pointer :: sampler => null ()
    class(mci_vamp_instance_t), pointer :: instance => null ()
  end type mci_workspace_t

```

21.6.7 Integrator instance

The history entries should point to the corresponding history entry in the `pass_t` object. If there is none, we may allocate a local history, which is then just transient.

```

<MCI vamp: public>+≡
  public :: mci_vamp_instance_t

<MCI vamp: types>+≡
  type, extends (mci_instance_t) :: mci_vamp_instance_t
    type(mci_vamp_t), pointer :: mci => null ()
    logical :: grids_defined = .false.
    logical :: grids_from_file = .false.
    integer :: n_it = 0
    integer :: it = 0
    logical :: pass_complete = .false.
    integer :: n_calls = 0
    integer :: calls = 0
    integer :: calls_valid = 0
    logical :: it_complete = .false.
    logical :: enable_adapt_grids = .false.
    logical :: enable_adapt_weights = .false.
    logical :: allow_adapt_grids = .false.
    logical :: allow_adapt_weights = .false.
    integer :: n_adapt_grids = 0
    integer :: n_adapt_weights = 0
    logical :: generating_events = .false.
    real(default) :: safety_factor = 1
    type(vamp_grids) :: grids
    real(default) :: g = 0
    real(default), dimension(:), allocatable :: gi
    real(default) :: integral = 0
    real(default) :: error = 0
    real(default) :: efficiency = 0
    real(default), dimension(:), allocatable :: vamp_x
    logical :: vamp_weight_set = .false.
    real(default) :: vamp_weight = 0
    real(default) :: vamp_excess = 0
    logical :: allocate_global_history = .false.
    type(vamp_history), dimension(:), pointer :: v_history => null ()
    logical :: allocate_channel_history = .false.
    type(vamp_history), dimension(:,,:), pointer :: v_histories => null ()
  contains
    <MCI vamp: mci vamp instance: TBP>

```

```
end type mci_vamp_instance_t
```

Output.

```
<MCI vamp: mci vamp instance: TBP>≡
```

```
  procedure :: write => mci_vamp_instance_write
```

```
<MCI vamp: sub interfaces>+≡
```

```
  module subroutine mci_vamp_instance_write (object, unit, pacify)
    class(mci_vamp_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
  end subroutine mci_vamp_instance_write
```

```
<MCI vamp: procedures>+≡
```

```
  module subroutine mci_vamp_instance_write (object, unit, pacify)
    class(mci_vamp_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3x,A," // FMT_19 // ")") "Integrand = ", object%integrand
    write (u, "(3x,A," // FMT_19 // ")") "Weight      = ", object%mci_weight
    if (object%vamp_weight_set) then
      write (u, "(3x,A," // FMT_19 // ")") "VAMP wgt  = ", object%vamp_weight
      if (object%vamp_excess /= 0) then
        write (u, "(3x,A," // FMT_19 // ")") "VAMP exc  = ", &
          object%vamp_excess
      end if
    end if
    write (u, "(3x,A,L1)") "adapt grids  = ", object%enable_adapt_grids
    write (u, "(3x,A,L1)") "adapt weights = ", object%enable_adapt_weights
    if (object%grids_defined) then
      if (object%grids_from_file) then
        write (u, "(3x,A)") "VAMP grids: read from file"
      else
        write (u, "(3x,A)") "VAMP grids: defined"
      end if
    else
      write (u, "(3x,A)") "VAMP grids: [undefined]"
    end if
    write (u, "(3x,A,I0)") "n_it          = ", object%n_it
    write (u, "(3x,A,I0)") "it            = ", object%it
    write (u, "(3x,A,L1)") "pass complete = ", object%it_complete
    write (u, "(3x,A,I0)") "n_calls       = ", object%n_calls
    write (u, "(3x,A,I0)") "calls         = ", object%calls
    write (u, "(3x,A,I0)") "calls_valid   = ", object%calls_valid
    write (u, "(3x,A,L1)") "it complete   = ", object%it_complete
    write (u, "(3x,A,I0)") "n adapt.(g)   = ", object%n_adapt_grids
    write (u, "(3x,A,I0)") "n adapt.(w)   = ", object%n_adapt_weights
    write (u, "(3x,A,L1)") "gen. events   = ", object%generating_events
    write (u, "(3x,A,L1)") "neg. weights  = ", object%negative_weights
    if (object%safety_factor /= 1) write &
      (u, "(3x,A," // fmt // ")") "safety f = ", object%safety_factor
```

```

write (u, "(3x,A," // fmt // ")") "integral = ", object%integral
write (u, "(3x,A," // fmt // ")") "error    = ", object%error
write (u, "(3x,A," // fmt // ")") "eff.     = ", object%efficiency
write (u, "(3x,A)") "weights:"
do i = 1, size (object%w)
    write (u, "(5x,I0,1x," // FMT_12 // ")") i, object%w(i)
end do
end subroutine mci_vamp_instance_write

```

Write the grids to the specified unit.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: write_grids => mci_vamp_instance_write_grids

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_write_grids (object, unit)
        class(mci_vamp_instance_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine mci_vamp_instance_write_grids

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_write_grids (object, unit)
        class(mci_vamp_instance_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%grids_defined) then
            call vamp_write_grids (object%grids, u, write_integrals = .true.)
        end if
    end subroutine mci_vamp_instance_write_grids

```

Finalizer: the history arrays are pointer arrays and need finalization.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: final => mci_vamp_instance_final

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_final (object)
        class(mci_vamp_instance_t), intent(inout) :: object
    end subroutine mci_vamp_instance_final

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_final (object)
        class(mci_vamp_instance_t), intent(inout) :: object
        if (object%allocate_global_history) then
            if (associated (object%v_history)) then
                call vamp_delete_history (object%v_history)
                deallocate (object%v_history)
            end if
        end if
        if (object%allocate_channel_history) then
            if (associated (object%v_histories)) then
                call vamp_delete_history (object%v_histories)
                deallocate (object%v_histories)
            end if
        end if
        if (object%grids_defined) then

```

```

        call vamp_delete_grids (object%grids)
        object%grids_defined = .false.
    end if
end subroutine mci_vamp_instance_final

```

Initializer.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: init => mci_vamp_instance_init

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_init (mci_instance, mci)
        class(mci_vamp_instance_t), intent(out) :: mci_instance
        class(mci_t), intent(in), target :: mci
    end subroutine mci_vamp_instance_init

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_init (mci_instance, mci)
        class(mci_vamp_instance_t), intent(out) :: mci_instance
        class(mci_t), intent(in), target :: mci
        call mci_instance%base_init (mci)
        select type (mci)
            type is (mci_vamp_t)
                mci_instance%mci => mci
                allocate (mci_instance%gi (mci%n_channel))
                mci_instance%allocate_global_history = .not. mci%history_par%global
                mci_instance%allocate_channel_history = .not. mci%history_par%channel
                mci_instance%negative_weights = mci%negative_weights
            end select
    end subroutine mci_vamp_instance_init

```

Prepare a new integration pass: write the pass-specific settings to the `instance` object. This should be called initially, together with the `create_grids` procedure, and whenever we start a new integration pass.

Set `reshape` if the number of calls is different than previously (unless it was zero, indicating the first pass).

We link VAMP histories to the allocated histories in the current pass object, so the recorded results are persistent. However, if there are no histories present there, we allocate them locally. In that case, the histories will disappear together with the MCI instance object.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: new_pass => mci_vamp_instance_new_pass

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_new_pass (instance, reshape)
        class(mci_vamp_instance_t), intent(inout) :: instance
        logical, intent(out) :: reshape
    end subroutine mci_vamp_instance_new_pass

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_new_pass (instance, reshape)
        class(mci_vamp_instance_t), intent(inout) :: instance
        logical, intent(out) :: reshape
        type(pass_t), pointer :: current
        associate (mci => instance%mci)

```

```

current => mci%current_pass
instance%n_it = current%n_it
if (instance%n_calls == 0) then
    reshape = .false.
    instance%n_calls = current%n_calls
else if (instance%n_calls == current%n_calls) then
    reshape = .false.
else
    reshape = .true.
    instance%n_calls = current%n_calls
end if
instance%it = 0
instance%calls = 0
instance%calls_valid = 0
instance%enable_adapt_grids = current%adapt_grids
instance%enable_adapt_weights = current%adapt_weights
instance%generating_events = .false.
if (instance%allocate_global_history) then
    if (associated (instance%v_history)) then
        call vamp_delete_history (instance%v_history)
        deallocate (instance%v_history)
    end if
    allocate (instance%v_history (instance%n_it))
    call vamp_create_history (instance%v_history, verbose = .false.)
else
    instance%v_history => current%v_history
end if
if (instance%allocate_channel_history) then
    if (associated (instance%v_histories)) then
        call vamp_delete_history (instance%v_histories)
        deallocate (instance%v_histories)
    end if
    allocate (instance%v_histories (instance%n_it, mci%n_channel))
    call vamp_create_history (instance%v_histories, verbose = .false.)
else
    instance%v_histories => current%v_histories
end if
end associate
end subroutine mci_vamp_instance_new_pass

```

Create a grid set within the `instance` object, using the data of the current integration pass. Also reset counters that track this grid set.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: create_grids => mci_vamp_instance_create_grids

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_create_grids (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        end subroutine mci_vamp_instance_create_grids

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_create_grids (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        type (pass_t), pointer :: current
        integer, dimension(:), allocatable :: num_div

```



```

real(default), dimension(:,:), allocatable :: region
associate (mci => instance%mci)
  current => mci%current_pass
  allocate (num_div (mci%n_dim))
  allocate (region (2, mci%n_dim))
  region(1,:) = 0
  region(2,:) = 1
  num_div = current%n_bins
  instance%n_adapt_grids = 0
  instance%n_adapt_weights = 0
  if (.not. instance%grids_defined) then
    call vamp_create_grids (instance%grids, &
      region, &
      current%n_calls, &
      weights = instance%w, &
      num_div = num_div, &
      stratified = mci%grid_par%stratified)
    instance%grids_defined = .true.
  else
    call msg_bug ("VAMP: create grids: grids already defined")
  end if
end associate
end subroutine mci_vamp_instance_create_grids

```

Reset a grid set, so we can start a fresh integration pass. In effect, we delete results of previous integrations, but keep the grid shapes, weights, and variance arrays, so adaptation is still possible. The grids are prepared for a specific number of calls (per iteration) and sampling mode (stratified/importance).

The `vamp_discard_integrals` implementation will reshape the grids only if the argument `num_calls` is present.

```

<MCI vamp: mci vamp instance: TBP>+≡
  procedure :: discard_integrals => mci_vamp_instance_discard_integrals

<MCI vamp: sub interfaces>+≡
  module subroutine mci_vamp_instance_discard_integrals (instance, reshape)
    class(mci_vamp_instance_t), intent(inout) :: instance
    logical, intent(in) :: reshape
  end subroutine mci_vamp_instance_discard_integrals

<MCI vamp: procedures>+≡
  module subroutine mci_vamp_instance_discard_integrals (instance, reshape)
    class(mci_vamp_instance_t), intent(inout) :: instance
    logical, intent(in) :: reshape
    instance%calls = 0
    instance%calls_valid = 0
    instance%integral = 0
    instance%error = 0
    instance%efficiency = 0
    associate (mci => instance%mci)
      if (instance%grids_defined) then
        if (mci%grid_par%use_vamp_equivalences) then
          if (reshape) then
            call vamp_discard_integrals (instance%grids, &
              num_calls = instance%n_calls, &

```

```

        stratified = mci%grid_par%stratified, &
        eq = mci%equivalences)
    else
        call vamp_discard_integrals (instance%grids, &
            stratified = mci%grid_par%stratified, &
            eq = mci%equivalences)
    end if
else
    if (reshape) then
        call vamp_discard_integrals (instance%grids, &
            num_calls = instance%n_calls, &
            stratified = mci%grid_par%stratified)
    else
        call vamp_discard_integrals (instance%grids, &
            stratified = mci%grid_par%stratified)
    end if
end if
else
    call msg_bug ("VAMP: discard integrals: grids undefined")
end if
end associate
end subroutine mci_vamp_instance_discard_integrals

```

After grids are created (with equidistant binning and equal weight), adaptation is redundant. Therefore, we should allow it only after a complete integration step has been performed, calling this.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: allow_adaptation => mci_vamp_instance_allow_adaptation

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_allow_adaptation (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
    end subroutine mci_vamp_instance_allow_adaptation

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_allow_adaptation (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        instance%allow_adapt_grids = .true.
        instance%allow_adapt_weights = .true.
    end subroutine mci_vamp_instance_allow_adaptation

```

Adapt grids.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: adapt_grids => mci_vamp_instance_adapt_grids

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_adapt_grids (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
    end subroutine mci_vamp_instance_adapt_grids

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_adapt_grids (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        if (instance%enable_adapt_grids .and. instance%allow_adapt_grids) then
            if (instance%grids_defined) then

```

```

        call vamp_refine_grids (instance%grids)
        instance%n_adapt_grids = instance%n_adapt_grids + 1
    else
        call msg_bug ("VAMP: adapt grids: grids undefined")
    end if
end if
end subroutine mci_vamp_instance_adapt_grids

```

Adapt weights. Use the variance array returned by VAMP for recalculating the weight array. The parameter `channel_weights_power` dampens fluctuations.

If the number of calls in a given channel falls below a user-defined threshold, the weight is not lowered further but kept at this threshold. The other channel weights are reduced accordingly. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: adapt_weights => mci_vamp_instance_adapt_weights
<MCI vamp: main procedures>+≡
    subroutine mci_vamp_instance_adapt_weights (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        real(default) :: w_sum, w_avg_ch, sum_w_underflow, w_min
        real(default), dimension(:), allocatable :: weights
        integer :: n_ch, ch, n_underflow
        logical, dimension(:), allocatable :: mask, underflow
        type(exception) :: vamp_exception
        logical :: wsum_non_zero
        if (instance%enable_adapt_weights .and. instance%allow_adapt_weights) then
            associate (mci => instance%mci)
                if (instance%grids_defined) then
                    allocate (weights (size (instance%grids%weights)))
                    weights = instance%grids%weights &
                        * vamp_get_variance (instance%grids%grids) &
                        ** mci%grid_par%channel_weights_power
                    w_sum = sum (weights)
                    if (w_sum /= 0) then
                        weights = weights / w_sum
                        if (mci%n_chain /= 0) then
                            allocate (mask (mci%n_channel))
                            do ch = 1, mci%n_chain
                                mask = mci%chain == ch
                                n_ch = count (mask)
                                if (n_ch /= 0) then
                                    w_avg_ch = sum (weights, mask) / n_ch
                                    where (mask) weights = w_avg_ch
                                end if
                            end do
                        end if
                    end if
                    if (mci%grid_par%threshold_calls /= 0) then
                        w_min = &
                            real (mci%grid_par%threshold_calls, default) &
                            / instance%n_calls
                        allocate (underflow (mci%n_channel))
                        underflow = weights /= 0 .and. abs (weights) < w_min
                        n_underflow = count (underflow)
                    end if
                end if
            end associate
        end if
    end subroutine mci_vamp_instance_adapt_weights

```

```

        sum_w_underflow = sum (weights, mask=underflow)
        if (sum_w_underflow /= 1) then
            where (underflow)
                weights = w_min
            elsewhere
                weights = weights &
                    * (1 - n_underflow * w_min) / (1 - sum_w_underflow)
            end where
        end if
    end if
end if
call instance%set_channel_weights (weights, wsum_non_zero)
if (wsum_non_zero) call vamp_update_weights &
    (instance%grids, weights, exc = vamp_exception)
call handle_vamp_exception (vamp_exception, mci%verbose)
else
    call msg_bug ("VAMP: adapt weights: grids undefined")
end if
end associate
instance%n_adapt_weights = instance%n_adapt_weights + 1
end if
end subroutine mci_vamp_instance_adapt_weights

```

Integration: sample the VAMP grids. The number of calls etc. are already stored inside the grids. We provide the random-number generator, the sampling function, and a link to the workspace object, which happens to contain a pointer to the sampler object. The sampler object thus becomes the workspace of the sampling function.

Note: in the current implementation, the random-number generator must be the TAO generator. This explicit dependence should be removed from the VAMP implementation. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: sample_grids => mci_vamp_instance_sample_grids

<MCI vamp: main procedures>+≡
    subroutine mci_vamp_instance_sample_grids &
        (instance, rng, sampler, eq)
        class(mci_vamp_instance_t), intent(inout), target :: instance
        class(rng_t), intent(inout) :: rng
        class(mci_sampler_t), intent(inout), target :: sampler
        type(vamp_equivalences_t), intent(in), optional :: eq
        class(vamp_data_t), allocatable :: data
        type(exception) :: vamp_exception
        allocate (mci_workspace_t :: data)
        select type (data)
            type is (mci_workspace_t)
                data%sampler => sampler
                data%instance => instance
            end select
        select type (rng)
            type is (rng_tao_t)
                instance%it = instance%it + 1
                instance%calls = 0

```

```

    if (instance%grids_defined) then
        call vamp_sample_grids ( &
            rng%state, &
            instance%grids, &
            vamp_sampling_function, &
            data, &
            1, &
            eq = eq, &
            history = instance%v_history(instance%it:), &
            histories = instance%v_histories(instance%it:,:), &
            integral = instance%integral, &
            std_dev = instance%error, &
            exc = vamp_exception, &
            negative_weights = instance%negative_weights)
        call handle_vamp_exception (vamp_exception, instance%nci%verbose)
        instance%efficiency = instance%get_efficiency ()
    else
        call msg_bug ("VAMP: sample grids: grids undefined")
    end if
class default
    call msg_fatal ("VAMP integration: random-number generator must be TAO")
end select
end subroutine mci_vamp_instance_sample_grids

```

Compute the reweighting efficiency for the current grids, suitable averaged over all active channels.

(MCI vamp: mci vamp instance: TBP)+≡

```

    procedure :: get_efficiency_array => mci_vamp_instance_get_efficiency_array
    procedure :: get_efficiency => mci_vamp_instance_get_efficiency

```

(MCI vamp: sub interfaces)+≡

```

    module function mci_vamp_instance_get_efficiency_array &
        (mci) result (efficiency)
        class(mci_vamp_instance_t), intent(in) :: mci
        real(default), dimension(:), allocatable :: efficiency
    end function mci_vamp_instance_get_efficiency_array
    module function mci_vamp_instance_get_efficiency (mci) result (efficiency)
        class(mci_vamp_instance_t), intent(in) :: mci
        real(default) :: efficiency
    end function mci_vamp_instance_get_efficiency

```

(MCI vamp: procedures)+≡

```

    module function mci_vamp_instance_get_efficiency_array &
        (mci) result (efficiency)
        class(mci_vamp_instance_t), intent(in) :: mci
        real(default), dimension(:), allocatable :: efficiency
        allocate (efficiency (mci%nci%n_channel))
        if (.not. mci%negative_weights) then
            where (mci%grids%grids%f_max /= 0)
                efficiency = mci%grids%grids%mu(1) / abs (mci%grids%grids%f_max)
            elsewhere
                efficiency = 0
            end where
        else
            where (mci%grids%grids%f_max /= 0)

```

```

        efficiency = &
            (mci%grids%grids%mu_plus(1) - mci%grids%grids%mu_minus(1)) &
            / abs (mci%grids%grids%f_max)
    elsewhere
        efficiency = 0
    end where
end if
end function mci_vamp_instance_get_efficiency_array

module function mci_vamp_instance_get_efficiency (mci) result (efficiency)
    class(mci_vamp_instance_t), intent(in) :: mci
    real(default) :: efficiency
    real(default), dimension(:), allocatable :: weight
    real(default) :: norm
    allocate (weight (mci%mci%n_channel))
    weight = mci%grids%weights * abs (mci%grids%grids%f_max)
    norm = sum (weight)
    if (norm /= 0) then
        efficiency = dot_product (mci%get_efficiency_array (), weight) / norm
    else
        efficiency = 1
    end if
end function mci_vamp_instance_get_efficiency

```

Prepare an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

The pass-specific data of the previous integration pass are retained, but we reset the number of iterations and calls to zero. The latter now counts the number of events (calls to the sampling function, actually).

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: init_simulation => mci_vamp_instance_init_simulation

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_init_simulation &
        (instance, safety_factor)
        class(mci_vamp_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: safety_factor
    end subroutine mci_vamp_instance_init_simulation

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_init_simulation &
        (instance, safety_factor)
        class(mci_vamp_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: safety_factor
        associate (mci => instance%mci)
            allocate (instance%vamp_x (mci%n_dim))
            instance%it = 0
            instance%calls = 0
            instance%generating_events = .true.
            if (present (safety_factor)) instance%safety_factor = safety_factor
            if (.not. instance%grids_defined) then
                if (mci%grid_filename_set) then
                    if (.not. mci%check_grid_file) &
                        call msg_warning ("Reading grid file: MD5 sum check disabled")

```

```

    call msg_message ("Simulate: " &
        // "using integration grids from file '" &
        // char (mci%grid_filename) // "'")
    call mci%read_grids_data (instance)
    if (instance%safety_factor /= 1) then
        write (msg_buffer, "(A,ES10.3,A)") "Simulate: &
            &applying safety factor", instance%safety_factor, &
            " to event rejection"
        call msg_message ()
        instance%grids%grids%f_max = &
            instance%grids%grids%f_max * instance%safety_factor
    end if
    else
        call msg_bug ("VAMP: simulation: no grids, no grid filename")
    end if
end if
end associate
end subroutine mci_vamp_instance_init_simulation

```

Finalize an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: final_simulation => mci_vamp_instance_final_simulation

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_final_simulation (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
    end subroutine mci_vamp_instance_final_simulation

<MCI vamp: procedures>+≡
    module subroutine mci_vamp_instance_final_simulation (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        if (allocated (instance%vamp_x)) deallocate (instance%vamp_x)
    end subroutine mci_vamp_instance_final_simulation

```

21.6.8 Integrator instance: evaluation

Here, we compute the multi-channel reweighting factor for the current channel, that accounts for the Jacobians of the transformations from/to all other channels.

The computation of the VAMP probabilities may consume considerable time, therefore we enable parallel evaluation. (Collecting the contributions to `mci%g` is a reduction, which we should also implement via OpenMP.)

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: compute_weight => mci_vamp_instance_compute_weight

<MCI vamp: sub interfaces>+≡
    module subroutine mci_vamp_instance_compute_weight (mci, c)
        class(mci_vamp_instance_t), intent(inout) :: mci
        integer, intent(in) :: c
    end subroutine mci_vamp_instance_compute_weight

```

```

<MCI vamp: procedures>+=
module subroutine mci_vamp_instance_compute_weight (mci, c)
  class(mci_vamp_instance_t), intent(inout) :: mci
  integer, intent(in) :: c
  integer :: i
  mci%selected_channel = c
  !$OMP PARALLEL PRIVATE(i) SHARED(mci)
  !$OMP DO
  do i = 1, mci%nc_channel
    if (mci%w(i) /= 0) then
      mci%gi(i) = vamp_probability (mci%grids%grids(i), mci%x(:,i))
    else
      mci%gi(i) = 0
    end if
  end do
  !$OMP END DO
  !$OMP END PARALLEL
  mci%g = 0
  if (mci%gi(c) /= 0) then
    do i = 1, mci%nc_channel
      if (mci%w(i) /= 0 .and. mci%f(i) /= 0) then
        mci%g = mci%g + mci%w(i) * mci%gi(i) / mci%f(i)
      end if
    end do
  end if
  if (mci%g /= 0) then
    mci%weight = mci%gi(c) / mci%g
  else
    mci%weight = 0
  end if
end subroutine mci_vamp_instance_compute_weight

```

Record the integrand.

```

<MCI vamp: mci vamp instance: TBP>+=
  procedure :: record_integrand => mci_vamp_instance_record_integrand

<MCI vamp: sub interfaces>+=
  module subroutine mci_vamp_instance_record_integrand (mci, integrand)
    class(mci_vamp_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    end subroutine mci_vamp_instance_record_integrand

<MCI vamp: procedures>+=
  module subroutine mci_vamp_instance_record_integrand (mci, integrand)
    class(mci_vamp_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    mci%integrand = integrand
  end subroutine mci_vamp_instance_record_integrand

```

Get the event weight. The default routine returns the same value that we would use for integration. This is correct if we select the integration channel according to the channel weight. `vamp_next_event` does differently, so we should rather rely on the weight that VAMP returns. This is the value stored in `vamp_weight`.

We override the default TBP accordingly.

```

<MCI vamp: mci vamp instance: TBP>+≡
  procedure :: get_event_weight => mci_vamp_instance_get_event_weight
  procedure :: get_event_excess => mci_vamp_instance_get_event_excess

<MCI vamp: sub interfaces>+≡
  module function mci_vamp_instance_get_event_weight (mci) result (value)
    class(mci_vamp_instance_t), intent(in) :: mci
    real(default) :: value
  end function mci_vamp_instance_get_event_weight
  module function mci_vamp_instance_get_event_excess (mci) result (value)
    class(mci_vamp_instance_t), intent(in) :: mci
    real(default) :: value
  end function mci_vamp_instance_get_event_excess

<MCI vamp: procedures>+≡
  module function mci_vamp_instance_get_event_weight (mci) result (value)
    class(mci_vamp_instance_t), intent(in) :: mci
    real(default) :: value
    if (mci%vamp_weight_set) then
      value = mci%vamp_weight
    else
      call msg_bug ("VAMP: attempt to read undefined event weight")
    end if
  end function mci_vamp_instance_get_event_weight

  module function mci_vamp_instance_get_event_excess (mci) result (value)
    class(mci_vamp_instance_t), intent(in) :: mci
    real(default) :: value
    if (mci%vamp_weight_set) then
      value = mci%vamp_excess
    else
      call msg_bug ("VAMP: attempt to read undefined event excess weight")
    end if
  end function mci_vamp_instance_get_event_excess

```

21.6.9 VAMP exceptions

A VAMP routine may have raised an exception. Turn this into a WHIZARD error message.

An external signal could raise a fatal exception, but this should be delayed and handled by the correct termination routine. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp: main procedures>+≡
  subroutine handle_vamp_exception (exc, verbose)
    type(exception), intent(in) :: exc
    logical, intent(in) :: verbose
    integer :: exc_level
    if (verbose) then
      exc_level = EXC_INFO
    else
      exc_level = EXC_ERROR
    end if

```

```

    if (exc%level >= exc_level) then
        write (msg_buffer, "(A,':',1x,A)" trim (exc%origin), trim (exc%message)
        select case (exc%level)
            case (EXC_INFO); call msg_message ()
            case (EXC_WARN); call msg_warning ()
            case (EXC_ERROR); call msg_error ()
            case (EXC_FATAL)
                if (signal_is_pending ()) then
                    call msg_message ()
                else
                    call msg_fatal ()
                end if
            end select
        end if
    end subroutine handle_vamp_exception

```

21.6.10 Unit tests

Test module, followed by the corresponding implementation module.

<mci_vamp_ut.f90>≡

<File header>

```

module mci_vamp_ut
    use unit_tests
    use mci_vamp_uti

```

<Standard module head>

<MCI vamp: public test>

contains

<MCI vamp: test driver>

```

end module mci_vamp_ut

```

<mci_vamp_uti.f90>≡

<File header>

```

module mci_vamp_uti

```

<Use kinds>

<Use strings>

```

    use io_units
    use constants, only: PI, TWOPI
    use rng_base
    use rng_tao
    use phs_base
    use mci_base
    use vamp, only: vamp_write_grids !NODEP!

```

```

    use mci_vamp

```

```

<Standard module head>

<MCI vamp: test declarations>

<MCI vamp: test types>

contains

<MCI vamp: tests>

end module mci_vamp_util
API: driver for the unit tests below.
<MCI vamp: public test>≡
    public :: mci_vamp_test
<MCI vamp: test driver>≡
    subroutine mci_vamp_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <MCI vamp: execute tests>
    end subroutine mci_vamp_test

```

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

In mode 1, the function is $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

In mode 2, the function is $11x^{10}$, also with integral 1.

Mode 4 includes ranges of zero and negative function value, the integral is negative. The results should be identical to the results of `mci_midpoint_4`, where the same function is evaluated. The function is $f(x) = (1 - 3x^2) \theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$.

```

<MCI vamp: test types>≡
    type, extends (mci_sampler_t) :: test_sampler_1_t
        real(default), dimension(:), allocatable :: x
        real(default) :: val
        integer :: mode = 1
    contains
    <MCI vamp: test sampler 1: TBP>
    end type test_sampler_1_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI vamp: test sampler 1: TBP>≡
    procedure :: write => test_sampler_1_write
<MCI vamp: tests>≡
    subroutine test_sampler_1_write (object, unit, testflag)
        class(test_sampler_1_t), intent(in) :: object

```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
integer :: u
u = given_output_unit (unit)
select case (object%mode)
case (1)
  write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"
case (2)
  write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10"
case (3)
  write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10 * 2 * cos^2 (2 pi y)"
case (4)
  write (u, "(1x,A)") "Test sampler: f(x) = (1 - 3 x^2) theta(x - 1/2)"
end select
end subroutine test_sampler_1_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

(MCI vamp: test sampler 1: TBP)+≡

```

procedure :: evaluate => test_sampler_1_evaluate

```

(MCI vamp: tests)+≡

```

subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
  class(test_sampler_1_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  if (allocated (sampler%x)) deallocate (sampler%x)
  allocate (sampler%x (size (x_in)))
  sampler%x = x_in
  select case (sampler%mode)
  case (1)
    sampler%val = 3 * x_in(1) ** 2
  case (2)
    sampler%val = 11 * x_in(1) ** 10
  case (3)
    sampler%val = 11 * x_in(1) ** 10 * 2 * cos (twopi * x_in(2)) ** 2
  case (4)
    if (x_in(1) >= .5_default) then
      sampler%val = 1 - 3 * x_in(1) ** 2
    else
      sampler%val = 0
    end if
  end select
  call sampler%fetch (val, x, f)
end subroutine test_sampler_1_evaluate

```

The point is always valid.

(MCI vamp: test sampler 1: TBP)+≡

```

procedure :: is_valid => test_sampler_1_is_valid

```

```

<MCI vamp: tests>+≡
function test_sampler_1_is_valid (sampler) result (valid)
  class(test_sampler_1_t), intent(in) :: sampler
  logical :: valid
  valid = .true.
end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp: test sampler 1: TBP>+≡
  procedure :: rebuild => test_sampler_1_rebuild
<MCI vamp: tests>+≡
  subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_1_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_1_rebuild

```

Extract the results.

```

<MCI vamp: test sampler 1: TBP>+≡
  procedure :: fetch => test_sampler_1_fetch
<MCI vamp: tests>+≡
  subroutine test_sampler_1_fetch (sampler, val, x, f)
    class(test_sampler_1_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_1_fetch

```

Two-channel, two dimension test sampler

This sampler implements the function

$$f(x, y) = 4 \sin^2(\pi x) \sin^2(\pi y) + 2 \sin^2(\pi v) \quad (21.11)$$

where

$$x = u^v \quad u = xy \quad (21.12)$$

$$y = u^{(1-v)} \quad v = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log xy} \right) \quad (21.13)$$

Each term contributes 1 to the integral. The first term in the function is peaked along a cross aligned to the coordinates x and y , while the second term is peaked along the diagonal $x = y$.

The Jacobian is

$$\frac{\partial(x,y)}{\partial(u,v)} = |\log u| \quad (21.14)$$

```

<MCI vamp: test types>+≡
  type, extends (mci_sampler_t) :: test_sampler_2_t
    real(default), dimension(:,:), allocatable :: x
    real(default), dimension(:), allocatable :: f
    real(default) :: val
  contains
    <MCI vamp: test sampler 2: TBP>
  end type test_sampler_2_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI vamp: test sampler 2: TBP>≡
  procedure :: write => test_sampler_2_write

<MCI vamp: tests>+≡
  subroutine test_sampler_2_write (object, unit, testflag)
    class(test_sampler_2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Two-channel test sampler 2"
  end subroutine test_sampler_2_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

<MCI vamp: test sampler 2: TBP>+≡
  procedure :: compute => test_sampler_2_compute

<MCI vamp: tests>+≡
  subroutine test_sampler_2_compute (sampler, c, x_in)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default) :: xx, yy, uu, vv
    if (.not. allocated (sampler%x)) &
      allocate (sampler%x (size (x_in), 2))
    if (.not. allocated (sampler%f)) &
      allocate (sampler%f (2))
    select case (c)
    case (1)
      xx = x_in(1)
      yy = x_in(2)
      uu = xx * yy
      vv = (1 + log (xx/yy) / log (xx*yy)) / 2
    case (2)
      uu = x_in(1)
      vv = x_in(2)
      xx = uu ** vv

```

```

        yy = uu ** (1 - vv)
    end select
    sampler%val = (2 * sin (pi * xx) * sin (pi * yy)) ** 2 &
        + 2 * sin (pi * vv) ** 2
    sampler%f(1) = 1
    sampler%f(2) = abs (log (uu))
    sampler%x(:,1) = [xx, yy]
    sampler%x(:,2) = [uu, vv]
end subroutine test_sampler_2_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: evaluate => test_sampler_2_evaluate

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
        class(test_sampler_2_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        call sampler%fetch (val, x, f)
    end subroutine test_sampler_2_evaluate

```

The point is always valid.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: is_valid => test_sampler_2_is_valid

⟨MCI vamp: tests⟩+≡
    function test_sampler_2_is_valid (sampler) result (valid)
        class(test_sampler_2_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_2_is_valid

```

Rebuild: compute all but the function value.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: rebuild => test_sampler_2_rebuild

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_2_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_2_rebuild

```

```
end subroutine test_sampler_2_rebuild
```

Extract the results.

```
<MCI vamp: test sampler 2: TBP>+=
  procedure :: fetch => test_sampler_2_fetch

<MCI vamp: tests>+=
  subroutine test_sampler_2_fetch (sampler, val, x, f)
    class(test_sampler_2_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x = sampler%x
    f = sampler%f
  end subroutine test_sampler_2_fetch
```

Two-channel, one dimension test sampler

This sampler implements the function

$$f(x, y) = a * 5x^4 + b * 5(1 - x)^4 \quad (21.15)$$

Each term contributes 1 to the integral, multiplied by a or b , respectively. The first term is peaked at $x = 1$, the second one at $x = 0$.

We implement the two mappings

$$x = u^{1/5} \quad \text{and} \quad x = 1 - v^{1/5}, \quad (21.16)$$

with Jacobians

$$\frac{\partial(x)}{\partial(u)} = u^{-4/5}/5 \quad \text{and} \quad v^{-4/5}/5, \quad (21.17)$$

respectively. The first mapping concentrates points near $x = 1$, the second one near $x = 0$.

```
<MCI vamp: test types>+=
  type, extends (mci_sampler_t) :: test_sampler_3_t
    real(default), dimension(:,:), allocatable :: x
    real(default), dimension(:), allocatable :: f
    real(default) :: val
    real(default) :: a = 1
    real(default) :: b = 1
  contains
    <MCI vamp: test sampler 3: TBP>
  end type test_sampler_3_t
```

Output: display a and b

```
<MCI vamp: test sampler 3: TBP>=
  procedure :: write => test_sampler_3_write
```



```

<MCI vamp: tests>+=
subroutine test_sampler_3_write (object, unit, testflag)
  class(test_sampler_3_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Two-channel test sampler 3"
  write (u, "(3x,A,F5.2)") "a = ", object%a
  write (u, "(3x,A,F5.2)") "b = ", object%b
end subroutine test_sampler_3_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

<MCI vamp: test sampler 3: TBP>+=
  procedure :: compute => test_sampler_3_compute

<MCI vamp: tests>+=
subroutine test_sampler_3_compute (sampler, c, x_in)
  class(test_sampler_3_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default) :: u, v, xx
  if (.not. allocated (sampler%x)) &
    allocate (sampler%x (size (x_in), 2))
  if (.not. allocated (sampler%f)) &
    allocate (sampler%f (2))
  select case (c)
  case (1)
    u = x_in(1)
    xx = u ** 0.2_default
    v = (1 - xx) ** 5._default
  case (2)
    v = x_in(1)
    xx = 1 - v ** 0.2_default
    u = xx ** 5._default
  end select
  sampler%val = sampler%a * 5 * xx ** 4 + sampler%b * 5 * (1 - xx) ** 4
  sampler%f(1) = 0.2_default * u ** (-0.8_default)
  sampler%f(2) = 0.2_default * v ** (-0.8_default)
  sampler%x(:,1) = [u]
  sampler%x(:,2) = [v]
end subroutine test_sampler_3_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI vamp: test sampler 3: TBP>+=
  procedure :: evaluate => test_sampler_3_evaluate

<MCI vamp: tests>+=
subroutine test_sampler_3_evaluate (sampler, c, x_in, val, x, f)
  class(test_sampler_3_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(out) :: val

```

```

    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    call sampler%fetch (val, x, f)
end subroutine test_sampler_3_evaluate

```

The point is always valid.

```

⟨MCI vamp: test sampler 3: TBP⟩+≡
    procedure :: is_valid => test_sampler_3_is_valid

⟨MCI vamp: tests⟩+≡
    function test_sampler_3_is_valid (sampler) result (valid)
        class(test_sampler_3_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_3_is_valid

```

Rebuild: compute all but the function value.

```

⟨MCI vamp: test sampler 3: TBP⟩+≡
    procedure :: rebuild => test_sampler_3_rebuild

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_3_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_3_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_3_rebuild

```

Extract the results.

```

⟨MCI vamp: test sampler 3: TBP⟩+≡
    procedure :: fetch => test_sampler_3_fetch

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_3_fetch (sampler, val, x, f)
        class(test_sampler_3_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_3_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

Note: We would like to check the precise contents of the grid allocated during integration, but the output format for reals is very long (for good reasons), so the last digits in the grid content display are numerical noise. So, we just check the integration results.

```

<MCI vamp: execute tests>≡
  call test (mci_vamp_1, "mci_vamp_1", &
    "one-dimensional integral", &
    u, results)

<MCI vamp: test declarations>≡
  public :: mci_vamp_1

<MCI vamp: tests>+≡
  subroutine mci_vamp_1 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_1"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(single channel)"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 1)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize instance"
    write (u, "(A)")

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    write (u, "(A)")  "* Initialize test sampler"
    write (u, "(A)")

    allocate (test_sampler_1_t :: sampler)
    call sampler%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "  (lower precision to avoid"
write (u, "(A)")  "    numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 1, 1000, pacify = .true.)
call mci%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_1"

end subroutine mci_vamp_1

```

Multiple iterations

Construct an integrator and use it for a one-dimensional sampler. Integrate with five iterations without grid adaptation.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_2, "mci_vamp_2", &
    "multiple iterations", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_2

<MCI vamp: tests>+≡
  subroutine mci_vamp_2 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_2"

```

```

write (u, "(A)")  "* Purpose: integrate function in one dimension &
                  &(single channel)"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 1)
select type (mci)
type is (mci_vamp_t)
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .false.)
end select
call mci%integrate (mci_instance, sampler, 3, 100)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_2"

```

```
end subroutine mci_vamp_2
```

Grid adaptation

Construct an integrator and use it for a one-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_3, "mci_vamp_3", &
    "grid adaptation", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_3

<MCI vamp: tests>+≡
  subroutine mci_vamp_3 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_3"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(single channel)"
    write (u, "(A)")  "*           and adapt grid"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 1)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_1_t :: sampler)
    select type (sampler)
    type is (test_sampler_1_t)
      sampler%mode = 2
    end select

```

```

call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 100)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_3"

end subroutine mci_vamp_3

```

Two-dimensional integral

Construct an integrator and use it for a two-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_4, "mci_vamp_4", &
    "two-dimensional integration", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_4

<MCI vamp: tests>+≡
  subroutine mci_vamp_4 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_4"
    write (u, "(A)")  "* Purpose: integrate function in two dimensions &

```

```

        &(single channel)"
write (u, "(A)")  "*"                and adapt grid"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 1)
select type (mci)
type is (mci_vamp_t)
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 3
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_4"

```



```
end subroutine mci_vamp_4
```

Two-channel integral

Construct an integrator and use it for a two-dimensional sampler with two channels.

Integrate with three iterations and in-between grid adaptations.

```
<MCI vamp: execute tests>+≡
  call test (mci_vamp_5, "mci_vamp_5", &
    "two-dimensional integration", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_5

<MCI vamp: tests>+≡
  subroutine mci_vamp_5 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_5"
    write (u, "(A)")  "* Purpose: integrate function in two dimensions &
      &(two channels)"
    write (u, "(A)")  "*           and adapt grid"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_2_t :: sampler)
    call sampler%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_5"

end subroutine mci_vamp_5

```

Weight adaptation

Construct an integrator and use it for a one-dimensional sampler with two channels.

Integrate with three iterations and in-between weight adaptations.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_6, "mci_vamp_6", &
    "weight adaptation", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_6

<MCI vamp: tests>+≡
  subroutine mci_vamp_6 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_6"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(two channels)"

```

```

write (u, "(A)")  "*"                and adapt weights"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_3_t :: sampler)
select type (sampler)
type is (test_sampler_3_t)
    sampler%a = 0.9_default
    sampler%b = 0.1_default
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()
deallocate (mci_instance)
deallocate (mci)

```

```

write (u, "(A)")
write (u, "(A)")  "* Re-initialize with chained channels"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
call mci%declare_chains ([1,1])
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_6"

end subroutine mci_vamp_6

```

Equivalences

Construct an integrator and use it for a one-dimensional sampler with two channels.

Integrate with three iterations and in-between grid adaptations. Apply an equivalence between the two channels, so the binning of the two channels is forced to coincide. Compare this with the behavior without equivalences.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_7, "mci_vamp_7", &
    "use channel equivalences", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_7

<MCI vamp: tests>+≡
  subroutine mci_vamp_7 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    type(phs_channel_t), dimension(:), allocatable :: channel
    class(rng_t), allocatable :: rng
    real(default), dimension(:,:), allocatable :: x
    integer :: u_grid, iostat, i, div, ch
    character(16) :: buffer

    write (u, "(A)")  "* Test output: mci_vamp_7"
    write (u, "(A)")  "* Purpose: check effect of channel equivalences"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_3_t :: sampler)
    select type (sampler)
    type is (test_sampler_3_t)
      sampler%a = 0.7_default
      sampler%b = 0.3_default
    end select
    call sampler%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 2 and n_calls = 1000, &
    &adapt grids"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 2, 1000)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write grids and extract binning"
write (u, "(A)")

u_grid = free_unit ()
open (u_grid, status = "scratch", action = "readwrite")
select type (mci_instance)
type is (mci_vamp_instance_t)
    call vamp_write_grids (mci_instance%grids, u_grid)
end select
rewind (u_grid)
allocate (x (0:20, 2))
do div = 1, 2
    FIND_BINS1: do
        read (u_grid, "(A)")  buffer
        if (trim (adjustl (buffer)) == "begin d%x") then
            do
                read (u_grid, *, iostat = iostat)  i, x(i,div)
                if (iostat /= 0)  exit FIND_BINS1
            end do
        end if
    end do FIND_BINS1
end do
close (u_grid)

write (u, "(1x,A,L1)")  "Equal binning in both channels = ", &
    all (x(:,1) == x(:,2))
deallocate (x)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()
deallocate (mci_instance)
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Re-initialize integrator, instance"
write (u, "(A)")

```

```

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .true.
    call mci%set_grid_parameters (grid_par)
end select

write (u, "(A)")  "* Define equivalences"
write (u, "(A)")

allocate (channel (2))
do ch = 1, 2
    allocate (channel(ch)%eq (2))
    do i = 1, 2
        associate (eq => channel(ch)%eq(i))
            call eq%init (1)
            eq%c = i
            eq%perm = [1]
            eq%mode = [0]
        end associate
    end do
    write (u, "(1x,I0,':')", advance = "no")  ch
    call channel(ch)%write (u)
end do
call mci%declare_equivalences (channel, dim_offset = 0)

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 2 and n_calls = 1000, &
    &adapt grids"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 2, 1000)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write grids and extract binning"
write (u, "(A)")

u_grid = free_unit ()
open (u_grid, status = "scratch", action = "readwrite")

```

```

select type (mci_instance)
type is (mci_vamp_instance_t)
  call vamp_write_grids (mci_instance%grids, u_grid)
end select
rewind (u_grid)
allocate (x (0:20, 2))
do div = 1, 2
  FIND_BINS2: do
    read (u_grid, "(A)") buffer
    if (trim (adjustl (buffer)) == "begin d%x") then
      do
        read (u_grid, *, iostat = iostat) i, x(i,div)
        if (iostat /= 0) exit FIND_BINS2
      end do
    end if
  end do FIND_BINS2
end do
close (u_grid)

write (u, "(1x,A,L1)") "Equal binning in both channels = ", &
  all (x(:,1) == x(:,2))
deallocate (x)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_7"

end subroutine mci_vamp_7

```

Multiple passes

Integrate with three passes and different settings for weight and grid adaptation.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_8, "mci_vamp_8", &
    "integration passes", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_8

<MCI vamp: tests>+≡
  subroutine mci_vamp_8 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

```



```

write (u, "(A)")  "* Test output: mci_vamp_8"
write (u, "(A)")  "* Purpose: integrate function in one dimension &
                    &(two channels)"
write (u, "(A)")  "*           in three passes"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_3_t :: sampler)
select type (sampler)
type is (test_sampler_3_t)
    sampler%a = 0.9_default
    sampler%b = 0.1_default
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with grid and weight adaptation"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true., adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with grid adaptation"
write (u, "(A)")

```

```

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate without adaptation"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_8"

end subroutine mci_vamp_8

```

Weighted events

Construct an integrator and use it for a two-dimensional sampler with two channels. Integrate and generate a weighted event.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_9, "mci_vamp_9", &
    "weighted event", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_9

```

```

<MCI vamp: tests>+≡
subroutine mci_vamp_9 (u)
  integer, intent(in) :: u
  type(grid_parameters_t) :: grid_par
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng

  write (u, "(A)")  "* Test output: mci_vamp_9"
  write (u, "(A)")  "* Purpose: integrate function in two dimensions &
    &(two channels)"
  write (u, "(A)")  "*           and generate a weighted event"

  write (u, "(A)")
  write (u, "(A)")  "* Initialize integrator, sampler, instance"
  write (u, "(A)")

  allocate (mci_vamp_t :: mci)
  call mci%set_dimensions (2, 2)
  select type (mci)
  type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
  end select

  allocate (rng_tao_t :: rng)
  call rng%init ()
  call mci%import_rng (rng)

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  allocate (test_sampler_2_t :: sampler)
  call sampler%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
  write (u, "(A)")

  call mci%add_pass ()
  call mci%integrate (mci_instance, sampler, 1, 1000)
  call mci%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Generate a weighted event"
  write (u, "(A)")

  call mci_instance%init_simulation ()
  call mci%generate_weighted_event (mci_instance, sampler)

  write (u, "(1x,A)")  "MCI instance:"
  call mci_instance%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_9"

end subroutine mci_vamp_9

```

Grids I/O

Construct an integrator and allocate grids. Write grids to file, read them in again and compare.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_10, "mci_vamp_10", &
    "grids I/O", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_10

<MCI vamp: tests>+≡
  subroutine mci_vamp_10 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng
    type(string_t) :: file1, file2
    character(80) :: buffer1, buffer2
    integer :: u1, u2, iostat1, iostat2
    logical :: equal, success

    write (u, "(A)")  "* Test output: mci_vamp_10"
    write (u, "(A)")  "* Purpose: write and read VAMP grids"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

```

```

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

mci%md5sum = "1234567890abcdef1234567890abcdef"

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)

write (u, "(A)")  "* Write grids to file"
write (u, "(A)")

file1 = "mci_vamp_10.1"
select type (mci)
type is (mci_vamp_t)
    call mci%set_grid_filename (file1)
    call mci%write_grids (mci_instance)
end select

call mci_instance%final ()
call mci%final ()
deallocate (mci)

write (u, "(A)")  "* Read grids from file"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

mci%md5sum = "1234567890abcdef1234567890abcdef"

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

select type (mci)

```

```

type is (mci_vamp_t)
  call mci%set_grid_filename (file1)
  call mci%add_pass ()
  call mci%current_pass%configure (1, 1000, &
    mci%min_calls, &
    mci%grid_par%min_bins, mci%grid_par%max_bins, &
    mci%grid_par%min_calls_per_channel * mci%n_channel)
  call mci%read_grids_header (success)
  call mci%compute_md5sum ()
  call mci%read_grids_data (mci_instance, read_integrals = .true.)
end select
write (u, "(1x,A,L1)") "success = ", success

write (u, "(A)")
write (u, "(A)")  "* Write grids again"
write (u, "(A)")

file2 = "mci_vamp_10.2"
select type (mci)
type is (mci_vamp_t)
  call mci%set_grid_filename (file2)
  call mci%write_grids (mci_instance)
end select

u1 = free_unit ()
open (u1, file = char (file1) // ".vg", action = "read", status = "old")
u2 = free_unit ()
open (u2, file = char (file2) // ".vg", action = "read", status = "old")

equal = .true.
iostat1 = 0
iostat2 = 0
do while (equal .and. iostat1 == 0 .and. iostat2 == 0)
  read (u1, "(A)", iostat = iostat1) buffer1
  read (u2, "(A)", iostat = iostat2) buffer2
  equal = buffer1 == buffer2 .and. iostat1 == iostat2
end do
close (u1)
close (u2)

if (equal) then
  write (u, "(1x,A)") "Success: grid files are identical"
else
  write (u, "(1x,A)") "Failure: grid files differ"
end if

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_10"

```

```
end subroutine mci_vamp_10
```

Weighted events with grid I/O

Construct an integrator and use it for a two-dimensional sampler with two channels. Integrate, write grids, and generate a weighted event using the grids from file.

```
<MCI vamp: execute tests>+≡
  call test (mci_vamp_11, "mci_vamp_11", &
    "weighted events with grid I/O", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_11

<MCI vamp: tests>+≡
  subroutine mci_vamp_11 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_11"
    write (u, "(A)")  "* Purpose: integrate function in two dimensions &
      &(two channels)"
    write (u, "(A)")  "*           and generate a weighted event"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
      call mci%set_grid_filename (var_str ("mci_vamp_11"))
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_2_t :: sampler)
```

```

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)

write (u, "(A)")  "* Reset instance"
write (u, "(A)")

call mci_instance%final ()
call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Generate a weighted event"
write (u, "(A)")

call mci_instance%init_simulation ()
call mci%generate_weighted_event (mci_instance, sampler)

write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_11"

end subroutine mci_vamp_11

```

Unweighted events with grid I/O

Construct an integrator and use it for a two-dimensional sampler with two channels.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_12, "mci_vamp_12", &
    "unweighted events with grid I/O", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_12

<MCI vamp: tests>+≡
  subroutine mci_vamp_12 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_12"
    write (u, "(A)")  "* Purpose: integrate function in two dimensions &

```



```

        &(two channels)"
write (u, "(A)")  "*"                and generate an unweighted event"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
    call mci%set_grid_filename (var_str ("mci_vamp_12"))
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)

write (u, "(A)")  "* Reset instance"
write (u, "(A)")

call mci_instance%final ()
call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Generate an unweighted event"
write (u, "(A)")

call mci_instance%init_simulation ()
call mci%generate_unweighted_event (mci_instance, sampler)

write (u, "(1x,A)")  "MCI instance:"
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_12"

end subroutine mci_vamp_12

```

Update integration results

Compare two mci objects; match the two and update the first if successful.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_13, "mci_vamp_13", &
    "updating integration results", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_13

<MCI vamp: tests>+≡
  subroutine mci_vamp_13 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci, mci_ref
    logical :: success

    write (u, "(A)")  "* Test output: mci_vamp_13"
    write (u, "(A)")  "* Purpose: match and update integrators"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator with no passes"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select
    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize reference"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci_ref)
    call mci_ref%set_dimensions (2, 2)
    select type (mci_ref)
    type is (mci_vamp_t)
      call mci_ref%set_grid_parameters (grid_par)
    end select

    select type (mci_ref)
    type is (mci_vamp_t)

```

```

call mci_ref%add_pass (adapt_grids = .true.)
call mci_ref%current_pass%configure (2, 1000, 0, 1, 5, 0)
mci_ref%current_pass%calls = [77, 77]
mci_ref%current_pass%integral = [1.23_default, 3.45_default]
mci_ref%current_pass%error = [0.23_default, 0.45_default]
mci_ref%current_pass%efficiency = [0.1_default, 0.6_default]
mci_ref%current_pass%integral_defined = .true.

call mci_ref%add_pass ()
call mci_ref%current_pass%configure (2, 2000, 0, 1, 7, 0)
mci_ref%current_pass%calls = [99, 0]
mci_ref%current_pass%integral = [7.89_default, 0._default]
mci_ref%current_pass%error = [0.89_default, 0._default]
mci_ref%current_pass%efficiency = [0.86_default, 0._default]
mci_ref%current_pass%integral_defined = .true.
end select

call mci_ref%write (u)

write (u, "(A)")
write (u, "(A)")  "* Update integrator (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)")  "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add pass to integrator"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_grids = .true.)
  call mci%current_pass%configure (2, 1000, 0, 1, 5, 0)
  mci%current_pass%calls = [77, 77]
  mci%current_pass%integral = [1.23_default, 3.45_default]
  mci%current_pass%error = [0.23_default, 0.45_default]
  mci%current_pass%efficiency = [0.1_default, 0.6_default]
  mci%current_pass%integral_defined = .true.
end select

write (u, "(A)")  "* Update integrator (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

```

```

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add pass to integrator, wrong parameters"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass ()
  call mci%current_pass%configure (2, 1000, 0, 1, 7, 0)
end select

write (u, "(A)")  "* Update integrator (should fail)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Reset and add passes to integrator"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%reset ()
  call mci%add_pass (adapt_grids = .true.)
  call mci%current_pass%configure (2, 1000, 0, 1, 5, 0)
  mci%current_pass%calls = [77, 77]
  mci%current_pass%integral = [1.23_default, 3.45_default]
  mci%current_pass%error = [0.23_default, 0.45_default]
  mci%current_pass%efficiency = [0.1_default, 0.6_default]
  mci%current_pass%integral_defined = .true.

  call mci%add_pass ()
  call mci%current_pass%configure (2, 2000, 0, 1, 7, 0)
end select

write (u, "(A)")  "* Update integrator (should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

```

```

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Update again (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add extra result to integrator"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  mci%current_pass%calls(2) = 1234
end select

write (u, "(A)")  "* Update integrator (should fail)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci%final ()
call mci_ref%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_13"

end subroutine mci_vamp_13

```

Accuracy Goal

Integrate with multiple iterations. Skip iterations once an accuracy goal has been reached.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_14, "mci_vamp_14", &
        "accuracy goal", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_14

<MCI vamp: tests>+≡
    subroutine mci_vamp_14 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_vamp_14"
        write (u, "(A)")  "* Purpose: integrate function in one dimension &
            &(single channel)"
        write (u, "(A)")  "*               and check accuracy goal"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator, sampler, instance"
        write (u, "(A)")

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (1, 1)
        select type (mci)
        type is (mci_vamp_t)
            grid_par%use_vamp_equivalences = .false.
            grid_par%accuracy_goal = 5E-2_default
            call mci%set_grid_parameters (grid_par)
        end select

        allocate (rng_tao_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        allocate (test_sampler_1_t :: sampler)
        select type (sampler)
        type is (test_sampler_1_t)
            sampler%mode = 2
        end select
        call sampler%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Integrate with n_it = 5 and n_calls = 100"
        write (u, "(A)")

        select type (mci)
        type is (mci_vamp_t)

```

```

        call mci%add_pass (adapt_grids = .true.)
    end select
    call mci%integrate (mci_instance, sampler, 5, 100)
    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call mci_instance%final ()
    call mci%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: mci_vamp_14"

end subroutine mci_vamp_14

```

VAMP history

Integrate with three passes and different settings for weight and grid adaptation. Then show the VAMP history.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_15, "mci_vamp_15", &
        "VAMP history", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_15

<MCI vamp: tests>+≡
    subroutine mci_vamp_15 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        type(history_parameters_t) :: history_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_vamp_15"
        write (u, "(A)")  "*   Purpose: integrate function in one dimension &
            &(two channels)"
        write (u, "(A)")  "*               in three passes, show history"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator, sampler, instance"
        write (u, "(A)")

        history_par%channel = .true.

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (1, 2)
        select type (mci)
        type is (mci_vamp_t)

```

```

        grid_par%stratified = .false.
        grid_par%use_vamp_equivalences = .false.
        call mci%set_grid_parameters (grid_par)
        call mci%set_history_parameters (history_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

    allocate (test_sampler_3_t :: sampler)
    select type (sampler)
    type is (test_sampler_3_t)
        sampler%a = 0.9_default
        sampler%b = 0.1_default
    end select
    call sampler%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Pass 1: grid and weight adaptation"

    select type (mci)
    type is (mci_vamp_t)
        call mci%add_pass (adapt_grids = .true., adapt_weights = .true.)
    end select
    call mci%integrate (mci_instance, sampler, 3, 1000)

    write (u, "(A)")
    write (u, "(A)")  "* Pass 2: grid adaptation"

    select type (mci)
    type is (mci_vamp_t)
        call mci%add_pass (adapt_grids = .true.)
    end select
    call mci%integrate (mci_instance, sampler, 3, 1000)

    write (u, "(A)")
    write (u, "(A)")  "* Pass 3: without adaptation"

    select type (mci)
    type is (mci_vamp_t)
        call mci%add_pass ()
    end select
    call mci%integrate (mci_instance, sampler, 3, 1000)

    write (u, "(A)")
    write (u, "(A)")  "* Contents of MCI record, with history"
    write (u, "(A)")

    call mci%write (u)
    select type (mci)

```



```

type is (mci_vamp_t)
  call mci%write_history (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_15"

end subroutine mci_vamp_15

```

One-dimensional integration with sign change

Construct an integrator and use it for a one-dimensional sampler.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_16, "mci_vamp_16", &
    "1-D integral with sign change", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_16

<MCI vamp: tests>+≡
  subroutine mci_vamp_16 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_16"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(single channel)"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 1)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
      mci%negative_weights = .true.
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()

```

```

call mci%import_rng (rng)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 4
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "    (lower precision to avoid"
write (u, "(A)")  "        numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 1, 1000, pacify = .true.)
call mci%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_16"

end subroutine mci_vamp_16

```

21.7 Multi-channel integration with VAMP2

The multi-channel integration uses VEGAS as backbone integrator. The base interface for the multi-channel integration is given by `mci_base` module.

We interface the VAMP2 interface given by `vamp2` module.

```
<mci_vamp2.f90>≡  
<File header>  
  
module mci_vamp2  
  
  <Use kinds>  
  <Use strings>  
  use phs_base  
  use rng_base  
  use mci_base  
  use vamp2  
  
  <Standard module head>  
  
  <MCI vamp2: public>  
  
  <MCI vamp2: types>  
  
  <MCI vamp2: interfaces>  
  
    interface  
  <MCI vamp2: sub interfaces>  
    end interface  
  
  contains  
  
  <MCI vamp2: main procedures>  
  
end module mci_vamp2  
  
<mci_vamp2_sub.f90>≡  
<File header>  
  
submodule (mci_vamp2) mci_vamp2_s  
  
  use io_units  
  use format_utils, only: pac_fmt  
  use format_utils, only: write_separator, write_indent  
  use format_defs, only: FMT_12, FMT_14, FMT_17, FMT_19  
  use constants, only: tiny_13  
  use diagnostics  
  use md5  
  use os_interface, only: mpi_get_comm_id  
  use rng_stream, only: rng_stream_t  
  use vegas, only: VEGAS_MODE_IMPORTANCE, VEGAS_MODE_IMPORTANCE_ONLY  
  
  <Use mpi f08>  
  
  implicit none
```

```

contains

<MCI vamp2: procedures>

end submodule mci_vamp2_s

```

21.7.1 Type: mci_vamp2_func_t

```

<MCI vamp2: types>≡
type, extends (vamp2_func_t) :: mci_vamp2_func_t
  private
  real(default) :: integrand = 0._default
  class(mci_sampler_t), pointer :: sampler => null ()
  class(mci_vamp2_instance_t), pointer :: instance => null ()
contains
  <MCI vamp2: mci vamp2 func: TBP>
end type mci_vamp2_func_t

```

Set instance and sampler aka workspace. Also, reset number of n_calls.

```

<MCI vamp2: mci vamp2 func: TBP>≡
  procedure, public :: set_workspace => mci_vamp2_func_set_workspace

<MCI vamp2: sub interfaces>≡
  module subroutine mci_vamp2_func_set_workspace (self, instance, sampler)
    class(mci_vamp2_func_t), intent(inout) :: self
    class(mci_vamp2_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
  end subroutine mci_vamp2_func_set_workspace

<MCI vamp2: procedures>≡
  module subroutine mci_vamp2_func_set_workspace (self, instance, sampler)
    class(mci_vamp2_func_t), intent(inout) :: self
    class(mci_vamp2_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    self%instance => instance
    self%sampler => sampler
  end subroutine mci_vamp2_func_set_workspace

```

Get the different channel probabilities.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: get_probabilities => mci_vamp2_func_get_probabilities

<MCI vamp2: sub interfaces>+≡
  module function mci_vamp2_func_get_probabilities (self) result (gi)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(self%n_channel) :: gi
  end function mci_vamp2_func_get_probabilities

<MCI vamp2: procedures>+≡
  module function mci_vamp2_func_get_probabilities (self) result (gi)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(self%n_channel) :: gi
  end function mci_vamp2_func_get_probabilities

```

```

    gi = self%gi
end function mci_vamp2_func_get_probabilities

```

Get multi-channel weight.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: get_weight => mci_vamp2_func_get_weight

<MCI vamp2: sub interfaces>+≡
  module function mci_vamp2_func_get_weight (self) result (g)
    class(mci_vamp2_func_t), intent(in) :: self
    real(default) :: g
  end function mci_vamp2_func_get_weight

<MCI vamp2: procedures>+≡
  module function mci_vamp2_func_get_weight (self) result (g)
    class(mci_vamp2_func_t), intent(in) :: self
    real(default) :: g
    g = self%g
  end function mci_vamp2_func_get_weight

```

Set integrand.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: set_integrand => mci_vamp2_func_set_integrand

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_func_set_integrand (self, integrand)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), intent(in) :: integrand
  end subroutine mci_vamp2_func_set_integrand

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_func_set_integrand (self, integrand)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), intent(in) :: integrand
    self%integrand = integrand
  end subroutine mci_vamp2_func_set_integrand

```

Evaluate the mappings.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: evaluate_maps => mci_vamp2_func_evaluate_maps

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_func_evaluate_maps (self, x)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
  end subroutine mci_vamp2_func_evaluate_maps

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_func_evaluate_maps (self, x)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    select type (self)
      type is (mci_vamp2_func_t)
        call self%instance%evaluate (self%sampler, self%current_channel, x)
      end select
  end subroutine

```

```

    self%valid_x = self%instance%valid
    self%xi = self%instance%x
    self%det = self%instance%f
end subroutine mci_vamp2_func_evaluate_maps

```

Evaluate the function, more or less.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
    procedure, public :: evaluate_func => mci_vamp2_func_evaluate_func

<MCI vamp2: sub interfaces>+≡
    module function mci_vamp2_func_evaluate_func (self, x) result (f)
        class(mci_vamp2_func_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: f
    end function mci_vamp2_func_evaluate_func

<MCI vamp2: procedures>+≡
    module function mci_vamp2_func_evaluate_func (self, x) result (f)
        class(mci_vamp2_func_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: f
        f = self%integrand
        if (signal_is_pending ()) then
            call msg_message ("VAMP2: function evaluate_func: signal received")
            call terminate_now_if_signal ()
        end if
        call terminate_now_if_single_event ()
    end function mci_vamp2_func_evaluate_func

```

21.7.2 Type: mci_vamp2_config_t

We extend vamp2_config_t.

```

<MCI vamp2: public>≡
    public :: mci_vamp2_config_t

<MCI vamp2: types>+≡
    type, extends (vamp2_config_t) :: mci_vamp2_config_t
    !
end type mci_vamp2_config_t

```

21.7.3 Integration pass

The list of passes is organized in a separate container. We store the parameters and results for each integration pass in `pass_t` and the linked list is stored in `list_pass_t`.

```

<MCI vamp2: types>+≡
    type :: list_pass_t
        type(pass_t), pointer :: first => null ()
        type(pass_t), pointer :: current => null ()
    contains
    <MCI vamp2: list pass: TBP>

```

```
end type list_pass_t
```

Finalizer. Deallocate each element of the list beginning by the first.

```
<MCI vamp2: list pass: TBP>≡
  procedure :: final => list_pass_final

<MCI vamp2: sub interfaces>+≡
  module subroutine list_pass_final (self)
    class(list_pass_t), intent(inout) :: self
  end subroutine list_pass_final

<MCI vamp2: procedures>+≡
  module subroutine list_pass_final (self)
    class(list_pass_t), intent(inout) :: self
    type(pass_t), pointer :: current
    current => self%first
    do while (associated (current))
      self%first => current%next
      deallocate (current)
      current => self%first
    end do
  end subroutine list_pass_final
```

Add a new pass.

```
<MCI vamp2: list pass: TBP>+≡
  procedure :: add => list_pass_add

<MCI vamp2: sub interfaces>+≡
  module subroutine list_pass_add &
    (self, adapt_grids, adapt_weights, final_pass)
    class(list_pass_t), intent(inout) :: self
    logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
  end subroutine list_pass_add

<MCI vamp2: procedures>+≡
  module subroutine list_pass_add &
    (self, adapt_grids, adapt_weights, final_pass)
    class(list_pass_t), intent(inout) :: self
    logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
    type(pass_t), pointer :: new_pass
    allocate (new_pass)
    new_pass%i_pass = 1
    new_pass%i_first_it = 1
    new_pass%adapt_grids = .false.; if (present (adapt_grids)) &
      & new_pass%adapt_grids = adapt_grids
    new_pass%adapt_weights = .false.; if (present (adapt_weights)) &
      & new_pass%adapt_weights = adapt_weights
    new_pass%is_final_pass = .false.; if (present (final_pass)) &
      & new_pass%is_final_pass = final_pass
    if (.not. associated (self%first)) then
      self%first => new_pass
    else
      new_pass%i_pass = new_pass%i_pass + self%current%i_pass
      new_pass%i_first_it = self%current%i_first_it + self%current%n_it
      self%current%next => new_pass
```

```

end if
self%current => new_pass
end subroutine list_pass_add

```

Update list from a reference. All passes except for the last one must match exactly. For the last one, integration results are updated. The reference output may contain extra passes, these are ignored.

```

<MCI vamp2: list pass: TBP>+≡
  procedure :: update_from_ref => list_pass_update_from_ref

<MCI vamp2: sub interfaces>+≡
  module subroutine list_pass_update_from_ref (self, ref, success)
    class(list_pass_t), intent(inout) :: self
    type(list_pass_t), intent(in) :: ref
    logical, intent(out) :: success
  end subroutine list_pass_update_from_ref

<MCI vamp2: procedures>+≡
  module subroutine list_pass_update_from_ref (self, ref, success)
    class(list_pass_t), intent(inout) :: self
    type(list_pass_t), intent(in) :: ref
    logical, intent(out) :: success
    type(pass_t), pointer :: current, ref_current
    current => self%first
    ref_current => ref%first
    success = .true.
    do while (success .and. associated (current))
      if (associated (ref_current)) then
        if (associated (current%next)) then
          success = current .matches. ref_current
        else
          call current%update (ref_current, success)
        end if
        current => current%next
        ref_current => ref_current%next
      else
        success = .false.
      end if
    end do
  end subroutine list_pass_update_from_ref

<MCI vamp2: list pass: TBP>+≡
  procedure :: has_last_integral => list_pass_has_last_integral
  procedure :: get_last_integral => list_pass_get_last_integral

<MCI vamp2: sub interfaces>+≡
  module function list_pass_has_last_integral(self) result (flag)
    class(list_pass_t), intent(in) :: self
    logical :: flag
  end function list_pass_has_last_integral
  module subroutine list_pass_get_last_integral &
    (self, integral, error, efficiency)
    class(list_pass_t), intent(in) :: self
    real(default), intent(out) :: integral
    real(default), intent(out) :: error

```



```

        real(default), intent(out) :: efficiency
    end subroutine list_pass_get_last_integral
<MCI vamp2: procedures>+≡
module function list_pass_has_last_integral(self) result (flag)
    class(list_pass_t), intent(in) :: self
    logical :: flag
    flag = associated(self%current)
    if (flag) flag = self%current%integral_defined
end function list_pass_has_last_integral

module subroutine list_pass_get_last_integral &
    (self, integral, error, efficiency)
    class(list_pass_t), intent(in) :: self
    real(default), intent(out) :: integral
    real(default), intent(out) :: error
    real(default), intent(out) :: efficiency
    if (self%has_last_integral()) then
        integral = self%current%get_integral()
        error = self%current%get_error()
        efficiency = self%current%get_efficiency()
    else
        integral = 0
        error = 0
        efficiency = 0
    end if
end subroutine list_pass_get_last_integral

```

Output. Write the complete linked list to the specified unit.

```

<MCI vamp2: list pass: TBP>+≡
    procedure :: write => list_pass_write
<MCI vamp2: sub interfaces>+≡
    module subroutine list_pass_write (self, unit, pacify)
        class(list_pass_t), intent(in) :: self
        integer, intent(in) :: unit
        logical, intent(in), optional :: pacify
    end subroutine list_pass_write
<MCI vamp2: procedures>+≡
module subroutine list_pass_write (self, unit, pacify)
    class(list_pass_t), intent(in) :: self
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    type(pass_t), pointer :: current
    current => self%first
    do while (associated (current))
        write (unit, "(1X,A)") "Integration pass:"
        call current%write (unit, pacify)
        current => current%next
    end do
end subroutine list_pass_write

```

The parameters and results are stored in the nodes `pass_t` of the linked list.

```

<MCI vamp2: types>+≡

```

```

type :: pass_t
  integer :: i_pass = 0
  integer :: i_first_it = 0
  integer :: n_it = 0
  integer :: n_calls = 0
  logical :: adapt_grids = .false.
  logical :: adapt_weights = .false.
  logical :: is_final_pass = .false.
  logical :: integral_defined = .false.
  integer, dimension(:), allocatable :: calls
  integer, dimension(:), allocatable :: calls_valid
  real(default), dimension(:), allocatable :: integral
  real(default), dimension(:), allocatable :: error
  real(default), dimension(:), allocatable :: efficiency
  type(pass_t), pointer :: next => null ()
contains
  <MCI vamp2: pass: TBP>
end type pass_t

```

Output. Note that the precision of the numerical values should match the precision for comparing output from file with data.

```

<MCI vamp2: pass: TBP>≡
  procedure :: write => pass_write

<MCI vamp2: sub interfaces>+≡
  module subroutine pass_write (self, unit, pacify)
    class(pass_t), intent(in) :: self
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
  end subroutine pass_write

<MCI vamp2: procedures>+≡
  module subroutine pass_write (self, unit, pacify)
    class(pass_t), intent(in) :: self
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    real(default) :: pac_error
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3X,A,I0)") "n_it           = ", self%n_it
    write (u, "(3X,A,I0)") "n_calls        = ", self%n_calls
    write (u, "(3X,A,L1)") "adapt grids   = ", self%adapt_grids
    write (u, "(3X,A,L1)") "adapt weights = ", self%adapt_weights
    if (self%integral_defined) then
      write (u, "(3X,A)") "Results: [it, calls, valid, integral, error, efficiency]"
      do i = 1, self%n_it
        if (abs (self%error(i)) > tiny_13) then
          pac_error = self%error(i)
        else
          pac_error = 0
        end if
        write (u, "(5x,I0,2(1x,I0),3(1x," // fmt // ")") &
          i, self%calls(i), self%calls_valid(i), self%integral(i), &

```

```

        pac_error, self%efficiency(i)
    end do
else
    write (u, "(3x,A)") "Results: [undefined]"
end if
end subroutine pass_write

```

Read and reconstruct the pass.

(MCI vamp2: pass: TBP)+≡

```

    procedure :: read => pass_read

```

(MCI vamp2: sub interfaces)+≡

```

    module subroutine pass_read (self, u, n_pass, n_it)
        class(pass_t), intent(out) :: self
        integer, intent(in) :: u, n_pass, n_it
    end subroutine pass_read

```

(MCI vamp2: procedures)+≡

```

    module subroutine pass_read (self, u, n_pass, n_it)
        class(pass_t), intent(out) :: self
        integer, intent(in) :: u, n_pass, n_it
        integer :: i, j
        character(80) :: buffer
        self%i_pass = n_pass + 1
        self%i_first_it = n_it + 1
        call read_ival (u, self%n_it)
        call read_ival (u, self%n_calls)
        call read_lval (u, self%adapt_grids)
        call read_lval (u, self%adapt_weights)
        allocate (self%calls (self%n_it), source = 0)
        allocate (self%calls_valid (self%n_it), source = 0)
        allocate (self%integral (self%n_it), source = 0._default)
        allocate (self%error (self%n_it), source = 0._default)
        allocate (self%efficiency (self%n_it), source = 0._default)
        read (u, "(A)") buffer
        select case (trim (adjustl (buffer)))
        case ("Results: [it, calls, valid, integral, error, efficiency]")
            do i = 1, self%n_it
                read (u, *) &
                    j, self%calls(i), self%calls_valid(i), self%integral(i), self%error(i), &
                    self%efficiency(i)
            end do
            self%integral_defined = .true.
        case ("Results: [undefined]")
            self%integral_defined = .false.
        case default
            call msg_fatal ("Reading integration pass: corrupted file")
        end select
    end subroutine pass_read

```

Auxiliary: Read real, integer, string value. We search for an equals sign, the value must follow.

(MCI vamp2: procedures)+≡

```

    subroutine read_rval (u, rval)

```

```

integer, intent(in) :: u
real(default), intent(out) :: rval
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) rval
end subroutine read_rval

subroutine read_ival (u, ival)
integer, intent(in) :: u
integer, intent(out) :: ival
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) ival
end subroutine read_ival

subroutine read_sval (u, sval)
integer, intent(in) :: u
character(*), intent(out) :: sval
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) sval
end subroutine read_sval

subroutine read_lval (u, lval)
integer, intent(in) :: u
logical, intent(out) :: lval
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) lval
end subroutine read_lval

```

Configure. We adjust the number of `n_calls`, if it is lower than `n_calls_min_per_channel` times `b_channel`, and print a warning message.

<MCI vamp2: pass: TBP>+≡

```
procedure :: configure => pass_configure
```

<MCI vamp2: sub interfaces>+≡

```

module subroutine pass_configure (pass, n_it, n_calls, n_calls_min)
class(pass_t), intent(inout) :: pass
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
integer, intent(in) :: n_calls_min
end subroutine pass_configure

```

<MCI vamp2: procedures>+≡

```

module subroutine pass_configure (pass, n_it, n_calls, n_calls_min)
class(pass_t), intent(inout) :: pass
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
integer, intent(in) :: n_calls_min
pass%n_it = n_it

```

```

pass%n_calls = max (n_calls, n_calls_min)
if (pass%n_calls /= n_calls) then
    write (msg_buffer, "(A,I0)") "VAMP2: too few calls, resetting " &
        // "n_calls to ", pass%n_calls
    call msg_warning ()
end if
allocate (pass%calls (n_it), source = 0)
allocate (pass%calls_valid (n_it), source = 0)
allocate (pass%integral (n_it), source = 0._default)
allocate (pass%error (n_it), source = 0._default)
allocate (pass%efficiency (n_it), source = 0._default)
end subroutine pass_configure

```

Given two pass objects, compare them. All parameters must match. Where integrations are done in both (number of calls nonzero), the results must be equal (up to numerical noise).

The allocated array sizes might be different, but should match up to the common `n_it` value.

```

<MCI vamp2: interfaces>≡
interface operator (.matches.)
    module procedure pass_matches
end interface operator (.matches.)

<MCI vamp2: sub interfaces>+≡
module function pass_matches (pass, ref) result (ok)
    type(pass_t), intent(in) :: pass, ref
    logical :: ok
end function pass_matches

<MCI vamp2: procedures>+≡
module function pass_matches (pass, ref) result (ok)
    type(pass_t), intent(in) :: pass, ref
    integer :: n
    logical :: ok
    ok = .true.
    if (ok) ok = pass%i_pass == ref%i_pass
    if (ok) ok = pass%i_first_it == ref%i_first_it
    if (ok) ok = pass%n_it == ref%n_it
    if (ok) ok = pass%n_calls == ref%n_calls
    if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
    if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
    if (ok) ok = pass%integral_defined .eqv. ref%integral_defined
    if (pass%integral_defined) then
        n = pass%n_it
        if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
        if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
        if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
        if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
        if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
    end if
end function pass_matches

```

Update a pass object, given a reference. The parameters must match, except for the `n_it` entry. The number of complete iterations must be less or equal to

the reference, and the number of complete iterations in the reference must be no larger than `n_it`. Where results are present in both passes, they must match. Where results are present in the reference only, the pass is updated accordingly.

```

(MCI vamp2: pass: TBP)+≡
    procedure :: update => pass_update

(MCI vamp2: sub interfaces)+≡
    module subroutine pass_update (pass, ref, ok)
        class(pass_t), intent(inout) :: pass
        type(pass_t), intent(in) :: ref
        logical, intent(out) :: ok
    end subroutine pass_update

(MCI vamp2: procedures)+≡
    module subroutine pass_update (pass, ref, ok)
        class(pass_t), intent(inout) :: pass
        type(pass_t), intent(in) :: ref
        logical, intent(out) :: ok
        integer :: n, n_ref
        ok = .true.
        if (ok) ok = pass%i_pass == ref%i_pass
        if (ok) ok = pass%i_first_it == ref%i_first_it
        if (ok) ok = pass%n_calls == ref%n_calls
        if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
        if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
        if (ok) then
            if (ref%integral_defined) then
                if (.not. allocated (pass%calls)) then
                    allocate (pass%calls (pass%n_it), source = 0)
                    allocate (pass%calls_valid (pass%n_it), source = 0)
                    allocate (pass%integral (pass%n_it), source = 0._default)
                    allocate (pass%error (pass%n_it), source = 0._default)
                    allocate (pass%efficiency (pass%n_it), source = 0._default)
                end if
                n = count (pass%calls /= 0)
                n_ref = count (ref%calls /= 0)
                ok = n <= n_ref .and. n_ref <= pass%n_it
                if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
                if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
                if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
                if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
                if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
                if (ok) then
                    pass%calls(n+1:n_ref) = ref%calls(n+1:n_ref)
                    pass%calls_valid(n+1:n_ref) = ref%calls_valid(n+1:n_ref)
                    pass%integral(n+1:n_ref) = ref%integral(n+1:n_ref)
                    pass%error(n+1:n_ref) = ref%error(n+1:n_ref)
                    pass%efficiency(n+1:n_ref) = ref%efficiency(n+1:n_ref)
                    pass%integral_defined = any (pass%calls /= 0)
                end if
            end if
        end if
    end subroutine pass_update

```

Match two real numbers: they are equal up to a tolerance, which is 10^{-8} , matching the number of digits that are output by `pass_write`. In particular, if one number is exactly zero, the other one must also be zero.

```

(MCI vamp2: interfaces)+≡
  interface operator (.matches.)
    module procedure real_matches
  end interface operator (.matches.)

(MCI vamp2: sub interfaces)+≡
  elemental module function real_matches (x, y) result (ok)
    real(default), intent(in) :: x, y
    logical :: ok
  end function real_matches

(MCI vamp2: procedures)+≡
  elemental module function real_matches (x, y) result (ok)
    real(default), intent(in) :: x, y
    logical :: ok
    real(default), parameter :: tolerance = 1.e-8_default
    ok = abs (x - y) <= tolerance * max (abs (x), abs (y))
  end function real_matches

```

Return the index of the most recent complete integration. If there is none, return zero.

```

(MCI vamp2: pass: TBP)+≡
  procedure :: get_integration_index => pass_get_integration_index

(MCI vamp2: sub interfaces)+≡
  module function pass_get_integration_index (pass) result (n)
    class (pass_t), intent(in) :: pass
    integer :: n
  end function pass_get_integration_index

(MCI vamp2: procedures)+≡
  module function pass_get_integration_index (pass) result (n)
    class (pass_t), intent(in) :: pass
    integer :: n
    integer :: i
    n = 0
    if (allocated (pass%calls)) then
      do i = 1, pass%n_it
        if (pass%calls(i) == 0) exit
        n = i
      end do
    end if
  end function pass_get_integration_index

```

Return the most recent integral and error, if available.

```

(MCI vamp2: pass: TBP)+≡
  procedure :: get_calls => pass_get_calls
  procedure :: get_calls_valid => pass_get_calls_valid
  procedure :: get_integral => pass_get_integral
  procedure :: get_error => pass_get_error
  procedure :: get_efficiency => pass_get_efficiency

```

```

(MCI vamp2: sub interfaces)+≡
  module function pass_get_calls (pass) result (calls)
    class(pass_t), intent(in) :: pass
    integer :: calls
  end function pass_get_calls
  module function pass_get_calls_valid (pass) result (valid)
    class(pass_t), intent(in) :: pass
    integer :: valid
  end function pass_get_calls_valid
  module function pass_get_integral (pass) result (integral)
    class(pass_t), intent(in) :: pass
    real(default) :: integral
  end function pass_get_integral
  module function pass_get_error (pass) result (error)
    class(pass_t), intent(in) :: pass
    real(default) :: error
  end function pass_get_error
  module function pass_get_efficiency (pass) result (efficiency)
    class(pass_t), intent(in) :: pass
    real(default) :: efficiency
  end function pass_get_efficiency

(MCI vamp2: procedures)+≡
  module function pass_get_calls (pass) result (calls)
    class(pass_t), intent(in) :: pass
    integer :: calls
    integer :: n
    n = pass%get_integration_index ()
    calls = 0
    if (n /= 0) then
      calls = pass%calls(n)
    end if
  end function pass_get_calls

  module function pass_get_calls_valid (pass) result (valid)
    class(pass_t), intent(in) :: pass
    integer :: valid
    integer :: n
    n = pass%get_integration_index ()
    valid = 0
    if (n /= 0) then
      valid = pass%calls_valid(n)
    end if
  end function pass_get_calls_valid

  module function pass_get_integral (pass) result (integral)
    class(pass_t), intent(in) :: pass
    real(default) :: integral
    integer :: n
    n = pass%get_integration_index ()
    integral = 0
    if (n /= 0) then
      integral = pass%integral(n)
    end if
  end function pass_get_integral

```



```

module function pass_get_error (pass) result (error)
  class(pass_t), intent(in) :: pass
  real(default) :: error
  integer :: n
  n = pass%get_integration_index ()
  error = 0
  if (n /= 0) then
    error = pass%error(n)
  end if
end function pass_get_error

module function pass_get_efficiency (pass) result (efficiency)
  class(pass_t), intent(in) :: pass
  real(default) :: efficiency
  integer :: n
  n = pass%get_integration_index ()
  efficiency = 0
  if (n /= 0) then
    efficiency = pass%efficiency(n)
  end if
end function pass_get_efficiency

```

21.7.4 Integrator

We store the different passes of integration, adaptation and actual sampling, in a linked list.

We store the total number of calls `n_calls` and the minimal number of calls `n_calls_min`. The latter is calculated based on `n_channel` and `min_calls_per_channel`. If `n_calls` is smaller than `n_calls_min`, then we replace `n_calls` with `n_min_calls`.

```

<MCI vamp2: public>+=
  public :: mci_vamp2_t

<MCI vamp2: types>+=
  type, extends(mci_t) :: mci_vamp2_t
    type(mci_vamp2_config_t) :: config
    type(vamp2_t) :: integrator
    type(vamp2_equivalences_t) :: equivalences
    logical :: integrator_defined = .false.
    logical :: integrator_from_file = .false.
    logical :: adapt_grids = .false.
    logical :: adapt_weights = .false.
    integer :: n_adapt_grids = 0
    integer :: n_adapt_weights = 0
    integer :: n_calls = 0
    type(list_pass_t) :: list_pass
    logical :: rebuild = .true.
    logical :: check_grid_file = .true.
    logical :: grid_filename_set = .false.
    logical :: negative_weights = .false.
    logical :: verbose = .false.
    logical :: pass_complete = .false.

```

```

        logical :: it_complete = .false.
        type(string_t) :: grid_filename
        integer :: grid_checkpoint = 1
        logical :: binary_grid_format = .false.
        type(string_t) :: parallel_method
        character(32) :: md5sum_adapted = ""
contains
    <MCI vamp2: mci vamp2: TBP>
end type mci_vamp2_t

```

Finalizer: call to base and list finalizer.

```

<MCI vamp2: mci vamp2: TBP>≡
    procedure, public :: final => mci_vamp2_final

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_final (object)
        class(mci_vamp2_t), intent(inout) :: object
    end subroutine mci_vamp2_final

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_final (object)
        class(mci_vamp2_t), intent(inout) :: object
        call object%list_pass%final ()
        call object%base_final ()
    end subroutine mci_vamp2_final

```

Output. Do not output the grids themselves, this may result in tons of data.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: write => mci_vamp2_write

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_write (object, unit, pacify, md5sum_version)
        class(mci_vamp2_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
    end subroutine mci_vamp2_write

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_write (object, unit, pacify, md5sum_version)
        class(mci_vamp2_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1X,A)") "VAMP2 integrator:"
        call object%base_write (u, pacify, md5sum_version)
        write (u, "(1X,A)") "Grid config:"
        call object%config%write (u)
        write (u, "(3X,A,L1)") "Integrator defined      = ", object%integrator_defined
        write (u, "(3X,A,L1)") "Integrator from file = ", object%integrator_from_file
        write (u, "(3X,A,L1)") "Adapt grids          = ", object%adapt_grids
        write (u, "(3X,A,L1)") "Adapt weights        = ", object%adapt_weights
        write (u, "(3X,A,I0)") "No. of adapt grids   = ", object%n_adapt_grids

```

```

write (u, "(3X,A,I0)") "No. of adapt weights = ", object%n_adapt_weights
write (u, "(3X,A,L1)") "Verbose           = ", object%verbose
if (object%config%equivalences) then
  call object%equivalences%write (u)
end if
call object%list_pass%write (u, pacify)
if (object%md5sum_adapted /= "") then
  write (u, "(1X,A,A,A)") "MD5 sum (including results) = ', &
    & object%md5sum_adapted, "'"
end if
end subroutine mci_vamp2_write

```

Compute the (adapted) MD5 sum, including the configuration MD5 sum and the printout, which incorporates the current results.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: compute_md5sum => mci_vamp2_compute_md5sum

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_compute_md5sum (mci, pacify)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
  end subroutine mci_vamp2_compute_md5sum

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_compute_md5sum (mci, pacify)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
    integer :: u
    mci%md5sum_adapted = ""
    u = free_unit ()
    open (u, status = "scratch", action = "readwrite")
    write (u, "(A)") mci%md5sum
    call mci%write (u, pacify, md5sum_version = .true.)
    rewind (u)
    mci%md5sum_adapted = md5sum (u)
    close (u)
  end subroutine mci_vamp2_compute_md5sum

```

Return the MD5 sum: If available, return the adapted one.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: get_md5sum => mci_vamp2_get_md5sum

<MCI vamp2: sub interfaces>+≡
  pure module function mci_vamp2_get_md5sum (mci) result (md5sum)
    class(mci_vamp2_t), intent(in) :: mci
    character(32) :: md5sum
  end function mci_vamp2_get_md5sum

<MCI vamp2: procedures>+≡
  pure module function mci_vamp2_get_md5sum (mci) result (md5sum)
    class(mci_vamp2_t), intent(in) :: mci
    character(32) :: md5sum
    if (mci%md5sum_adapted /= "") then
      md5sum = mci%md5sum_adapted
    else

```

```

        md5sum = mci%md5sum
    end if
end function mci_vamp2_get_md5sum

```

Startup message: short version. Make a call to the base function and print additional information about the multi-channel parameters.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: startup_message => mci_vamp2_startup_message

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_startup_message (mci, unit, n_calls)
        class(mci_vamp2_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
    end subroutine mci_vamp2_startup_message

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_startup_message (mci, unit, n_calls)
        class(mci_vamp2_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
        integer :: num_calls, n_bins
        num_calls = 0; if (present (n_calls)) num_calls = n_calls
        n_bins = mci%config%n_bins_max
        call mci%base_startup_message (unit = unit, n_calls = n_calls)
        if (mci%config%equivalences) then
            write (msg_buffer, "(A)") &
                "Integrator: Using VAMP2 channel equivalences"
            call msg_message (unit = unit)
        end if
        if (mci%binary_grid_format) then
            write (msg_buffer, "(A,A,A,A)") &
                "Integrator: Write grid header to '" // char (mci%get_grid_filename ()) // &
                "' and grids to '" // char (mci%get_grid_filename (binary_grid_format = .true.)) // "
        else
            write (msg_buffer, "(A,A,A)") &
                "Integrator: Write grid header and grids to '" // char (mci%get_grid_filename ()) // "
        end if
        call msg_message (unit = unit)
        select case (mci%grid_checkpoint)
        case (0)
            write (msg_buffer, "(A)") &
                "Integrator: Grid checkpoint after each pass"
        case (1)
            write (msg_buffer, "(A)") &
                "Integrator: Grid checkpoint after each iteration"
        case (2:)
            write (msg_buffer, "(A,1X,I0,1X,A)") &
                "Integrator: Grid checkpoint after", mci%grid_checkpoint, &
                "iterations and after each pass"
        case default
            call msg_bug ("Integrator: Cannot assign grid checkpoint (value is negative).")
        end select
        call msg_message (unit = unit)
        write (msg_buffer, "(A,2(1x,I0,1x,A),L1)") &
            "Integrator:", num_calls, &
            "initial calls,", n_bins, &

```

```

        "max. bins, stratified = ", &
        mci%config%stratified
    call msg_message (unit = unit)
    write (msg_buffer, "(A,2(1x,I0,1x,A))") &
        "Integrator: VAMP2"
    call msg_message (unit = unit)
end subroutine mci_vamp2_startup_message

```

Log entry: just headline.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: write_log_entry => mci_vamp2_write_log_entry

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_write_log_entry (mci, u)
        class(mci_vamp2_t), intent(in) :: mci
        integer, intent(in) :: u
    end subroutine mci_vamp2_write_log_entry

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_write_log_entry (mci, u)
        class(mci_vamp2_t), intent(in) :: mci
        integer, intent(in) :: u
        write (u, "(1x,A)") "MC Integrator is VAMP2"
        call write_separator (u)
        if (mci%config%equivalences) then
            call mci%equivalences%write (u)
        else
            write (u, "(3x,A)") "No channel equivalences have been used."
        end if
        call write_separator (u)
        call mci%write_chain_weights (u)
    end subroutine mci_vamp2_write_log_entry

```

Set the MCI index (necessary for processes with multiple components). We append the index to the grid filename, just before the final dotted suffix.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: record_index => mci_vamp2_record_index

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_record_index (mci, i_mci)
        class(mci_vamp2_t), intent(inout) :: mci
        integer, intent(in) :: i_mci
    end subroutine mci_vamp2_record_index

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_record_index (mci, i_mci)
        class(mci_vamp2_t), intent(inout) :: mci
        integer, intent(in) :: i_mci
        type(string_t) :: basename, suffix
        character(32) :: buffer
        if (mci%grid_filename_set) then
            write (buffer, "(I0)") i_mci
            mci%grid_filename = mci%grid_filename // ".m" // trim (buffer)
        end if
    end subroutine mci_vamp2_record_index

```

Set the configuration object. We adjust the maximum number of bins `n_bins_max` according to `n_calls`

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: set_config => mci_vamp2_set_config

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_set_config (mci, config)
    class(mci_vamp2_t), intent(inout) :: mci
    type(mci_vamp2_config_t), intent(in) :: config
  end subroutine mci_vamp2_set_config

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_set_config (mci, config)
    class(mci_vamp2_t), intent(inout) :: mci
    type(mci_vamp2_config_t), intent(in) :: config
    mci%config = config
  end subroutine mci_vamp2_set_config

```

Set the the rebuild flag, also the for checking the grid.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: set_rebuild_flag => mci_vamp2_set_rebuild_flag

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_set_rebuild_flag (mci, rebuild, check_grid_file)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(in) :: rebuild
    logical, intent(in) :: check_grid_file
  end subroutine mci_vamp2_set_rebuild_flag

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_set_rebuild_flag (mci, rebuild, check_grid_file)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(in) :: rebuild
    logical, intent(in) :: check_grid_file
    mci%rebuild = rebuild
    mci%check_grid_file = check_grid_file
  end subroutine mci_vamp2_set_rebuild_flag

```

Set the filename.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: set_grid_filename => mci_vamp2_set_grid_filename
  procedure, public :: get_grid_filename => mci_vamp2_get_grid_filename

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_set_grid_filename (mci, name, run_id)
    class(mci_vamp2_t), intent(inout) :: mci
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: run_id
  end subroutine mci_vamp2_set_grid_filename
  module function mci_vamp2_get_grid_filename (mci, binary_grid_format) &
    result (filename)
    class(mci_vamp2_t), intent(in) :: mci
    logical, intent(in), optional :: binary_grid_format
    type(string_t) :: filename
  end function mci_vamp2_get_grid_filename

```

```

<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_set_grid_filename (mci, name, run_id)
  class(mci_vamp2_t), intent(inout) :: mci
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: run_id
  mci%grid_filename = name
  if (present (run_id)) then
    mci%grid_filename = name // "." // run_id
  end if
  mci%grid_filename_set = .true.
end subroutine mci_vamp2_set_grid_filename

module function mci_vamp2_get_grid_filename (mci, binary_grid_format) &
  result (filename)
  class(mci_vamp2_t), intent(in) :: mci
  logical, intent(in), optional :: binary_grid_format
  type(string_t) :: filename
  filename = mci%grid_filename // ".vg2"
  if (present (binary_grid_format)) then
    if (binary_grid_format) then
      filename = mci%grid_filename // ".vgx2"
    end if
  end if
end function mci_vamp2_get_grid_filename

```

To simplify the interface, we prepend a grid path in a separate subroutine.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure :: prepend_grid_path => mci_vamp2_prepend_grid_path

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_prepend_grid_path (mci, prefix)
    class(mci_vamp2_t), intent(inout) :: mci
    type(string_t), intent(in) :: prefix
  end subroutine mci_vamp2_prepend_grid_path

<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_prepend_grid_path (mci, prefix)
  class(mci_vamp2_t), intent(inout) :: mci
  type(string_t), intent(in) :: prefix
  if (.not. mci%grid_filename_set) then
    call msg_warning &
      ("VAMP2: Cannot add prefix to invalid integrator filename!")
  end if
  mci%grid_filename = prefix // "/" // mci%grid_filename
end subroutine mci_vamp2_prepend_grid_path

```

Not implemented.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: declare_flat_dimensions => &
    mci_vamp2_declare_flat_dimensions

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_declare_flat_dimensions (mci, dim_flat)
    class(mci_vamp2_t), intent(inout) :: mci

```

```

        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_vamp2_declare_flat_dimensions

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_declare_flat_dimensions (mci, dim_flat)
        class(mci_vamp2_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_vamp2_declare_flat_dimensions

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: declare_equivalences => mci_vamp2_declare_equivalences

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_declare_equivalences (mci, channel, dim_offset)
        class(mci_vamp2_t), intent(inout) :: mci
        type(phps_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_vamp2_declare_equivalences

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_declare_equivalences (mci, channel, dim_offset)
        class(mci_vamp2_t), intent(inout) :: mci
        type(phps_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
        integer, dimension(:), allocatable :: perm, mode
        integer :: n_channels, n_dim, n_equivalences
        integer :: c, i, j, dest, src
        integer :: n_dim_perm
        n_channels = mci%n_channel
        n_dim = mci%n_dim
        n_equivalences = 0
        do c = 1, n_channels
            n_equivalences = n_equivalences + size (channel(c)%eq)
        end do
        mci%equivalences = vamp2_equivalences_t (&
            n_eqv = n_equivalences, n_channel = n_channels, n_dim = n_dim)
        allocate (perm (n_dim))
        allocate (mode (n_dim))
        perm = [(i, i = 1, n_dim)]
        mode = 0
        c = 1
        j = 0
        do i = 1, n_equivalences
            if (j < size (channel(c)%eq)) then
                j = j + 1
            else
                c = c + 1
                j = 1
            end if
            associate (eq => channel(c)%eq(j))
                dest = c
                src = eq%c
                n_dim_perm = size (eq%perm)
                perm(dim_offset+1:dim_offset+n_dim_perm) = eq%perm + dim_offset
                mode(dim_offset+1:dim_offset+n_dim_perm) = eq%mode
            end associate
        end do
    end subroutine mci_vamp2_declare_equivalences

```



```

        call mci%equivalences%set_equivalence &
            (i, dest, src, perm, mode)
    end associate
end do
call mci%equivalences%freeze ()
end subroutine mci_vamp2_declare_equivalences

```

Allocate instance with matching type. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: allocate_instance => mci_vamp2_allocate_instance

<MCI vamp2: main procedures>≡
    subroutine mci_vamp2_allocate_instance (mci, mci_instance)
        class(mci_vamp2_t), intent(in) :: mci
        class(mci_instance_t), intent(out), pointer :: mci_instance
        allocate (mci_vamp2_instance_t :: mci_instance)
    end subroutine mci_vamp2_allocate_instance

```

Allocate a new integration pass. We can preset everything that does not depend on the number of iterations and calls. This is postponed to the integrate method.

In the final pass, we do not check accuracy goal etc., since we can assume that the user wants to perform and average all iterations in this pass.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: add_pass => mci_vamp2_add_pass

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_add_pass &
        (mci, adapt_grids, adapt_weights, final_pass)
        class(mci_vamp2_t), intent(inout) :: mci
        logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
    end subroutine mci_vamp2_add_pass

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_add_pass &
        (mci, adapt_grids, adapt_weights, final_pass)
        class(mci_vamp2_t), intent(inout) :: mci
        logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
        call mci%list_pass%add (adapt_grids, adapt_weights, final_pass)
    end subroutine mci_vamp2_add_pass

```

Update the list of integration passes.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: update_from_ref => mci_vamp2_update_from_ref

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_update_from_ref (mci, mci_ref, success)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_t), intent(in) :: mci_ref
        logical, intent(out) :: success
    end subroutine mci_vamp2_update_from_ref

```

```

<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_update_from_ref (mci, mci_ref, success)
  class(mci_vamp2_t), intent(inout) :: mci
  class(mci_t), intent(in) :: mci_ref
  logical, intent(out) :: success
  select type (mci_ref)
  type is (mci_vamp2_t)
    call mci%list_pass%update_from_ref (mci_ref%list_pass, success)
    if (mci%list_pass%has_last_integral()) then
      call mci%list_pass%get_last_integral( &
        integral = mci%integral, &
        error = mci%error, &
        efficiency = mci%efficiency)
      mci%integral_known = .true.
      mci%error_known = .true.
      mci%efficiency_known = .true.
    end if
  end select
end subroutine mci_vamp2_update_from_ref

```

Update the MCI record (i.e., the integration passes) by reading from input stream. The stream should contain a write output from a previous run. We first check the MD5 sum of the configuration parameters. If that matches, we proceed directly to the stored integration passes. If successful, we may continue to read the file; the position will be after a blank line that must follow the MCI record.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: update => mci_vamp2_update

<MCI vamp2: sub interfaces>+≡
module subroutine mci_vamp2_update (mci, u, success)
  class(mci_vamp2_t), intent(inout) :: mci
  integer, intent(in) :: u
  logical, intent(out) :: success
end subroutine mci_vamp2_update

<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_update (mci, u, success)
  class(mci_vamp2_t), intent(inout) :: mci
  integer, intent(in) :: u
  logical, intent(out) :: success
  character(80) :: buffer
  character(32) :: md5sum_file
  type(mci_vamp2_t) :: mci_file
  integer :: n_pass, n_it
  call read_sval (u, md5sum_file)
  success = .true.; if (mci%check_grid_file) &
    & success = (md5sum_file == mci%md5sum)
  if (success) then
    read (u, *)
    read (u, "(A)") buffer
    if (trim (adjustl (buffer)) /= "VAMP2 integrator:") then
      call msg_fatal ("VAMP2: reading grid file: corrupted data")
    end if
  end if

```

```

n_pass = 0
n_it = 0
do
  read (u, "(A)") buffer
  select case (trim (adjustl (buffer)))
  case ("")
    exit
  case ("Integration pass:")
    call mci_file%list_pass%add ()
    call mci_file%list_pass%current%read (u, n_pass, n_it)
    n_pass = n_pass + 1
    n_it = n_it + mci_file%list_pass%current%n_it
  end select
end do
call mci%update_from_ref (mci_file, success)
call mci_file%final ()
end if
end subroutine mci_vamp2_update

```

Read / write grids from / to file.

We split the reading process in two parts. First, we check on the header where we check (and update) all relevant pass data using `mci_vamp2_update`. In the second part we only read the integrator data. We implement `mci_vamp2_read` for completeness.

The writing of the MCI object is split into two parts, a header with the relevant process configuration regarding the integration and the results of the different passes and their iterations. The other part is the actual grid. The header will always be written in ASCII format, including a md5 hash, in order to testify against unwilling changes to the setup. The grid part can be either added to the ASCII file, or to an additional binary file.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure :: write_grids => mci_vamp2_write_grids
  procedure :: read_header => mci_vamp2_read_header
  procedure :: read_data => mci_vamp2_read_data
  procedure, private :: advance_to_data => mci_vamp2_advance_to_data

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_write_grids (mci)
    class(mci_vamp2_t), intent(in) :: mci
  end subroutine mci_vamp2_write_grids
  module subroutine mci_vamp2_read_header (mci, success)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(out) :: success
  end subroutine mci_vamp2_read_header
  module subroutine mci_vamp2_read_data (mci)
    class(mci_vamp2_t), intent(inout) :: mci
  end subroutine mci_vamp2_read_data
  module subroutine mci_vamp2_advance_to_data (mci, u, binary_grid_format)
    class(mci_vamp2_t), intent(in) :: mci
    integer, intent(in) :: u
    logical, intent(out) :: binary_grid_format
  end subroutine mci_vamp2_advance_to_data

```

<MCI vamp2: procedures>+≡

```

module subroutine mci_vamp2_write_grids (mci)
  class(mci_vamp2_t), intent(in) :: mci
  integer :: u
  if (.not. mci%grid_filename_set) then
    call msg_bug ("VAMP2: write grids: filename undefined")
  end if
  if (.not. mci%integrator_defined) then
    call msg_bug ("VAMP2: write grids: grids undefined")
  end if
  open (newunit = u, file = char (mci%get_grid_filename ()), &
        action = "write", status = "replace")
  write (u, "(1X,A,A,A)") "MD5sum = '", mci%md5sum, "'"
  write (u, *)
  call mci%write (u)
  write (u, *)
  if (mci%binary_grid_format) then
    write (u, "(1X,2A)") "VAMP2 grids: binary file: ", &
      char (mci%get_grid_filename (binary_grid_format = .true.))
    close (u)
    open (newunit = u, &
          file = char (mci%get_grid_filename (binary_grid_format = .true.)), &
          action = "write", &
          access = "stream", &
          form = "unformatted", &
          status = "replace")
    call mci%integrator%write_binary_grids (u)
  else
    write (u, "(1X,A)") "VAMP2 grids:"
    call mci%integrator%write_grids (u)
  end if
  close (u)
end subroutine mci_vamp2_write_grids

module subroutine mci_vamp2_read_header (mci, success)
  class(mci_vamp2_t), intent(inout) :: mci
  logical, intent(out) :: success
  logical :: exist, binary_grid_format, exist_binary
  integer :: u
  success = .false.
  if (.not. mci%grid_filename_set) then
    call msg_bug ("VAMP2: read grids: filename undefined")
  end if
  !! First, check for existence of the (usual) grid file.
  inquire (file = char (mci%get_grid_filename ()), exist = exist)
  if (.not. exist) return !! success = .false.
  open (newunit = u, file = char (mci%get_grid_filename ()), &
        action = "read", status = "old")
  !! Second, check for existence of a (possible) binary grid file.
  call mci%advance_to_data (u, binary_grid_format)
  rewind (u) !! Rewind header file, after line search.
  if (binary_grid_format) then
    inquire (file = char &
      (mci%get_grid_filename (binary_grid_format = .true.)), &

```

```

        exist = exist)
    if (.not. exist) then
        write (msg_buffer, "(3A)") &
            "VAMP2: header: binary grid file not found, discarding " // &
            "grid file '", char (mci%get_grid_filename ()), "'."
        call msg_message ()
        return !! success = .false.
    end if
end if
!! The grid file (ending *.vg) exists and, if binary file is listed, it
!! exists, too.
call mci%update (u, success)
close (u)
if (.not. success) then
    write (msg_buffer, "(A,A,A)") &
        "VAMP2: header: parameter mismatch, discarding pass from file '", &
        char (mci%get_grid_filename ()), "'."
    call msg_message ()
end if
end subroutine mci_vamp2_read_header

module subroutine mci_vamp2_read_data (mci)
    class(mci_vamp2_t), intent(inout) :: mci
    integer :: u
    logical :: binary_grid_format
    if (mci%integrator_defined) then
        call msg_bug ("VAMP2: read grids: grids already defined")
    end if
    open (newunit = u, &
        file = char (mci%get_grid_filename ()), &
        action = "read", &
        status = "old")
    call mci%advance_to_data (u, binary_grid_format)
    if (binary_grid_format) then
        close (u)
        write (msg_buffer, "(3A)") &
            "VAMP2: Reading from binary grid file '", &
            char (mci%get_grid_filename (binary_grid_format = .true.)), "'."
        call msg_message ()
        open (newunit = u, &
            file = char (mci%get_grid_filename (binary_grid_format = .true.)), &
            action = "read", &
            access = "stream", &
            form = "unformatted", &
            status = "old")
        call mci%integrator%read_binary_grids (u)
    else
        call mci%integrator%read_grids (u)
    end if
    mci%integrator_defined = .true.
    close (u)
end subroutine mci_vamp2_read_data

module subroutine mci_vamp2_advance_to_data (mci, u, binary_grid_format)

```

```

class(mci_vamp2_t), intent(in) :: mci
integer, intent(in) :: u
logical, intent(out) :: binary_grid_format
character(80) :: buffer
type(string_t) :: search_string_binary, search_string_ascii
search_string_binary = "VAMP2 grids: binary file: " // &
    mci%get_grid_filename (binary_grid_format = .true.)
search_string_ascii = "VAMP2 grids:"
SEARCH: do
    read (u, "(A)") buffer
    if (trim (adjustl (buffer)) == char (search_string_binary)) then
        binary_grid_format = .true.
        exit SEARCH
    else if (trim (adjustl (buffer)) == char (search_string_ascii)) then
        binary_grid_format = .false.
        exit SEARCH
    end if
end do SEARCH
end subroutine mci_vamp2_advance_to_data

```

Interface: VAMP2

We define the interfacing procedures, as such, initialising the VAMP2 integrator or resetting the results.

Initialise the VAMP2 integrator which is stored within the `mci` object, using the data of the current integration pass. Furthermore, reset the counters that track this set of integrator.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: init_integrator => mci_vamp2_init_integrator

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_init_integrator (mci)
        class(mci_vamp2_t), intent(inout) :: mci
    end subroutine mci_vamp2_init_integrator

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_init_integrator (mci)
        class(mci_vamp2_t), intent(inout) :: mci
        type (pass_t), pointer :: current
        integer :: ch, vegas_mode
        current => mci%list_pass%current
        vegas_mode = merge (VEGAS_MODE_IMPORTANCE, VEGAS_MODE_IMPORTANCE_ONLY, &
            & mci%config%stratified)
        mci%n_adapt_grids = 0
        mci%n_adapt_weights = 0
        if (mci%integrator_defined) then
            call msg_bug ("VAMP2: init integrator: &
                & integrator is already initialised.")
        end if
        mci%integrator = vamp2_t (mci%n_channel, mci%n_dim, &
            & n_bins_max = mci%config%n_bins_max, &
            & iterations = 1, &
            & mode = vegas_mode)
    end subroutine

```

```

    if (mci%has_chains ()) &
        call mci%integrator%set_chain (mci%n_chain, mci%chain)
    call mci%integrator%set_config (mci%config)
    mci%integrator_defined = .true.
end subroutine mci_vamp2_init_integrator

```

Reset a grid set. Purge the accumulated results.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: reset_result => mci_vamp2_reset_result

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_reset_result (mci)
        class(mci_vamp2_t), intent(inout) :: mci
    end subroutine mci_vamp2_reset_result

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_reset_result (mci)
        class(mci_vamp2_t), intent(inout) :: mci
        if (.not. mci%integrator_defined) then
            call msg_bug ("VAMP2: reset results: integrator undefined")
        end if
        call mci%integrator%reset_result ()
    end subroutine mci_vamp2_reset_result

```

Set calls per channel. The number of calls to each channel is defined by the channel weight

$$\alpha_i = \frac{N_i}{\sum N_i}. \quad (21.18)$$

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: set_calls => mci_vamp2_set_calls

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_set_calls (mci, n_calls)
        class(mci_vamp2_t), intent(inout) :: mci
        integer :: n_calls
    end subroutine mci_vamp2_set_calls

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_set_calls (mci, n_calls)
        class(mci_vamp2_t), intent(inout) :: mci
        integer :: n_calls
        if (.not. mci%integrator_defined) then
            call msg_bug ("VAMP2: set calls: grids undefined")
        end if
        call mci%integrator%set_calls (n_calls)
    end subroutine mci_vamp2_set_calls

```

Integration

Initialize. We prepare the integrator from a previous pass, or from file, or with new objects.

At the end, we update the number of calls either when we got the integration grids from file and we added new iterations to the current pass, or we allocated a new integrator.

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, private :: init_integration => mci_vamp2_init_integration

(MCI vamp2: sub interfaces)+≡
  module subroutine mci_vamp2_init_integration (mci, n_it, n_calls, instance)
    class(mci_vamp2_t), intent(inout) :: mci
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    class(mci_instance_t), intent(inout) :: instance
  end subroutine mci_vamp2_init_integration

(MCI vamp2: procedures)+≡
  module subroutine mci_vamp2_init_integration (mci, n_it, n_calls, instance)
    class(mci_vamp2_t), intent(inout) :: mci
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    class(mci_instance_t), intent(inout) :: instance
    logical :: from_file, success
    if (.not. associated (mci%list_pass%current)) then
      call msg_bug ("MCI integrate: current_pass object not allocated")
    end if
    associate (current_pass => mci%list_pass%current)
      current_pass%integral_defined = .false.
      mci%config%n_calls_min = mci%config%n_calls_min_per_channel * &
        mci%config%n_channel
      call current_pass%configure (n_it, n_calls, mci%config%n_calls_min)
      mci%adapt_grids = current_pass%adapt_grids
      mci%adapt_weights = current_pass%adapt_weights
      mci%pass_complete = .false.
      mci%it_complete = .false.
      from_file = .false.
      if (.not. mci%integrator_defined .or. mci%integrator_from_file) then
        if (mci%grid_filename_set .and. .not. mci%rebuild) then
          call mci%read_header (success)
          from_file = success
          if (.not. mci%integrator_defined .and. success) &
            call mci%read_data ()
        end if
      end if
      if (from_file) then
        if (.not. mci%check_grid_file) &
          & call msg_warning ("Reading grid file: MD5 sum check disabled")
        call msg_message ("VAMP2: " &
          // "Using grids and results from file '" &
          // char (mci%get_grid_filename ()) // "'.")
      else if (.not. mci%integrator_defined) then
        call msg_message ("VAMP2: " &
          // "Initialize new grids and write to file '" &
          // char (mci%get_grid_filename ()) // "'.")
        call mci%init_integrator ()
      end if
      mci%integrator_from_file = from_file
    end associate
  end subroutine mci_vamp2_init_integration

```



```

        if (.not. mci%integrator_from_file .or. (n_it > current_pass%get_integration_index ())) then
            call mci%integrator%set_calls (current_pass%n_calls)
        end if
        call mci%integrator%set_equivalences (mci%equivalences)
    end associate
<MCI vamp2: mci vamp2 init integration: allocate request>
end subroutine mci_vamp2_init_integration

```

Allocate request object and load into integrator object.

```

<MPI: MCI vamp2: mci vamp2 init integration: allocate request>≡
    if (mci%parallel_method /= "") then
        call mci%integrator%allocate_request (method = char (mci%parallel_method))
    else
        call msg_message ("VAMP2: Use default parallel method: simple.")
        call mci%integrator%allocate_request (method = "simple")
    end if

```

Integrate. Perform a new integration pass (possibly reusing previous results), which may consist of several iterations. We reinitialise the sampling new each time and set the workspace again. Note: we record the integral once per iteration. The integral stored in the mci record itself is the last integral of the current iteration, no averaging done. The results record may average results. Note: recording the efficiency is not supported yet.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: integrate => mci_vamp2_integrate

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_integrate (mci, instance, sampler, &
        n_it, n_calls, results, pacify)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        class(mci_results_t), intent(inout), optional :: results
        logical, intent(in), optional :: pacify
    end subroutine mci_vamp2_integrate

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_integrate (mci, instance, sampler, &
        n_it, n_calls, results, pacify)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        class(mci_results_t), intent(inout), optional :: results
        logical, intent(in), optional :: pacify
        integer :: it
        logical :: from_file, success
    <MCI vamp2: mci vamp2 integrate: variables>
    <MCI vamp2: mci vamp2 integrate: initialization>
        call mci%init_integration (n_it, n_calls, instance)
        from_file = mci%integrator_from_file
        select type (instance)

```

```

type is (mci_vamp2_instance_t)
    call instance%set_workspace (sampler)
end select
associate (current_pass => mci%list_pass%current)
    do it = 1, current_pass%n_it
        if (signal_is_pending ()) return
        mci%integrator_from_file = from_file .and. &
            it <= current_pass%get_integration_index ()
        if (.not. mci%integrator_from_file) then
            mci%it_complete = .false.
            select type (instance)
                type is (mci_vamp2_instance_t)
                    call mci%integrator%integrate (instance%func, mci%rng, &
                        & iterations = 1, &
                        & reset_result = .true., &
                        & refine_grids = mci%adapt_grids, &
                        & adapt_weights = mci%adapt_weights, &
                        & verbose = mci%verbose)
                end select
            if (signal_is_pending ()) return
            mci%it_complete = .true.
            integral = mci%integrator%get_integral ()
            calls = mci%integrator%get_n_calls ()
            select type (instance)
                type is (mci_vamp2_instance_t)
                    calls_valid = instance%func%get_n_calls ()
                    call instance%func%reset_n_calls ()
                end select
            error = sqrt (mci%integrator%get_variance ())
            efficiency = mci%integrator%get_efficiency ()
            {MCI vamp2: mci vamp2 integrate: sampling}
            if (integral /= 0) then
                current_pass%integral(it) = integral
                current_pass%calls(it) = calls
                current_pass%calls_valid(it) = calls_valid
                current_pass%error(it) = error
                current_pass%efficiency(it) = efficiency
            end if
            current_pass%integral_defined = .true.
        end if
    end if
    if (present (results)) then
        if (mci%has_chains ()) then
            call mci%collect_chain_weights (instance%w)
            call results%record (1, &
                n_calls = current_pass%calls(it), &
                n_calls_valid = current_pass%calls_valid(it), &
                integral = current_pass%integral(it), &
                error = current_pass%error(it), &
                efficiency = current_pass%efficiency(it), &
                efficiency_pos = current_pass%efficiency(it), &
                efficiency_neg = 0._default, &
                chain_weights = mci%chain_weights, &
                suppress = pacify)
        else

```

```

        call results%record (1, &
            n_calls = current_pass%calls(it), &
            n_calls_valid = current_pass%calls_valid(it), &
            integral = current_pass%integral(it), &
            error = current_pass%error(it), &
            efficiency = current_pass%efficiency(it), &
            efficiency_pos = current_pass%efficiency(it), &
            efficiency_neg = 0._default, &
            suppress = pacify)
    end if
end if
if (.not. mci%integrator_from_file &
    .and. mci%grid_filename_set) then
    <MCI vamp2: mci vamp2 integrate: post sampling>
    call checkpoint_and_write_grids (it = it, &
        final_it = (it == current_pass%n_it))
end if
if (.not. current_pass%is_final_pass) then
    call check_goals (it, success)
    if (success) exit
end if
end do
if (signal_is_pending ()) return
mci%pass_complete = .true.
mci%integral = current_pass%get_integral()
mci%error = current_pass%get_error()
mci%efficiency = current_pass%get_efficiency()
mci%integral_known = .true.
mci%error_known = .true.
mci%efficiency_known = .true.
call mci%compute_md5sum (pacify)
end associate
contains
    <MCI vamp2: mci vamp2 integrate: procedures>
end subroutine mci_vamp2_integrate

<MCI vamp2: mci vamp2 integrate: variables>≡
    real(default) :: integral, error, efficiency
    integer :: calls, calls_valid

<MCI vamp2: mci vamp2 integrate: initialization>≡

<MCI vamp2: mci vamp2 integrate: sampling>≡

<MCI vamp2: mci vamp2 integrate: post sampling>≡

<MPI: MCI vamp2: mci vamp2 integrate: variables>≡
    integer :: rank, n_size
    type(MPI_Request), dimension(6) :: request
MPI procedure-specific initialization.

<MPI: MCI vamp2: mci vamp2 integrate: initialization>≡
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)

```

We broadcast the current results to all worker, such that they can store them in to the pass list.

```
<MPI: MCI vamp2: mci vamp2 integrate: sampling>≡
  call MPI_Ibcast (integral, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(1))
  call MPI_Ibcast (calls, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, request(2))
  call MPI_Ibcast (calls_valid, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, request(3))
  call MPI_Ibcast (error, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(4))
  call MPI_Ibcast (efficiency, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(5))
  call MPI_Waitall (5, request, MPI_STATUSES_IGNORE)
```

We only allow the master to write the grids to file.

```
<MPI: MCI vamp2: mci vamp2 integrate: post sampling>≡
  if (rank == 0) &
```

Write grids to `grid_filename` at a given checkpoint.

We qualify each iteration and pass as possible checkpoint. However, we allow the user to alter the checkpoint behavior:

- after every iteration,
- after every pass,
- after a N iterations and every pass.

The user sets the Sindarin variable `vamp_grid_checkpoint` to an integer value where the value 0 represents each pass, value 1 each iteration, and a value > 1 means after N iterations (or at the last iteration of a pass).

```
<MCI vamp2: mci vamp2 integrate: procedures>≡
  subroutine checkpoint_and_write_grids (it, final_it)
    integer, intent(in) :: it
    logical, intent(in) :: final_it
    select case (mci%grid_checkpoint)
    case (0)
      if (.not. final_it) return
    case (1)
    case (2:)
      if (.not. (final_it &
        .or. mod (it, mci%grid_checkpoint) == 0)) return
    case default
      call msg_bug ("VAMP2: Grid checkpoint must be a positive integer.")
    end select
    call mci%write_grids ()
  end subroutine checkpoint_and_write_grids
```

Check whether we are already finished with this pass.

```
<MCI vamp2: mci vamp2 integrate: procedures>+≡
  subroutine check_goals (it, success)
    integer, intent(in) :: it
    logical, intent(out) :: success
    success = .false.
    associate (current_pass => mci%list_pass%current)
      if (error_reached (it)) then
        current_pass%n_it = it
        call msg_message ("VAMP2: error goal reached; &
```

```

        &skipping iterations")
    success = .true.
    return
end if
if (rel_error_reached (it)) then
    current_pass%n_it = it
    call msg_message ("VAMP2: relative error goal reached; &
        &skipping iterations")
    success = .true.
    return
end if
if (accuracy_reached (it)) then
    current_pass%n_it = it
    call msg_message ("VAMP2: accuracy goal reached; &
        &skipping iterations")
    success = .true.
    return
end if
end associate
end subroutine check_goals

```

Return true if the error, relative error or accuracy goals have been reached, if any.

(MCI vamp2: mci vamp2 integrate: procedures)+≡

```

function error_reached (it) result (flag)
    integer, intent(in) :: it
    logical :: flag
    real(default) :: error_goal, error
    error_goal = mci%config%error_goal
    flag = .false.
    associate (current_pass => mci%list_pass%current)
        if (error_goal > 0 .and. current_pass%integral_defined) then
            error = abs (current_pass%error(it))
            flag = error < error_goal
        end if
    end associate
end function error_reached

function rel_error_reached (it) result (flag)
    integer, intent(in) :: it
    logical :: flag
    real(default) :: rel_error_goal, rel_error
    rel_error_goal = mci%config%rel_error_goal
    flag = .false.
    associate (current_pass => mci%list_pass%current)
        if (rel_error_goal > 0 .and. current_pass%integral_defined) then
            rel_error = abs (current_pass%error(it) / current_pass%integral(it))
            flag = rel_error < rel_error_goal
        end if
    end associate
end function rel_error_reached

function accuracy_reached (it) result (flag)

```

```

integer, intent(in) :: it
logical :: flag
real(default) :: accuracy_goal, accuracy
accuracy_goal = mci%config%accuracy_goal
flag = .false.
associate (current_pass => mci%list_pass%current)
  if (accuracy_goal > 0 .and. current_pass%integral_defined) then
    if (current_pass%integral(it) /= 0) then
      accuracy = abs (current_pass%error(it) / current_pass%integral(it)) &
        * sqrt (real (current_pass%calls(it), default))
      flag = accuracy < accuracy_goal
    else
      flag = .true.
    end if
  end if
end associate
end function accuracy_reached

```

21.7.5 Event generation

Prepare simulation. We check the grids and reread them from file, if necessary.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: prepare_simulation => mci_vamp2_prepare_simulation

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_prepare_simulation (mci)
    class(mci_vamp2_t), intent(inout) :: mci
  end subroutine mci_vamp2_prepare_simulation

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_prepare_simulation (mci)
    class(mci_vamp2_t), intent(inout) :: mci
    logical :: success
    if (.not. mci%grid_filename_set) then
      call msg_bug ("VAMP2: preapre simulation: integrator filename not set.")
    end if
    call mci%read_header (success)
    call mci%compute_md5sum ()
    if (.not. success) then
      call msg_fatal ("Simulate: " &
        // "reading integration grids from file '" &
        // char (mci%get_grid_filename ()) // "' failed")
    end if
    if (.not. mci%integrator_defined) then
      call mci%read_data ()
    end if
    call groom_rng (mci%rng)
  contains
    subroutine groom_rng (rng)
      class(rng_t), intent(inout) :: rng
      integer :: i, rank, n_size
      call mpi_get_comm_id (n_size, rank)
      do i = 2, rank + 1
        select type (rng)

```

```

        type is (rng_stream_t)
        call rng%next_substream ()
        if (i == rank) &
            call msg_message ("MCI: Advance RNG for parallel event simulation")
        class default
            call msg_bug ("Use of any random number generator &
                &beside rng_stream for parallel event generation not supported.")
        end select
    end do
end subroutine groom_rng
end subroutine mci_vamp2_prepare_simulation

```

Generate an unweighted event. We only set the workspace again before generating an event.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: generate_weighted_event => &
        mci_vamp2_generate_weighted_event

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_generate_weighted_event (mci, instance, sampler)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_vamp2_generate_weighted_event

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_generate_weighted_event (mci, instance, sampler)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        if (.not. mci%integrator_defined) then
            call msg_bug ("VAMP2: generate weighted event: undefined integrator")
        end if
        select type (instance)
        type is (mci_vamp2_instance_t)
            instance%event_generated = .false.
            call instance%set_workspace (sampler)
            call mci%integrator%generate_weighted (&
                & instance%func, mci%rng, instance%event_x)
            instance%event_weight = mci%integrator%get_evt_weight ()
            instance%event_excess = 0
            instance%n_events = instance%n_events + 1
            instance%event_generated = .true.
        end select
    end subroutine mci_vamp2_generate_weighted_event

```

We apply an additional rescaling factor for `f_max` (either for the positive or negative distribution).

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: generate_unweighted_event => &
        mci_vamp2_generate_unweighted_event

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_generate_unweighted_event &

```

```

        (mci, instance, sampler)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_vamp2_generate_unweighted_event
<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_generate_unweighted_event (mci, instance, sampler)
    class(mci_vamp2_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    if (.not. mci%integrator_defined) then
        call msg_bug ("VAMP2: generate unweighted event: undefined integrator")
    end if
    select type (instance)
    type is (mci_vamp2_instance_t)
        instance%event_generated = .false.
        call instance%set_workspace (sampler)
        generate: do
            call mci%integrator%generate_unweighted (&
                & instance%func, mci%rng, instance%event_x, &
                & opt_event_rescale = instance%event_rescale_f_max)
            instance%event_excess = mci%integrator%get_evt_weight_excess ()
            if (signal_is_pending ()) return
            if (sampler%is_valid ()) exit generate
        end do generate
        if (mci%integrator%get_evt_weight () < 0._default) then
            if (.not. mci%negative_weights) then
                call msg_fatal ("VAMP2: cannot sample negative weights!")
            end if
            instance%event_weight = -1._default
        else
            instance%event_weight = 1._default
        end if
        instance%n_events = instance%n_events + 1
        instance%event_generated = .true.
    end select
end subroutine mci_vamp2_generate_unweighted_event

<MCI vamp2: mci vamp2: TBP>+≡
procedure, public :: rebuild_event => mci_vamp2_rebuild_event
<MCI vamp2: sub interfaces>+≡
module subroutine mci_vamp2_rebuild_event (mci, instance, sampler, state)
    class(mci_vamp2_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
end subroutine mci_vamp2_rebuild_event
<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_rebuild_event (mci, instance, sampler, state)
    class(mci_vamp2_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler

```



```

class(mci_state_t), intent(in) :: state
call msg_bug ("VAMP2: rebuild event not implemented yet.")
end subroutine mci_vamp2_rebuild_event

```

21.7.6 Integrator instance

We store all information relevant for simulation. The event weight is stored, when a weighted event is generated, and the event excess, when a larger weight occurs than actual stored max. weight.

We give the possibility to rescale the `f_max` within the integrator object with `event_rescale_f_max`.

```

<MCI vamp2: public>+≡
public :: mci_vamp2_instance_t

<MCI vamp2: types>+≡
type, extends (mci_instance_t) :: mci_vamp2_instance_t
class(mci_vamp2_func_t), allocatable :: func
real(default), dimension(:), allocatable :: gi
integer :: n_events = 0
logical :: event_generated = .false.
real(default) :: event_weight = 0._default
real(default) :: event_excess = 0._default
real(default) :: event_rescale_f_max = 1._default
real(default), dimension(:), allocatable :: event_x
contains
<MCI vamp2: mci vamp2 instance: TBP>
end type mci_vamp2_instance_t

```

Output.

```

<MCI vamp2: mci vamp2 instance: TBP>≡
procedure, public :: write => mci_vamp2_instance_write

<MCI vamp2: sub interfaces>+≡
module subroutine mci_vamp2_instance_write (object, unit, pacify)
class(mci_vamp2_instance_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: pacify
end subroutine mci_vamp2_instance_write

<MCI vamp2: procedures>+≡
module subroutine mci_vamp2_instance_write (object, unit, pacify)
class(mci_vamp2_instance_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: pacify
integer :: u, ch, j
character(len=7) :: fmt
call pac_fmt (fmt, FMT_17, FMT_14, pacify)
u = given_output_unit (unit)
write (u, "(1X,A)") "MCI VAMP2 instance:"
write (u, "(1X,A,I0)") &
& "Selected channel" = ", object%selected_channel"
write (u, "(1X,A25,1X," // fmt // ")") &
& "Integrand" = ", object%integrand"

```

```

write (u, "(1X,A25,1X," // fmt // ")") &
    & "MCI weight" = ", object%mc_i_weight
write (u, "(1X,A,L1)") &
    & "Valid" = ", object%valid
write (u, "(1X,A)") "MCI a-priori weight:"
do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%w(ch)
end do
write (u, "(1X,A)") "MCI jacobian:"
do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%f(ch)
end do
write (u, "(1X,A)") "MCI mapped x:"
do ch = 1, size (object%w)
    do j = 1, size (object%x, 1)
        write (u, "(3X,2(1X,I8),1X," // fmt // ")") j, ch, object%x(j, ch)
    end do
end do
write (u, "(1X,A)") "MCI channel weight:"
do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%gi(ch)
end do
write (u, "(1X,A,I0)") &
    & "Number of event" = ", object%n_events
write (u, "(1X,A,L1)") &
    & "Event generated" = ", object%event_generated
write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event weight" = ", object%event_weight
write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event excess" = ", object%event_excess
write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event rescale f max" = ", object%event_rescale_f_max
write (u, "(1X,A,L1)") &
    & "Negative (event) weight" = ", object%negative_weights
write (u, "(1X,A)") "MCI event"
do j = 1, size (object%event_x)
    write (u, "(3X,I25,1X," // fmt // ")") j, object%event_x(j)
end do
end subroutine mci_vamp2_instance_write

```

Finalizer. We are only using allocatable, so there is nothing to do here.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
    procedure, public :: final => mci_vamp2_instance_final

<MCI vamp2: sub interfaces>+≡
    module subroutine mci_vamp2_instance_final (object)
        class(mci_vamp2_instance_t), intent(inout) :: object
    end subroutine mci_vamp2_instance_final

<MCI vamp2: procedures>+≡
    module subroutine mci_vamp2_instance_final (object)
        class(mci_vamp2_instance_t), intent(inout) :: object
    !
    end subroutine mci_vamp2_instance_final

```

Initializer. Gfortran 7/8/9 bug, has to remain in the main module:

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: init => mci_vamp2_instance_init

<MCI vamp2: main procedures>+≡
  subroutine mci_vamp2_instance_init (mci_instance, mci)
    class(mci_vamp2_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
    call mci_instance%base_init (mci)
    allocate (mci_instance%gi(mci%n_channel), source=0._default)
    allocate (mci_instance%event_x(mci%n_dim), source=0._default)
    allocate (mci_vamp2_func_t :: mci_instance%func)
    call mci_instance%func%init (n_dim = mci%n_dim, n_channel = mci%n_channel)
  end subroutine mci_vamp2_instance_init

```

Set workspace for mci_vamp2_func_t.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: set_workspace => mci_vamp2_instance_set_workspace

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_instance_set_workspace (instance, sampler)
    class(mci_vamp2_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
  end subroutine mci_vamp2_instance_set_workspace

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_instance_set_workspace (instance, sampler)
    class(mci_vamp2_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    call instance%func%set_workspace (instance, sampler)
  end subroutine mci_vamp2_instance_set_workspace

```

Evaluation

Compute multi-channel weight. The computation of the multi-channel weight is done by the VAMP2 function. We retrieve the information.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: compute_weight => mci_vamp2_instance_compute_weight

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_instance_compute_weight (mci, c)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
  end subroutine mci_vamp2_instance_compute_weight

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_instance_compute_weight (mci, c)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
    mci%gi = mci%func%get_probabilities ()
    mci%mc_weight = mci%func%get_weight ()
  end subroutine mci_vamp2_instance_compute_weight

```

Record the integrand.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: record_integrand => mci_vamp2_instance_record_integrand

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_instance_record_integrand (mci, integrand)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
  end subroutine mci_vamp2_instance_record_integrand

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_instance_record_integrand (mci, integrand)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    mci%integrand = integrand
    call mci%func%set_integrand (integrand)
  end subroutine mci_vamp2_instance_record_integrand

```

Event simulation

In contrast to VAMP, we reset only counters and set the safety factor, which will then will be applied each time an event is generated. In that way we do not rescale the actual values in the integrator, but more the current value!

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: init_simulation => mci_vamp2_instance_init_simulation

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_instance_init_simulation &
    (instance, safety_factor)
    class(mci_vamp2_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
  end subroutine mci_vamp2_instance_init_simulation

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_instance_init_simulation (instance, safety_factor)
    class(mci_vamp2_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
    if (present (safety_factor)) instance%event_rescale_f_max = safety_factor
    instance%n_events = 0
    instance%event_generated = .false.
    if (instance%event_rescale_f_max /= 1) then
      write (msg_buffer, "(A,ES10.3,A)") "Simulate: &
        &applying safety factor ", instance%event_rescale_f_max, &
        & " to event rejection."
      call msg_message ()
    end if
  end subroutine mci_vamp2_instance_init_simulation

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: final_simulation => mci_vamp2_instance_final_simulation

<MCI vamp2: sub interfaces>+≡
  module subroutine mci_vamp2_instance_final_simulation (instance)
    class(mci_vamp2_instance_t), intent(inout) :: instance
  end subroutine mci_vamp2_instance_final_simulation

```

```

<MCI vamp2: procedures>+≡
  module subroutine mci_vamp2_instance_final_simulation (instance)
    class(mci_vamp2_instance_t), intent(inout) :: instance
    !
  end subroutine mci_vamp2_instance_final_simulation

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: get_event_weight => mci_vamp2_instance_get_event_weight

<MCI vamp2: sub interfaces>+≡
  module function mci_vamp2_instance_get_event_weight (mci) result (weight)
    class(mci_vamp2_instance_t), intent(in) :: mci
    real(default) :: weight
  end function mci_vamp2_instance_get_event_weight

<MCI vamp2: procedures>+≡
  module function mci_vamp2_instance_get_event_weight (mci) result (weight)
    class(mci_vamp2_instance_t), intent(in) :: mci
    real(default) :: weight
    if (.not. mci%event_generated) then
      call msg_bug ("VAMP2: get event weight: no event generated")
    end if
    weight = mci%event_weight
  end function mci_vamp2_instance_get_event_weight

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: get_event_excess => mci_vamp2_instance_get_event_excess

<MCI vamp2: sub interfaces>+≡
  module function mci_vamp2_instance_get_event_excess (mci) result (excess)
    class(mci_vamp2_instance_t), intent(in) :: mci
    real(default) :: excess
  end function mci_vamp2_instance_get_event_excess

<MCI vamp2: procedures>+≡
  module function mci_vamp2_instance_get_event_excess (mci) result (excess)
    class(mci_vamp2_instance_t), intent(in) :: mci
    real(default) :: excess
    if (.not. mci%event_generated) then
      call msg_bug ("VAMP2: get event excess: no event generated")
    end if
    excess = mci%event_excess
  end function mci_vamp2_instance_get_event_excess

```

21.7.7 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_vamp2_ut.f90>≡  
  <File header>  
  
  module mci_vamp2_ut  
    use unit_tests  
    use mci_vamp2_uti  
  
    <Standard module head>  
  
    <MCI vamp2: public test>  
  
    contains  
  
    <MCI vamp2: test driver>  
  
  end module mci_vamp2_ut  
<mci_vamp2_uti.f90>≡  
  <File header>  
  
  module mci_vamp2_uti  
  
    <Use kinds>  
    <Use strings>  
  
    use io_units  
    use constants, only: PI, TWOPI  
    use rng_base  
    use rng_tao  
    use rng_stream  
    use mci_base  
  
    use mci_vamp2  
  
    <Standard module head>  
  
    <MCI vamp2: test declarations>  
  
    <MCI vamp2: test types>  
  
    contains  
  
    <MCI vamp2: tests>  
  
  end module mci_vamp2_uti  
API: driver for the unit tests below.  
<MCI vamp2: public test>≡  
  public :: mci_vamp2_test  
<MCI vamp2: test driver>≡  
  subroutine mci_vamp2_test (u, results)  
    integer, intent(in) :: u
```

```

    type(test_results_t), intent(inout) :: results
    <MCI vamp2: execute tests>
end subroutine mci_vamp2_test

```

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

In mode 1, the function is $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

In mode 2, the function is $11x^{10}$, also with integral 1.

Mode 4 includes ranges of zero and negative function value, the integral is negative. The results should be identical to the results of `mci_midpoint_4`, where the same function is evaluated. The function is $f(x) = (1 - 3x^2) \theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$.

```

<MCI vamp2: test types>≡
    type, extends (mci_sampler_t) :: test_sampler_1_t
        real(default), dimension(:), allocatable :: x
        real(default) :: val
        integer :: mode = 1
    contains
        <MCI vamp2: test sampler 1: TBP>
    end type test_sampler_1_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI vamp2: test sampler 1: TBP>≡
    procedure, public :: write => test_sampler_1_write

<MCI vamp2: tests>≡
    subroutine test_sampler_1_write (object, unit, testflag)
        class(test_sampler_1_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        select case (object%mode)
            case (1)
                write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"
            case (2)
                write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10"
            case (3)
                write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10 * 2 * cos^2 (2 pi y)"
            case (4)
                write (u, "(1x,A)") "Test sampler: f(x) = (1 - 3 x^2) theta(x - 1/2)"
        end select
    end subroutine test_sampler_1_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

(MCI vamp2: test_sampler_1: TBP)+≡
  procedure, public :: evaluate => test_sampler_1_evaluate

(MCI vamp2: tests)+≡
  subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_1_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    select case (sampler%mode)
    case (1)
      sampler%val = 3 * x_in(1) ** 2
    case (2)
      sampler%val = 11 * x_in(1) ** 10
    case (3)
      sampler%val = 11 * x_in(1) ** 10 * 2 * cos (twopi * x_in(2)) ** 2
    case (4)
      if (x_in(1) >= .5_default) then
        sampler%val = 1 - 3 * x_in(1) ** 2
      else
        sampler%val = 0
      end if
    end select
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_1_evaluate

```

The point is always valid.

```

(MCI vamp2: test_sampler_1: TBP)+≡
  procedure, public :: is_valid => test_sampler_1_is_valid

(MCI vamp2: tests)+≡
  function test_sampler_1_is_valid (sampler) result (valid)
    class(test_sampler_1_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

(MCI vamp2: test_sampler_1: TBP)+≡
  procedure, public :: rebuild => test_sampler_1_rebuild

(MCI vamp2: tests)+≡
  subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_1_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val

```



```

    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
end subroutine test_sampler_1_rebuild

```

Extract the results.

```

⟨MCI vamp2: test sampler 1: TBP⟩+≡
    procedure, public :: fetch => test_sampler_1_fetch

⟨MCI vamp2: tests⟩+≡
    subroutine test_sampler_1_fetch (sampler, val, x, f)
        class(test_sampler_1_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x(:,1) = sampler%x
        f = 1
    end subroutine test_sampler_1_fetch

```

Two-channel, two dimension test sampler

This sampler implements the function

$$f(x, y) = 4 \sin^2(\pi x) \sin^2(\pi y) + 2 \sin^2(\pi v) \quad (21.19)$$

where

$$x = u^v \quad u = xy \quad (21.20)$$

$$y = u^{(1-v)} \quad v = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log xy} \right) \quad (21.21)$$

Each term contributes 1 to the integral. The first term in the function is peaked along a cross aligned to the coordinates x and y , while the second term is peaked along the diagonal $x = y$.

The Jacobian is

$$\frac{\partial(x, y)}{\partial(u, v)} = |\log u| \quad (21.22)$$

```

⟨MCI vamp2: test types⟩+≡
    type, extends (mci_sampler_t) :: test_sampler_2_t
        real(default), dimension(:,:), allocatable :: x
        real(default), dimension(:), allocatable :: f
        real(default) :: val
    contains
        ⟨MCI vamp2: test sampler 2: TBP⟩
    end type test_sampler_2_t

```

Output: There is nothing stored inside, so just print an informative line.

```

(MCI vamp2: test_sampler_2: TBP)+≡
  procedure, public :: write => test_sampler_2_write

(MCI vamp2: tests)+≡
  subroutine test_sampler_2_write (object, unit, testflag)
    class(test_sampler_2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Two-channel test sampler 2"
  end subroutine test_sampler_2_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

(MCI vamp2: test_sampler_2: TBP)+≡
  procedure, public :: compute => test_sampler_2_compute

(MCI vamp2: tests)+≡
  subroutine test_sampler_2_compute (sampler, c, x_in)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default) :: xx, yy, uu, vv
    if (.not. allocated (sampler%x)) &
      allocate (sampler%x (size (x_in), 2))
    if (.not. allocated (sampler%f)) &
      allocate (sampler%f (2))
    select case (c)
    case (1)
      xx = x_in(1)
      yy = x_in(2)
      uu = xx * yy
      vv = (1 + log (xx/yy) / log (xx*yy)) / 2
    case (2)
      uu = x_in(1)
      vv = x_in(2)
      xx = uu ** vv
      yy = uu ** (1 - vv)
    end select
    sampler%val = (2 * sin (pi * xx) * sin (pi * yy)) ** 2 &
      + 2 * sin (pi * vv) ** 2
    sampler%f(1) = 1
    sampler%f(2) = abs (log (uu))
    sampler%x(:,1) = [xx, yy]
    sampler%x(:,2) = [uu, vv]
  end subroutine test_sampler_2_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

(MCI vamp2: test_sampler_2: TBP)+≡
  procedure, public :: evaluate => test_sampler_2_evaluate

```

```

<MCI vamp2: tests>+=
  subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_2_evaluate

```

The point is always valid.

```

<MCI vamp2: test sampler 2: TBP>+=
  procedure, public :: is_valid => test_sampler_2_is_valid

<MCI vamp2: tests>+=
  function test_sampler_2_is_valid (sampler) result (valid)
    class(test_sampler_2_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_2_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp2: test sampler 2: TBP>+=
  procedure, public :: rebuild => test_sampler_2_rebuild

<MCI vamp2: tests>+=
  subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    x = sampler%x
    f = sampler%f
  end subroutine test_sampler_2_rebuild

```

Extract the results.

```

<MCI vamp2: test sampler 2: TBP>+=
  procedure, public :: fetch => test_sampler_2_fetch

<MCI vamp2: tests>+=
  subroutine test_sampler_2_fetch (sampler, val, x, f)
    class(test_sampler_2_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x = sampler%x
    f = sampler%f
  end subroutine test_sampler_2_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

```
<MCI vamp2: execute tests>≡
    call test (mci_vamp2_1, "mci_vamp2_1", "one-dimensional integral", u, results)

<MCI vamp2: test declarations>≡
    public :: mci_vamp2_1

<MCI vamp2: tests>+≡
    subroutine mci_vamp2_1 (u)
        integer, intent(in) :: u
        type(mci_vamp2_config_t) :: config
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable, target :: mci_sampler
        class(rng_t), allocatable :: rng
        type(string_t) :: filename

        write (u, "(A)") "* Test output: mci_vamp2_1"
        write (u, "(A)") "* Purpose: integrate function in one dimension (single channel)"

        write (u, "(A)")
        write (u, "(A)") "* Initialise integrator"
        write (u, "(A)")

        allocate (mci_vamp2_t :: mci)
        call mci%set_dimensions (1, 1)

        filename = "mci_vamp2_1"
        select type (mci)
            type is (mci_vamp2_t)
                call mci%set_config (config)
                call mci%set_grid_filename (filename)
            end select

        allocate (rng_stream_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        call mci%write (u, pacify = .true.)

        write (u, "(A)")
        write (u, "(A)") "* Initialise instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")
        write (u, "(A)") "* Initialise test sampler"
        write (u, "(A)")

        allocate (test_sampler_1_t :: mci_sampler)
        call mci_sampler%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "  (lower precision to avoid"
write (u, "(A)")  "    numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp2_t)
  call mci%add_pass ()
end select
call mci%integrate (mci_instance, mci_sampler, 1, 1000, pacify = .true.)
call mci%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
  call mci%write_grids ()
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp2_1"

end subroutine mci_vamp2_1

```

Multiple iterations

Construct an integrator and use it for a one-dimensional sampler. Integrate with five iterations without grid adaptation.

```

<MCI vamp2: execute tests>+≡
  call test (mci_vamp2_2, "mci_vamp2_2", &
    "multiple iterations", &
    u, results)

<MCI vamp2: test declarations>+≡
  public :: mci_vamp2_2

```

(MCI vamp2: tests) +=

```

subroutine mci_vamp2_2 (u)
  type(mci_vamp2_config_t) :: config
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng
  type(string_t) :: filename

  write (u, "(A)")  "* Test output: mci_vamp2_2"
  write (u, "(A)")  "* Purpose: integrate function in one dimension &
    &(single channel), but multiple iterations."

  write (u, "(A)")
  write (u, "(A)")  "* Initialize integrator, sampler, instance"
  write (u, "(A)")

  allocate (mci_vamp2_t :: mci)
  call mci%set_dimensions (1, 1)
  filename = "mci_vamp2_2"
  select type (mci)
    type is (mci_vamp2_t)
      call mci%set_config (config)
      call mci%set_grid_filename (filename)
  end select

  allocate (rng_stream_t :: rng)
  call rng%init ()
  call mci%import_rng (rng)

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  allocate (test_sampler_1_t :: sampler)
  select type (sampler)
    type is (test_sampler_1_t)
      sampler%mode = 2
  end select
  call sampler%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
  write (u, "(A)")

  select type (mci)
    type is (mci_vamp2_t)
      call mci%add_pass (adapt_grids = .false.)
  end select
  call mci%integrate (mci_instance, sampler, 3, 1000, pacify = .true.)
  call mci%write (u, pacify = .true.)

  write (u, "(A)")
  write (u, "(A)")  "* Contents of mci_instance:"

```

```

write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
    call mci%write_grids ()
end select

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: mci_vamp2_2"

end subroutine mci_vamp2_2

```

Grid adaptation

Construct an integrator and use it for a one-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp2: execute tests>+≡
    call test (mci_vamp2_3, "mci_vamp2_3", &
        "grid adaptation", &
        u, results)

<MCI vamp2: test declarations>+≡
    public :: mci_vamp2_3

<MCI vamp2: tests>+≡
    subroutine mci_vamp2_3 (u)
        integer, intent(in) :: u
        type(mci_vamp2_config_t) :: config
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng
        type(string_t) :: filename

        write (u, "(A)") "* Test output: mci_vamp2_3"
        write (u, "(A)") "* Purpose: integrate function in one dimension &
            &(single channel)"
        write (u, "(A)") "* and adapt grid"

        write (u, "(A)")
    end subroutine mci_vamp2_3

```

```

write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp2_t :: mci)
call mci%set_dimensions (1, 1)
filename = "mci_vamp2_3"
select type (mci)
type is (mci_vamp2_t)
    call mci%set_grid_filename (filename)
    call mci%set_config (config)
end select

allocate (rng_stream_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp2_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000, pacify = .true.)
call mci%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
    call mci%write_grids ()
end select

write (u, "(A)")

```



```

        write (u, "(A)")  "* Cleanup"
        write (u, "(A)")

        call mci_instance%final ()
        call mci%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: mci_vamp2_3"

    end subroutine mci_vamp2_3

```

21.8 Dispatch

```

⟨dispatch_mci.f90⟩≡
  ⟨File header⟩

  module dispatch_mci

    ⟨Use strings⟩
    use variables
    use mci_base

    ⟨Standard module head⟩

    ⟨Dispatch mci: public⟩

    interface
    ⟨Dispatch mci: sub interfaces⟩
    end interface

  end module dispatch_mci

⟨dispatch_mci_sub.f90⟩≡
  ⟨File header⟩

  submodule (dispatch_mci) dispatch_mci_s

    use diagnostics
    use os_interface
    use mci_none
    use mci_midpoint
    use mci_vamp
    use mci_vamp2

    implicit none

    ⟨Dispatch mci: parameters⟩

    contains

    ⟨Dispatch mci: procedures⟩

```

```
end submodule dispatch_mci_s
```

Allocate an integrator according to the variable `$integration_method`.

```
<Dispatch mci: public>≡
```

```
public :: dispatch_mci_setup
```

```
<Dispatch mci: sub interfaces>≡
```

```
module subroutine dispatch_mci_setup (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
end subroutine dispatch_mci_setup
```

```
<Dispatch mci: procedures>≡
```

```
module subroutine dispatch_mci_setup (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  type(string_t) :: run_id
  type(string_t) :: integration_method
  type(grid_parameters_t) :: grid_par
  type(history_parameters_t) :: history_par
  type(mci_vamp2_config_t) :: mci_vamp2_config
  integer :: grid_checkpoint
  logical :: rebuild_grids, check_grid_file, negative_weights, verbose
  logical :: dispatch_nlo, binary_grid_format
  type(string_t) :: grid_path, parallel_method
  dispatch_nlo = .false.; if (present(is_nlo)) dispatch_nlo = is_nlo
  integration_method = &
    var_list%get_sval (var_str ("integration_method"))
  select case (char (integration_method))
  case ("none")
    allocate (mci_none_t :: mci)
  case ("midpoint")
    allocate (mci_midpoint_t :: mci)
  case ("vamp", "default")
    call unpack_options_vamp ()
    allocate (mci_vamp_t :: mci)
    select type (mci)
    type is (mci_vamp_t)
      call mci%set_grid_parameters (grid_par)
      if (run_id /= "") then
        call mci%set_grid_filename (process_id, run_id)
      else
        call mci%set_grid_filename (process_id)
      end if
      grid_path = var_list%get_sval (var_str ("integrate_workspace"))
      if (grid_path /= "") then
        call setup_grid_path (grid_path)
        call mci%prepend_grid_path (grid_path)
      end if
      call mci%set_history_parameters (history_par)
      call mci%set_rebuild_flag (rebuild_grids, check_grid_file)
```

```

        mci%negative_weights = negative_weights
        mci%verbose = verbose
    end select
case ("vamp2")
    call unpack_options_vamp2 ()
    allocate (mci_vamp2_t :: mci)
    select type (mci)
    type is (mci_vamp2_t)
        call mci%set_config (mci_vamp2_config)
        if (run_id /= "") then
            call mci%set_grid_filename (process_id, run_id)
        else
            call mci%set_grid_filename (process_id)
        end if
        grid_path = var_list%get_sval (var_str ("integrate_workspace"))
        if (grid_path /= "") then
            call setup_grid_path (grid_path)
            call mci%prepend_grid_path (grid_path)
        end if
        call mci%set_rebuild_flag (rebuild_grids, check_grid_file)
        mci%negative_weights = negative_weights
        mci%verbose = verbose
        mci%grid_checkpoint = grid_checkpoint
        mci%binary_grid_format = binary_grid_format
        mci%parallel_method = parallel_method
    end select
case default
    call msg_fatal ("Integrator '" &
        // char (integration_method) // "' not implemented")
end select
contains
    <Dispatch mci s: procedures>
end subroutine dispatch_mci_setup

```

<Dispatch mci s: procedures>≡

```

subroutine unpack_options_vamp ()
    grid_par%threshold_calls = &
        var_list%get_ival (var_str ("threshold_calls"))
    grid_par%min_calls_per_channel = &
        var_list%get_ival (var_str ("min_calls_per_channel"))
    grid_par%min_calls_per_bin = &
        var_list%get_ival (var_str ("min_calls_per_bin"))
    grid_par%min_bins = &
        var_list%get_ival (var_str ("min_bins"))
    grid_par%max_bins = &
        var_list%get_ival (var_str ("max_bins"))
    grid_par%stratified = &
        var_list%get_lval (var_str ("?stratified"))
    select case (char (var_list%get_sval (var_str ("phs_method"))))
    case ("rambo")
        grid_par%use_vamp_equivalences = .false.
    case default
        grid_par%use_vamp_equivalences = &
            var_list%get_lval (var_str ("?use_vamp_equivalences"))
    end select
end subroutine

```

```

end select
grid_par%channel_weights_power = &
    var_list%get_rval (var_str ("channel_weights_power"))
grid_par%accuracy_goal = &
    var_list%get_rval (var_str ("accuracy_goal"))
grid_par%error_goal = &
    var_list%get_rval (var_str ("error_goal"))
grid_par%rel_error_goal = &
    var_list%get_rval (var_str ("relative_error_goal"))
history_par%global = &
    var_list%get_lval (var_str ("?vamp_history_global"))
history_par%global_verbose = &
    var_list%get_lval (var_str ("?vamp_history_global_verbose"))
history_par%channel = &
    var_list%get_lval (var_str ("?vamp_history_channels"))
history_par%channel_verbose = &
    var_list%get_lval (var_str ("?vamp_history_channels_verbose"))
verbose = &
    var_list%get_lval (var_str ("?vamp_verbose"))
check_grid_file = &
    var_list%get_lval (var_str ("?check_grid_file"))
run_id = &
    var_list%get_sval (var_str ("$run_id"))
rebuild_grids = &
    var_list%get_lval (var_str ("?rebuild_grids"))
negative_weights = &
    var_list%get_lval (var_str ("?negative_weights")) .or. dispatch_nlo
end subroutine unpack_options_vamp

subroutine unpack_options_vamp2 ()
    mci_vamp2_config%n_bins_max = &
        var_list%get_ival (var_str ("max_bins"))
    mci_vamp2_config%n_calls_min_per_channel = &
        var_list%get_ival (var_str ("min_calls_per_channel"))
    mci_vamp2_config%n_calls_threshold = &
        var_list%get_ival (var_str ("threshold_calls"))
    mci_vamp2_config%beta = &
        var_list%get_rval (var_str ("channel_weights_power"))
    mci_vamp2_config%stratified = &
        var_list%get_lval (var_str ("?stratified"))
    select case (char (var_list%get_sval (var_str ("phs_method"))))
    case ("rambo")
        mci_vamp2_config%equivalences = .false.
    case default
        mci_vamp2_config%equivalences = &
            var_list%get_lval (var_str ("?use_vamp_equivalences"))
    end select
    mci_vamp2_config%accuracy_goal = &
        var_list%get_rval (var_str ("accuracy_goal"))
    mci_vamp2_config%error_goal = &
        var_list%get_rval (var_str ("error_goal"))
    mci_vamp2_config%rel_error_goal = &
        var_list%get_rval (var_str ("relative_error_goal"))
    verbose = &

```

```

        var_list%get_lval (var_str ("?vamp_verbose"))
check_grid_file = &
        var_list%get_lval (var_str ("?check_grid_file"))
run_id = &
        var_list%get_sval (var_str ("$run_id"))
rebuild_grids = &
        var_list%get_lval (var_str ("?rebuild_grids"))
negative_weights = &
        var_list%get_lval (var_str ("?negative_weights")) .or. dispatch_nlo
grid_checkpoint = &
        var_list%get_ival (var_str ("vamp_grid_checkpoint"))
select case (char (var_list%get_sval (var_str ("$vamp_grid_format"))))
case ("binary","Binary","BINARY")
        binary_grid_format = .true.
case ("ascii","Ascii","ASCII")
        binary_grid_format = .false.
case default
        binary_grid_format = .false.
end select
select case (char (var_list%get_sval (var_str ("$vamp_parallel_method"))))
case ("simple","Simple","SIMPLE")
        parallel_method = var_str ("simple")
case ("load","Load","LOAD")
        parallel_method = var_str ("load")
case default
        parallel_method = var_str ("simple")
end select
end subroutine unpack_options_vamp2

```

Make sure that the VAMP grid subdirectory, if requested, exists before it is used. Also include a sanity check on the directory name.

```

<Dispatch mci: parameters>≡
character(*), parameter :: ALLOWED_IN_DIRNAME = &
        "abcdefghijklmnopqrstuvwxyz&
        &ABCDEFGHIJKLMNOPQRSTUVWXYZ&
        &1234567890&
        &.,_-= "

<Dispatch mci: public>+≡
public :: setup_grid_path

<Dispatch mci: sub interfaces>+≡
module subroutine setup_grid_path (grid_path)
        type(string_t), intent(in) :: grid_path
end subroutine setup_grid_path

<Dispatch mci: procedures>+≡
module subroutine setup_grid_path (grid_path)
        type(string_t), intent(in) :: grid_path
        if (verify (grid_path, ALLOWED_IN_DIRNAME) == 0) then
                call msg_message ("Integrator: preparing VAMP grid directory '" &
                        // char (grid_path) // "'")
                call os_system_call ("mkdir -p '" // grid_path // "'")
        else
                call msg_fatal ("Integrator: VAMP grid_path '" &

```

```

        // char (grid_path) // '' contains illegal characters")
    end if
end subroutine setup_grid_path

```

21.8.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_mci_ut.f90>≡
  <File header>

  module dispatch_mci_ut
    use unit_tests
    use dispatch_mci_uti

    <Standard module head>

    <Dispatch mci: public test>

    contains

    <Dispatch mci: test driver>

  end module dispatch_mci_ut

<dispatch_mci_uti.f90>≡
  <File header>

  module dispatch_mci_uti

    <Use kinds>
    <Use strings>
    use variables
    use mci_base
    use mci_none
    use mci_midpoint
    use mci_vamp
    use dispatch_mci

    <Standard module head>

    <Dispatch mci: test declarations>

    contains

    <Dispatch mci: tests>

  end module dispatch_mci_uti
API: driver for the unit tests below.
<Dispatch mci: public test>≡
  public ::dispatch_mci_test

```

```

<Dispatch mci: test driver>≡
  subroutine dispatch_mci_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Dispatch mci: execute tests>
  end subroutine dispatch_mci_test

```

Select type: integrator core

```

<Dispatch mci: execute tests>≡
  call test (dispatch_mci_1, "dispatch_mci_1", &
    "integration method", &
    u, results)

<Dispatch mci: test declarations>≡
  public :: dispatch_mci_1

<Dispatch mci: tests>≡
  subroutine dispatch_mci_1 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    class(mci_t), allocatable :: mci
    type(string_t) :: process_id

    write (u, "(A)")  "* Test output: dispatch_mci_1"
    write (u, "(A)")  "* Purpose: select integration method"
    write (u, "(A)")

    call var_list%init_defaults (0)

    process_id = "dispatch_mci_1"

    write (u, "(A)")  "* Allocate MCI as none_t"
    write (u, "(A)")

    call var_list%set_string (&
      var_str ("integration_method"), &
      var_str ("none"), is_known = .true.)
    call dispatch_mci_setup (mci, var_list, process_id)
    select type (mci)
      type is (mci_none_t)
        call mci%write (u)
    end select

    call mci%final ()
    deallocate (mci)

    write (u, "(A)")
    write (u, "(A)")  "* Allocate MCI as midpoint_t"
    write (u, "(A)")

    call var_list%set_string (&
      var_str ("integration_method"), &
      var_str ("midpoint"), is_known = .true.)

```

```

call dispatch_mci_setup (mci, var_list, process_id)
select type (mci)
type is (mci_midpoint_t)
    call mci%write (u)
end select

call mci%final ()
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Allocate MCI as vamp_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("vamp"), is_known = .true.)
call var_list%set_int (var_str ("threshold_calls"), &
    1, is_known = .true.)
call var_list%set_int (var_str ("min_calls_per_channel"), &
    2, is_known = .true.)
call var_list%set_int (var_str ("min_calls_per_bin"), &
    3, is_known = .true.)
call var_list%set_int (var_str ("min_bins"), &
    4, is_known = .true.)
call var_list%set_int (var_str ("max_bins"), &
    5, is_known = .true.)
call var_list%set_log (var_str ("?stratified"), &
    .false., is_known = .true.)
call var_list%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
call var_list%set_real (var_str ("channel_weights_power"), &
    4._default, is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_global_verbos"), &
    .true., is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_channels"), &
    .true., is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_channels_verbos"), &
    .true., is_known = .true.)
call var_list%set_log (var_str ("?stratified"), &
    .false., is_known = .true.)

call dispatch_mci_setup (mci, var_list, process_id)
select type (mci)
type is (mci_vamp_t)
    call mci%write (u)
    call mci%write_history_parameters (u)
end select

call mci%final ()
deallocate (mci)

```



```

write (u, "(A)")
write (u, "(A)")  "* Allocate MCI as vamp_t, allow for negative weights"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("vamp"), is_known = .true.)
call var_list%set_log (var_str ("?negative_weights"), &
    .true., is_known = .true.)

call dispatch_mci_setup (mci, var_list, process_id)
select type (mci)
type is (mci_vamp_t)
    call mci%write (u)
    call mci%write_history_parameters (u)
end select

call mci%final ()
deallocate (mci)

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_mci_1"

end subroutine dispatch_mci_1

```

Chapter 22

Parton shower and interface to PYTHIA6

This is the code for the WHIZARD QCD parton shower for final state radiation (FSR) and initial state radiation (ISR) as well as the interface to the PYTHIA module for showering and hadronization.

22.1 Basics of the shower

```
<shower_base.f90>≡  
  <File header>  
  
  module shower_base  
  
    <Use kinds>  
    <Use strings>  
    use lorentz  
    use particles  
    use os_interface  
    use rng_base  
    use variables  
    use model_data  
    use pdf  
    use tauola_interface  
  
    <Standard module head>  
  
    <Shower base: public>  
  
    <Shower base: parameters>  
  
    <Shower base: types>  
  
    <Shower base: interfaces>  
  
    interface  
    <Shower base: sub interfaces>
```

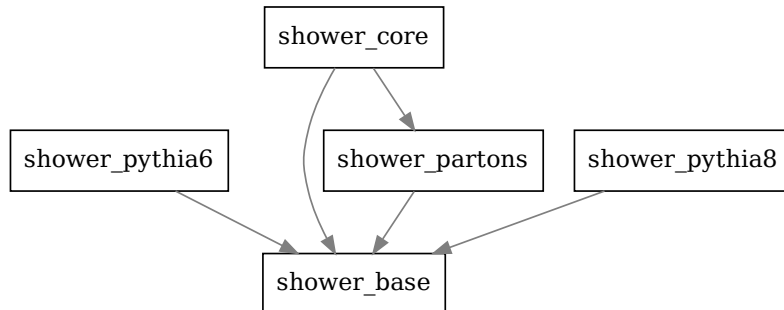


Figure 22.1: Module dependencies in `src/shower`.

```

end interface

end module shower_base

<shower_base_sub.f90>≡
  <File header>

  submodule (shower_base) shower_base_s

    use io_units
    use constants
    use diagnostics
    use format_utils, only: write_separator
    use physics_defs
    use sm_physics, only: running_as_lam

    implicit none

  contains

    <Shower base: procedures>

  end submodule shower_base_s

```

22.1.1 Shower implementations

```

<Shower base: public>≡
  public :: PS_WHIZARD, PS_PYTHIA6, PS_PYTHIA8, PS_UNDEFINED

<Shower base: parameters>≡
  integer, parameter :: PS_UNDEFINED = 0
  integer, parameter :: PS_WHIZARD = 1
  integer, parameter :: PS_PYTHIA6 = 2
  integer, parameter :: PS_PYTHIA8 = 3

```

A dictionary

```
<Shower base: public>+≡
    public :: shower_method_of_string

<Shower base: sub interfaces>≡
    elemental module function shower_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
    end function shower_method_of_string

<Shower base: procedures>≡
    elemental module function shower_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
        select case (char(string))
        case ("WHIZARD")
            i = PS_WHIZARD
        case ("PYTHIA6")
            i = PS_PYTHIA6
        case ("PYTHIA8")
            i = PS_PYTHIA8
        case default
            i = PS_UNDEFINED
        end select
    end function shower_method_of_string

<Shower base: public>+≡
    public :: shower_method_to_string

<Shower base: sub interfaces>+≡
    elemental module function shower_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
    end function shower_method_to_string

<Shower base: procedures>+≡
    elemental module function shower_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
        case (PS_WHIZARD)
            string = "WHIZARD"
        case (PS_PYTHIA6)
            string = "PYTHIA6"
        case (PS_PYTHIA8)
            string = "PYTHIA8"
        case default
            string = "UNDEFINED"
        end select
    end function shower_method_to_string
```

22.1.2 Shower settings

These the general shower settings, the settings and parameters for the matching are defined in the corresponding matching modules. The width and the

cutoff of the Gaussian primordial k_t distribution, PARP(91) and PARP(93), in GeV, are called `isr_primordial_kt_width` and `isr_primordial_kt_cutoff` in WHIZARD. The parameter MSTJ(45) gives the maximum number of flavors in gluon decay to quarks, and is here called `max_n_flavors`.

The two parameters `isr_alphas_running` and `fsr_alphas_running` decide whether to use constant or running α_s in the form of the function $D_{\alpha_s}(t)$ for the FSR and ISR (MSTJ(44), MSTP(64)), respectively. The next parameter, `fixed_alpha_s` is the parameter PARU(111), which sets the value for constant α_s , and the flag whether to use P_t -ordered ISR is `isr_pt_ordered`. From the entry `min_voirtuality` on, parameters have meanings both for the PYTHIA and WHIZARD parton shower(s), where PYTHIA values are denoted at the end of the line.

```

(Shower base: public)+≡
    public :: shower_settings_t

(Shower base: types)≡
    type :: shower_settings_t
        logical :: active = .false.
        logical :: isr_active = .false.
        logical :: fsr_active = .false.
        logical :: muli_active = .false.
        logical :: hadronization_active = .false.
        logical :: tau_dec = .false.
        logical :: verbose = .false.
        integer :: method = PS_UNDEFINED
        logical :: hadron_collision = .false.
        logical :: mlm_matching = .false.
        logical :: ckkw_matching = .false.
        logical :: powheg_matching = .false.
        type(string_t) :: pythia6_pygive
        type(string_t) :: pythia8_config
        type(string_t) :: pythia8_config_file
        real(default) :: min_virtuality = 1._default      ! PARJ(82)^2
        real(default) :: fsr_lambda = 0.29_default      ! PARP(72)
        real(default) :: isr_lambda = 0.29_default      ! PARP(61)
        integer :: max_n_flavors = 5                    ! MSTJ(45)
        logical :: isr_alphas_running = .true.          ! MSTP(64)
        logical :: fsr_alphas_running = .true.          ! MSTJ(44)
        real(default) :: fixed_alpha_s = 0.2_default    ! PARU(111)
        logical :: alpha_s_fudged = .true.
        logical :: isr_pt_ordered = .false.
        logical :: isr_angular_ordered = .true.         ! MSTP(62)
        real(default) :: isr_primordial_kt_width = 1.5_default ! PARP(91)
        real(default) :: isr_primordial_kt_cutoff = 5._default ! PARP(93)
        real(default) :: isr_z_cutoff = 0.999_default    ! 1-PARP(66)
        real(default) :: isr_minenergy = 2._default     ! PARP(65)
        real(default) :: isr_tscalefactor = 1._default
        logical :: isr_only_onshell_emitted_partons = .true. ! MSTP(63)
    contains
        (Shower base: shower settings: TBP)
end type shower_settings_t

```

Read in the shower settings (and flags whether matching and hadronization are

switched on).

(Shower base: shower settings: TBP)≡

```
procedure :: init => shower_settings_init
```

(Shower base: sub interfaces)+≡

```
module subroutine shower_settings_init (settings, var_list)
  class(shower_settings_t), intent(out) :: settings
  type(var_list_t), intent(in) :: var_list
end subroutine shower_settings_init
```

(Shower base: procedures)+≡

```
module subroutine shower_settings_init (settings, var_list)
  class(shower_settings_t), intent(out) :: settings
  type(var_list_t), intent(in) :: var_list

  settings%fsr_active = &
    var_list%get_lval (var_str ("?ps_fsr_active"))
  settings%isr_active = &
    var_list%get_lval (var_str ("?ps_isr_active"))
  settings%tau_dec = &
    var_list%get_lval (var_str ("?ps_taudec_active"))
  settings%mul_active = &
    var_list%get_lval (var_str ("?mul_active"))
  settings%hadronization_active = &
    var_list%get_lval (var_str ("?hadronization_active"))
  settings%mlm_matching = &
    var_list%get_lval (var_str ("?mlm_matching"))
  settings%ckkw_matching = &
    var_list%get_lval (var_str ("?ckkw_matching"))
  settings%powheg_matching = &
    var_list%get_lval (var_str ("?powheg_matching"))
  settings%method = shower_method_of_string ( &
    var_list%get_sval (var_str ("$shower_method")))
  settings%active = settings%isr_active .or. &
    settings%fsr_active .or. &
    settings%powheg_matching .or. &
    settings%mul_active .or. &
    settings%hadronization_active
  if (.not. settings%active) return
  settings%verbose = &
    var_list%get_lval (var_str ("?shower_verbose"))
  settings%pythia6_pygive = &
    var_list%get_sval (var_str ("$ps_PYTHIA_PYGIVE"))
  settings%pythia8_config = &
    var_list%get_sval (var_str ("$ps_PYTHIA8_config"))
  settings%pythia8_config_file = &
    var_list%get_sval (var_str ("$ps_PYTHIA8_config_file"))
  settings%min_virtuality = &
    (var_list%get_rval (var_str ("ps_mass_cutoff"))**2)
  settings%fsr_lambda = &
    var_list%get_rval (var_str ("ps_fsr_lambda"))
  settings%isr_lambda = &
    var_list%get_rval (var_str ("ps_isr_lambda"))
  settings%max_n_flavors = &
    var_list%get_ival (var_str ("ps_max_n_flavors"))
```

```

settings%isr_alphas_running = &
    var_list%get_lval (var_str ("?ps_isr_alphas_running"))
settings%fsr_alphas_running = &
    var_list%get_lval (var_str ("?ps_fsr_alphas_running"))
settings%fixed_alpha_s = &
    var_list%get_rval (var_str ("ps_fixed_alphas"))
settings%isr_pt_ordered = &
    var_list%get_lval (var_str ("?ps_isr_pt_ordered"))
settings%isr_angular_ordered = &
    var_list%get_lval (var_str ("?ps_isr_angular_ordered"))
settings%isr_primordial_kt_width = &
    var_list%get_rval (var_str ("ps_isr_primordial_kt_width"))
settings%isr_primordial_kt_cutoff = &
    var_list%get_rval (var_str ("ps_isr_primordial_kt_cutoff"))
settings%isr_z_cutoff = &
    var_list%get_rval (var_str ("ps_isr_z_cutoff"))
settings%isr_minenergy = &
    var_list%get_rval (var_str ("ps_isr_minenergy"))
settings%isr_tscalefactor = &
    var_list%get_rval (var_str ("ps_isr_tscalefactor"))
settings%isr_only_onshell_emitted_partons = &
    var_list%get_lval (&
        var_str ("?ps_isr_only_onshell_emitted_partons"))
end subroutine shower_settings_init

```

(Shower base: shower settings: TBP)+≡

```

procedure :: write => shower_settings_write

```

(Shower base: sub interfaces)+≡

```

module subroutine shower_settings_write (settings, unit)
    class(shower_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
end subroutine shower_settings_write

```

(Shower base: procedures)+≡

```

module subroutine shower_settings_write (settings, unit)
    class(shower_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Shower settings:"
    call write_separator (u)
    write (u, "(1x,A)") "Master switches:"
    write (u, "(3x,A,1x,L1)") &
        "ps_isr_active" = ", settings%isr_active
    write (u, "(3x,A,1x,L1)") &
        "ps_fsr_active" = ", settings%fsr_active
    write (u, "(3x,A,1x,L1)") &
        "ps_tau_dec" = ", settings%tau_dec
    write (u, "(3x,A,1x,L1)") &
        "muli_active" = ", settings%muli_active
    write (u, "(3x,A,1x,L1)") &
        "hadronization_active" = ", settings%hadronization_active
    write (u, "(1x,A)") "General settings:"
    if (settings%isr_active .or. settings%fsr_active) then

```

```

write (u, "(3x,A)") &
    "method" = " // &
    char (shower_method_to_string (settings%method))
write (u, "(3x,A,1x,L1)") &
    "shower_verbose" = ", settings%verbose
write (u, "(3x,A,ES19.12)") &
    "ps_mass_cutoff" = ", &
    sqrt (abs (settings%min_virtuality))
write (u, "(3x,A,1x,I1)") &
    "ps_max_n_flavors" = ", settings%max_n_flavors
else
    write (u, "(3x,A)") " [ISR and FSR off]"
end if
if (settings%isr_active) then
    write (u, "(1x,A)") "ISR settings:"
    write (u, "(3x,A,1x,L1)") &
        "ps_isr_pt_ordered" = ", settings%isr_pt_ordered
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_lambda" = ", settings%isr_lambda
    write (u, "(3x,A,1x,L1)") &
        "ps_isr_alphas_running" = ", settings%isr_alphas_running
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_primordial_kt_width" = ", settings%isr_primordial_kt_width
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_primordial_kt_cutoff" = ", &
        settings%isr_primordial_kt_cutoff
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_z_cutoff" = ", settings%isr_z_cutoff
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_minenergy" = ", settings%isr_minenergy
    write (u, "(3x,A,ES19.12)") &
        "ps_isr_tscalefactor" = ", settings%isr_tscalefactor
else if (settings%fsr_active) then
    write (u, "(3x,A)") " [ISR off]"
end if
if (settings%fsr_active) then
    write (u, "(1x,A)") "FSR settings:"
    write (u, "(3x,A,ES19.12)") &
        "ps_fsr_lambda" = ", settings%fsr_lambda
    write (u, "(3x,A,1x,L1)") &
        "ps_fsr_alphas_running" = ", settings%fsr_alphas_running
else if (settings%isr_active) then
    write (u, "(3x,A)") " [FSR off]"
end if
write (u, "(1x,A)") "Matching Settings:"
write (u, "(3x,A,1x,L1)") &
    "mlm_matching" = ", settings%mlm_matching
write (u, "(3x,A,1x,L1)") &
    "cckw_matching" = ", settings%cckw_matching
write (u, "(1x,A)") "PYTHIA6 specific settings:"
write (u, "(3x,A,A,A)") &
    "ps_PYTHIA_PYGIVE" = ', &
    char(settings%pythia6_pygive), ""
write (u, "(1x,A)") "PYTHIA8 specific settings:"

```



```

write (u, "(3x,A,A,A)") &
    "ps_PYTHIA8_config" = ', ' &
    char (settings%pythia8_config), ""
write (u, "(3x,A,A,A)") &
    "ps_PYTHIA8_config_file" = ', ' &
    char (settings%pythia8_config_file), ""
end subroutine shower_settings_write

```

22.1.3 Abstract Shower Type

Any parton shower implementation will use random numbers to generate emissions.

```

⟨Shower base: public⟩+≡
    public :: shower_base_t

⟨Shower base: types⟩+≡
    type, abstract :: shower_base_t
        class(rng_t), allocatable :: rng
        type(string_t) :: name
        type(pdf_data_t) :: pdf_data
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings
        type(os_data_t) :: os_data
        real(default) :: fac_scale
        real(default) :: alpha_s
    contains
        ⟨Shower base: shower base: TBP⟩
    end type shower_base_t

⟨Shower base: shower base: TBP⟩≡
    procedure :: write_msg => shower_base_write_msg

⟨Shower base: sub interfaces⟩+≡
    module subroutine shower_base_write_msg (shower)
        class(shower_base_t), intent(inout) :: shower
    end subroutine shower_base_write_msg

⟨Shower base: procedures⟩+≡
    module subroutine shower_base_write_msg (shower)
        class(shower_base_t), intent(inout) :: shower
        call msg_message ("Shower: Using " // char(shower%name) // " shower")
    end subroutine shower_base_write_msg

⟨Shower base: shower base: TBP⟩+≡
    procedure :: import_rng => shower_base_import_rng

⟨Shower base: sub interfaces⟩+≡
    pure module subroutine shower_base_import_rng (shower, rng)
        class(shower_base_t), intent(inout) :: shower
        class(rng_t), intent(inout), allocatable :: rng
    end subroutine shower_base_import_rng

```

```

<Shower base: procedures>+≡
  pure module subroutine shower_base_import_rng (shower, rng)
    class(shower_base_t), intent(inout) :: shower
    class(rng_t), intent(inout), allocatable :: rng
    call move_alloc (from = rng, to = shower%rng)
  end subroutine shower_base_import_rng

```

Shower implementations need to know the overall settings as well as pdf_data_t if ISR needs to be simulated. In order to use external files or tools we need access to os_data.

```

<Shower base: shower base: TBP>+≡
  procedure (shower_base_init), deferred :: init

<Shower base: interfaces>≡
  abstract interface
    subroutine shower_base_init (shower, settings, taudec_settings, pdf_data, os_data)
      import
      class(shower_base_t), intent(out) :: shower
      type(shower_settings_t), intent(in) :: settings
      type(taudec_settings_t), intent(in) :: taudec_settings
      type(pdf_data_t), intent(in) :: pdf_data
      type(os_data_t), intent(in) :: os_data
    end subroutine shower_base_init
  end interface

```

Prepare a new event.

Set event parameters: fac_scale, alpha_s

```

<Shower base: shower base: TBP>+≡
  procedure :: prepare_new_event => shower_base_prepare_new_event

<Shower base: sub interfaces>+≡
  module subroutine shower_base_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_base_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
  end subroutine shower_base_prepare_new_event

<Shower base: procedures>+≡
  module subroutine shower_base_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_base_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
    shower%fac_scale = fac_scale
    shower%alpha_s = alpha_s
  end subroutine shower_base_prepare_new_event

```

```

<Shower base: shower base: TBP>+≡
  procedure (shower_base_import_particle_set), deferred :: import_particle_set

<Shower base: interfaces>+≡
  abstract interface
    subroutine shower_base_import_particle_set &
      (shower, particle_set)
      import
      class(shower_base_t), target, intent(inout) :: shower
      type(particle_set_t), intent(in) :: particle_set

```

```

        end subroutine shower_base_import_particle_set
    end interface

    <Shower base: shower base: TBP>+≡
        procedure (shower_base_generate_emissions), deferred :: generate_emissions
    <Shower base: interfaces>+≡
        abstract interface
            subroutine shower_base_generate_emissions &
                (shower, valid, number_of_emissions)
            import
            class(shower_base_t), intent(inout), target :: shower
            logical, intent(out) :: valid
            integer, optional, intent(in) :: number_of_emissions
            end subroutine shower_base_generate_emissions
        end interface

    <Shower base: shower base: TBP>+≡
        procedure (shower_base_make_particle_set), deferred :: make_particle_set
    <Shower base: interfaces>+≡
        abstract interface
            subroutine shower_base_make_particle_set &
                (shower, particle_set, model, model_hadrons)
            import
            class(shower_base_t), intent(in) :: shower
            type(particle_set_t), intent(inout) :: particle_set
            class(model_data_t), intent(in), target :: model
            class(model_data_t), intent(in), target :: model_hadrons
            end subroutine shower_base_make_particle_set
        end interface

    <Shower base: shower base: TBP>+≡
        procedure (shower_base_get_final_colored_ME_momenta), deferred :: &
            get_final_colored_ME_momenta
    <Shower base: interfaces>+≡
        abstract interface
            subroutine shower_base_get_final_colored_ME_momenta &
                (shower, momenta)
            import
            class(shower_base_t), intent(in) :: shower
            type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
            end subroutine shower_base_get_final_colored_ME_momenta
        end interface

```

22.1.4 Additional parameters

These parameters are the cut-off scale t_{cut} , given in GeV^2 (PARJ(82)), the cut-off scale for the P_t^2 -ordered shower in GeV^2 , and the two shower parameters PARP(72) and PARP(61), respectively.

```

    <Shower base: parameters>+≡
        real(default), public :: D_min_scale = 0.5_default

```

Treating either u and d , or all quarks except t as massless:

```
<Shower base: parameters>+≡
  logical, public :: treat_light_quarks_massless = .true.
  logical, public :: treat_duscb_quarks_massless = .false.
```

Temporary parameters for the P_t -ordered shower:

```
<Shower base: parameters>+≡
  real(default), public :: scalefactor1 = 0.02_default
  real(default), public :: scalefactor2 = 0.02_default

<Shower base: public>+≡
  public :: D_alpha_s_isr
  public :: D_alpha_s_fsr

<Shower base: sub interfaces>+≡
  module function D_alpha_s_isr (tin, settings) result (alpha_s)
    real(default), intent(in) :: tin
    type(shower_settings_t), intent(in) :: settings
    real(default) :: alpha_s
  end function D_alpha_s_isr
  module function D_alpha_s_fsr (tin, settings) result (alpha_s)
    real(default), intent(in) :: tin
    type(shower_settings_t), intent(in) :: settings
    real(default) :: alpha_s
  end function D_alpha_s_fsr

<Shower base: procedures>+≡
  module function D_alpha_s_isr (tin, settings) result (alpha_s)
    real(default), intent(in) :: tin
    type(shower_settings_t), intent(in) :: settings
    real(default) :: min_virtuality, d_constalpha_s, d_lambda_isr
    integer :: d_nf
    real(default) :: t
    real(default) :: alpha_s
    min_virtuality = settings%min_virtuality
    d_lambda_isr = settings%isr_lambda
    d_constalpha_s = settings%fixed_alpha_s
    d_nf = settings%max_n_flavors
    if (settings%alpha_s_fudged) then
      t = max (max (0.1_default * min_virtuality, &
        1.1_default * d_lambda_isr**2), abs(tin))
    else
      t = abs(tin)
    end if
    if (settings%isr_alphas_running) then
      alpha_s = running_as_lam (number_of_flavors(t, d_nf, min_virtuality), &
        sqrt(t), d_lambda_isr, 0)
    else
      alpha_s = d_constalpha_s
    end if
  end function D_alpha_s_isr

  module function D_alpha_s_fsr (tin, settings) result (alpha_s)
    real(default), intent(in) :: tin
    type(shower_settings_t), intent(in) :: settings
    real(default) :: min_virtuality, d_lambda_fsr, d_constalpha_s
```

```

integer :: d_nf
real(default) :: t
real(default) :: alpha_s
min_virtuality = settings%min_virtuality
d_lambda_fsr = settings%fsr_lambda
d_constalpha_s = settings%fixed_alpha_s
d_nf = settings%max_n_flavors
if (settings%alpha_s_fudged) then
    t = max (max (0.1_default * min_virtuality, &
                  1.1_default * d_lambda_fsr**2), abs(tin))
else
    t = abs(tin)
end if
if (settings%fsr_alphas_running) then
    alpha_s = running_as_lam (number_of_flavors (t, d_nf, min_virtuality), &
                              sqrt(t), d_lambda_fsr, 0)
else
    alpha_s = d_constalpha_s
end if
end function D_alpha_s_fsr

```

Mass and mass squared selection functions. All masses are in GeV. Light quarks are assumed to be ordered, $m_1 < m_2 < m_3 \dots$, and they get current masses, not elementary ones. Mesons and baryons other than proton and neutron are needed as beam-remnants. Particles with PDG number zero are taken massless, as well as proper beam remnants and any other particles.

(Shower base: public)+≡

```

public :: mass_type
public :: mass_squared_type

```

(Shower base: sub interfaces)+≡

```

elemental module function mass_type (type, m2_default) result (mass)
    integer, intent(in) :: type
    real(default), intent(in) :: m2_default
    real(default) :: mass
end function mass_type
elemental module function mass_squared_type &
    (type, m2_default) result (mass2)
    integer, intent(in) :: type
    real(default), intent(in) :: m2_default
    real(default) :: mass2
end function mass_squared_type

```

(Shower base: procedures)+≡

```

elemental module function mass_type (type, m2_default) result (mass)
    integer, intent(in) :: type
    real(default), intent(in) :: m2_default
    real(default) :: mass
    mass = sqrt (mass_squared_type (type, m2_default))
end function mass_type

elemental module function mass_squared_type &
    (type, m2_default) result (mass2)
    integer, intent(in) :: type

```

```

real(default), intent(in) :: m2_default
real(default) :: mass2
select case (abs (type))
!!!   case (1,2)
!!!       if (treat_light_quarks_massless .or. &
!!!           treat_duscb_quarks_massless) then
!!!           mass2 = zero
!!!       else
!!!           mass2 = 0.330_default**2
!!!       end if
!!!   case (3)
!!!       if (treat_duscb_quarks_massless) then
!!!           mass2 = zero
!!!       else
!!!           mass2 = 0.500_default**2
!!!       end if
!!!   case (4)
!!!       if (treat_duscb_quarks_massless) then
!!!           mass2 = zero
!!!       else
!!!           mass2 = 1.500_default**2
!!!       end if
!!!   case (5)
!!!       if (treat_duscb_quarks_massless) then
!!!           mass2 = zero
!!!       else
!!!           mass2 = 4.800_default**2
!!!       end if
!!!   case (GLUON)
!!!       mass2 = zero
case (NEUTRON)
    mass2 = 0.939565_default**2
case (PROTON)
    mass2 = 0.93827_default**2
case (DPLUS)
    mass2 = 1.86960_default**2
case (D0)
    mass2 = 1.86483_default**2
case (B0)
    mass2 = 5.27950_default**2
case (BPLUS)
    mass2 = 5.27917_default**2
case (DELTAPLUSPLUS)
    mass2 = 1.232_default**2
case (SIGMA0)
    mass2 = 1.192642_default**2
case (SIGMAPLUS)
    mass2 = 1.18937_default**2
case (SIGMACPLUS)
    mass2 = 2.4529_default**2
case (SIGMACPLUSPLUS)
    mass2 = 2.45402_default**2
case (SIGMAB0)
    mass2 = 5.8152_default**2

```

```

case (SIGMABPLUS)
  mass2 = 5.8078_default**2
case (BEAM_REMNANT)
  mass2 = zero !!! don't know how to handle the beamremnant
case default
  mass2 = m2_default
end select
end function mass_squared_type

```

The number of flavors active at a certain scale (virtuality) t .

```

⟨Shower base: public⟩+≡
  public :: number_of_flavors

⟨Shower base: sub interfaces⟩+≡
  elemental module function number_of_flavors &
    (t, d_nf, min_virtuality) result (nr)
    real(default), intent(in) :: t, min_virtuality
    integer, intent(in) :: d_nf
    real(default) :: nr
  end function number_of_flavors

⟨Shower base: procedures⟩+≡
  elemental module function number_of_flavors &
    (t, d_nf, min_virtuality) result (nr)
    real(default), intent(in) :: t, min_virtuality
    integer, intent(in) :: d_nf
    real(default) :: nr
    integer :: i
    nr = 0
    if (t < min_virtuality) return ! arbitrary cut off
    ! TODO: do i = 1, min (max (3, d_nf), 6)
    do i = 1, min (3, d_nf)
      !!! to do: take heavier quarks(-> cuts on allowed costheta in g->qq)
      !!! into account
      if ((four * mass_squared_type (i, zero) + min_virtuality) < t ) then
        nr = i
      else
        exit
      end if
    end do
  end function number_of_flavors

```

22.1.5 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨shower_base_ut.f90⟩≡
  ⟨File header⟩

  module shower_base_ut
    use unit_tests
    use shower_base_util

  ⟨Standard module head⟩

```

```

    <Shower base: public test>

contains

    <Shower base: test driver>

end module shower_base_ut
<shower_base_uti.f90>≡
    <File header>

module shower_base_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use variables
    use shower_base

    <Standard module head>

    <Shower base: test declarations>

contains

    <Shower base: tests>

end module shower_base_uti
API: driver for the unit tests below.
<Shower base: public test>≡
    public :: shower_base_test
<Shower base: test driver>≡
    subroutine shower_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Shower base: execute tests>
    end subroutine shower_base_test

```

Shower settings

This test dispatches an `shower_settings` object, which is used to steer the initial and final state showers.

```

<Shower base: execute tests>≡
    call test (shower_base_1, "shower_base_1", &
        "Shower settings", &
        u, results)
<Shower base: test declarations>≡
    public :: shower_base_1

```



```

(Shower base: tests)=
subroutine shower_base_1 (u)
  integer, intent(in) :: u
  type(var_list_t) :: var_list
  type(shower_settings_t) :: shower_settings

  write (u, "(A)")  "* Test output: shower_base_1"
  write (u, "(A)")  "* Purpose: setting ISR/FSR shower"
  write (u, "(A)")

  write (u, "(A)")  "* Default settings"
  write (u, "(A)")

  call var_list%init_defaults (0)
  call var_list%set_log (var_str ("?alphas_is_fixed"), &
    .true., is_known = .true.)
  call shower_settings%init (var_list)
  call write_separator (u)
  call shower_settings%write (u)
  call write_separator (u)

  write (u, "(A)")
  write (u, "(A)")  "* Switch on ISR/FSR showers, hadronization"
  write (u, "(A)")  "      and MLM matching"
  write (u, "(A)")

  call var_list%set_string (var_str ("$shower_method"), &
    var_str ("PYTHIA6"), is_known = .true.)
  call var_list%set_log (var_str ("?ps_fsr_active"), &
    .true., is_known = .true.)
  call var_list%set_log (var_str ("?ps_isr_active"), &
    .true., is_known = .true.)
  call var_list%set_log (var_str ("?hadronization_active"), &
    .true., is_known = .true.)
  call var_list%set_log (var_str ("?mlm_matching"), &
    .true., is_known = .true.)
  call var_list%set_int &
    (var_str ("ps_max_n_flavors"), 4, is_known = .true.)
  call var_list%set_real &
    (var_str ("ps_isr_z_cutoff"), 0.1234_default, &
    is_known=.true.)
  call var_list%set_real (&
    var_str ("mlm_etamax"), 3.456_default, is_known=.true.)
  call var_list%set_string (&
    var_str ("ps_PYTHIA_PYGIVE"), var_str ("abcdefgh"), is_known=.true.)
  call shower_settings%init (var_list)
  call write_separator (u)
  call shower_settings%write (u)
  call write_separator (u)

  call var_list%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: shower_base_1"

```

```
end subroutine shower_base_1
```

22.2 Parton module for the shower

```
<shower_partons.f90>≡
  <File header>

  module shower_partons

    <Use kinds with double>
    use constants
    use lorentz
    use particles
    use model_data
    use shower_base
    use rng_base

    <Standard module head>

    <Shower partons: public>

    <Shower partons: types>

    interface
    <Shower partons: sub interfaces>
    end interface

  end module shower_partons

<shower_partons_sub.f90>≡
  <File header>

  submodule (shower_partons) shower_partons_s

    <Use debug>
    use io_units
    use system_defs, only: TAB
    use diagnostics
    use physics_defs
    use sm_physics
    use colors
    use flavors
    use subevents

    implicit none

  contains

    <Shower partons: procedures>

  end submodule shower_partons_s
```

22.2.1 The basic type defintions

The type `parton_t` defines a parton for the shower. The `x` value of the parton is only needed for spacelike showers. The pointer `initial` is only needed for partons in initial showers, it points to the hadron the parton is coming from. An auxiliary value for the P_t -ordered ISR is `aux_pt`. Then, there are two auxiliary entries for the clustering of CKKW pseudo weights and CKKW matching, `ckkwlabel` and `ckkwscale`. In order to make shower settings available to all operations on the shower partons, we endow the `parton_t` type with a pointer to `shower_settings_t`.

```

<Shower partons: public>≡
    public :: parton_t

<Shower partons: types>≡
    type :: parton_t
        integer :: nr = 0
        integer :: type = 0
        type(shower_settings_t), pointer :: settings => null()
        type(vector4_t) :: momentum = vector4_null
        real(default) :: t = zero
        real(default) :: mass2 = zero
        real(default) :: scale = zero
        real(default) :: z = zero
        real(default) :: costheta = zero
        real(default) :: x = zero
        logical :: simulated = .false.
        logical :: belongstoFSR = .true.
        logical :: belongstointeraction = .false.
        type(parton_t), pointer :: parent => null ()
        type(parton_t), pointer :: child1 => null ()
        type(parton_t), pointer :: child2 => null ()
        type(parton_t), pointer :: initial => null ()
        integer :: c1 = 0, c2 = 0
        integer :: aux_pt = 0
        integer :: ckkwlabel = 0
        real(default) :: ckkwscale = zero
        integer :: ckkwtype = -1
        integer :: interactionnr = 0
    contains
        <Shower partons: parton: TBP>
    end type parton_t

<Shower partons: public>+≡
    public :: parton_pointer_t

<Shower partons: types>+≡
    type :: parton_pointer_t
        type(parton_t), pointer :: p => null ()
    end type parton_pointer_t

```

22.2.2 Routines

```
<Shower partons: parton: TBP>≡
  procedure :: to_particle => parton_to_particle

<Shower partons: sub interfaces>≡
  module function parton_to_particle &
    (parton, model, from_hard_int) result (particle)
    type(particle_t) :: particle
    class(parton_t), intent(in) :: parton
    class(model_data_t), pointer, intent(in) :: model
    logical, intent(in), optional :: from_hard_int
  end function parton_to_particle

<Shower partons: procedures>≡
  module function parton_to_particle &
    (parton, model, from_hard_int) result (particle)
    type(particle_t) :: particle
    class(parton_t), intent(in) :: parton
    class(model_data_t), pointer, intent(in) :: model
    logical, intent(in), optional :: from_hard_int
    integer :: col, anti_col
    call parton%to_color (col, anti_col, from_hard_int)
    call particle%init (parton%to_status (from_hard_int), parton%type, &
      model, col, anti_col, parton%momentum)
  end function parton_to_particle

<Shower partons: public>+≡
  public :: parton_of_particle

<Shower partons: sub interfaces>+≡
  pure module function parton_of_particle (particle, nr) result (parton)
    type(parton_t) :: parton
    type(particle_t), intent(in) :: particle
    integer, intent(in) :: nr
  end function parton_of_particle

<Shower partons: procedures>+≡
  pure module function parton_of_particle (particle, nr) result (parton)
    type(parton_t) :: parton
    type(particle_t), intent(in) :: particle
    integer, intent(in) :: nr
    integer, dimension(2) :: col_array
    parton%nr = nr
    parton%momentum = particle%p
    parton%t = particle%p2
    parton%type = particle%flv%get_pdg ()
    col_array = particle%get_color ()
    parton%c1 = col_array (1)
    parton%c2 = col_array (2)
    parton%interactionnr = 1
    parton%mass2 = particle%flv%get_mass () ** 2
  end function parton_of_particle

<Shower partons: parton: TBP>+≡
  procedure :: to_status => parton_to_status
```

```

<Shower partons: sub interfaces>+≡
  pure module function parton_to_status &
    (parton, from_hard_int) result (status)
    integer :: status
    class(parton_t), intent(in) :: parton
    logical, intent(in), optional :: from_hard_int
  end function parton_to_status

<Shower partons: procedures>+≡
  pure module function parton_to_status &
    (parton, from_hard_int) result (status)
    integer :: status
    class(parton_t), intent(in) :: parton
    logical, intent(in), optional :: from_hard_int
    logical :: fhi
    fhi = .false.; if (present (from_hard_int)) fhi = from_hard_int
    if (fhi .or. parton%is_colored ()) then
      if (associated (parton%initial) .and. .not. parton%belongstoFSR) then
        status = PRT_INCOMING
      else
        status = PRT_OUTGOING
      end if
    else
      status = PRT_BEAM_REMNANT
    end if
  end function parton_to_status

<Shower partons: parton: TBP>+≡
  procedure :: to_color => parton_to_color

<Shower partons: sub interfaces>+≡
  pure module subroutine parton_to_color (parton, c1, c2, from_hard_int)
    class(parton_t), intent(in) :: parton
    integer, intent(out) :: c1, c2
    logical, intent(in), optional :: from_hard_int
  end subroutine parton_to_color

<Shower partons: procedures>+≡
  pure module subroutine parton_to_color (parton, c1, c2, from_hard_int)
    class(parton_t), intent(in) :: parton
    integer, intent(out) :: c1, c2
    logical, intent(in), optional :: from_hard_int
    logical :: fhi
    fhi = .false.; if (present (from_hard_int)) fhi = from_hard_int
    c1 = 0
    c2 = 0
    if (parton%is_colored ()) then
      if (fhi) then
        if (parton%c1 /= 0) c1 = parton%c1
        if (parton%c2 /= 0) c2 = parton%c2
      else
        if (parton%c1 /= 0) c1 = 500 + parton%c1
        if (parton%c2 /= 0) c2 = 500 + parton%c2
      end if
    end if
  end if

```

```

        end subroutine parton_to_color

    <Shower partons: public>+≡
        public :: parton_copy

    <Shower partons: sub interfaces>+≡
        module subroutine parton_copy (prt1, prt2)
            type(parton_t), intent(in) :: prt1
            type(parton_t), intent(out) :: prt2
        end subroutine parton_copy

    <Shower partons: procedures>+≡
        module subroutine parton_copy (prt1, prt2)
            type(parton_t), intent(in) :: prt1
            type(parton_t), intent(out) :: prt2
            if (associated (prt1%settings)) prt2%settings => prt1%settings
            prt2%nr = prt1%nr
            prt2%type = prt1%type
            prt2%momentum = prt1%momentum
            prt2%t = prt1%t
            prt2%mass2 = prt1%mass2
            prt2%scale = prt1%scale
            prt2%z = prt1%z
            prt2%costheta = prt1%costheta
            prt2%x = prt1%x
            prt2%simulated = prt1%simulated
            prt2%belongstoFSR = prt1%belongstoFSR
            prt2%belongstointeraction = prt1%belongstointeraction
            prt2%interactionnr = prt1%interactionnr
            if (associated (prt1%parent)) prt2%parent => prt1%parent
            if (associated (prt1%child1)) prt2%child1 => prt1%child1
            if (associated (prt1%child2)) prt2%child2 => prt1%child2
            if (associated (prt1%initial)) prt2%initial => prt1%initial
            prt2%c1 = prt1%c1
            prt2%c2 = prt1%c2
            prt2%aux_pt = prt1%aux_pt
        end subroutine parton_copy

```

This returns the angle between the daughters assuming them to be massless.

```

    <Shower partons: parton: TBP>+≡
        procedure :: get_costheta => parton_get_costheta

    <Shower partons: sub interfaces>+≡
        elemental module function parton_get_costheta (prt) result (costheta)
            class(parton_t), intent(in) :: prt
            real(default) :: costheta
        end function parton_get_costheta

    <Shower partons: procedures>+≡
        elemental module function parton_get_costheta (prt) result (costheta)
            class(parton_t), intent(in) :: prt
            real(default) :: costheta
            real(default) :: denom
            denom = two * prt%z * (one - prt%z) * prt%momentum%p(0)**2
            if (denom > eps0) then

```

```

        costheta = one - prt%t / denom
    else
        costheta = - one
    end if
end function parton_get_costheta

```

The same for massive daughters.

```

<Shower partons: parton: TBP>+≡
    procedure :: get_costheta_mass => parton_get_costheta_mass

<Shower partons: sub interfaces>+≡
    elemental module function parton_get_costheta_mass (prt) result (costheta)
        class(parton_t), intent(in) :: prt
        real(default) :: costheta
    end function parton_get_costheta_mass

<Shower partons: procedures>+≡
    elemental module function parton_get_costheta_mass (prt) result (costheta)
        class(parton_t), intent(in) :: prt
        real(default) :: costheta
        real(default) :: sqrt12
        if (prt%is_branched ()) then
            if (prt%child1%simulated .and. &
                prt%child2%simulated) then
                sqrt12 = sqrt (max (zero, (prt%z)**2 * prt%momentum%p(0)**2 &
                    - prt%child1%t)) * &
                    sqrt (max (zero, (one - prt%z)**2 * prt%momentum%p(0)**2 &
                        - prt%child2%t))

                if (sqrt12 > eps0) then
                    costheta = (prt%t - prt%child1%t - prt%child2%t - &
                        two * prt%z * (one - prt%z) * prt%momentum%p(0)**2) / &
                        (- two * sqrt12)
                    return
                end if
            end if
        end if
        costheta = prt%get_costheta ()
    end function parton_get_costheta_mass

```

This function returns the angle between the momentum vectors of the parton and first daughter. This is only used for debugging.

```

<Shower partons: parton: TBP>+≡
    procedure :: get_costheta_motherfirst => parton_get_costheta_motherfirst

<Shower partons: sub interfaces>+≡
    elemental module function parton_get_costheta_motherfirst &
        (prt) result (costheta)
        class(parton_t), intent(in) :: prt
        real(default) :: costheta
    end function parton_get_costheta_motherfirst

<Shower partons: procedures>+≡
    elemental module function parton_get_costheta_motherfirst &
        (prt) result (costheta)
        class(parton_t), intent(in) :: prt

```

```

real(default) :: costheta
if (prt%is_branched ()) then
  if ((prt%child1%simulated .or. &
      prt%child1%is_final () .or. &
      prt%child1%is_branched ()) .and. &
      (prt%child2%simulated .or. &
      prt%child2%is_final () .or. &
      prt%child2%is_branched ())) then
    costheta = enclosed_angle_ct (prt%momentum, prt%child1%momentum)
    return
  end if
end if
costheta = - two
end function parton_get_costheta_motherfirst

```

Get the parton velocities.

```

<Shower partons: parton: TBP>+≡
  procedure :: get_beta => parton_get_beta

<Shower partons: sub interfaces>+≡
  elemental module function parton_get_beta (prt) result (beta)
    class(parton_t), intent(in) :: prt
    real(default) :: beta
  end function parton_get_beta

<Shower partons: procedures>+≡
  pure function get_beta (t,E) result (beta)
    real(default), intent(in) :: t,E
    real(default) :: beta
    beta = sqrt (max (tiny_07, one - t /(E**2)))
  end function get_beta

  elemental module function parton_get_beta (prt) result (beta)
    class(parton_t), intent(in) :: prt
    real(default) :: beta
    beta = sqrt (max (tiny_07, one - prt%t / prt%momentum%p(0)**2))
  end function parton_get_beta

```

Write routine.

```

<Shower partons: parton: TBP>+≡
  procedure :: write => parton_write

<Shower partons: sub interfaces>+≡
  module subroutine parton_write (prt, unit)
    class(parton_t), intent(in) :: prt
    integer, intent(in), optional :: unit
  end subroutine parton_write

<Shower partons: procedures>+≡
  module subroutine parton_write (prt, unit)
    class(parton_t), intent(in) :: prt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return

```



```

write (u, "(1x,7A)") "Shower parton <nr>", TAB, "<type>", TAB // TAB, &
    "<parent>", TAB, "<mom(0:3)>"
write (u, "(2x,I5,3A)", advance = "no") prt%nr, TAB, TAB, TAB
if (prt%is_final ()) then
    write (u, "(1x,I5,1x,A)", advance = "no") prt%type, TAB // TAB
else
    write (u, "( '[',I5,' ]',A)", advance = "no") prt%type, TAB // TAB
end if
if (associated (prt%parent)) then
    write (u, "(I5,A)", advance = "no") prt%parent%nr, TAB // TAB
else
    write (u, "(5x,2A)", advance = "no") TAB, TAB
end if
write (u, "(4(ES12.5,A))") prt%momentum%p(0), TAB, &
    prt%momentum%p(1), TAB, &
    prt%momentum%p(2), TAB, &
    prt%momentum%p(3)
write (u, "(1x,9A)") "<p4square>", TAB // TAB, "<t>", TAB // TAB, &
    "<scale>", TAB // TAB, "<c1>", TAB, "<c2>", TAB, "<mass2>"
write (u, "(1x,3(ES12.5,A))", advance = "no") &
    prt%momentum ** 2, TAB // TAB, prt%t, TAB, prt%scale, TAB, prt%mass2
write (u, "(2(I4,A))") prt%c1, TAB, prt%c2, TAB
if (prt%is_branched ()) then
    if (prt%belongstoFSR) then
        write (u, "(1x,9A)") "costheta(prt)", TAB, &
            "costheta_correct(prt)", TAB, &
            "prt%costheta", TAB, "prt%z", TAB, &
            "costheta_motherfirst(prt)"
        write (u, "(1X,5(ES12.5,A))") &
            prt%get_costheta (), TAB, &
            prt%get_costheta_mass (), TAB // TAB, &
            prt%costheta, TAB, prt%z, TAB, &
            prt%get_costheta_motherfirst (), TAB
    else
        write (u, "(1x,9A)") "prt%z", TAB, "prt%x", TAB, &
            "costheta_correct(prt)", TAB, &
            "prt%costheta", TAB, &
            "costheta_motherfirst(prt)"
        write (u, "(1X,5(ES12.5,A))") &
            prt%z, TAB, prt%x, TAB, &
            prt%get_costheta_mass (), TAB, &
            prt%costheta, TAB, &
            prt%get_costheta_motherfirst (), TAB
    end if
else
    if (prt%belongstoFSR) then
        write (u, "(1X,A)") "not branched."
    else
        write (u, "(1X,A,ES12.5)") "not branched. x = ", prt%x
    end if
end if
write (u, "(A)", advance = "no") " Parton"
if (prt%belongstoFSR) then
    write (u, "(A)", advance = "no") " is FSR,"

```

```

else
  if (associated (prt%initial)) then
    write (u, "(A,I1)", advance = "no") " from hadron,", prt%initial%nr
  else
    write (u, "(A)", advance = "no") ""
  end if
end if
if (prt%is_final ()) then
  write (u, "(A)", advance = "no") " is final,"
else
  write (u, "(A)", advance = "no") ""
end if
if (prt%simulated) then
  write (u, "(A)", advance = "no") " is simulated,"
else
  write (u, "(A)", advance = "no") ""
end if
if (associated (prt%child1) .and. associated (prt%child2)) then
  write (u, "(A,2(I5),A)", advance = "no") &
    " has children: ", prt%child1%nr, prt%child2%nr, ","
else if (associated (prt%child1)) then
  write (u, "(A,1(I5),A)", advance = "no") &
    " has one child: ", prt%child1%nr, ", "
end if
if (prt%belongstointeraction) then
  write (u, "(A,I2)") " belongs to interaction ", &
    prt%interactionnr
else
  write (u, "(A,I2)") " does not belong to interaction ", &
    prt%interactionnr
end if
write (u, "(A)") TAB
end subroutine parton_write

```

<Shower partons: parton: TBP>+≡

```

procedure :: is_final => parton_is_final

```

<Shower partons: sub interfaces>+≡

```

elemental module function parton_is_final (prt) result (is_final)
  class(parton_t), intent(in) :: prt
  logical :: is_final
end function parton_is_final

```

<Shower partons: procedures>+≡

```

elemental module function parton_is_final (prt) result (is_final)
  class(parton_t), intent(in) :: prt
  logical :: is_final
  is_final = .false.
  if (prt%belongstoFSR) then
    is_final = .not. associated (prt%child1) .and. &
      (.not. prt%belongstointeraction .or. &
        (prt%belongstointeraction .and. prt%simulated))
  end if
end function parton_is_final

```

```

<Shower partons: parton: TBP>+=
  procedure :: is_branched => parton_is_branched

<Shower partons: sub interfaces>+=
  elemental module function parton_is_branched (prt) result (is_branched)
    class(parton_t), intent(in) :: prt
    logical :: is_branched
  end function parton_is_branched

<Shower partons: procedures>+=
  elemental module function parton_is_branched (prt) result (is_branched)
    class(parton_t), intent(in) :: prt
    logical :: is_branched
    is_branched = associated (prt%child1) .and. associated (prt%child2)
  end function parton_is_branched

<Shower partons: parton: TBP>+=
  procedure :: set_simulated => parton_set_simulated

<Shower partons: sub interfaces>+=
  pure module subroutine parton_set_simulated (prt, sim)
    class(parton_t), intent(inout) :: prt
    logical, intent(in), optional :: sim
  end subroutine parton_set_simulated

<Shower partons: procedures>+=
  pure module subroutine parton_set_simulated (prt, sim)
    class(parton_t), intent(inout) :: prt
    logical, intent(in), optional :: sim
    if (present (sim)) then
      prt%simulated = sim
    else
      prt%simulated = .true.
    end if
  end subroutine parton_set_simulated

<Shower partons: public>+=
  public :: parton_set_parent

<Shower partons: sub interfaces>+=
  module subroutine parton_set_parent (prt, parent)
    type(parton_t), intent(inout) :: prt
    type(parton_t), intent(in) , target :: parent
  end subroutine parton_set_parent

<Shower partons: procedures>+=
  module subroutine parton_set_parent (prt, parent)
    type(parton_t), intent(inout) :: prt
    type(parton_t), intent(in) , target :: parent
    prt%parent => parent
  end subroutine parton_set_parent

<Shower partons: public>+=
  public :: parton_get_parent

```

```

<Shower partons: sub interfaces>+≡
    module function parton_get_parent (prt) result (parent)
        type(parton_t), intent(in) :: prt
        type(parton_t), pointer :: parent
    end function parton_get_parent

<Shower partons: procedures>+≡
    module function parton_get_parent (prt) result (parent)
        type(parton_t), intent(in) :: prt
        type(parton_t), pointer :: parent
        parent => prt%parent
    end function parton_get_parent

<Shower partons: public>+≡
    public :: parton_set_initial

<Shower partons: sub interfaces>+≡
    module subroutine parton_set_initial (prt, initial)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in) , target :: initial
    end subroutine parton_set_initial

<Shower partons: procedures>+≡
    module subroutine parton_set_initial (prt, initial)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in) , target :: initial
        prt%initial => initial
    end subroutine parton_set_initial

<Shower partons: public>+≡
    public :: parton_get_initial

<Shower partons: sub interfaces>+≡
    module function parton_get_initial (prt) result (initial)
        type(parton_t), intent(in) :: prt
        type(parton_t), pointer :: initial
    end function parton_get_initial

<Shower partons: procedures>+≡
    module function parton_get_initial (prt) result (initial)
        type(parton_t), intent(in) :: prt
        type(parton_t), pointer :: initial
        initial => prt%initial
    end function parton_get_initial

<Shower partons: public>+≡
    public :: parton_set_child

<Shower partons: sub interfaces>+≡
    module subroutine parton_set_child (prt, child, i)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in), target :: child
        integer, intent(in) :: i
    end subroutine parton_set_child

```

```

<Shower partons: procedures>+≡
  module subroutine parton_set_child (prt, child, i)
    type(parton_t), intent(inout) :: prt
    type(parton_t), intent(in), target :: child
    integer, intent(in) :: i
    if (i == 1) then
      prt%child1 => child
    else
      prt%child2 => child
    end if
  end subroutine parton_set_child

<Shower partons: public>+≡
  public :: parton_get_child

<Shower partons: sub interfaces>+≡
  module function parton_get_child (prt, i) result (child)
    type(parton_t), pointer :: child
    type(parton_t), intent(in) :: prt
    integer, intent(in) :: i
  end function parton_get_child

<Shower partons: procedures>+≡
  module function parton_get_child (prt, i) result (child)
    type(parton_t), pointer :: child
    type(parton_t), intent(in) :: prt
    integer, intent(in) :: i
    child => null ()
    if (i == 1) then
      child => prt%child1
    else
      child => prt%child2
    end if
  end function parton_get_child

<Shower partons: parton: TBP>+≡
  procedure :: is_quark => parton_is_quark

<Shower partons: sub interfaces>+≡
  elemental module function parton_is_quark (prt) result (is_quark)
    class(parton_t), intent(in) :: prt
    logical :: is_quark
  end function parton_is_quark

<Shower partons: procedures>+≡
  elemental module function parton_is_quark (prt) result (is_quark)
    class(parton_t), intent(in) :: prt
    logical :: is_quark
    is_quark = abs (prt%type) <= 6 .and. prt%type /= 0
  end function parton_is_quark

<Shower partons: parton: TBP>+≡
  procedure :: is_squark => parton_is_squark

```

```

<Shower partons: sub interfaces>+≡
    elemental module function parton_is_squark (prt) result (is_squark)
        class(parton_t), intent(in) :: prt
        logical :: is_squark
    end function parton_is_squark

<Shower partons: procedures>+≡
    elemental module function parton_is_squark (prt) result (is_squark)
        class(parton_t), intent(in) :: prt
        logical :: is_squark
        is_squark = ((abs(prt%type) >= 1000001) .and. (abs(prt%type) <= 1000006)) &
            .or. ((abs(prt%type) >= 2000001) .and. (abs(prt%type) <= 2000006))
    end function parton_is_squark

```

9 can be used for gluons in codes for glueballs

```

<Shower partons: parton: TBP>+≡
    procedure :: is_gluon => parton_is_gluon

<Shower partons: sub interfaces>+≡
    elemental module function parton_is_gluon (prt) result (is_gluon)
        class(parton_t), intent(in) :: prt
        logical :: is_gluon
    end function parton_is_gluon

<Shower partons: procedures>+≡
    elemental module function parton_is_gluon (prt) result (is_gluon)
        class(parton_t), intent(in) :: prt
        logical :: is_gluon
        is_gluon = prt%type == GLUON .or. prt%type == 9
    end function parton_is_gluon

<Shower partons: parton: TBP>+≡
    procedure :: is_gluino => parton_is_gluino

<Shower partons: sub interfaces>+≡
    elemental module function parton_is_gluino (prt) result (is_gluino)
        class(parton_t), intent(in) :: prt
        logical :: is_gluino
    end function parton_is_gluino

<Shower partons: procedures>+≡
    elemental module function parton_is_gluino (prt) result (is_gluino)
        class(parton_t), intent(in) :: prt
        logical :: is_gluino
        is_gluino = prt%type == 1000021
    end function parton_is_gluino

<Shower partons: parton: TBP>+≡
    procedure :: is_proton => parton_is_proton

<Shower partons: sub interfaces>+≡
    elemental module function parton_is_proton (prt) result (is_hadron)
        class(parton_t), intent(in) :: prt
        logical :: is_hadron
    end function parton_is_proton

```

```

<Shower partons: procedures>+≡
  elemental module function parton_is_proton (prt) result (is_hadron)
    class(parton_t), intent(in) :: prt
    logical :: is_hadron
    is_hadron = abs (prt%type) == PROTON
  end function parton_is_proton

```

TODO: SUSY partons.

```

<Shower partons: parton: TBP>+≡
  procedure :: is_colored => parton_is_colored

```

```

<Shower partons: sub interfaces>+≡
  pure module function parton_is_colored (parton) result (is_colored)
    logical :: is_colored
    class(parton_t), intent(in) :: parton
  end function parton_is_colored

```

```

<Shower partons: procedures>+≡
  pure module function parton_is_colored (parton) result (is_colored)
    logical :: is_colored
    class(parton_t), intent(in) :: parton
    is_colored = parton_is_quark (parton) .or. parton_is_gluon (parton)
  end function parton_is_colored

```

```

<Shower partons: parton: TBP>+≡
  procedure :: mass => parton_mass

```

```

<Shower partons: sub interfaces>+≡
  elemental module function parton_mass (prt) result (mass)
    class(parton_t), intent(in) :: prt
    real(default) :: mass
  end function parton_mass

```

```

<Shower partons: procedures>+≡
  elemental module function parton_mass (prt) result (mass)
    class(parton_t), intent(in) :: prt
    real(default) :: mass
    mass = mass_type (prt%type, prt%mass2)
  end function parton_mass

```

```

<Shower partons: parton: TBP>+≡
  procedure :: mass_squared => parton_mass_squared

```

```

<Shower partons: sub interfaces>+≡
  elemental module function parton_mass_squared (prt) result (mass_squared)
    class(parton_t), intent(in) :: prt
    real(default) :: mass_squared
  end function parton_mass_squared

```

```

<Shower partons: procedures>+≡
  elemental module function parton_mass_squared (prt) result (mass_squared)
    class(parton_t), intent(in) :: prt
    real(default) :: mass_squared
    mass_squared = mass_squared_type (prt%type, prt%mass2)
  end function parton_mass_squared

```

```

<Shower partons: parton: TBP>+≡
  procedure :: momentum_to_pythia6 => parton_momentum_to_pythia6

<Shower partons: sub interfaces>+≡
  pure module function parton_momentum_to_pythia6 (prt) result (p)
    real(double), dimension(1:5) :: p
    class(parton_t), intent(in) :: prt
  end function parton_momentum_to_pythia6

<Shower partons: procedures>+≡
  pure module function parton_momentum_to_pythia6 (prt) result (p)
    real(double), dimension(1:5) :: p
    class(parton_t), intent(in) :: prt
    p = prt%momentum%to_pythia6 (prt%mass ())
  end function parton_momentum_to_pythia6

<Shower partons: public>+≡
  public :: P_prt_to_child1

<Shower partons: sub interfaces>+≡
  module function P_prt_to_child1 (prt) result (retvalue)
    type(parton_t), intent(in) :: prt
    real(default) :: retvalue
  end function P_prt_to_child1

<Shower partons: procedures>+≡
  module function P_prt_to_child1 (prt) result (retvalue)
    type(parton_t), intent(in) :: prt
    real(default) :: retvalue
    retvalue = zero
    if (prt%is_gluon ()) then
      if (prt%child1%is_quark ()) then
        retvalue = P_gqq (prt%z)
      else if (prt%child1%is_gluon ()) then
        retvalue = P_ggg (prt%z) + P_ggg (one - prt%z)
      end if
    else if (prt%is_quark ()) then
      if (prt%child1%is_quark ()) then
        retvalue = P_qqg (prt%z)
      else if (prt%child1%is_gluon ()) then
        retvalue = P_qqg (one - prt%z)
      end if
    end if
  end function P_prt_to_child1

```

This function returns whether the kinematics of the branching of parton prt into its daughters are allowed or not.

```

<Shower partons: public>+≡
  public :: thetabar

<Shower partons: sub interfaces>+≡
  module function thetabar (prt, recoiler, isr_ang, E3out) result (retvalue)
    type(parton_t), intent(inout) :: prt
    type(parton_t), intent(in) :: recoiler
    real(default), intent(out), optional :: E3out

```



```

        logical, intent(in) :: isr_ang
        logical :: retvalue
    end function thetabar

<Shower partons: procedures>+≡
    module function thetabar (prt, recoiler, isr_ang, E3out) result (retvalue)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in) :: recoiler
        real(default), intent(out), optional :: E3out
        logical, intent(in) :: isr_ang
        logical :: retvalue
        real(default) :: ctheta, cthetachild1
        real(default) p1, p4, p3, E3, shat

        shat = (prt%child1%momentum + recoiler%momentum)**2
        E3 = 0.5_default * (shat / prt%z - recoiler%t + prt%child1%t - &
            prt%child2%mass_squared ()) / sqrt(shat)
        if (present (E3out)) then
            E3out = E3
        end if
        !!! absolute values of momenta in a 3 -> 1 + 4 branching
        p3 = sqrt (E3**2 - prt%t)
        p1 = sqrt (prt%child1%momentum%p(0)**2 - prt%child1%t)
        p4 = sqrt (max (zero, (E3 - prt%child1%momentum%p(0))**2 &
            - prt%child2%t))
        if (p3 > zero) then
            retvalue = ((p1 + p4 >= p3) .and. (p3 >= abs(p1 - p4)) )
            if (retvalue .and. isr_ang) then
                !!! check angular ordering
                if (associated (prt%child1)) then
                    if (associated (prt%child1%child2)) then
                        ctheta = (E3**2 - p1**2 - p4**2 + prt%t) / (two * p1 * p4)
                        cthetachild1 = (prt%child1%momentum%p(0)**2 - &
                            space_part (prt%child1%child1%momentum)**2 &
                            - space_part (prt%child1%child2%momentum)**2 + prt%child1%t) &
                            / (two * space_part (prt%child1%child1%momentum)**1 * &
                                space_part (prt%child1%child2%momentum)**1)
                        retvalue = (ctheta > cthetachild1)
                    end if
                end if
            end if
        else
            retvalue = .false.
        end if
    end function thetabar

<Shower partons: public>+≡
    public :: parton_apply_cstheta

<Shower partons: sub interfaces>+≡
    recursive module subroutine parton_apply_cstheta (prt, rng)
        type(parton_t), intent(inout) :: prt
        class(rng_t), intent(inout), allocatable :: rng
    end subroutine parton_apply_cstheta

```

<Shower partons: procedures>+≡

```

recursive module subroutine parton_apply_costheta (prt, rng)
  type(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
  if (debug2_active (D_SHOWER)) then
    print *, "D: parton_apply_costheta for parton " , prt%nr
    print *, 'prt%momentum%p = ', prt%momentum%p
    if (debug_on) call msg_debug2 (D_SHOWER, "prt%type", prt%type)
  end if
  prt%z = 0.5_default * (one + prt%get_beta () * prt%costheta)
  if (associated (prt%child1) .and. associated (prt%child2)) then
    if (prt%child1%simulated .and. prt%child2%simulated) then
      prt%z = 0.5_default * (one + (prt%child1%t - prt%child2%t) / &
        prt%t + prt%get_beta () * prt%costheta * &
        sqrt((prt%t - prt%child1%t - prt%child2%t)**2 - &
          4 * prt%child1%t * prt%child2%t) / prt%t)
      if (prt%type /= INTERNAL) then
        prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
        prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
      end if
      call prt%generate_ps (rng)
      call parton_apply_costheta (prt%child1, rng)
      call parton_apply_costheta (prt%child2, rng)
    end if
  end if
end subroutine parton_apply_costheta

```

<Shower partons: public>+≡

```

public :: parton_apply_lorentztrafo

```

<Shower partons: sub interfaces>+≡

```

module subroutine parton_apply_lorentztrafo (prt, L)
  type(parton_t), intent(inout) :: prt
  type(lorentz_transformation_t), intent(in) :: L
end subroutine parton_apply_lorentztrafo

```

<Shower partons: procedures>+≡

```

module subroutine parton_apply_lorentztrafo (prt, L)
  type(parton_t), intent(inout) :: prt
  type(lorentz_transformation_t), intent(in) :: L
  prt%momentum = L * prt%momentum
end subroutine parton_apply_lorentztrafo

```

<Shower partons: public>+≡

```

public :: parton_apply_lorentztrafo_recursive

```

<Shower partons: sub interfaces>+≡

```

recursive module subroutine parton_apply_lorentztrafo_recursive (prt, L)
  type(parton_t), intent(inout) :: prt
  type(lorentz_transformation_t), intent(in) :: L
end subroutine parton_apply_lorentztrafo_recursive

```

<Shower partons: procedures>+≡

```

recursive module subroutine parton_apply_lorentztrafo_recursive (prt, L)
  type(parton_t), intent(inout) :: prt

```

```

type(lorentz_transformation_t) ,intent(in) :: L
if (prt%type /= PROTON .and. prt%type /= BEAM_REMNANT) then
  !!! don't boost hadrons and beam-remnants
  call parton_apply_lorentztrafo (prt, L)
end if
if (associated (prt%child1) .and. associated (prt%child2)) then
  if ((space_part_norm (prt%child1%momentum) < eps0) .and. &
      (space_part_norm (prt%child2%momentum) < eps0) .and. &
      (.not. prt%child1%belongstointeraction) .and. &
      (.not. prt%child2%belongstointeraction)) then
    !!! don't boost unevolved timelike partons
  else
    call parton_apply_lorentztrafo_recursive (prt%child1, L)
    call parton_apply_lorentztrafo_recursive (prt%child2, L)
  end if
else
  if (associated (prt%child1)) then
    call parton_apply_lorentztrafo_recursive (prt%child1, L)
  end if
  if (associated (prt%child2)) then
    call parton_apply_lorentztrafo_recursive (prt%child2, L)
  end if
end if
end subroutine parton_apply_lorentztrafo_recursive

```

This takes the three-momentum of a parton and generates three-momenta of its children given their energy and virtuality

<Shower partons: parton: TBP>+≡

```

procedure :: generate_ps => parton_generate_ps

```

<Shower partons: sub interfaces>+≡

```

module subroutine parton_generate_ps (prt, rng)
  class(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
end subroutine parton_generate_ps

```

<Shower partons: procedures>+≡

```

module subroutine parton_generate_ps (prt, rng)
  class(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
  real(default), dimension(1:3, 1:3) :: directions
  integer i,j
  real(default) :: scproduct, pabs, plabs, p2abs, x, ptabs, phi
  real(default), dimension(1:3) :: momentum
  type(vector3_t) :: pchild1_direction
  type(lorentz_transformation_t) :: L, rotation
  if (debug2_active (D_SHOWER)) &
    print *, "D: parton_generate_ps for parton " , prt%nr
  if (debug_active (D_SHOWER)) then
    if (.not. (associated (prt%child1) .and. associated (prt%child2))) then
      call msg_fatal ("no children for generate_ps")
    end if
  end if
  !!! test if parton is a virtual parton from the imagined parton shower history
  if (prt%type == INTERNAL) then

```

```

L = inverse (boost (prt%momentum, sqrt(prt%t)))
!!! boost to restframe of mother
call parton_apply_lorentztrafo (prt, L)
call parton_apply_lorentztrafo (prt%child1, L)
call parton_apply_lorentztrafo (prt%child2, L)
!!! Store child1's momenta
pchild1_direction = direction (space_part (prt%child1%momentum))
!!! Redistribute energy
prt%child1%momentum%p(0) = (prt%momentum%p(0)**2 - &
    prt%child2%t + prt%child1%t) / (two * prt%momentum%p(0))
prt%child2%momentum%p(0) = prt%momentum%p(0) - &
    prt%child1%momentum%p(0)

! rescale momenta and set momenta to be along z-axis
prt%child1%momentum = vector4_moving (prt%child1%momentum%p(0), &
    vector3_canonical(3) * &
    sqrt(prt%child1%momentum%p(0)**2 - prt%child1%t))
prt%child2%momentum = vector4_moving (prt%child2%momentum%p(0), &
    - vector3_canonical(3) * &
    sqrt(prt%child2%momentum%p(0)**2 - prt%child2%t))

!!! rotate so that total momentum is along former total momentum
rotation = rotation_to_2nd (space_part (prt%child1%momentum), &
    pchild1_direction)
call parton_apply_lorentztrafo (prt%child1, rotation)
call parton_apply_lorentztrafo (prt%child2, rotation)

L = inverse (L)          !!! inverse of the boost to restframe of mother
call parton_apply_lorentztrafo (prt, L)
call parton_apply_lorentztrafo (prt%child1, L)
call parton_apply_lorentztrafo (prt%child2, L)
else
!!! directions(1,:) -> direction of the parent parton
if (space_part_norm (prt%momentum) < eps0) return
directions(1,1:3) = prt%momentum%p(1:3) / space_part_norm (prt%momentum)
!!! directions(2,:) and directions(3,:) -> two random directions
!!! perpendicular to the direction of the parent parton
do j = 2, 3
    call rng%generate (directions(j,:))
end do
do i = 2, 3
    scproduct = zero
    do j = 1, i - 1
        scproduct = directions(i,1) * directions(j,1) + &
            directions(i,2) * directions(j,2) + &
            directions(i,3) * directions(j,3)
        directions(i,1) = directions(i,1) - directions(j,1) * scproduct
        directions(i,2) = directions(i,2) - directions(j,2) * scproduct
        directions(i,3) = directions(i,3) - directions(j,3) * scproduct
    end do
    scproduct = directions(i,1)**2 + directions(i,2)**2 + &
        directions(i,3)**2
    do j = 1, 3
        directions(i,j) = directions(i,j) / sqrt(scproduct)
    end do
end do

```

```

        end do
    end do
    <Enforce right-handed system for directions>

    pabs = space_part_norm (prt%momentum)
    if ((prt%child1%momentum%p(0)**2 - prt%child1%t < 0) .or. &
        (prt%child2%momentum%p(0)**2 - prt%child2%t < 0)) then
        if (debug_on) call msg_debug(D_SHOWER, "generate_ps error at E^2 < t")
        return
    end if
    plabs = sqrt (prt%child1%momentum%p(0)**2 - prt%child1%t)
    p2abs = sqrt (prt%child2%momentum%p(0)**2 - prt%child2%t)
    x = (pabs**2 + plabs**2 - p2abs**2) / (two * pabs)
    if (pabs > plabs + p2abs .or. &
        pabs < abs(plabs - p2abs)) then
        if (debug_active (D_SHOWER)) then
            print *, "D: parton_generate_ps Dreiecksungleichung error &
                &for parton ", prt%nr, " ", &
                space_part_norm (prt%momentum), " ", plabs, " ", p2abs
            call prt%write ()
            call prt%child1%write ()
            call prt%child2%write ()
        end if
        return
    end if
    !!! Due to numerical problems transverse momentum could be imaginary ->
    !!! set transverse momentum to zero
    ptabs = sqrt (max (plabs * plabs - x * x, zero))
    call rng%generate (phi)
    phi = twopi * phi
    do i = 1, 3
        momentum(i) = x * directions(1,i) + ptabs * &
            (cos(phi) * directions(2,i) + sin(phi) * directions(3,i))
    end do
    prt%child1%momentum%p(1:3) = momentum(1:3)
    do i = 1, 3
        momentum(i) = (space_part_norm (prt%momentum) - x) * directions(1,i) - &
            ptabs * (cos(phi) * directions(2,i) + sin(phi) * directions(3,i))
    end do
    prt%child2%momentum%p(1:3) = momentum(1:3)
end if
end subroutine parton_generate_ps

```

```

<Enforce right-handed system for directions>≡
    if ((directions(1,1) * (directions(2,2) * directions(3,3) - &
        directions(2,3) * directions(3,2)) + &
        directions(1,2) * (directions(2,3) * directions(3,1) - &
        directions(2,1) * directions(3,3)) + &
        directions(1,3) * (directions(2,1) * directions(3,2) - &
        directions(2,2) * directions(3,1))) < 0) then
        directions(3,:) = - directions(3,:)
    end if

```

This routine is similar to parton_generate_ps, but now for the ISR. It takes

the three-momentum of a parton's first child as fixed and generates the two remaining three-momenta.

```

(Shower partons: parton: TBP)+≡
  procedure :: generate_ps_ini => parton_generate_ps_ini

(Shower partons: sub interfaces)+≡
  module subroutine parton_generate_ps_ini (prt, rng)
    class(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
  end subroutine parton_generate_ps_ini

(Shower partons: procedures)+≡
  module subroutine parton_generate_ps_ini (prt, rng)
    class(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
    real(default), dimension(1:3, 1:3) :: directions
    integer :: i,j
    real(default) :: scproduct, pabs, plabs, p2abs, x, ptabs, phi
    real(default), dimension(1:3) :: momentum
    if (debug_active (D_SHOWER)) &
      print *, "D: parton_generate_ps_ini: for parton " , prt%nr
    if (debug_active (D_SHOWER)) then
      if (.not. (associated (prt%child1) .and. associated (prt%child2))) then
        call msg_fatal ("no children for generate_ps")
      end if
    end if

    if (.not. prt%is_proton()) then
      !!! generate ps for normal partons
      do i = 1, 3
        directions(1,i) = prt%child1%momentum%p(i) / &
          space_part_norm(prt%child1%momentum)
      end do
      do j = 2, 3
        call rng%generate (directions(j,:))
      end do
      do i = 2, 3
        scproduct = zero
        do j = 1, i - 1
          scproduct = directions(i,1) * directions(j,1) + &
            directions(i,2) * directions(j,2) + &
            directions(i,3) * directions(j,3)
          directions(i,1) = directions(i,1) - directions(j,1) * scproduct
          directions(i,2) = directions(i,2) - directions(j,2) * scproduct
          directions(i,3) = directions(i,3) - directions(j,3) * scproduct
        end do
        scproduct = directions(i,1)**2 + directions(i,2)**2 + &
          directions(i,3)**2
        do j = 1, 3
          directions(i,j) = directions(i,j) / sqrt(scproduct)
        end do
      end do
      (Enforce right-handed system for directions)

      pabs = space_part_norm (prt%child1%momentum)

```

```

p1abs = sqrt (prt%momentum%p(0)**2 - prt%t)
p2abs = sqrt (max(zero, prt%child2%momentum%p(0)**2 - &
prt%child2%t))

x = (pabs**2 + p1abs**2 - p2abs**2) / (two * pabs)
if (debug_active (D_SHOWER)) then
  if (pabs > p1abs + p2abs .or. pabs < abs(p1abs - p2abs)) then
    print *, "error at generate_ps, Dreiecksungleichung for parton ", &
      prt%nr, " ", pabs," ",p1abs," ",p2abs
    call prt%write ()
    call prt%child1%write ()
    call prt%child2%write ()
    call msg_fatal ("parton_generate_ps_ini: Dreiecksungleichung")
  end if
end if
if (debug_active (D_SHOWER)) print *, "D: parton_generate_ps_ini: x = ", x
ptabs = sqrt (p1abs * p1abs - x**2)
call rng%generate (phi)
phi = twopi * phi
do i = 1,3
  momentum(i) = x * directions(1,i) + ptabs * (cos(phi) * &
    directions(2,i) + sin(phi) * directions(3,i))
end do
prt%momentum%p(1:3) = momentum
do i = 1, 3
  momentum(i) = (x - pabs) * directions(1,i) + ptabs * (cos(phi) * &
    directions(2,i) + sin(phi) * directions(3,i))
end do
prt%child2%momentum%p(1:3) = momentum(1:3)
else
  !!! for first partons just set beam remnants momentum
  prt%child2%momentum = prt%momentum - prt%child1%momentum
end if
end subroutine parton_generate_ps_ini

```

22.2.3 The analytic FSR

```

<Shower partons: parton: TBP>+≡
  procedure :: next_t_ana => parton_next_t_ana

<Shower partons: sub interfaces>+≡
  module subroutine parton_next_t_ana (prt, rng)
    class(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
  end subroutine parton_next_t_ana

<Shower partons: procedures>+≡
  module subroutine parton_next_t_ana (prt, rng)
    class(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
    integer :: gtoqq
    real(default) :: integral, random
    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_SHOWER, "next_t_ana")

```

```

! check if branchings are possible at all
if (min (prt%t, prt%momentum%p(0)**2) < &
    prt%mass_squared () + prt%settings%min_virtuality) then
    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
    return
end if
integral = zero
call rng%generate (random)
do
    call parton_simulate_stept (prt, rng, integral, random, gtoqq, .false.)
    if (prt%simulated) then
        if (prt%is_gluon ()) then
            !!! Abusing the x-variable to store the information to which
            !!! quark flavor the gluon branches (if any)
            prt%x = one * gtoqq + 0.1_default
            !!! x = gtoqq + 0.1 -> int(x) will be the quark flavor or
            !!! zero for g -> gg
        end if
        exit
    end if
end do
end subroutine parton_next_t_ana

```

The shower is actually sensitive to how close we go to the one here.

(Shower partons: procedures)+≡

```

function cmax (prt, tt) result (cmaxx)
    type(parton_t), intent(in) :: prt
    real(default), intent(in), optional :: tt
    real(default) :: t, cost, cmaxx, radicand
    t = prt%t; if (present (tt)) t = tt
    if (associated (prt%parent)) then
        cost = prt%parent%get_costheta ()
        radicand = max(zero, one - &
            t / (prt%get_beta () * prt%momentum%p(0)**2 * &
            (one + cost) / (one - cost))
        if (debug_on) call msg_debug2 (D_SHOWER, "cmax: sqrt (radicand)", sqrt (radicand))
        cmaxx = min (0.99999_default, sqrt (radicand))
    else
        cmaxx = 0.99999_default
    end if
end function cmax

```

Simulation routine. The variable `lookatsister` takes constraints from the sister parton into account, if not given it is assumed `.true.`. `a` and `x` are three-dimensional arrays for values used for the integration.

(Shower partons: public)+≡

```

public :: parton_simulate_stept

```

(Shower partons: sub interfaces)+≡

```

module subroutine parton_simulate_stept &
    (prt, rng, integral, random, gtoqq, lookatsister)
    type(parton_t), intent(inout) :: prt

```



```

class(rng_t), intent(inout), allocatable :: rng
real(default), intent(inout) :: integral
real(default), intent(inout) :: random
integer, intent(out) :: gtoqq
logical, intent(in), optional :: lookatsister
end subroutine parton_simulate_stept

<Shower partons: procedures>+≡
module subroutine parton_simulate_stept &
  (prt, rng, integral, random, gtoqq, lookatsister)
  type(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
  real(default), intent(inout) :: integral
  real(default), intent(inout) :: random
  integer, intent(out) :: gtoqq
  logical, intent(in), optional :: lookatsister

  type(parton_t), pointer :: sister
  real(default) :: tstep, tmin, oldt
  real(default) :: c, cstep
  real(default), dimension(3) :: z, P
  real(default) :: to_integral
  real(default) :: a11,a12,a13,a21,a22,a23
  real(default) :: cmax_t
  real(default) :: temprand
  real(default), dimension(3) :: a, x

  ! higher values -> faster but coarser
  real(default), parameter :: tstepfactor = 0.02_default
  real(default), parameter :: tstepmin = 0.5_default
  real(default), parameter :: cstepfactor = 0.8_default
  real(default), parameter :: cstepmin = 0.03_default

  if (signal_is_pending ()) return
  if (debug_on) call msg_debug (D_SHOWER, "parton_simulate_stept")
  gtoqq = 111 ! illegal value
  call prt%set_simulated (.false.)

  <Set sister if lookatsister is true or not given>

  tmin = prt%settings%min_virtuality + prt%mass_squared ()
  if (prt%is_quark ()) then
    to_integral = three *pi * log(one / random)
  else if (prt%is_gluon ()) then
    to_integral = four *pi * log(one / random)
  else
    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
    return
  end if

  if (associated (sister)) then
    if (sqrt(prt%t) > sqrt(prt%parent%t) - &
      sqrt(sister%mass_squared ())) then
      prt%t = (sqrt (prt%parent%t) - sqrt (sister%mass_squared ()))**2
    end if
  end if

```

```

        end if
    end if
    if (prt%t > prt%momentum%p(0)**2) then
        prt%t = prt%momentum%p(0)**2
    end if

    if (prt%t <= tmin) then
        prt%t = prt%mass_squared ()
        call prt%set_simulated ()
        return
    end if

    ! simulate the branchings between prt%t and prt%t - tstep
    tstep = max(tstepfactor * (prt%t - 0.9_default * tmin), tstepmin)
    cmax_t = cmax(prt)
    c = - cmax_t ! take highest t -> minimal constraint
    cstep = max(cstepfactor * (one - abs(c)), cstepmin)
    ! get values at border of "previous" bin -> to be used in first bin
    z(3) = 0.5_default + 0.5_default * get_beta (prt%t - &
        0.5_default * tstep, prt%momentum%p(0)) * c
    if (prt%is_gluon ()) then
        P(3) = P_ggg (z(3)) + P_gqq (z(3)) * number_of_flavors &
            (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
    else
        P(3) = P_qqg (z(3))
    end if
    a(3) = D_alpha_s_fsr (z(3) * (one - z(3)) * prt%t, &
        prt%settings) * P(3) / (prt%t - 0.5_default * tstep)

    do while (c < cmax_t .and. (integral < to_integral))
        if (signal_is_pending ()) return
        cmax_t = cmax (prt)
        cstep = max (cstepfactor * (one - abs(c)**2), cstepmin)
        if (c + cstep > cmax_t) then
            cstep = cmax_t - c
        end if
        if (cstep < 1E-9_default) then
            !!! reject too small bins
            exit
        end if
        z(1) = z(3)
        z(2) = 0.5_default + 0.5_default * get_beta &
            (prt%t - 0.5_default * tstep, prt%momentum%p(0)) * &
            (c + 0.5_default * cstep)
        z(3) = 0.5_default + 0.5_default * get_beta &
            (prt%t - 0.5_default * tstep, prt%momentum%p(0)) * (c + cstep)
        P(1) = P(3)
        if (prt%is_gluon ()) then
            P(2) = P_ggg(z(2)) + P_gqq(z(2)) * number_of_flavors &
                (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
            P(3) = P_ggg(z(3)) + P_gqq(z(3)) * number_of_flavors &
                (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
        else
            P(2) = P_qqg(z(2))
        end if
    end while

```

```

P(3) = P_qqg(z(3))
end if
! get values at borders of the integral and in the middle
a(1) = a(3)
a(2) = D_alpha_s_fsr (z(2) * (one - z(2)) * prt%t, &
    prt%settings) * P(2) / &
    (prt%t - 0.5_default * tstep)
a(3) = D_alpha_s_fsr (z(3) * (one - z(3)) * prt%t, &
    prt%settings) * P(3) / &
    (prt%t - 0.5_default * tstep)

!!! a little tricky:
!!! fit  $x(1) + x(2)/(1 + c) + x(3)/(1 - c)$  to these values
a11 = (one+c+0.5_default*cstep) * (one-c-0.5_default*cstep) - &
    (one-c) * (one+c+0.5_default*cstep)
a12 = (one-c-0.5_default*cstep) - (one+c+0.5_default*cstep) * &
    (one-c) / (one+c)
a13 = a(2) * (one+c+0.5_default*cstep) * (one-c-0.5_default*cstep) - &
    a(1) * (one-c) * (one+c+0.5_default*cstep)
a21 = (one+c+cstep) * (one-c-cstep) - (one+c+cstep) * (one-c)
a22 = (one-c-cstep) - (one+c+cstep) * (one-c) / (one+c)
a23 = a(3) * (one+c+cstep) * (one-c-cstep) - &
    a(1) * (one-c) * (one+c+cstep)

x(2) = (a23 - a21 * a13 / a11) / (a22 - a12 * a21 / a11)
x(1) = (a13 - a12 * x(2)) / a11
x(3) = a(1) * (one - c) - x(1) * (one - c) - x(2) * (one - c) / (one + c)

integral = integral + tstep * (x(1) * cstep + x(2) * &
    log((one + c + cstep) / (one + c)) - x(3) * &
    log((one - c - cstep) / (one - c)))

if (integral > to_integral) then
    oldt = prt%t
    call rng%generate (temprand)
    prt%t = prt%t - temprand * tstep
    call rng%generate (temprand)
    prt%costheta = c + (0.5_default - temprand) * cstep
    call prt%set_simulated ()

    if (prt%t < prt%settings%min_virtuality + prt%mass_squared ()) then
        prt%t = prt%mass_squared ()
    end if
    if (abs(prt%costheta) > cmax_t) then
        ! reject branching due to violation of costheta-limits
        call rng%generate (random)
        if (prt%is_quark ()) then
            to_integral = three * pi * log(one / random)
        else if (prt%is_gluon ()) then
            to_integral = four * pi * log(one / random)
        end if
        integral = zero
        prt%t = oldt
        call prt%set_simulated (.false.)
    end if
end if

```

```

end if
if (prt%is_gluon ()) then
! decide between g->gg and g->qqbar splitting
z(1) = 0.5_default + 0.5_default * prt%costheta
call rng%generate (temprand)
if (P_ggg(z(1)) > temprand * (P_ggg (z(1)) + P_gqq (z(1)) * &
    number_of_flavors(prt%t, prt%settings%max_n_flavors, &
    prt%settings%min_virtuality))) then
    gtoqq = 0
else
    call rng%generate (temprand)
    gtoqq = 1 + int (temprand * number_of_flavors &
        (prt%t, prt%settings%max_n_flavors, &
        prt%settings%min_virtuality))
end if
end if
else
    c = c + cstep
end if
cmax_t = cmax (prt)
end do
if (integral <= to_integral) then
    prt%t = prt%t - tstep
    if (prt%t < prt%settings%min_virtuality + prt%mass_squared ()) then
        prt%t = prt%mass_squared ()
        call prt%set_simulated ()
    end if
end if
end if
end subroutine parton_simulate_step

```

<Set sister if lookatsister is true or not given>≡

```

sister => null()
SET_SISTER: do
    if (present (lookatsister)) then
        if (.not. lookatsister) then
            exit SET_SISTER
        end if
    end if
    if (prt%nr == prt%parent%child1%nr) then
        sister => prt%parent%child2
    else
        sister => prt%parent%child1
    end if
    exit SET_SISTER
end do SET_SISTER

```

From the whole ISR algorithm all functionality has been moved to `shower_core.f90`.

Only `maxzz` remains here, because more than one module needs to access it.

<Shower partons: public>+≡

```

public :: maxzz

```

<Shower partons: sub interfaces>+≡

```

module function maxzz (shat, s, maxz_isr, minenergy_timelike) result (maxz)
    real(default), intent(in) :: shat, s, minenergy_timelike, maxz_isr

```

```

        real(default) :: maxz
    end function maxzz
<Shower partons: procedures>+≡
    module function maxzz (shat, s, maxz_isr, minenergy_timelike) result (maxz)
        real(default), intent(in) :: shat, s, minenergy_timelike, maxz_isr
        real(default) :: maxz
        maxz = min (maxz_isr, one - (two * minenergy_timelike * sqrt(shat)) / s)
    end function maxzz

```

22.3 Main shower module

```

<shower_core.f90>≡
    <File header>

    module shower_core

        <Use kinds with double>
        <Use strings>
        <Use debug>
        use os_interface
        use lorentz
        use particles
        use model_data
        use pdf
        use rng_base
        use shower_base
        use shower_partons
        use muli, only: muli_t
        use tauola_interface

        <Standard module head>

        <Shower core: public>

        <Shower core: types>

        <Shower core: interfaces>

        interface
        <Shower core: sub interfaces>
        end interface

    end module shower_core

<shower_core_sub.f90>≡
    <File header>

    submodule (shower_core) shower_core_s

        use io_units
        use constants
        use format_utils, only: write_separator

```

```

    use numeric_utils
    use diagnostics
    use physics_defs
    use sm_physics
    use hep_common
    use flavors
    use colors
    use subevents

    implicit none

    <Shower core: parameters>

    contains

    <Shower core: procedures>

    end submodule shower_core_s

    <Shower core: public>≡
        public :: shower_interaction_t
    <Shower core: types>≡
        type :: shower_interaction_t
            type(parton_pointer_t), dimension(:), allocatable :: partons
        end type shower_interaction_t

        type :: shower_interaction_pointer_t
            type(shower_interaction_t), pointer :: i => null ()
        end type shower_interaction_pointer_t

    The WHIZARD internal shower. Flags distinguish between analytic and  $k_T$ -
    ordered showers.

    <Shower core: public>+≡
        public :: shower_t
    <Shower core: types>+≡
        type, extends (shower_base_t) :: shower_t
            type(shower_interaction_pointer_t), dimension(:), allocatable :: &
                interactions
            type(parton_pointer_t), dimension(:), allocatable :: partons
            type(multi_t) :: mi
            integer :: next_free_nr
            integer :: next_color_nr
            logical :: valid
            contains
                <Shower core: shower: TBP>
            end type shower_t

    <Shower core: shower: TBP>≡
        procedure :: init => shower_init

```

```

<Shower core: sub interfaces>≡
  module subroutine shower_init &
    (shower, settings, taudec_settings, pdf_data, os_data)
    class(shower_t), intent(out) :: shower
    type(shower_settings_t), intent(in) :: settings
    type(taudec_settings_t), intent(in) :: taudec_settings
    type(pdf_data_t), intent(in) :: pdf_data
    type(os_data_t), intent(in) :: os_data
  end subroutine shower_init

<Shower core: procedures>≡
  module subroutine shower_init &
    (shower, settings, taudec_settings, pdf_data, os_data)
    class(shower_t), intent(out) :: shower
    type(shower_settings_t), intent(in) :: settings
    type(taudec_settings_t), intent(in) :: taudec_settings
    type(pdf_data_t), intent(in) :: pdf_data
    type(os_data_t), intent(in) :: os_data
    if (debug_on) call msg_debug (D_SHOWER, "shower_init")
    shower%settings = settings
    shower%taudec_settings = taudec_settings
    shower%os_data = os_data
    call shower%pdf_data%init (pdf_data)
    shower%name = "WHIZARD internal"
    call shower%write_msg ()
  end subroutine shower_init

<Shower core: shower: TBP>+≡
  procedure :: prepare_new_event => shower_prepare_new_event

<Shower core: sub interfaces>+≡
  module subroutine shower_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
  end subroutine shower_prepare_new_event

<Shower core: procedures>+≡
  module subroutine shower_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
    call shower%cleanup ()
    shower%next_free_nr = 1
    shower%next_color_nr = 1
    if (debug_active (D_SHOWER)) then
      if (allocated (shower%interactions)) then
        call msg_bug ("Shower: creating new shower while old one " // &
          "is still associated (interactions)")
      end if
      if (allocated (shower%partons)) then
        call msg_bug ("Shower: creating new shower while old one " // &
          "is still associated (partons)")
      end if
    end if
    treat_light_quarks_massless = .true.
    treat_duscb_quarks_massless = .false.
  end subroutine shower_prepare_new_event

```

```

        shower%valid = .true.
    end subroutine shower_prepare_new_event

```

It would be better to have the multi type outside of the shower.

```

<Shower core: shower: TBP>+≡
    procedure :: activate_multiple_interactions => &
        shower_activate_multiple_interactions

<Shower core: sub interfaces>+≡
    module subroutine shower_activate_multiple_interactions (shower)
        class(shower_t), intent(inout) :: shower
    end subroutine shower_activate_multiple_interactions

<Shower core: procedures>+≡
    module subroutine shower_activate_multiple_interactions (shower)
        class(shower_t), intent(inout) :: shower
        if (shower%mi%is_initialized ()) then
            call shower%mi%restart ()
        else
            call shower%mi%initialize (&
                GeV2_scale_cutoff=shower%settings%min_virtuality, &
                GeV2_s=shower_interaction_get_s &
                (shower%interactions(1)%i), &
                multi_dir=char(shower%os_data%whizard_mulpath))
        end if
        call shower%mi%apply_initial_interaction ( &
            GeV2_s=shower_interaction_get_s(shower%interactions(1)%i), &
            x1=shower%interactions(1)%i%partons(1)%p%parent%x, &
            x2=shower%interactions(1)%i%partons(2)%p%parent%x, &
            pdg_f1=shower%interactions(1)%i%partons(1)%p%parent%type, &
            pdg_f2=shower%interactions(1)%i%partons(2)%p%parent%type, &
            n1=shower%interactions(1)%i%partons(1)%p%parent%nr, &
            n2=shower%interactions(1)%i%partons(2)%p%parent%nr)
    end subroutine shower_activate_multiple_interactions

<Shower core: shower: TBP>+≡
    procedure :: import_particle_set => shower_import_particle_set

<Shower core: sub interfaces>+≡
    module subroutine shower_import_particle_set (shower, particle_set)
        class(shower_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
    end subroutine shower_import_particle_set

<Shower core: procedures>+≡
    module subroutine shower_import_particle_set (shower, particle_set)
        class(shower_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
        !integer, dimension(:), allocatable :: connections
        type(parton_t), dimension(:), allocatable, target, save :: partons, hadrons
        type(parton_pointer_t), dimension(:), allocatable :: &
            parton_pointers
        integer :: n_beam, n_in, n_out, n_tot
        integer :: i, j, nr, max_color_nr
        if (debug_on) call msg_debug (D_SHOWER, 'shower_import_particle_set')

```



```

call count_and_allocate ()
call setup_hadrons_from_particle_set ()
call setup_partons_from_particle_set ()
call shower%update_max_color_nr (1 + max_color_nr)
call shower%add_interaction_2ton (parton_pointers)
if (shower%settings%multi_active) then
    call shower%activate_multiple_interactions ()
end if
if (debug_on) call msg_debug2 (D_SHOWER, 'shower%write() after shower_import_particle_set')
if (debug2_active (D_SHOWER)) then
    call shower%write ()
end if
contains
<Shower core: shower import particle set: procedures>
end subroutine shower_import_particle_set

```

<Shower core: shower import particle set: procedures>≡

```

subroutine count_and_allocate ()
    max_color_nr = 0
    n_beam = particle_set%get_n_beam ()
    n_in = particle_set%get_n_in ()
    n_out = particle_set%get_n_out ()
    n_tot = particle_set%get_n_tot ()
    if (allocated (partons)) deallocate (partons)
    allocate (partons (n_in + n_out))
    allocate (parton_pointers (n_in+n_out))
end subroutine count_and_allocate

```

<Shower core: shower import particle set: procedures>+≡

```

subroutine setup_hadrons_from_particle_set ()
    j = 0
    !!! !!! !!! Workaround for Portland 16.1 compiler bug
    !!! if (n_beam > 0 .and. all (particle_set%prt(1:2)%flv%get_pdg_abs () > TAU)) then
    if (n_beam > 0 .and. particle_set%prt(1)%flv%get_pdg_abs () > TAU .and. &
        particle_set%prt(2)%flv%get_pdg_abs () > TAU) then
        if (debug_on) call msg_debug (D_SHOWER, 'Copy hadrons from particle_set to hadrons')
        if (.not. allocated (hadrons)) allocate (hadrons (1:2))
        do i = 1, n_tot
            if (particle_set%prt(i)%status == PRT_BEAM) then
                j = j + 1
                nr = shower%get_next_free_nr ()
                hadrons(j) = parton_of_particle (particle_set%prt(i), nr)
                hadrons(j)%settings => shower%settings
                max_color_nr = max (max_color_nr, abs(hadrons(j)%c1), &
                    abs(hadrons(j)%c2))
            end if
        end do
    end if
end subroutine setup_hadrons_from_particle_set

```

<Shower core: shower import particle set: procedures>+≡

```

subroutine setup_partons_from_particle_set ()
    integer, dimension(1) :: parent

```

```

j = 0
if (debug_on) call msg_debug (D_SHOWER, "Copy partons from particle_set to partons")
do i = 1, n_tot
  if (particle_set%prt(i)%get_status () == PRT_INCOMING .or. &
      particle_set%prt(i)%get_status () == PRT_OUTGOING) then
    j = j + 1
    nr = shower%get_next_free_nr ()
    partons(j) = parton_of_particle (particle_set%prt(i), nr)
    partons(j)%settings => shower%settings
    parton_pointers(j)%p => partons(j)
    max_color_nr = max (max_color_nr, abs (partons(j)%c1), &
                        abs (partons(j)%c2))
    if (particle_set%prt(i)%get_status () == PRT_INCOMING .and. &
        particle_set%prt(i)%get_n_parents () == 1 .and. &
        allocated (hadrons)) then
      parent = particle_set%prt(i)%get_parents ()
      partons(j)%initial => hadrons (parent(1))
      partons(j)%x = space_part_norm (partons(j)%momentum) / &
                    space_part_norm (partons(j)%initial%momentum)
    end if
  end if
end do
end subroutine setup_partons_from_particle_set

```

(Shower core: shower: TBP)+≡

```

procedure :: generate_emissions => shower_generate_emissions

```

(Shower core: sub interfaces)+≡

```

module subroutine shower_generate_emissions &
  (shower, valid, number_of_emissions)
  class(shower_t), intent(inout), target :: shower
  logical, intent(out) :: valid
  integer, optional, intent(in) :: number_of_emissions
end subroutine shower_generate_emissions

```

(Shower core: procedures)+≡

```

module subroutine shower_generate_emissions &
  (shower, valid, number_of_emissions)
  class(shower_t), intent(inout), target :: shower
  logical, intent(out) :: valid
  integer, optional, intent(in) :: number_of_emissions

  type(parton_t), dimension(:), allocatable, target :: partons
  type(parton_pointer_t), dimension(:), allocatable :: &
    parton_pointers
  real(default) :: mi_scale, ps_scale, shat, phi
  type(parton_pointer_t) :: temppp
  integer :: i, j, k
  integer :: n_int, max_color_nr
  integer, dimension(2,4) :: color_corr
  if (debug_on) call msg_debug (D_SHOWER, "shower_generate_emissions")
  if (shower%settings%isr_active) then
    if (debug_on) call msg_debug (D_SHOWER, "Generate ISR with FSR")
    i = 0
    BRANCHINGS: do

```

```

i = i + 1
if (signal_is_pending ()) return
if (shower%settings%multi_active) then
call shower%mi%generate_gev2_pt2 &
      (shower%get_ISR_scale (), mi_scale)
else
      mi_scale = 0.0
end if

!!! Shower: debugging
!!! shower%generate_next_isr_branching returns a pointer to
!!! the parton with the next ISR-branching, this parton's
!!! scale is the scale of the next branching
! temppp=shower%generate_next_isr_branching_veto ()
temppp = shower%generate_next_isr_branching ()

if (.not. associated (temppp%p) .and. &
      mi_scale < shower%settings%min_virtuality) then
      exit BRANCHINGS
end if
!!! check if branching or interaction occurs next
if (associated (temppp%p)) then
      ps_scale = abs(temppp%p%t)
else
      ps_scale = 0._default
end if
if (mi_scale > ps_scale) then
      !!! discard branching evolution lower than mi_scale
      call shower%set_max_ISR_scale (mi_scale)
      if (associated (temppp%p)) &
            call temppp%p%set_simulated (.false.)

      !!! execute new interaction
      deallocate (partons)
      deallocate (parton_pointers)
      allocate (partons(1:4))
      allocate (parton_pointers(1:4))
      do j = 1, 4
            partons(j)%nr = shower%get_next_free_nr ()
            partons(j)%belongstointeraction = .true.
            parton_pointers(j)%p => partons(j)
      end do
      call shower%mi%generate_partons (partons(1)%nr, partons(2)%nr, &
            partons(1)%x, partons(2)%x, &
            partons(1)%type, partons(2)%type, &
            partons(3)%type, partons(4)%type)
      !!! calculate momenta
      shat = partons(1)%x * partons(2)%x * &
            shower_interaction_get_s (shower%interactions(1)%i)
      partons(1)%momentum = [0.5_default * sqrt(shat), &
            zero, zero, 0.5_default*sqrt(shat)]
      partons(2)%momentum = [0.5_default * sqrt(shat), &
            zero, zero, -0.5_default*sqrt(shat)]
      call parton_set_initial (partons(1), &

```

```

        shower%interactions(1)%i%partons(1)%p%initial)
    call parton_set_initial (partons(2), &
        shower%interactions(1)%i%partons(2)%p%initial)
    partons(1)%belongstoFSR = .false.
    partons(2)%belongstoFSR = .false.
    !!! calculate color connection
call shower%mi%get_color_correlations &
    (shower%get_next_color_nr (), &
        max_color_nr,color_corr)
call shower%update_max_color_nr (max_color_nr)

    partons(1)%c1 = color_corr(1,1)
    partons(1)%c2 = color_corr(2,1)
    partons(2)%c1 = color_corr(1,2)
    partons(2)%c2 = color_corr(2,2)
    partons(3)%c1 = color_corr(1,3)
    partons(3)%c2 = color_corr(2,3)
    partons(4)%c1 = color_corr(1,4)
    partons(4)%c2 = color_corr(2,4)

    call shower%rng%generate (phi)
    phi = 2 * pi * phi
    partons(3)%momentum = [0.5_default*sqrt(shat), &
        sqrt(mi_scale)*cos(phi), &
        sqrt(mi_scale)*sin(phi), &
        sqrt(0.25_default*shat - mi_scale)]
    partons(4)%momentum = [ 0.5_default*sqrt(shat), &
        -sqrt(mi_scale)*cos(phi), &
        -sqrt(mi_scale)*sin(phi), &
        -sqrt(0.25_default*shat - mi_scale)]
    partons(3)%belongstoFSR = .true.
    partons(4)%belongstoFSR = .true.

    call shower%add_interaction_2ton (parton_pointers)
    n_int = size (shower%interactions)
    do k = 1, 2
    call shower%mi%replace_parton &
        (shower%interactions(n_int)%i%partons(k)%p%initial%nr, &
            shower%interactions(n_int)%i%partons(k)%p%nr, &
            shower%interactions(n_int)%i%partons(k)%p%parent%nr, &
            shower%interactions(n_int)%i%partons(k)%p%type, &
            shower%interactions(n_int)%i%partons(k)%p%x, &
            mi_scale)
        end do
    else
    !!! execute the next branching 'found' in the previous step
    call shower%execute_next_isr_branching (temppp)
    if (shower%settings%multi_active) then
    call shower%mi%replace_parton (temppp%p%initial%nr, &
        temppp%p%child1%nr, temppp%p%nr, &
        temppp%p%type, temppp%p%x, ps_scale)
    end if
    end if
end if

```

```

        end do BRANCHINGS

        call shower%generate_fsr_for_isr_partons ()
    else
        if (signal_is_pending ()) return
        if (debug_on) call msg_debug (D_SHOWER, "Generate FSR without ISR")
        call shower%simulate_no_isr_shower ()
    end if

    !!! some bookkeeping, needed after the shower is done
    call shower%boost_to_labframe ()
    call shower%generate_primordial_kt ()
    call shower%update_beamremnants ()

    if (shower%settings%fsr_active) then
        do i = 1, size (shower%interactions)
            if (signal_is_pending ()) return
            call shower%interaction_generate_fsr_2ton &
                (shower%interactions(i)%i)
        end do
    else
        call shower%simulate_no_fsr_shower ()
    end if
    if (debug_on) call msg_debug (D_SHOWER, "Shower finished:")
    if (debug_active (D_SHOWER)) call shower%write ()

    valid = shower%valid
    !!! clean-up muli: we should finalize the muli pdf sets
    !!!      when _all_ runs are done. Not after every event if possible
    ! call shower%mi%finalize()
end subroutine shower_generate_emissions

```

<Shower core: shower: TBP>+≡

```

    procedure :: make_particle_set => shower_make_particle_set

```

<Shower core: sub interfaces>+≡

```

    module subroutine shower_make_particle_set &
        (shower, particle_set, model, model_hadrons)
        class(shower_t), intent(in) :: shower
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        class(model_data_t), intent(in), target :: model_hadrons
    end subroutine shower_make_particle_set

```

<Shower core: procedures>+≡

```

    module subroutine shower_make_particle_set &
        (shower, particle_set, model, model_hadrons)
        class(shower_t), intent(in) :: shower
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        class(model_data_t), intent(in), target :: model_hadrons
        call shower%combine_with_particle_set (particle_set, model, &
            model_hadrons)
    if (shower%settings%hadronization_active) then
        call shower%converttopythia ()
    end if

```

```

        end if
    end subroutine shower_make_particle_set

```

The parameters of the shower module:

```

<Shower core: parameters>≡
    real(default), save :: alphaspdfmax = 12._default

```

In this routine, *y* and *ymin* are the jet measures, *w* and *wmax* are weights, *s* is the kinematic energy squared of the interaction. The flag *isr_is_possible_and_allowed* checks whether the initial parton is set, lepton-hadron collisions are not implemented (yet).

As a workaround: as WHIZARD can treat partons as massless, there might be partons with $E < m$: if such a parton is found, quarks will be treated massless.

```

<Shower core: shower: TBP>+≡
    procedure :: add_interaction_2ton => shower_add_interaction_2ton

<Shower core: sub interfaces>+≡
    module subroutine shower_add_interaction_2ton (shower, partons)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(in), dimension(:), allocatable :: partons
    end subroutine shower_add_interaction_2ton

<Shower core: procedures>+≡
    module subroutine shower_add_interaction_2ton (shower, partons)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(in), dimension(:), allocatable :: partons
        !type(ckkw_pseudo_shower_weights_t), intent(in) :: ckkw_pseudo_weights

        integer :: n_partons, n_out
        integer :: i, j, imin, jmin
        real(default) :: y, ymin
        !real(default) :: w, wmax
        !real(default) :: random, sum
        type(parton_pointer_t), dimension(:), allocatable :: new_partons
        type(parton_t), pointer :: prt
        integer :: n_int
        type(shower_interaction_pointer_t), dimension(:), allocatable :: temp
        type(vector4_t) :: prtmomentum, childmomentum
        logical :: isr_is_possible_and_allowed
        type(lorentz_transformation_t) :: L

        if (signal_is_pending ()) return
        if (debug_on) call msg_debug (D_SHOWER, "Add interaction2toN")
        n_partons = size (partons)
        n_out = n_partons - 2
        if (n_out < 2) then
            call msg_bug &
                ("Shower core: trying to add a 2-> (something<2) interaction")
        end if

        isr_is_possible_and_allowed = (associated (partons(1)%p%initial) &
            .and. associated (partons(2)%p%initial)) .and. &

```

```

        shower%settings%isr_active
if (debug_on) call msg_debug (D_SHOWER, "isr_is_possible_and_allowed", &
    isr_is_possible_and_allowed)

if (associated (partons(1)%p%initial) .and. &
    partons(1)%p%is_quark ()) then
    if (partons(1)%p%momentum%p(0) < &
        two * partons(1)%p%mass()) then
        if (abs(partons(1)%p%type) < 2) then
            treat_light_quarks_massless = .true.
        else
            treat_duscb_quarks_massless = .true.
        end if
    end if
end if
if (associated (partons(2)%p%initial) .and. &
    partons(2)%p%is_quark ()) then
    if (partons(2)%p%momentum%p(0) < &
        two * partons(2)%p%mass()) then
        if (abs(partons(2)%p%type) < 2) then
            treat_light_quarks_massless = .true.
        else
            treat_duscb_quarks_massless = .true.
        end if
    end if
end if

<Add a new interaction to shower%interactions>

if (associated (shower%interactions(n_int)%i%partons(1)%p%initial)) &
    call shower%interactions(n_int)%i%partons(1)%p%initial%set_simulated ()
if (associated (shower%interactions(n_int)%i%partons(2)%p%initial)) &
    call shower%interactions(n_int)%i%partons(2)%p%initial%set_simulated ()
if (isr_is_possible_and_allowed) then
    !!! boost to the CMFrame of the incoming partons
    L = boost (-(shower%interactions(n_int)%i%partons(1)%p%momentum + &
        shower%interactions(n_int)%i%partons(2)%p%momentum), &
        (shower%interactions(n_int)%i%partons(1)%p%momentum + &
        shower%interactions(n_int)%i%partons(2)%p%momentum)**1 )
    do i = 1, n_partons
        call parton_apply_lorentztrafo &
            (shower%interactions(n_int)%i%partons(i)%p, L)
    end do
end if
do i = 1, size (partons)
    if (signal_is_pending ()) return
    !!! partons are marked as belonging to the hard interaction
    shower%interactions(n_int)%i%partons(i)%p%belongstointeraction &
        = .true.
    shower%interactions(n_int)%i%partons(i)%p%belongstoFSR = i > 2
    shower%interactions(n_int)%i%partons(i)%p%interactionnr = n_int
    !!! include a 2^(i - 1) number as a label for the ckkw clustering
    shower%interactions(n_int)%i%partons(i)%p%ckkwlabel = 2**(i - 1)
end do

```

```

    <Add partons from shower%interactions to shower%partons>

    if (isr_is_possible_and_allowed) then
        if (shower%settings%isr_pt_ordered) then
            call shower_prepare_for_simulate_isr_pt &
                (shower, shower%interactions(size (shower%interactions))%i)
        else
            call shower_prepare_for_simulate_isr_ana_test &
                (shower, shower%interactions(n_int)%i%partons(1)%p, &
                shower%interactions(n_int)%i%partons(2)%p)
        end if
    end if

    !!! generate pseudo parton shower history and add all partons to
    !!!         shower%partons-array
    !!! TODO initial -> initial + final branchings ??
    allocate (new_partons(1:(n_partons - 2)))
    do i = 1, size (new_partons)
        nullify (new_partons(i)%p)
    end do
    do i = 1, size (new_partons)
        new_partons(i)%p => shower%interactions(n_int)%i%partons(i + 2)%p
    end do
    imin = 0
    jmin = 0

    ! TODO: (bcn 2015-04-24) make this a clustering step of the matching
    !   if (allocated (ckkw_pseudo_weights%weights)) then
    !       !<Perform clustering using the CKKW weights>
    !   else
    !       <Perform clustering in the usual way>
    !   end if

    !!! set the FSR starting scale for all partons
    do i = 1, size (new_partons)
        !!! the imaginary mother is the only parton remaining in new_partons
        if (.not. associated (new_partons(i)%p)) cycle
        call set_starting_scale (new_partons(i)%p, &
            get_starting_scale (new_partons(i)%p))
        exit
    end do

contains

    <Procedures of shower_add_interaction_2ton>
    end subroutine shower_add_interaction_2ton

<Add a new interaction to shower%interactions>≡
    if (allocated (shower%interactions)) then
        n_int = size (shower%interactions) + 1
    else
        n_int = 1
    end if

```



```

allocate (temp (1:n_int))
do i = 1, n_int - 1
    allocate (temp(i)%i)
    temp(i)%i = shower%interactions(i)%i
end do
allocate (temp(n_int)%i)
allocate (temp(n_int)%i%partons(1:n_partons))
do i = 1, n_partons
    allocate (temp(n_int)%i%partons(i)%p)
    call parton_copy (partons(i)%p, temp(n_int)%i%partons(i)%p)
end do
if (allocated (shower%interactions)) deallocate(shower%interactions)
allocate (shower%interactions(1:n_int))
do i = 1, n_int
    shower%interactions(i)%i => temp(i)%i
end do
deallocate (temp)

<Add partons from shower%interactions to shower%partons>≡
if (allocated (shower%partons)) then
    allocate (new_partons(1:size(shower%partons) + &
        size(shower%interactions(n_int)%i%partons)))
    do i = 1, size (shower%partons)
        new_partons(i)%p => shower%partons(i)%p
    end do
    do i = 1, size (shower%interactions(n_int)%i%partons)
        new_partons(size(shower%partons) + i)%p => &
            shower%interactions(n_int)%i%partons(i)%p
    end do
    deallocate (shower%partons)
else
    allocate (new_partons(1:size(shower%interactions(n_int)%i%partons)))
    do i = 1, size (partons)
        new_partons(i)%p => shower%interactions(n_int)%i%partons(i)%p
    end do
end if
allocate (shower%partons(1:size (new_partons)))
do i = 1, size (new_partons)
    shower%partons(i)%p => new_partons(i)%p
end do
deallocate (new_partons)

<Perform clustering using the CKKW weights>≡
CKKW_CLUSTERING: do
    !!! search for the combination with the highest weight
    wmax = zero
    CKKW_OUTER: do i = 1, size (new_partons)
        CKKW_INNER: do j = i + 1, size (new_partons)
            if (.not. associated (new_partons(i)%p)) cycle
            if (.not. associated (new_partons(j)%p)) cycle
            w = ckkw_pseudo_weights%weights(new_partons(i)%p%ckkwlabel + &
                new_partons(j)%p%ckkwlabel)
            if (w > wmax .or. vanishes(wmax)) then
                wmax = w
                imin = i
            end if
        end do
    end do
end do

```

```

        jmin = j
    end if
end do CKKW_INNER
end do CKKW_OUTER
if (wmax > zero) then
    call shower%add_parent (new_partons(imin)%p)
    call parton_set_child (new_partons(imin)%p%parent, &
        new_partons(jmin)%p, 2)
    call parton_set_parent (new_partons(jmin)%p, &
        new_partons(imin)%p%parent)
    prt => new_partons(imin)%p%parent
    prt%nr = shower_get_next_free_nr (shower)
    prt%type = INTERNAL

    prt%momentum = new_partons(imin)%p%momentum + &
        new_partons(jmin)%p%momentum
    prt%t = prt%momentum**2

    !!! auxilliary values for the ckkw matching
    !!! for now, randomly choose the type of the intermediate
    prt%ckkwlabel = new_partons(imin)%p%ckkwlabel + &
        new_partons(jmin)%p%ckkwlabel
    sum = zero
    call shower%rng%generate (random)
    CKKW_TYPE: do i = 0, 4
        if (sum + &
            ckkw_pseudo_weights%weights_by_type(prt%ckkwlabel, i) > &
            random * ckkw_pseudo_weights%weights(prt%ckkwlabel) ) then
            prt%ckkwtype = i
            exit ckkw_type
        end if
        sum = sum + &
            ckkw_pseudo_weights%weights_by_type(prt%ckkwlabel, i)
    end do CKKW_TYPE

    !!! TODO -> calculate costheta and store it for
    !!!         later use in generate_ps

    if (space_part_norm(prt%momentum) > tiny_10) then
        prtmomentum = prt%momentum
        childmomentum = prt%child1%momentum
        prtmomentum = boost (- prt%get_beta() / &
            sqrt (one - &
                (prt%get_beta ())**2), space_part (prt%momentum) / &
            space_part_norm(prt%momentum)) * prtmomentum
        childmomentum = boost (- prt%get_beta () / &
            sqrt(one - &
                (prt%get_beta ())**2), space_part (prt%momentum) / &
            space_part_norm(prt%momentum)) * childmomentum
        prt%costheta = enclosed_angle_ct(prtmomentum, childmomentum)
    else
        prt%costheta = - one
    end if
end if

```

```

prt%belongstointeraction = .true.
prt%belongstoFSR = &
    new_partons(imin)%p%belongstoFSR .and. &
    new_partons(jmin)%p%belongstoFSR

nullify (new_partons(imin)%p)
nullify (new_partons(jmin)%p)
new_partons(imin)%p => prt
else
    exit CKKW_CLUSTERING
end if
end do CKKW_CLUSTERING
(Perform clustering in the usual way)==
CLUSTERING: do
    !!! search for the partons to be clustered together
    ymin = zero
    OUTER: do i = 1, size (new_partons)
        INNER: do j = i + 1, size (new_partons)
            !!! calculate the jet measure
            if (.not.associated (new_partons(i)%p)) cycle INNER
            if (.not.associated (new_partons(j)%p)) cycle INNER
            !if (.not. shower_clustering_allowed &
                !(shower, new_partons, i,j)) &
                !cycle inner
            !!! Durham jet-measure ! don't care about constants
            y = min (new_partons(i)%p%momentum%p(0), &
                new_partons(j)%p%momentum%p(0)) * &
                (one - enclosed_angle_ct &
                (new_partons(i)%p%momentum, &
                new_partons(j)%p%momentum))
            if (y < ymin .or. vanishes(ymin)) then
                ymin = y
                imin = i
                jmin = j
            end if
        end do INNER
    end do OUTER
    if (ymin > zero) then
        call shower%add_parent (new_partons(imin)%p)
        call parton_set_child &
            (new_partons(imin)%p%parent, new_partons(jmin)%p, 2)
        call parton_set_parent &
            (new_partons(jmin)%p, new_partons(imin)%p%parent)
        prt => new_partons(imin)%p%parent
        prt%nr = shower_get_next_free_nr (shower)
        prt%type = INTERNAL

        prt%momentum = new_partons(imin)%p%momentum + &
            new_partons(jmin)%p%momentum
        prt%t = prt%momentum**2
        !!! TODO -> calculate costheta and store it for
        !!!         later use in generate_ps

        if (space_part_norm(prt%momentum) > tiny_10) then

```

```

prtmomentum = prt%momentum
childmomentum = prt%child1%momentum
prtmomentum = boost (- prt%get_beta () / sqrt(one - &
    (prt%get_beta ())**2), space_part(prt%momentum) / &
    space_part_norm(prt%momentum)) * prtmomentum
childmomentum = boost (- prt%get_beta() / &
    sqrt(one - &
    (prt%get_beta ())**2), space_part(prt%momentum) / &
    space_part_norm(prt%momentum)) * childmomentum
prt%costheta = enclosed_angle_ct (prtmomentum, childmomentum)
else
    prt%costheta = - one
end if

prt%belongstointeraction = .true.
nullify (new_partons(imin)%p)
nullify (new_partons(jmin)%p)
new_partons(imin)%p => prt
else
    exit CLUSTERING
end if
end do CLUSTERING

<Procedures of shower_add_interaction_2ton>≡
recursive subroutine transfer_pointers (destiny, start, prt)
    type(parton_pointer_t), dimension(:), allocatable :: destiny
    integer, intent(inout) :: start
    type(parton_t), pointer :: prt
    destiny(start)%p => prt
    start = start + 1
    if (associated (prt%child1)) then
        call transfer_pointers (destiny, start, prt%child1)
    end if
    if (associated (prt%child2)) then
        call transfer_pointers (destiny, start, prt%child2)
    end if
end subroutine transfer_pointers

<Procedures of shower_add_interaction_2ton>+≡
recursive function get_starting_scale (prt) result (scale)
    type(parton_t), pointer :: prt
    real(default) :: scale
    scale = huge (scale)
    if (associated (prt%child1) .and. associated (prt%child2)) then
        scale = min(scale, prt%t)
    end if
    if (associated (prt%child1)) then
        scale = min (scale, get_starting_scale (prt%child1))
    end if
    if (associated (prt%child2)) then
        scale = min (scale, get_starting_scale (prt%child2))
    end if
end function get_starting_scale

```

```

<Procedures of shower_add_interaction_2ton>+≡
recursive subroutine set_starting_scale (prt, scale)
  type(parton_t), pointer :: prt
  real(default) :: scale
  if (prt%type /= INTERNAL) then
    if (scale > prt%settings%min_virtuality + prt%mass_squared ()) then
      prt%t = scale
    else
      prt%t = prt%mass_squared ()
      call prt%set_simulated ()
    end if
  end if
  if (associated (prt%child1)) then
    call set_starting_scale (prt%child1, scale)
  end if
  if (associated (prt%child2)) then
    call set_starting_scale (prt%child2, scale)
  end if
end subroutine set_starting_scale

<Shower core: shower: TBP>+≡
procedure :: simulate_no_isr_shower => shower_simulate_no_isr_shower

<Shower core: sub interfaces>+≡
module subroutine shower_simulate_no_isr_shower (shower)
  class(shower_t), intent(inout) :: shower
  end subroutine shower_simulate_no_isr_shower

<Shower core: procedures>+≡
module subroutine shower_simulate_no_isr_shower (shower)
  class(shower_t), intent(inout) :: shower
  integer :: i, j
  type(parton_t), pointer :: prt
  if (debug_on) call msg_debug (D_SHOWER, "shower_simulate_no_isr_shower")
  do i = 1, size (shower%interactions)
    do j = 1, 2
      prt => shower%interactions(i)%i%partons(j)%p
      if (associated (prt%initial)) then
        !!! for virtuality ordered: remove unneeded partons
        if (associated (prt%parent)) then
          if (.not. prt%parent%is_proton ()) then
            if (associated (prt%parent%parent)) then
              if (.not. prt%parent%is_proton ()) then
                call shower_remove_parton_from_partons &
                  (shower, prt%parent%parent)
              end if
            end if
          end if
          call shower_remove_parton_from_partons &
            (shower, prt%parent)
        end if
      end if
      call parton_set_parent (prt, prt%initial)
      call parton_set_child (prt%initial, prt, 1)
      if (associated (prt%initial%child2)) then
        call shower_remove_parton_from_partons &

```

```

                (shower,prt%initial%child2)
                deallocate (prt%initial%child2)
            end if
            call shower%add_child (prt%initial, 2)
        end if
    end do
end do
end subroutine shower_simulate_no_isr_shower

```

(Shower core: shower: TBP)+≡

```

    procedure :: simulate_no_fsr_shower => shower_simulate_no_fsr_shower

```

(Shower core: sub interfaces)+≡

```

    module subroutine shower_simulate_no_fsr_shower (shower)
        class(shower_t), intent(inout) :: shower
        end subroutine shower_simulate_no_fsr_shower

```

(Shower core: procedures)+≡

```

    module subroutine shower_simulate_no_fsr_shower (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i, j
        type(parton_t), pointer :: prt
        do i = 1, size (shower%interactions)
            do j = 3, size (shower%interactions(i)%i%partons)
                prt => shower%interactions(i)%i%partons(j)%p
                call prt%set_simulated ()
                prt%scale = zero
                prt%t = prt%mass_squared ()
            end do
        end do
    end subroutine shower_simulate_no_fsr_shower

```

(Shower core: procedures)+≡

```

    subroutine swap_pointers (prtp1, prtp2)
        type(parton_pointer_t), intent(inout) :: prtp1, prtp2
        type(parton_pointer_t) :: prtptemp
        prtptemp%p => prtp1%p
        prtp1%p => prtp2%p
        prtp2%p => prtptemp%p
    end subroutine swap_pointers

```

This removes emitted timelike partons.

(Shower core: procedures)+≡

```

    recursive subroutine shower_remove_parton_from_partons (shower, prt)
        type(shower_t), intent(inout) :: shower
        type(parton_t), pointer :: prt
        integer :: i
        if (.not. prt%belongstoFSR .and. associated (prt%child2)) then
            call shower_remove_parton_from_partons_recursive (shower, prt%child2)
        end if
        do i = 1, size (shower%partons)
            if (associated (shower%partons(i)%p, prt)) then
                shower%partons(i)%p => null()
            end if
        end do
    end subroutine shower_remove_parton_from_partons

```

```

        ! TODO: (bcn 2015-05-05) memory leak here? no deallocation?
        exit
    end if
    if (debug_active (D_SHOWER)) then
        if (i == size (shower%partons)) then
            call msg_bug ("shower_remove_parton_from_partons: parton&
                &to be removed not found")
        end if
    end if
end do
end subroutine shower_remove_parton_from_partons

```

This removes the parton prt and all its children.

<Shower core: procedures>+≡

```

recursive subroutine shower_remove_parton_from_partons_recursive (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), pointer :: prt
    if (associated (prt%child1)) then
        call shower_remove_parton_from_partons_recursive (shower, prt%child1)
        deallocate (prt%child1)
    end if
    if (associated (prt%child2)) then
        call shower_remove_parton_from_partons_recursive (shower, prt%child2)
        deallocate (prt%child2)
    end if
    call shower_remove_parton_from_partons (shower, prt)
end subroutine shower_remove_parton_from_partons_recursive

```

<Shower core: shower: TBP>+≡

```

procedure :: sort_partons => shower_sort_partons

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_sort_partons (shower)
    class(shower_t), intent(inout) :: shower
end subroutine shower_sort_partons

```

<Shower core: procedures>+≡

```

module subroutine shower_sort_partons (shower)
    class(shower_t), intent(inout) :: shower
    integer :: i, j, maxsort, size_partons
    logical :: changed
    if (debug_on) call msg_debug2 (D_SHOWER, "shower_sort_partons")
    if (.not. allocated (shower%partons)) return
    size_partons = size (shower%partons)
    maxsort = 0
    do i = 1, size_partons
        if (associated (shower%partons(i)%p)) maxsort = i
    end do
    if (signal_is_pending ()) return
    size_partons = size (shower%partons)
    if (size_partons <= 1) return
    do i = 1, maxsort
        if (.not. associated (shower%partons(i)%p)) cycle
        if (.not. shower%settings%isr_pt_ordered) then

```

```

    !!! set unsimulated ISR partons to be "typeless" to prevent
    !!! influences from "wrong" masses
    if (.not. shower%partons(i)%p%belongstoFSR .and. &
        .not. shower%partons(i)%p%simulated .and. &
        .not. shower%partons(i)%p%belongstointeraction) then
        shower%partons(i)%p%type = 0
    end if
end if
end do
if (signal_is_pending ()) return
!!! Just a Bubblesort
!!! Different algorithms needed for t-ordered and pt^2-ordered shower
!!! Pt-ordered:
if (shower%settings%isr_pt_ordered) then
    OUTERDO_PT: do i = 1, maxsort - 1
        changed = .false.
        INNERDO_PT: do j = 1, maxsort - i
            if (.not. associated (shower%partons(j + 1)%p)) cycle
            if (.not. associated (shower%partons(j)%p)) then
                !!! change if j + 1 is associated and j is not
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (shower%partons(j)%p%scale < &
                shower%partons(j + 1)%p%scale) then
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (nearly_equal(shower%partons(j)%p%scale, &
                shower%partons(j + 1)%p%scale)) then
                if (shower%partons(j)%p%nr > shower%partons(j + 1)%p%nr) then
                    call swap_pointers (shower%partons(j), shower%partons(j + 1))
                    changed = .true.
                end if
            end if
        end do INNERDO_PT
        if (.not. changed) exit OUTERDO_PT
    end do outerdo_pt
    !!! |t|-ordered
else
    OUTERDO_T: do i = 1, maxsort - 1
        changed = .false.
        INNERDO_T: do j = 1, maxsort - i
            if (.not. associated (shower%partons(j + 1)%p)) cycle
            if (.not. associated (shower%partons(j)%p)) then
                !!! change if j+1 is associated and j isn't
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (.not. shower%partons(j)%p%belongstointeraction .and. &
                shower%partons(j + 1)%p%belongstointeraction) then
                !!! move partons belonging to the interaction to the front
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (.not. shower%partons(j)%p%belongstointeraction .and. &
                .not. shower%partons(j + 1)%p%belongstointeraction ) then
                if (abs (shower%partons(j)%p%t) - &

```



```

        shower%partons(j)%p%mass_squared () < &
        abs(shower%partons(j + 1)%p%t) - &
        shower%partons(j + 1)%p%mass_squared ()) then
        call swap_pointers (shower%partons(j), shower%partons(j + 1))
        changed = .true.
    else
        if (nearly_equal(abs (shower%partons(j)%p%t) - &
            shower%partons(j)%p%mass_squared (), &
            abs(shower%partons(j + 1)%p%t) - &
            shower%partons(j + 1)%p%mass_squared ())) then
            if (shower%partons(j)%p%nr > &
                shower%partons(j + 1)%p%nr) then
                call swap_pointers (shower%partons(j), &
                    shower%partons(j + 1))
                changed = .true.
            end if
        end if
    end if
end do INNERDO_T
if (.not. changed) exit OUTERDO_T
end do OUTERDO_T
end if
end subroutine shower_sort_partons

```

Deallocate the interaction pointers.

```

<Shower core: shower: TBP>+≡
    procedure :: cleanup => shower_cleanup

<Shower core: sub interfaces>+≡
    module subroutine shower_cleanup (shower)
        class(shower_t), intent(inout) :: shower
    end subroutine shower_cleanup

<Shower core: procedures>+≡
    module subroutine shower_cleanup (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i
        if (allocated (shower%interactions)) then
            do i = 1, size (shower%interactions)
                if (allocated (shower%interactions(i)%i%partons)) &
                    deallocate (shower%interactions(i)%i%partons)
                deallocate (shower%interactions(i)%i)
            end do
            deallocate (shower%interactions)
        end if
        if (allocated (shower%partons)) deallocate (shower%partons)
    end subroutine shower_cleanup

```

Bookkeeping functions.

```

<Shower core: shower: TBP>+≡
    procedure :: get_next_free_nr => shower_get_next_free_nr

```

```

<Shower core: sub interfaces>+≡
    module function shower_get_next_free_nr (shower) result (next_number)
        class(shower_t), intent(inout) :: shower
        integer :: next_number
    end function shower_get_next_free_nr

<Shower core: procedures>+≡
    module function shower_get_next_free_nr (shower) result (next_number)
        class(shower_t), intent(inout) :: shower
        integer :: next_number
        next_number = shower%next_free_nr
        shower%next_free_nr = shower%next_free_nr + 1
    end function shower_get_next_free_nr

<Shower core: shower: TBP>+≡
    procedure :: update_max_color_nr => shower_update_max_color_nr

<Shower core: sub interfaces>+≡
    pure module subroutine shower_update_max_color_nr (shower, index)
        class(shower_t), intent(inout) :: shower
        integer, intent(in) :: index
    end subroutine shower_update_max_color_nr

<Shower core: procedures>+≡
    pure module subroutine shower_update_max_color_nr (shower, index)
        class(shower_t), intent(inout) :: shower
        integer, intent(in) :: index
        if (index > shower%next_color_nr) then
            shower%next_color_nr = index
        end if
    end subroutine shower_update_max_color_nr

<Shower core: shower: TBP>+≡
    procedure :: get_next_color_nr => shower_get_next_color_nr

<Shower core: sub interfaces>+≡
    module function shower_get_next_color_nr (shower) result (next_color)
        class(shower_t), intent(inout) :: shower
        integer :: next_color
    end function shower_get_next_color_nr

<Shower core: procedures>+≡
    module function shower_get_next_color_nr (shower) result (next_color)
        class(shower_t), intent(inout) :: shower
        integer :: next_color
        next_color = shower%next_color_nr
        shower%next_color_nr = shower%next_color_nr + 1
    end function shower_get_next_color_nr

<Shower core: procedures>+≡
    subroutine shower_enlarge_partons_array (shower, custom_length)
        type(shower_t), intent(inout) :: shower
        integer, intent(in), optional :: custom_length
        integer :: i, length, oldlength
        type(parton_pointer_t), dimension(:), allocatable :: tmp_partons

```

```

if (debug_on) call msg_debug (D_SHOWER, "shower_enlarge_partons_array")
if (present(custom_length)) then
    length = custom_length
else
    length = 10
end if
if (debug_active (D_SHOWER)) then
    if (length < 1) then
        call msg_bug ("Shower: no parton_pointers added in shower%partons")
    end if
end if
if (allocated (shower%partons)) then
    oldlength = size (shower%partons)
    allocate (tmp_partons(1:oldlength))
    do i = 1, oldlength
        tmp_partons(i)%p => shower%partons(i)%p
    end do
    deallocate (shower%partons)
else
    oldlength = 0
end if
allocate (shower%partons(1:oldlength + length))
do i = 1, oldlength
    shower%partons(i)%p => tmp_partons(i)%p
end do
do i = oldlength + 1, oldlength + length
    shower%partons(i)%p => null()
end do
end subroutine shower_enlarge_partons_array

```

<Shower core: shower: TBP>+≡

```

procedure :: add_child => shower_add_child

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_add_child (shower, prt, child)
    class(shower_t), intent(inout) :: shower
    type(parton_t), pointer :: prt
    integer, intent(in) :: child
end subroutine shower_add_child

```

<Shower core: procedures>+≡

```

module subroutine shower_add_child (shower, prt, child)
    class(shower_t), intent(inout) :: shower
    type(parton_t), pointer :: prt
    integer, intent(in) :: child
    integer :: i, lastfree
    type(parton_pointer_t) :: newprt
    if (child /= 1 .and. child /= 2) then
        call msg_bug ("Shower: Adding child in nonexisting place")
    end if
    allocate (newprt%p)
    newprt%p%nr = shower%get_next_free_nr ()
    !!! add new parton as child
    if (child == 1) then
        prt%child1 => newprt%p
    end if
end subroutine shower_add_child

```

```

else
    prt%child2 => newprt%p
end if
newprt%p%parent => prt
if (associated (prt%settings)) then
    newprt%p%settings => prt%settings
end if
newprt%p%interactionnr = prt%interactionnr
!!! add new parton to shower%partons list
if (associated (shower%partons (size(shower%partons))%p)) then
    call shower_enlarge_partons_array (shower)
end if
!!! find last free pointer and let it point to the new parton
lastfree = 0
do i = size (shower%partons), 1, -1
    if (.not. associated (shower%partons(i)%p)) then
        lastfree = i
    end if
end do
if (lastfree == 0) then
    call msg_bug ("Shower: no free pointers found")
end if
shower%partons(lastfree)%p => newprt%p
end subroutine shower_add_child

```

<Shower core: shower: TBP>+≡

```

procedure :: add_parent => shower_add_parent

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_add_parent (shower, prt)
    class(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
end subroutine shower_add_parent

```

<Shower core: procedures>+≡

```

module subroutine shower_add_parent (shower, prt)
    class(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    integer :: i, lastfree
    type(parton_pointer_t) :: newprt
    if (debug_on) call msg_debug2 &
        (D_SHOWER, "shower_add_parent: for parton nr", prt%nr)
    allocate (newprt%p)
    newprt%p%nr = shower%get_next_free_nr ()
    !!! add new parton as parent
    newprt%p%child1 => prt
    prt%parent => newprt%p
    if (associated (prt%settings)) then
        newprt%p%settings => prt%settings
    end if
    newprt%p%interactionnr = prt%interactionnr
    !!! add new parton to shower%partons list
    if (.not. allocated (shower%partons) .or. &
        associated (shower%partons (size(shower%partons))%p)) then
        call shower_enlarge_partons_array (shower)
    end if

```

```

end if
!!! find last free pointer and let it point to the new parton
lastfree = 0
do i = size(shower%partons), 1, -1
  if (.not. associated (shower%partons(i)%p)) then
    lastfree = i
  end if
end do
if (debug_active (D_SHOWER)) then
  if (lastfree == 0) then
    call msg_bug ("Shower: no free pointers found")
  end if
end if
shower%partons(lastfree)%p => newprt%p
end subroutine shower_add_parent

```

For debugging:

```

<Shower core: procedures>+=
pure function shower_get_total_momentum (shower) result (mom)
  type(shower_t), intent(in) :: shower
  type(vector4_t) :: mom
  integer :: i
  if (.not. allocated (shower%partons)) return
  mom = vector4_null
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    if (shower%partons(i)%p%is_final ()) then
      mom = mom + shower%partons(i)%p%momentum
    end if
  end do
end function shower_get_total_momentum

```

Count the number of partons by going through `shower%partons` whereby you can require a minimum energy `mine` and specify whether to `include_remnants`, which is done if not given.

```

<Shower core: shower: TBP>+=
procedure :: get_nr_of_partons => shower_get_nr_of_partons

<Shower core: sub interfaces>+=
module function shower_get_nr_of_partons (shower, mine, &
  include_remnants, no_hard_prts, only_colored) result (nr)
  class(shower_t), intent(in) :: shower
  real(default), intent(in), optional :: mine
  logical, intent(in), optional :: include_remnants, no_hard_prts, &
    only_colored
  integer :: nr
end function shower_get_nr_of_partons

<Shower core: procedures>+=
module function shower_get_nr_of_partons (shower, mine, &
  include_remnants, no_hard_prts, only_colored) result (nr)
  class(shower_t), intent(in) :: shower
  real(default), intent(in), optional :: mine
  logical, intent(in), optional :: include_remnants, no_hard_prts, &

```

```

        only_colored
logical :: no_hard, only_col, include_rem
integer :: nr, i
nr = 0
no_hard = .false.; if (present (no_hard_prts)) &
    no_hard = no_hard_prts
only_col = .false.; if (present (only_colored)) &
    only_col = only_colored
include_rem = .true.; if (present (include_remnants)) &
    include_rem = include_remnants
do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    associate (prt => shower%partons(i)%p)
        if (.not. prt%is_final ()) cycle
        if (present (only_colored)) then
            if (only_col) then
                if (.not. prt%is_colored ()) cycle
            else
                if (prt%is_colored ()) cycle
            end if
        end if
        if (no_hard) then
            if (shower%partons(i)%p%belongstointeraction) cycle
        end if
        if (.not. include_rem) then
            if (prt%type == BEAM_REMNANT) cycle
        end if
        if (present(mine)) then
            if (prt%momentum%p(0) < mine) cycle
        end if
        nr = nr + 1
    end associate
end do
end function shower_get_nr_of_partons

```

(Shower core: procedures)+≡

```

function shower_get_nr_of_final_colored_ME_partons (shower) result (nr)
    type(shower_t), intent(in) :: shower
    integer :: nr
    integer :: i, j
    type(parton_t), pointer :: prt
    nr = 0
    do i = 1, size (shower%interactions)
        do j = 1, size (shower%interactions(i)%i%partons)
            prt => shower%interactions(i)%i%partons(j)%p
            if (.not. associated (prt)) cycle
            if (.not. prt%is_colored ()) cycle
            if (prt%belongstointeraction .and. prt%belongstoFSR .and. &
                (prt%type /= INTERNAL)) then
                nr = nr + 1
            end if
        end do
    end do
end function shower_get_nr_of_final_colored_ME_partons

```

```

(Shower core: shower: TBP)+≡
  procedure :: get_final_colored_ME_momenta => &
    shower_get_final_colored_ME_momenta

(Shower core: sub interfaces)+≡
  module subroutine shower_get_final_colored_ME_momenta (shower, momenta)
    class(shower_t), intent(in) :: shower
    type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
  end subroutine shower_get_final_colored_ME_momenta

(Shower core: procedures)+≡
  module subroutine shower_get_final_colored_ME_momenta (shower, momenta)
    class(shower_t), intent(in) :: shower
    type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
    type(parton_pointer_t), dimension(:), allocatable :: partons
    integer :: i, j, index, s
    type(parton_t), pointer :: prt
    s = shower_get_nr_of_final_colored_ME_partons (shower)
    if (s == 0) return
    allocate (partons(1:s))
    allocate (momenta(1:s))
    index = 0
    do i = 1, size (shower%interactions)
      do j = 1, size (shower%interactions(i)%i%partons)
        prt => shower%interactions(i)%i%partons(j)%p
        if (.not. associated (prt)) cycle
        if (.not. prt%is_colored ()) cycle
        if (prt%belongstointeraction .and. prt%belongstoFSR .and. &
          (prt%type /= INTERNAL)) then
          index = index + 1
          partons(index)%p => prt
        end if
      end do
    end do
    do i = 1, s ! pointers forbid array notation
      momenta(i) = partons(i)%p%momentum
    end do
  end subroutine shower_get_final_colored_ME_momenta

(Shower core: procedures)+≡
  recursive function interaction_fsr_is_finished_for_parton &
    (prt) result (finished)
  type(parton_t), intent(in) :: prt
  logical :: finished
  if (prt%belongstoFSR) then
    !!! FSR partons
    if (associated (prt%child1)) then
      finished = interaction_fsr_is_finished_for_parton (prt%child1) &
        .and. interaction_fsr_is_finished_for_parton (prt%child2)
    else
      finished = prt%t <= prt%mass_squared ()
    end if
  end if
  else

```

```

!!! search for emitted timelike partons in ISR shower
if (.not. associated (prt%initial)) then
  !!! no initial -> no ISR
  finished = .true.
else if (.not. associated (prt%parent)) then
  finished = .false.
else
  if (.not. prt%parent%is_proton ()) then
    if (associated (prt%child2)) then
      finished = interaction_fsr_is_finished_for_parton (prt%parent) .and. &
        interaction_fsr_is_finished_for_parton (prt%child2)
    else
      finished = interaction_fsr_is_finished_for_parton (prt%parent)
    end if
  else
    if (associated (prt%child2)) then
      finished = interaction_fsr_is_finished_for_parton (prt%child2)
    else
      !!! only second partons can come here -> if that happens FSR
      !!! evolution is not existing
      finished = .true.
    end if
  end if
end if
end function interaction_fsr_is_finished_for_parton

```

<Shower core: procedures>+≡

```

function interaction_fsr_is_finished (interaction) result (finished)
  type(shower_interaction_t), intent(in) :: interaction
  logical :: finished
  integer :: i
  finished = .true.
  if (.not. allocated (interaction%partons)) return
  do i = 1, size (interaction%partons)
    if (.not. interaction_fsr_is_finished_for_parton &
      (interaction%partons(i)%p)) then
      finished = .false.
    exit
  end if
end do
end function interaction_fsr_is_finished

```

<Shower core: public>+≡

```

public :: shower_interaction_get_s

```

<Shower core: sub interfaces>+≡

```

module function shower_interaction_get_s (interaction) result (s)
  type(shower_interaction_t), intent(in) :: interaction
  real(default) :: s
end function shower_interaction_get_s

```

<Shower core: procedures>+≡

```

module function shower_interaction_get_s (interaction) result (s)

```



```

type(shower_interaction_t), intent(in) :: interaction
real(default) :: s
s = (interaction%partons(1)%p%initial%momentum + &
      interaction%partons(2)%p%initial%momentum)**2
end function shower_interaction_get_s

```

(Shower core: procedures)+≡

```

function shower_fsr_is_finished (shower) result (finished)
type(shower_t), intent(in) :: shower
logical :: finished
integer :: i
finished = .true.
if (.not. allocated (shower%interactions)) return
do i = 1, size(shower%interactions)
  if (.not. interaction_fsr_is_finished (shower%interactions(i)%i)) then
    finished = .false.
    exit
  end if
end do
end function shower_fsr_is_finished

```

(Shower core: procedures)+≡

```

function shower_isr_is_finished (shower) result (finished)
type(shower_t), intent(in) :: shower
logical :: finished
integer :: i
type(parton_t), pointer :: prt
finished = .true.
if (.not.allocated (shower%partons)) return
do i = 1, size (shower%partons)
  if (.not. associated (shower%partons(i)%p)) cycle
  prt => shower%partons(i)%p
  if (shower%settings%isr_pt_ordered) then
    if (.not. prt%belongstoFSR .and. .not. prt%simulated &
        .and. prt%scale > zero) then
      finished = .false.
      exit
    end if
  else
    if (.not. prt%belongstoFSR .and. .not. prt%simulated &
        .and. prt%t < zero) then
      finished = .false.
      exit
    end if
  end if
end do
end function shower_isr_is_finished

```

(Shower core: procedures)+≡

```

subroutine interaction_find_partons_nearest_to_hadron &
  (interaction, prt1, prt2, isr_pt_ordered)
type(shower_interaction_t), intent(in) :: interaction

```

```

type(parton_t), pointer :: prt1, prt2
logical, intent(in) :: isr_pt_ordered
prt1 => null ()
prt2 => null ()
prt1 => interaction%partons(1)%p
do
  if (associated (prt1%parent)) then
    if (prt1%parent%is_proton ()) then
      exit
    else if ((.not. isr_pt_ordered .and. .not. prt1%parent%simulated) &
      .or. (isr_pt_ordered .and. .not. prt1%simulated)) then
      exit
    else
      prt1 => prt1%parent
    end if
  else
    exit
  end if
end do
prt2 => interaction%partons(2)%p
do
  if (associated (prt2%parent)) then
    if (prt2%parent%is_proton ()) then
      exit
    else if ((.not. isr_pt_ordered .and. .not. prt2%parent%simulated) &
      .or. (isr_pt_ordered .and. .not. prt2%simulated)) then
      exit
    else
      prt2 => prt2%parent
    end if
  else
    exit
  end if
end do
end subroutine interaction_find_partons_nearest_to_hadron

```

<Shower core: shower: TBP>+≡

```

procedure :: update_beamremnants => shower_update_beamremnants

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_update_beamremnants (shower)
  class(shower_t), intent(inout) :: shower
end subroutine shower_update_beamremnants

```

<Shower core: procedures>+≡

```

module subroutine shower_update_beamremnants (shower)
  class(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: hadron, remnant
  integer :: i
  real(default) :: random
  !!! only proton in first interaction !!!
  !!! currently only first beam-remnant will be updated
  do i = 1,2
    if (associated (shower%interactions(1)%i%partons(i)%p%initial)) then
      hadron => shower%interactions(1)%i%partons(i)%p%initial
    end if
  end do
end subroutine shower_update_beamremnants

```

```

else
  cycle
end if
remnant => hadron%child2
if (associated (remnant)) then
  remnant%momentum = hadron%momentum - hadron%child1%momentum
end if
!!! generate flavor of the beam-remnant if beam was proton
if (abs (hadron%type) == PROTON .and. associated (hadron%child1)) then
  if (hadron%child1%is_quark ()) then
    !!! decide if valence (u,d) or sea quark (s,c,b)
    if ((abs (hadron%child1%type) <= 2) .and. &
      (hadron%type * hadron%child1%type > zero)) then
      !!! valence quark
      if (abs (hadron%child1%type) == 1) then
        !!! if d then remaining diquark is uu_1
        remnant%type = sign (UU1, hadron%type)
      else
        call shower%rng%generate (random)
        !!! if u then remaining diquark is ud_0 or ud_1
        if (random < 0.75_default) then
          remnant%type = sign (UD0, hadron%type)
        else
          remnant%type = sign (UD1, hadron%type)
        end if
      end if
      remnant%c1 = hadron%child1%c2
      remnant%c2 = hadron%child1%c1
    else if ((hadron%type * hadron%child1%type) < zero) then
      !!! antiquark
      if (.not. associated (remnant%child1)) then
        call shower%add_child (remnant, 1)
      end if
      if (.not. associated (remnant%child2)) then
        call shower%add_child (remnant, 2)
      end if
      call shower%rng%generate (random)
      if (random < 0.6666_default) then
        !!! 2/3 into udq + u
        if (abs (hadron%child1%type) == 1) then
          remnant%child1%type = sign (NEUTRON, hadron%type)
        else if (abs (hadron%child1%type) == 2) then
          remnant%child1%type = sign (PROTON, hadron%type)
        else if (abs (hadron%child1%type) == 3) then
          remnant%child1%type = sign (SIGMA0, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
          remnant%child1%type = sign (SIGMACPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 5) then
          remnant%child1%type = sign (SIGMAB0, hadron%type)
        end if
        remnant%child2%type = sign (2, hadron%type)
      else
        !!! 1/3 into uuq + d
        if (abs (hadron%child1%type) == 1) then

```

```

        remnant%child1%type = sign (PROTON, hadron%type)
    else if (abs (hadron%child1%type) == 2) then
        remnant%child1%type = sign (DELTAPLUSPLUS, hadron%type)
    else if (abs (hadron%child1%type) == 3) then
        remnant%child1%type = sign (SIGMAPLUS, hadron%type)
    else if (abs (hadron%child1%type) == 4) then
        remnant%child1%type = sign (SIGMACPLUSPLUS, hadron%type)
    else if (abs (hadron%child1%type) == 5) then
        remnant%child1%type = sign (SIGMABPLUS, hadron%type)
    end if
    remnant%child2%type = sign (1, hadron%type)
end if
remnant%c1 = hadron%child1%c2
remnant%c2 = hadron%child1%c1
remnant%child1%c1 = 0
remnant%child1%c2 = 0
remnant%child2%c1 = remnant%c1
remnant%child2%c2 = remnant%c2
else
    !!! sea quark
    if (.not. associated (remnant%child1)) then
        call shower%add_child (remnant, 1)
    end if
    if (.not. associated (remnant%child2)) then
        call shower%add_child (remnant, 2)
    end if
    call shower%rng%generate (random)
    if (random < 0.5_default) then
        !!! 1/2 into usbar + ud_0
        if (abs (hadron%child1%type) == 3) then
            remnant%child1%type = sign (KPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
            remnant%child1%type = sign (D0, hadron%type)
        else if (abs (hadron%child1%type) == 5) then
            remnant%child1%type = sign (BPLUS, hadron%type)
        end if
        remnant%child2%type = sign (UD0, hadron%type)
    else if (random < 0.6666_default) then
        !!! 1/6 into usbar + ud_1
        if (abs (hadron%child1%type) == 3) then
            remnant%child1%type = sign (KPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
            remnant%child1%type = sign (D0, hadron%type)
        else if (abs (hadron%child1%type) == 5) then
            remnant%child1%type = sign (BPLUS, hadron%type)
        end if
        remnant%child2%type = sign (UD1, hadron%type)
    else
        !!! 1/3 into dsbar + uu_1
        if (abs (hadron%child1%type) == 3) then
            remnant%child1%type = sign (K0, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
            remnant%child1%type = sign (DPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 5) then

```

```

        remnant%child1%type = sign (B0, hadron%type)
    end if
    remnant%child2%type = sign (UU1, hadron%type)
end if
remnant%c1 = hadron%child1%c2
remnant%c2 = hadron%child1%c1
remnant%child1%c1 = 0
remnant%child1%c2 = 0
remnant%child2%c1 = remnant%c1
remnant%child2%c2 = remnant%c2
end if
else if (hadron%child1%is_gluon ()) then
    if (.not.associated (remnant%child1)) then
        call shower%add_child (remnant, 1)
    end if
    if (.not.associated (remnant%child2)) then
        call shower%add_child (remnant, 2)
    end if
    call shower%rng%generate (random)
    if (random < 0.5_default) then
        !!! 1/2 into u + ud_0
        remnant%child1%type = sign (2, hadron%type)
        remnant%child2%type = sign (UD0, hadron%type)
    else if (random < 0.6666_default) then
        !!! 1/6 into u + ud_1
        remnant%child1%type = sign (2, hadron%type)
        remnant%child2%type = sign (UD1, hadron%type)
    else
        !!! 1/3 into d + uu_1
        remnant%child1%type = sign (1, hadron%type)
        remnant%child2%type = sign (UU1, hadron%type)
    end if
    remnant%c1 = hadron%child1%c2
    remnant%c2 = hadron%child1%c1
    if (hadron%type > 0) then
        remnant%child1%c1 = remnant%c1
        remnant%child2%c2 = remnant%c2
    else
        remnant%child1%c2 = remnant%c2
        remnant%child2%c1 = remnant%c1
    end if
end if
remnant%initial => hadron
if (associated (remnant%child1)) then
    remnant%child1%initial => hadron
    remnant%child2%initial => hadron
    !!! don't care about on-shellness for now
    remnant%child1%momentum = 0.5_default * remnant%momentum
    remnant%child2%momentum = 0.5_default * remnant%momentum
    !!! but care about on-shellness for baryons
    if (mod (remnant%child1%type, 100) >= 10) then
        !!! check if the third quark is set -> meson or baryon
        remnant%child1%t = remnant%child1%mass_squared ()
        remnant%child1%momentum = [remnant%child1%momentum%p(0), &

```

```

        (remnant%child1%momentum%p(1:3) / &
        remnant%child1%momentum%p(1:3)**1) * &
        sqrt (remnant%child1%momentum%p(0)**2 - remnant%child1%t)]
        remnant%child2%momentum = remnant%momentum &
        - remnant%child1%momentum
    end if
end if
end if
end do
end subroutine shower_update_beamremnants

```

(Shower core: procedures)+≡

```

subroutine interaction_apply_lorentztrafo (interaction, L)
    type(shower_interaction_t), intent(inout) :: interaction
    type(lorentz_transformation_t), intent(in) :: L
    type(parton_t), pointer :: prt
    integer :: i
    !!! ISR part
    do i = 1,2
        prt => interaction%partons(i)%p
        !!! loop over ancestors
        MOTHERS: do
            !!! boost parton
            call parton_apply_lorentztrafo (prt, L)
            if (associated (prt%child2)) then
                !!! boost emitted timelike parton (and daughters)
                call parton_apply_lorentztrafo_recursive (prt%child2, L)
            end if
            if (associated (prt%parent)) then
                if (.not. prt%parent%is_proton ()) then
                    prt => prt%parent
                else
                    exit
                end if
            else
                exit
            end if
        end do MOTHERS
    end do
    !!! FSR part
    if (associated (interaction%partons(3)%p%parent)) then
        !!! pseudo Parton-Shower histora has been generated -> find
        !!! mother and go on from there recursively
        prt => interaction%partons(3)%p
        do while (associated (prt%parent))
            prt => prt%parent
        end do
        call parton_apply_lorentztrafo_recursive (prt, L)
    else
        do i = 3, size (interaction%partons)
            call parton_apply_lorentztrafo (interaction%partons(i)%p, L)
        end do
    end if
end subroutine interaction_apply_lorentztrafo

```

(Shower core: procedures)+≡

```

subroutine shower_apply_lorentztrafo (shower, L)
  type(shower_t), intent(inout) :: shower
  type(lorentz_transformation_t), intent(in) :: L
  integer :: i
  do i = 1, size (shower%interactions)
    call interaction_apply_lorentztrafo (shower%interactions(i)%i, L)
  end do
end subroutine shower_apply_lorentztrafo

```

This boosts partons belonging to the interaction to the center-of-mass frame of its partons nearest to the hadron.

(Shower core: procedures)+≡

```

subroutine interaction_boost_to_CMframe (interaction, isr_pt_ordered)
  type(shower_interaction_t), intent(inout) :: interaction
  logical, intent(in) :: isr_pt_ordered
  type(vector4_t) :: beta
  type(parton_t), pointer :: prt1, prt2
  call interaction_find_partons_nearest_to_hadron &
    (interaction, prt1, prt2, isr_pt_ordered)
  beta = prt1%momentum + prt2%momentum
  beta = beta / beta%p(0)
  if (debug_active (D_SHOWER)) then
    if (beta**2 > one) then
      call msg_error ("Shower: boost to CM frame: beta > 1")
      return
    end if
  end if
  if (space_part(beta)**2 > tiny_13) then
    call interaction_apply_lorentztrafo (interaction, &
      boost(space_part(beta)**1 / &
        sqrt (one - space_part(beta)**2), -direction(beta)))
  end if
end subroutine interaction_boost_to_CMframe

```

This boosts every interaction to the center-of-mass-frame of its partons nearest to the hadron.

(Shower core: shower: TBP)+≡

```

procedure :: boost_to_CMframe => shower_boost_to_CMframe

```

(Shower core: sub interfaces)+≡

```

module subroutine shower_boost_to_CMframe (shower)
  class(shower_t), intent(inout) :: shower
end subroutine shower_boost_to_CMframe

```

(Shower core: procedures)+≡

```

module subroutine shower_boost_to_CMframe (shower)
  class(shower_t), intent(inout) :: shower
  integer :: i
  do i = 1, size (shower%interactions)
    call interaction_boost_to_CMframe &
      (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
  end do
end module shower_boost_to_CMframe

```

```

end do
! TODO: (bcn 2015-03-23) this shouldnt be here !
call shower%update_beamremnants ()
end subroutine shower_boost_to_CMframe

```

This boost all partons so that initial partons have their assigned x -value.

```

<Shower core: shower: TBP>+=
  procedure :: boost_to_labframe => shower_boost_to_labframe

<Shower core: sub interfaces>+=
  module subroutine shower_boost_to_labframe (shower)
    class(shower_t), intent(inout) :: shower
  end subroutine shower_boost_to_labframe

<Shower core: procedures>+=
  module subroutine shower_boost_to_labframe (shower)
    class(shower_t), intent(inout) :: shower
    integer :: i
    do i = 1, size (shower%interactions)
      call interaction_boost_to_labframe &
        (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
    end do
  end subroutine shower_boost_to_labframe

```

This boosts all partons so that initial partons have their assigned x -value.

```

<Shower core: procedures>+=
  subroutine interaction_boost_to_labframe (interaction, isr_pt_ordered)
    type(shower_interaction_t), intent(inout) :: interaction
    logical, intent(in) :: isr_pt_ordered
    type(parton_t), pointer :: prt1, prt2
    type(vector3_t) :: beta
    call interaction_find_partons_nearest_to_hadron &
      (interaction, prt1, prt2, isr_pt_ordered)
    if (.not. associated (prt1%initial) .or. .not. &
      associated (prt2%initial)) then
      return
    end if
    !!! transform partons to overall labframe.
    beta = vector3_canonical(3) * &
      ((prt1%x * prt2%momentum%p(0) - &
        prt2%x * prt1%momentum%p(0)) / &
      (prt1%x * prt2%momentum%p(3) - &
        prt2%x * prt1%momentum%p(3)))
    if (beta**1 > tiny_10) &
      call interaction_apply_lorentztrafo (interaction, &
        boost (beta**1 / sqrt(one - beta**2), -direction(beta)))
  end subroutine interaction_boost_to_labframe

```

Only rotate to z if initial hadrons are given (and they are assumed to be aligned along the z -axis).

```

<Shower core: procedures>+=
  subroutine interaction_rotate_to_z (interaction, isr_pt_ordered)
    type(shower_interaction_t), intent(inout) :: interaction

```



```

logical, intent(in) :: isr_pt_ordered
type(parton_t), pointer :: prt1, prt2
call interaction_find_partons_nearest_to_hadron &
    (interaction, prt1, prt2, isr_pt_ordered)
if (associated (prt1%initial)) then
    call interaction_apply_lorentztrafo (interaction, &
        rotation_to_2nd (space_part (prt1%momentum), &
            vector3_canonical(3) * sign (one, &
                prt1%initial%momentum%p(3))))
end if
end subroutine interaction_rotate_to_z

```

Rotate initial partons to lie along $\pm z$ axis.

```

<Shower core: shower: TBP>+=
    procedure :: rotate_to_z => shower_rotate_to_z

<Shower core: sub interfaces>+=
    module subroutine shower_rotate_to_z (shower)
        class(shower_t), intent(inout) :: shower
    end subroutine shower_rotate_to_z

<Shower core: procedures>+=
    module subroutine shower_rotate_to_z (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i
        do i = 1, size (shower%interactions)
            call interaction_rotate_to_z &
                (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
        end do
        ! TODO: (bcn 2015-03-23) this shouldnt be here !
        call shower%update_beamremnants ()
    end subroutine shower_rotate_to_z

```

Return if there are no initials, electron-hadron collision not implemented.

```

<Shower core: procedures>+=
    subroutine interaction_generate_primordial_kt &
        (interaction, primordial_kt_width, primordial_kt_cutoff, rng)
        type(shower_interaction_t), intent(inout) :: interaction
        real(default), intent(in) :: primordial_kt_width, primordial_kt_cutoff
        class(rng_t), intent(inout), allocatable :: rng
        type(parton_t), pointer :: had1, had2
        type(vector4_t) :: momenta(2)
        type(vector3_t) :: beta
        real(default) :: pt (2), phi(2)
        real(default) :: shat
        real(default) :: btheta, bphi
        integer :: i
        if (vanishes (primordial_kt_width)) return
        if (.not. associated (interaction%partons(1)%p%initial) .or. &
            .not. associated (interaction%partons(2)%p%initial)) then
            return
        end if
        had1 => interaction%partons(1)%p%initial
        had2 => interaction%partons(2)%p%initial
    end subroutine

```

```

!!! copy momenta and energy
momenta(1) = had1%child1%momentum
momenta(2) = had2%child1%momentum
GENERATE_PT_PHI: do i = 1, 2
  !!! generate transverse momentum and phi
  GENERATE_PT: do
    call rng%generate (pt (i))
    pt(i) = primordial_kt_width * sqrt(-log(pt(i)))
    if (pt(i) < primordial_kt_cutoff) exit
  end do GENERATE_PT
  call rng%generate (phi (i))
  phi(i) = twopi * phi(i)
end do GENERATE_PT_PHI
!!! adjust momenta
shat = (momenta(1) + momenta(2))**2
momenta(1) = [momenta(1)%p(0), &
  pt(1) * cos(phi(1)), &
  pt(1) * sin(phi(1)), &
  momenta(1)%p(3)]
momenta(2) = [momenta(2)%p(0), &
  pt(2) * cos(phi(2)), &
  pt(2) * sin(phi(2)), &
  momenta(2)%p(3)]
beta = [momenta(1)%p(1) + momenta(2)%p(1), &
  momenta(1)%p(2) + momenta(2)%p(2), zero] / sqrt(shat)
momenta(1) = boost (beta**1 / sqrt(one - beta**2), -direction(beta)) &
  * momenta(1)
bphi = azimuthal_angle (momenta(1))
btheta = polar_angle (momenta(1))
call interaction_apply_lorentztrafo (interaction, &
  rotation (cos(bphi), sin(bphi), 3) * rotation(cos(btheta), &
  sin(btheta), 2) * rotation(cos(-bphi), sin(-bphi), 3))
call interaction_apply_lorentztrafo (interaction, &
  boost (beta**1 / sqrt(one - beta**2), -direction(beta)))
end subroutine interaction_generate_primordial_kt

```

<Shower core: shower: TBP>+≡

```

procedure :: generate_primordial_kt => shower_generate_primordial_kt

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_generate_primordial_kt (shower)
  class(shower_t), intent(inout) :: shower
end subroutine shower_generate_primordial_kt

```

<Shower core: procedures>+≡

```

module subroutine shower_generate_primordial_kt (shower)
  class(shower_t), intent(inout) :: shower
  integer :: i
  do i = 1, size (shower%interactions)
    call interaction_generate_primordial_kt (shower%interactions(i)%i, &
      shower%settings%isr_primordial_kt_width, &
      shower%settings%isr_primordial_kt_cutoff, shower%rng)
  end do
  ! TODO: (bcn 2015-03-23) this shouldnt be here !
  call shower%update_beamremnants ()

```

```
end subroutine shower_generate_primordial_kt
```

Output.

<Shower core: procedures>+≡

```
subroutine interaction_write (interaction, unit)
  type(shower_interaction_t), intent(in) :: interaction
  integer, intent(in), optional :: unit
  integer :: i, u
  u = given_output_unit (unit); if (u < 0) return
  if (associated (interaction%partons(1)%p)) then
    if (associated (interaction%partons(1)%p%initial)) &
      call interaction%partons(1)%p%initial%write (u)
    end if
  if (associated (interaction%partons(2)%p)) then
    if (associated (interaction%partons(2)%p%initial)) &
      call interaction%partons(2)%p%initial%write (u)
    end if
  if (allocated (interaction%partons)) then
    do i = 1, size (interaction%partons)
      call interaction%partons(i)%p%write (u)
    end do
  end if
  write (u, "(A)")
end subroutine interaction_write
```

<Shower core: shower: TBP>+≡

```
procedure :: write => shower_write
```

<Shower core: sub interfaces>+≡

```
module subroutine shower_write (shower, unit)
  class(shower_t), intent(in) :: shower
  integer, intent(in), optional :: unit
end subroutine shower_write
```

<Shower core: procedures>+≡

```
module subroutine shower_write (shower, unit)
  class(shower_t), intent(in) :: shower
  integer, intent(in), optional :: unit
  integer :: i, u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "-----"
  write (u, "(1x,A)") "WHIZARD internal parton shower"
  write (u, "(1x,A)") "-----"
  call shower%pdf_data%write (u)
  if (size (shower%interactions) > 0) then
    write (u, "(3x,A)") "Interactions: "
    do i = 1, size (shower%interactions)
      write (u, "(4x,A,I0)") "Interaction number ", i
      if (.not. associated (shower%interactions(i)%i)) then
        call msg_fatal ("Shower: missing interaction in shower")
      end if
      call interaction_write (shower%interactions(i)%i, u)
    end do
  else

```

```

        write (u, "(3x,A)") "[no interactions in shower]"
    end if
    write (u, "(A)")
    if (allocated (shower%partons)) then
        write (u, "(5x,A)") "Partons:"
        do i = 1, size (shower%partons)
            if (associated (shower%partons(i)%p)) then
                call shower%partons(i)%p%write (u)
                if (i < size (shower%partons)) then
                    if (associated (shower%partons(i + 1)%p)) then
                        if (shower%partons(i)%p%belongstointeraction .and. &
                            .not. shower%partons(i + 1)%p%belongstointeraction) then
                            call write_separator (u)
                        end if
                    end if
                end if
            end if
        end do
    else
        write (u, "(5x,A)") "[no partons in shower]"
    end if
    write (u, "(4x,A)") "Total Momentum: "
    call vector4_write (shower_get_total_momentum (shower))
    write (u, "(1x,A,L1)") "ISR finished: ", shower_isr_is_finished (shower)
    write (u, "(1x,A,L1)") "FSR finished: ", shower_fsr_is_finished (shower)
end subroutine shower_write

```

We combine the `particle_set` from the hard interaction with the partons of the shower. For simplicity, we do not maintain the mother-daughter-relations of the shower. Hadronic beam_remnants of the old `particle_set` are removed as they are provided, including proper flavor information, by the ISR shower.

(Shower core: shower: TBP)+≡

```

    procedure :: combine_with_particle_set => shower_combine_with_particle_set

```

(Shower core: sub interfaces)+≡

```

    module subroutine shower_combine_with_particle_set (shower, particle_set, &
        model_in, model_hadrons)
        class(shower_t), intent(in) :: shower
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
    end subroutine shower_combine_with_particle_set

```

(Shower core: procedures)+≡

```

    module subroutine shower_combine_with_particle_set (shower, particle_set, &
        model_in, model_hadrons)
        class(shower_t), intent(in) :: shower
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
        type(particle_t), dimension(:), allocatable :: particles
        integer, dimension(:), allocatable :: hard_colored_ids, &
            shower_partons_ids, incoming_ids, outgoing_ids
        class(model_data_t), pointer :: model

```

```

logical, dimension(:), allocatable :: hard_colored_mask
integer :: n_shower_partons, n_remnants, i, j
integer :: n_in, n_out, n_beam, n_tot_old
if (signal_is_pending ()) return
if (debug_on) call msg_debug (D_SHOWER, "shower_combine_with_particle_set")
if (debug_on) call msg_debug (D_SHOWER, "Particle set before replacing")
if (debug_active (D_SHOWER)) &
    call particle_set%write (summary=.true., compressed=.true.)

n_shower_partons = shower%get_nr_of_partons (only_colored = &
                                           .true., no_hard_prts = .true.)
n_remnants = shower%get_nr_of_partons (only_colored = .false., &
                                       no_hard_prts = .true.)

if (n_shower_partons + n_remnants > 0) then
    call particle_set%without_hadronic_remnants &
        (particles, n_tot_old, n_shower_partons + n_remnants)
    call count_and_allocate ()
    call replace_outgoings ()
    call set_hard_colored_as_resonant_parents_for_shower ()
    call add_to_pset (n_tot_old, .true.)
    call add_to_pset (n_tot_old + n_remnants, .false.)
    call particle_set%replace (particles)
end if

if (debug_on) call msg_debug (D_SHOWER, 'Particle set after replacing')
if (debug_active (D_SHOWER)) &
    call particle_set%write (summary=.true., compressed=.true.)

```

contains

<Shower core: shower combine with particle set: procedures>

end subroutine shower_combine_with_particle_set

<Shower core: shower combine with particle set: procedures>≡

```

subroutine count_and_allocate ()
    n_beam = particle_set%get_n_beam ()
    n_in = particle_set%get_n_in ()
    n_out = particle_set%get_n_out ()
    allocate (hard_colored_mask (size (particles)))
    hard_colored_mask = (particles%get_status () == PRT_INCOMING .or. &
                        particles%get_status () == PRT_OUTGOING) .and. &
                        particles%is_colored ()
    allocate (hard_colored_ids (count (hard_colored_mask)))
    hard_colored_ids = pack ([i, i=1, size (particles)], hard_colored_mask)
    allocate (shower_partons_ids (n_shower_partons))
    shower_partons_ids = [(n_tot_old + n_remnants + i, i=1, n_shower_partons)]
    allocate (incoming_ids(n_in))
    incoming_ids = [(n_beam + i, i=1, n_in)]
    allocate (outgoing_ids(n_out))
    outgoing_ids = [(n_tot_old - n_out + i, i=1, n_out)]
    if (debug_active (D_SHOWER)) then
        print *, 'n_remnants = ', n_remnants
        print *, 'n_shower_partons = ', n_shower_partons
    end if
end subroutine count_and_allocate

```

```

        print *, 'n_tot_old = ', n_tot_old
        print *, 'n_beam = ', n_beam
        print *, 'n_in, n_out = ', n_in, n_out
    end if
end subroutine count_and_allocate

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine replace_outgoings ()
    do i = 1, size (shower%interactions)
        if (i > 1) then
            call msg_bug ('shower_combine_with_particle_set assumes 1 interaction')
        end if
        associate (interaction => shower%interactions(i)%i)
            do j = 3, size (interaction%partons)
                if (associated (interaction%partons(j)%p)) then
                    call replace_parton_in_particles (j, interaction%partons(j)%p)
                end if
            end do
        end associate
    end do
end subroutine replace_outgoings

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine replace_parton_in_particles (j, prt)
    integer, intent(in) :: j
    type(parton_t), intent(in) :: prt
    integer :: idx
    if (j <= 2) then
        idx = n_beam + j
    else
        idx = n_tot_old - n_out - n_in + j
    end if
    call particles(idx)%set_momentum (prt%momentum)
end subroutine replace_parton_in_particles

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine set_hard_colored_as_resonant_parents_for_shower ()
    do i = 1, n_tot_old
        if (hard_colored_mask (i)) then
            if (hasSplitted (i)) then
                call particles(i)%add_children (shower_partons_ids)
                if (particles(i)%get_status () == PRT_OUTGOING) then
                    call particles(i)%set_status (PRT_RESONANT)
                end if
            end if
        end if
    end do
end subroutine set_hard_colored_as_resonant_parents_for_shower

```

(Shower core: shower combine with particle set: procedures)+≡

```

function hasSplitted (i) result (splitted)
    logical :: splitted

```

```

integer, intent(in) :: i
splitted = .false.
do j = 1, size (shower%partons)
  if (.not. associated (shower%partons(j)%p)) cycle
  if (particles(i)%flv%get_pdg () == shower%partons(j)%p%type) then
    if (all (nearly_equal (particles(i)%p%p, &
                          shower%partons(j)%p%momentum%p))) then
      splitted = shower%partons(j)%p%is_branched ()
    end if
  end if
end do
end function has_splitted

<Shower core: shower combine with particle set: procedures>+≡
subroutine add_to_pset (offset, remnants)
  integer, intent(in) :: offset
  logical, intent(in) :: remnants
  integer :: i, j
  j = offset
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    associate (prt => shower%partons(i)%p)
      if (.not. prt%is_final () .or. &
          prt%belongstointeraction) cycle
      if (remnants) then
        if (prt%is_colored ()) cycle
      else
        if (.not. (prt%is_colored ())) cycle
      end if
      j = j + 1
      call find_model (model, prt%type, model_in, model_hadrons)
      particles (j) = prt%to_particle (model)
      if (remnants) then
        call particles(j)%set_parents ([prt%initial%nr])
        call particles(prt%initial%nr)%add_child (j)
      else
        call particles(j)%set_parents (hard_colored_ids)
      end if
    end associate
  end do
end subroutine add_to_pset

<Shower core: shower: TBP>+≡
procedure :: write_lhef => shower_write_lhef

<Shower core: sub interfaces>+≡
module subroutine shower_write_lhef (shower, unit)
  class(shower_t), intent(in) :: shower
  integer, intent(in), optional :: unit
end subroutine shower_write_lhef

<Shower core: procedures>+≡
module subroutine shower_write_lhef (shower, unit)
  class(shower_t), intent(in) :: shower
  integer, intent(in), optional :: unit

```

```

integer :: u
integer :: i
integer :: c1, c2
u = given_output_unit (unit); if (u < 0) return
write(u,'(A)') '<LesHouchesEvents version="1.0">'
write(u,'(A)') '<- not a complete lhe file - just one event ->'
write(u,'(A)') '<event>'
write(u, *) 2 + shower%get_nr_of_partons (), 1, 1.0, 1.0, 1.0, 1.0
!!! write incoming partons
do i = 1, 2
  if (abs (shower%partons(i)%p%type) < 1000) then
    c1 = 0
    c2 = 0
    if (shower%partons(i)%p%is_colored ()) then
      if (shower%partons(i)%p%c1 /= 0) c1 = 500 + shower%partons(i)%p%c1
      if (shower%partons(i)%p%c2 /= 0) c2 = 500 + shower%partons(i)%p%c2
    end if
    write (u,*) shower%partons(i)%p%type, -1, 0, 0, c1, c2, &
      shower%partons(i)%p%momentum%p(1), &
      shower%partons(i)%p%momentum%p(2), &
      shower%partons(i)%p%momentum%p(3), &
      shower%partons(i)%p%momentum%p(0), &
      shower%partons(i)%p%momentum**2, zero, 9.0
  else
    write (u,*) shower%partons(i)%p%type, -9, 0, 0, 0, 0, &
      shower%partons(i)%p%momentum%p(1), &
      shower%partons(i)%p%momentum%p(2), &
      shower%partons(i)%p%momentum%p(3), &
      shower%partons(i)%p%momentum%p(0), &
      shower%partons(i)%p%momentum**2, zero, 9.0
  end if
end do
!!! write outgoing partons
do i = 3, size (shower%partons)
  if (.not. associated (shower%partons(i)%p)) cycle
  if (.not. shower%partons(i)%p%is_final ()) cycle
  c1 = 0
  c2 = 0
  if (shower%partons(i)%p%is_colored ()) then
    if (shower%partons(i)%p%c1 /= 0) c1 = 500 + shower%partons(i)%p%c1
    if (shower%partons(i)%p%c2 /= 0) c2 = 500 + shower%partons(i)%p%c2
  end if
  write (u,*) shower%partons(i)%p%type, 1, 1, 2, c1, c2, &
    shower%partons(i)%p%momentum%p(1), &
    shower%partons(i)%p%momentum%p(2), &
    shower%partons(i)%p%momentum%p(3), &
    shower%partons(i)%p%momentum%p(0), &
    shower%partons(i)%p%momentum**2, zero, 9.0
end do
write(u,'(A)') '</event>'
write(u,'(A)') '</LesHouchesEvents>'
end subroutine shower_write_lhef

```

(Shower core: procedures)+≡


```

subroutine shower_replace_parent_by_hadron (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt
  type(parton_t), pointer :: remnant => null()
  if (associated (prt%parent)) then
    call shower_remove_parton_from_partons (shower, prt%parent)
    deallocate (prt%parent)
  end if
  if (.not. associated (prt%initial%child2)) then
    call shower%add_child (prt%initial, 2)
  end if
  prt%parent => prt%initial
  prt%parent%child1 => prt
  ! make other child to be a beam-remnant
  remnant => prt%initial%child2
  remnant%type = BEAM_REMNANT
  remnant%momentum = prt%parent%momentum - prt%momentum
  remnant%x = one - prt%x
  remnant%parent => prt%initial
  remnant%t = zero
end subroutine shower_replace_parent_by_hadron

```

(Shower core: procedures)+≡

```

subroutine shower_get_first_ISR_scale_for_parton (shower, prt, tmax)
  type(shower_t), intent(inout), target :: shower
  type(parton_t), intent(inout), target :: prt
  real(default), intent(in), optional :: tmax
  real(default) :: t, tstep, random, integral, temp1
  real(default) :: temprand
  if (present(tmax)) then
    t = max (max (-shower%settings%isr_tscalefactor * prt%momentum%p(0)**2, &
      -abs(tmax)), prt%t)
  else
    t = max (-shower%settings%isr_tscalefactor * prt%momentum%p(0)**2, prt%t)
  end if
  call shower%rng%generate (random)
  random = -twopi * log(random)
  !!! compare Integral and log(random) instead of random and exp(-Integral)
  integral = zero
  call prt%set_simulated (.false.)
  do
    call shower%rng%generate (temprand)
    tstep = max (abs (0.01_default * t) * temprand, 0.1_default * &
      shower%settings%min_virtuality)
    if (t + 0.5_default * tstep > - shower%settings%min_virtuality) then
      prt%t = prt%mass_squared ()
      call prt%set_simulated ()
      exit
    end if
    prt%t = t + 0.5_default * tstep
    temp1 = integral_over_z_simple (prt, (random - integral) / tstep)
    integral = integral + tstep * temp1
    if (integral > random) then
      prt%t = t + 0.5_default * tstep
    end if
  end do

```

```

        exit
    end if
    t = t + tstep
end do
if (prt%t > - shower%settings%min_virtuality) then
    call shower_replace_parent_by_hadron (shower, prt)
end if

contains

function integral_over_z_simple (prt, final) result (integral)
    type(parton_t), intent(inout) :: prt
    real(default), intent(in) :: final
    real(default), volatile :: integral

    real(default), parameter :: zstepfactor = one
    real(default), parameter :: zstepmin = 0.0001_default
    real(default) :: z, zstep, minz, maxz
    real(default) :: pdfsum
    integer :: quark, d_nf

    integral = zero
    if (debug2_active (D_SHOWER)) then
        print *, "D: integral_over_z_simple: t = ", prt%t
    end if
    minz = prt%x
    ! maxz = maxx(shat, s, shower%settings%isr_z_cutoff, shower%settings%isr_minenergy)
    maxz = shower%settings%isr_z_cutoff
    z = minz
    d_nf = shower%settings%max_n_flavors
    !!! TODO -> Adapt zstep to structure of divergencies
    if (prt%child1%is_gluon ()) then
        !!! gluon coming from g->gg
        do
            call shower%rng%generate (temprand)
            zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
            zstep = min(zstep, maxz - z)
            integral = integral + zstep * (D_alpha_s_isr ((one - &
                (z + 0.5_default * zstep)) * abs(prt%t), &
                shower%settings) / (abs(prt%t))) * &
                P_ggg (z + 0.5_default * zstep) * &
                shower%get_pdf (prt%initial%type, &
                    prt%x / (z + 0.5_default * zstep), abs(prt%t), GLUON)
            if (integral > final) then
                exit
            end if
            z = z + zstep
            if (z >= maxz) then
                exit
            end if
        end do
        !!! gluon coming from q->qg ! correctly implemented yet?
        if (integral < final) then
            z = minz

```

```

do
  call shower%rng%generate (temprand)
  zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
  zstep = min(zstep, maxz - z)
  pdfsum = zero
  do quark = -d_nf, d_nf
    if (quark == 0) cycle
    pdfsum = pdfsum + shower%get_pdf (prt%initial%type, &
      prt%x / (z + 0.5_default * zstep), abs(prt%t), quark)
  end do
  integral = integral + zstep * (D_alpha_s_isr &
    ((z + 0.5_default * zstep) * abs(prt%t), &
    shower%settings) / (abs(prt%t))) * &
    P_qqg (one - (z + 0.5_default * zstep)) * pdfsum
  if (integral > final) then
    exit
  end if
  z = z + zstep
  if (z >= maxz) then
    exit
  end if
end do
end if
else if (prt%child1%is_quark ()) then
  !!! quark coming from q->qg
  do
    call shower%rng%generate(temprand)
    zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
    zstep = min(zstep, maxz - z)
    integral = integral + zstep * (D_alpha_s_isr ((one - &
      (z + 0.5_default * zstep)) * abs(prt%t), &
      shower%settings) / (abs(prt%t))) * &
      P_qqg (z + 0.5_default * zstep) * &
      shower%get_pdf (prt%initial%type, &
        prt%x / (z + 0.5_default * zstep), abs(prt%t), prt%type)
    if (integral > final) then
      exit
    end if
    z = z + zstep
    if (z >= maxz) then
      exit
    end if
  end do
  !!! quark coming from g->qqbar
  if (integral < final) then
    z = minz
    do
      call shower%rng%generate (temprand)
      zstep = max(zstepmin, temprand * zstepfactor * z*(one - z))
      zstep = min(zstep, maxz - z)
      integral = integral + zstep * (D_alpha_s_isr &
        ((one - (z + 0.5_default * zstep)) * abs(prt%t), &
        shower%settings) / (abs(prt%t))) * &
        P_gqq (z + 0.5_default * zstep) * &

```

```

        shower%get_pdf (prt%initial%type, &
        prt%x / (z + 0.5_default * zstep), abs(prt%t), GLUON)
    if (integral > final) then
        exit
    end if
    z = z + zstep
    if (z >= maxz) then
        exit
    end if
end do
end if

    end if
    integral = integral / shower%get_pdf (prt%initial%type, prt%x, &
    abs(prt%t), prt%type)
end function integral_over_z_simple

end subroutine shower_get_first_ISR_scale_for_parton

```

(Shower core: procedures)+≡

```

subroutine shower_prepare_for_simulate_isr_pt (shower, interaction)
    type(shower_t), intent(inout) :: shower
    type(shower_interaction_t), intent(inout) :: interaction
    real(default) :: s
    s = (interaction%partons(1)%p%momentum + &
        interaction%partons(2)%p%momentum)**2
    interaction%partons(1)%p%scale = shower%settings%isr_tscalefactor * 0.25_default * s
    interaction%partons(2)%p%scale = shower%settings%isr_tscalefactor * 0.25_default * s
end subroutine shower_prepare_for_simulate_isr_pt

```

(Shower core: procedures)+≡

```

subroutine shower_prepare_for_simulate_isr_ana_test (shower, prt1, prt2)
    type(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt1, prt2
    type(parton_t), pointer :: prt, prta, prtb
    real(default) :: scale, factor, E
    integer :: i
    if (.not. associated (prt1%initial) .or. .not. associated (prt2%initial)) then
        return
    end if
    scale = - (prt1%momentum + prt2%momentum) ** 2
    call prt1%set_simulated ()
    call prt2%set_simulated ()
    call shower%add_parent (prt1)
    call shower%add_parent (prt2)
    factor = sqrt (energy (prt1%momentum)**2 - scale) / &
        space_part_norm(prt1%momentum)
    prt1%parent%type = prt1%type
    prt1%parent%z = one
    prt1%parent%momentum = prt1%momentum
    prt1%parent%t = scale
    prt1%parent%x = prt1%x
    prt1%parent%initial => prt1%initial

```

```

prt1%parent%belongstoFSR = .false.
prt1%parent%c1 = prt1%c1
prt1%parent%c2 = prt1%c2

prt2%parent%type= prt2%type
prt2%parent%z = one
prt2%parent%momentum = prt2%momentum
prt2%parent%t = scale
prt2%parent%x = prt2%x
prt2%parent%initial => prt2%initial
prt2%parent%belongstoFSR = .false.
prt2%parent%c1 = prt2%c1
prt2%parent%c2 = prt2%c2

call shower_get_first_ISR_scale_for_parton (shower, prt1%parent)
call shower_get_first_ISR_scale_for_parton (shower, prt2%parent)

!!! redistribute energy among first partons
prta => prt1%parent
prtb => prt2%parent

E = energy (prt1%momentum + prt2%momentum)
prta%momentum%p(0) = (E**2 - prtb%t + prta%t) / (two * E)
prtb%momentum%p(0) = E - prta%momentum%p(0)

call prt1%parent%set_simulated ()
call prt2%parent%set_simulated ()
!!! rescale momenta
do i = 1, 2
  if (i == 1) then
    prt => prt1%parent
  else
    prt => prt2%parent
  end if
  factor = sqrt (energy (prt%momentum)**2 - prt%t) &
    / space_part_norm (prt%momentum)
  prt%momentum = vector4_moving (energy (prt%momentum), &
    factor * space_part (prt%momentum))
end do

if (prt1%parent%t < zero) then
  call shower%add_parent (prt1%parent)
  prt1%parent%parent%momentum = prt1%parent%momentum
  prt1%parent%parent%t = prt1%parent%t
  prt1%parent%parent%x = prt1%parent%x
  prt1%parent%parent%initial => prt1%parent%initial
  prt1%parent%parent%belongstoFSR = .false.
  call shower%add_child (prt1%parent%parent, 2)
end if

if (prt2%parent%t < zero) then
  call shower%add_parent (prt2%parent)
  prt2%parent%parent%momentum = prt2%parent%momentum
  prt2%parent%parent%t = prt2%parent%t

```

```

prt2%parent%parent%x = prt2%parent%x
prt2%parent%parent%initial => prt2%parent%initial
prt2%parent%parent%belongstoFSR = .false.
call shower%add_child (prt2%parent%parent, 2)
end if

end subroutine shower_prepare_for_simulate_isr_ana_test

```

(Shower core: procedures)+≡

```

subroutine shower_add_children_of_emitted_timelike_parton (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: prt

  if (prt%t > prt%mass_squared () + shower%settings%min_virtuality) then
    if (prt%is_quark ()) then
      !!! q -> qg
      call shower%add_child (prt, 1)
      prt%child1%type = prt%type
      prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
      prt%child1%t = prt%t
      call shower%add_child (prt, 2)
      prt%child2%type = GLUON
      prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
      prt%child2%t = prt%t
    else
      if (int (prt%x) > 0) then
        call shower%add_child (prt, 1)
        prt%child1%type = int (prt%x)
        prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
        prt%child1%t = prt%t
        call shower%add_child (prt, 2)
        prt%child2%type = -int (prt%x)
        prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
        prt%child2%t = prt%t
      else
        call shower%add_child (prt, 1)
        prt%child1%type = GLUON
        prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
        prt%child1%t = prt%t
        call shower%add_child (prt, 2)
        prt%child2%type = GLUON
        prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
        prt%child2%t = prt%t
      end if
    end if
  end if
end subroutine shower_add_children_of_emitted_timelike_parton

```

(Shower core: procedures)+≡

```

subroutine shower_simulate_children_ana (shower,prt)
  type(shower_t), intent(inout), target :: shower
  type(parton_t), intent(inout) :: prt
  real(default), dimension(1:2) :: random, integral

```

```

integer, dimension(1:2) :: gtoqq
integer :: daughter
type(parton_t), pointer :: daughterprt
integer :: n_loop

if (signal_is_pending ()) return
if (debug2_active (D_SHOWER)) &
    print *, "D: shower_simulate_children_ana: for parton " , prt%nr
gtoqq = 0
if (.not. associated (prt%child1) .or. .not. associated (prt%child2)) then
    call msg_error ("Shower: error in simulate_children_ana: no children.")
    return
end if

<Set beam-remnants and internal partons as simulated>

integral = zero

!!! impose constraints by angular ordering -> cf. (26) of Gaining analytic control
!!! check if no branchings are possible
if (.not. prt%child1%simulated) then
    prt%child1%t = min (prt%child1%t, &
        0.5_default * prt%child1%momentum%p(0)**2 * (one - &
        prt%get_cstheta ()))
    if (.not. associated (prt%child1%settings)) &
        prt%child1%settings => shower%settings
    if (min (prt%child1%t, prt%child1%momentum%p(0)**2) < &
        prt%child1%mass_squared () + &
        prt%child1%settings%min_virtuality) then
        prt%child1%t = prt%child1%mass_squared ()
        call prt%child1%set_simulated ()
    end if
end if
if (.not. prt%child2%simulated) then
    prt%child2%t = min (prt%child2%t, &
        0.5_default * prt%child2%momentum%p(0)**2 * (one - &
        prt%get_cstheta ()))
    if (.not. associated (prt%child2%settings)) &
        prt%child2%settings => shower%settings
    if (min (prt%child2%t, prt%child2%momentum%p(0)**2) < &
        prt%child2%mass_squared () + &
        prt%child2%settings%min_virtuality) then
        prt%child2%t = prt%child2%mass_squared ()
        call prt%child2%set_simulated ()
    end if
end if

call shower%rng%generate (random)

n_loop = 0
do
    if (signal_is_pending ()) return
    n_loop = n_loop + 1
    if (n_loop > 900) then

```

```

        !!! try with massless quarks
        treat_duscb_quarks_massless = .true.
    end if
    if (n_loop > 1000) then
        call msg_message ("simulate_children_ana failed for parton ", prt%nr)
        call msg_warning ("too many loops in simulate_children_ana")
        call shower%write ()
        shower%valid = .false.
        return
    end if

    !!! check if a branching in the range t(i) to t(i) - tstep(i) occurs
    if (.not. prt%child1%simulated) then
        call parton_simulate_stept &
            (prt%child1, shower%rng, integral(1), random(1), gtoqq(1))
    end if
    if (.not. prt%child2%simulated) then
        call parton_simulate_stept &
            (prt%child2, shower%rng, integral(2), random(2), gtoqq(2))
    end if

    if (prt%child1%simulated .and. prt%child2%simulated) then
        if (sqrt (prt%t) <= sqrt (prt%child1%t) + sqrt (prt%child2%t)) then
            <Repeat the simulation for the parton with the lower virtuality>
        else
            exit
        end if
    end if
end do

call parton_apply_costheta (prt, shower%rng)

<Add children>
call shower_parton_update_color_connections (shower, prt)
end subroutine shower_simulate_children_ana

<Set beam-remnants and internal partons as simulated>≡
if (HADRON_REMNANT <= abs (prt%type) .and. abs (prt%type) <= HADRON_REMNANT_OCTET) then
    !!! prt is beam-remnant
    call prt%set_simulated ()
    return
end if

!!! check if partons are "internal" -> fixed scale
if (prt%child1%type == INTERNAL) then
    call prt%child1%set_simulated ()
end if
if (prt%child2%type == INTERNAL) then
    call prt%child2%set_simulated ()
end if

<Repeat the simulation for the parton with the lower virtuality>≡
!!! virtuality : t - m**2 (assuming it's not fixed)
if (prt%child1%type == INTERNAL .and. prt%child2%type == INTERNAL) then

```



```

        call msg_fatal &
            ("Shower: both partons fixed, but momentum not conserved")
    else if (prt%child1%type == INTERNAL) then
        !!! reset child2
        call prt%child2%set_simulated (.false.)
        prt%child2%t = min (prt%child1%t, (sqrt (prt%t) - &
            sqrt (prt%child1%t))**2)
        integral(2) = zero
        call shower%rng%generate (random(2))
    else if (prt%child2%type == INTERNAL) then
        ! reset child1
        call prt%child1%set_simulated (.false.)
        prt%child1%t = min (prt%child2%t, (sqrt (prt%t) - &
            sqrt (prt%child2%t))**2)
        integral(1) = zero
        call shower%rng%generate (random(1))
    else if (prt%child1%t - prt%child1%mass_squared () > &
        prt%child2%t - prt%child2%mass_squared ()) then
        !!! reset child2
        call prt%child2%set_simulated (.false.)
        prt%child2%t = min (prt%child1%t, (sqrt (prt%t) - &
            sqrt (prt%child1%t))**2)
        integral(2) = zero
        call shower%rng%generate (random(2))
    else
        !!! reset child1 ! TODO choose child according to their t
        call prt%child1%set_simulated (.false.)
        prt%child1%t = min (prt%child2%t, (sqrt (prt%t) - &
            sqrt (prt%child2%t))**2)
        integral(1) = zero
        call shower%rng%generate (random(1))
    end if
<Add children>≡
    if (.not. associated (prt%child1%settings)) &
        prt%child1%settings => shower%settings
    if (.not. associated (prt%child2%settings)) &
        prt%child2%settings => shower%settings
    do daughter = 1, 2
        if (signal_is_pending ()) return
        if (daughter == 1) then
            daughterprt => prt%child1
        else
            daughterprt => prt%child2
        end if
        if (daughterprt%t < daughterprt%mass_squared () + &
            daughterprt%settings%min_virtuality) then
            cycle
        end if
        if (.not. (daughterprt%is_quark () .or. daughterprt%is_gluon ())) then
            cycle
        end if
        if (daughterprt%is_quark ()) then
            !!! q -> qg
            call shower%add_child (daughterprt, 1)

```

```

daughterprt%child1%type = daughterprt%type
daughterprt%child1%momentum%p(0) = daughterprt%z * &
    daughterprt%momentum%p(0)
daughterprt%child1%t = daughterprt%t
call shower%add_child (daughterprt, 2)
daughterprt%child2%type = GLUON
daughterprt%child2%momentum%p(0) = (one - daughterprt%z) * &
    daughterprt%momentum%p(0)
daughterprt%child2%t = daughterprt%t
else if (daughterprt%is_gluon ()) then
    if (gtoqq(daughter) > 0) then
        call shower%add_child (daughterprt, 1)
        daughterprt%child1%type = gtoqq (daughter)
        daughterprt%child1%momentum%p(0) = &
            daughterprt%z * daughterprt%momentum%p(0)
        daughterprt%child1%t = daughterprt%t
        call shower%add_child (daughterprt, 2)
        daughterprt%child2%type = - gtoqq (daughter)
        daughterprt%child2%momentum%p(0) = (one - &
            daughterprt%z) * daughterprt%momentum%p(0)
        daughterprt%child2%t = daughterprt%t
    else
        call shower%add_child (daughterprt, 1)
        daughterprt%child1%type = GLUON
        daughterprt%child1%momentum%p(0) = &
            daughterprt%z * daughterprt%momentum%p(0)
        daughterprt%child1%t = daughterprt%t
        call shower%add_child (daughterprt, 2)
        daughterprt%child2%type = GLUON
        daughterprt%child2%momentum%p(0) = (one - &
            daughterprt%z) * daughterprt%momentum%p(0)
        daughterprt%child2%t = daughterprt%t
    end if
end if
end do

```

The recoiler is `otherprt`. Instead of the random number and the exponential of the integral, we compare the logarithm of the random number and the integral.

(Shower core: procedures)+≡

```

subroutine shower_isr_step_pt (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), target, intent(inout) :: prt
    type(parton_t), pointer :: otherprt

    real(default) :: scale, scalestep
    real(default), volatile :: integral
    real(default) :: random, factor
    real(default) :: temprand1, temprand2

    otherprt => shower%find_recoiler (prt)

    scale = prt%scale
    call shower%rng%generate (temprand1)
    call shower%rng%generate (temprand2)

```

```

scalestep = max (abs (scalefactor1 * scale) * temprand1, &
    scalefactor2 * temprand2 * D_Min_scale)
call shower%rng%generate (random)
random = - twopi * log(random)
integral = zero

if (scale - 0.5_default * scalestep < D_Min_scale) then
    !!! close enough to cut-off scale -> ignore
    prt%scale = zero
    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
else
    prt%scale = scale - 0.5_default * scalestep
    factor = scalestep * (D_alpha_s_isr (prt%scale, &
        shower%settings) / (prt%scale * &
        shower%get_pdf (prt%initial%type, prt%x, prt%scale, prt%type)))
    integral = integral + factor * integral_over_z_isr_pt &
        (prt, otherprt, (random - integral) / factor)
    if (integral > random) then
        !!! prt%scale set above and prt%z set in integral_over_z_isr_pt
        call prt%set_simulated ()
        prt%t = - prt%scale / (one - prt%z)
    else
        prt%scale = scale - scalestep
    end if
end if

contains

function integral_over_z_isr_pt (prt, otherprt, final) &
    result (integral)
    type(parton_t), intent(inout) :: prt, otherprt
    real(default), intent(in) :: final
    real(default), volatile :: integral
    real(default) :: mbr, r
    real(default) :: zmin, zmax, z, zstep
    integer :: n_bin
    integer, parameter :: n_total_bins = 100
    real(default) :: quarkpdfsum
    real(default) :: temprand
    integer :: quark, d_nf

    quarkpdfsum = zero
    d_nf = shower%settings%max_n_flavors
    if (debug2_active (D_SHOWER)) then
        print *, "D: integral_over_z_isr_pt: for scale = ", prt%scale
    end if

    integral = zero
    mbr = (prt%momentum + otherprt%momentum)**1
    zmin = prt%x
    zmax = min (one - (sqrt (prt%scale) / mbr) * &
        (sqrt(one + 0.25_default * prt%scale / mbr**2) - &
        0.25_default * sqrt(prt%scale) / mbr), shower%settings%isr_z_cutoff)

```

```

zstep = (zmax - zmin) / n_total_bins

if (debug_active (D_SHOWER)) then
  if (zmin > zmax) then
    call msg_bug(" error in integral_over_z_isr_pt: zmin > zmax ")
    integral = zero
  end if
end if

!!! divide the range [zmin:zmax] in n_total_bins
BINS: do n_bin = 1, n_total_bins
  z = zmin + zstep * (n_bin - 0.5_default)
  !!! z-value in the middle of the bin

  if (prt%is_gluon ()) then
    QUARKS: do quark = -d_nf, d_nf
      if (quark == 0) cycle quarks
      quarkpdfsum = quarkpdfsum + shower%get_pdf &
        (prt%initial%type, prt%x / z, prt%scale, quark)
    end do QUARKS
    !!! g -> gg or q -> gq
    integral = integral + (zstep / z) * ((P_ggg (z) + &
      P_ggg (one - z)) * shower%get_pdf (prt%initial%type, &
      prt%x / z, prt%scale, GLUON) + P_qqg (one - z) * quarkpdfsum)
  else if (prt%is_quark ()) then
    !!! q -> qg or g -> qq
    integral = integral + (zstep / z) * ( P_qqg (z) * &
      shower%get_pdf (prt%initial%type, prt%x / z, prt%scale, &
      prt%type) + &
      P_gqq(z) * shower%get_pdf (prt%initial%type, prt%x / z, &
      prt%scale, GLUON))
  else
    ! call msg_fatal ("Bug neither quark nor gluon in" &
    ! // " integral_over_z_isr_pt")
  end if
  if (integral > final) then
    prt%z = z
    call shower%rng%generate (temprand)
    !!! decide type of father partons
    if (prt%is_gluon ()) then
      if (temprand > (P_qqg (one - z) * quarkpdfsum) / &
        ((P_ggg (z) + P_ggg (one - z)) * shower%get_pdf &
        (prt%initial%type, prt%x / z, prt%scale, GLUON) &
        + P_qqg (one - z) * quarkpdfsum)) then
        !!! gluon => gluon + gluon
        prt%aux_pt = GLUON
      else
        !!! quark => quark + gluon
        !!! decide which quark flavor the parent is
        r = temprand * quarkpdfsum
        WHICH_QUARK: do quark = -d_nf, d_nf
          if (quark == 0) cycle WHICH_QUARK
          if (r > quarkpdfsum - shower%get_pdf (prt%initial%type, &
            prt%x / z, prt%scale, quark)) then

```

```

        prt%aux_pt = quark
        exit WHICH_QUARK
    else
        quarkpdfsum = quarkpdfsum - shower%get_pdf &
            (prt%initial%type, prt%x / z, prt%scale, quark)
        end if
    end do WHICH_QUARK
end if

else if (prt%is_quark ()) then
    if (temprand > (P_qqg (z) * shower%get_pdf (prt%initial%type, &
        prt%x / z, prt%scale, prt%type)) / &
        (P_qqg (z) * shower%get_pdf (prt%initial%type, prt%x / z, &
        prt%scale, prt%type) + &
        P_gqq (z) * shower%get_pdf (prt%initial%type, prt%x / z, &
        prt%scale, GLUON))) then
        !!! gluon => quark + antiquark
        prt%aux_pt = GLUON
    else
        !!! quark => quark + gluon
        prt%aux_pt = prt%type
    end if
end if
exit BINS
end if
end do BINS
end function integral_over_z_isr_pt
end subroutine shower_isr_step_pt

```

This function returns a pointer to the parton with the next ISR branching, while FSR branchings are ignored.

(Shower core: shower: TBP)+≡

```

procedure :: generate_next_isr_branching_veto => &
    shower_generate_next_isr_branching_veto

```

(Shower core: sub interfaces)+≡

```

module function shower_generate_next_isr_branching_veto &
    (shower) result (next_brancher)
    class(shower_t), intent(inout) :: shower
    type(parton_pointer_t) :: next_brancher
end function shower_generate_next_isr_branching_veto

```

(Shower core: procedures)+≡

```

module function shower_generate_next_isr_branching_veto &
    (shower) result (next_brancher)
    class(shower_t), intent(inout) :: shower
    type(parton_pointer_t) :: next_brancher
    integer :: i
    type(parton_t), pointer :: prt
    real(default) :: random
    !!! pointers to branchable partons
    type(parton_pointer_t), dimension(:), allocatable :: partons
    integer :: n_partons
    real(default) :: weight
    real(default) :: temp1, temp2, temp3, E3

```

```

if (signal_is_pending ()) return

if (shower%settings%isr_pt_ordered) then
  next_brancher = shower%generate_next_isr_branching ()
  return
end if
next_brancher%p => null()
!!! branchable partons
n_partons = 0
do i = 1,size (shower%partons)
  prt => shower%partons(i)%p
  if (.not. associated (prt)) cycle
  if (prt%belongstoFSR) cycle
  if (prt%is_final ()) cycle
  if (.not. prt%belongstoFSR .and. prt%simulated) cycle
  n_partons = n_partons + 1
end do
if (n_partons == 0) then
  return
end if
allocate (partons(1:n_partons))
n_partons = 1
do i = 1, size (shower%partons)
  prt => shower%partons(i)%p
  if (.not. associated (prt)) cycle
  if (prt%belongstoFSR) cycle
  if (prt%is_final ()) cycle
  if (.not. prt%belongstoFSR .and. prt%simulated) cycle
  partons(n_partons)%p => shower%partons(i)%p
  n_partons = n_partons + 1
end do
!!! generate initial trial scales
do i = 1, size (partons)
  if (signal_is_pending ()) return
  call generate_next_trial_scale (partons(i)%p)
end do

do
  !!! search for parton with the highest trial scale
  prt => partons(1)%p
  do i = 1, size (partons)
    if (prt%t >= zero) cycle
    if (abs (partons(i)%p%t) > abs (prt%t)) then
      prt => partons(i)%p
    end if
  end do

  if (prt%t >= zero) then
    next_brancher%p => null()
    exit
  end if
  !!! generate trial z and type of mother prt
  call generate_trial_z_and_typ (prt)

```

```

!!! weight with pdf and alpha_s
temp1 = (D_alpha_s_isr ((one - prt%z) * abs(prt%t), &
    shower%settings) / sqrt (alphaspdfmax))
temp2 = shower%get_xpdf (prt%initial%type, prt%x, prt%t, &
    prt%type) / sqrt (alphaspdfmax)
temp3 = shower%get_xpdf (prt%initial%type, prt%child1%x, prt%child1%t, &
    prt%child1%type) / &
    shower%get_xpdf (prt%initial%type, prt%child1%x, prt%t, &
    prt%child1%type)
! TODO: (bcn 2015-02-19) ???
if (temp1 * temp2 * temp3 > one) then
    print *, "weights:", temp1, temp2, temp3
end if
weight = (D_alpha_s_isr ((one - prt%z) * abs(prt%t), &
    shower%settings)) * &
    shower%get_xpdf (prt%initial%type, prt%x, prt%t, prt%type) * &
    shower%get_xpdf (prt%initial%type, prt%child1%x, prt%child1%t, &
    prt%child1%type) / &
    shower%get_xpdf &
    (prt%initial%type, prt%child1%x, prt%t, prt%child1%type)
if (weight > alphaspdfmax) then
    print *, "Setting alphaspdfmax from ", alphaspdfmax, " to ", weight
    alphaspdfmax = weight
end if
weight = weight / alphaspdfmax
call shower%rng%generate (random)
if (weight < random) then
    !!! discard branching
    call generate_next_trial_scale (prt)
    cycle
end if
!!! branching accepted so far
!!! generate emitted parton
prt%child2%t = abs(prt%t)
prt%child2%momentum%p(0) = sqrt (abs(prt%t))
if (shower%settings%isr_only_onshell_emitted_partons) then
    prt%child2%t = prt%child2%mass_squared ()
else
    call prt%child2%next_t_ana (shower%rng)
end if

if (thetabar (prt, shower%find_recoiler (prt), &
    shower%settings%isr_angular_ordered, E3)) then
    prt%momentum%p(0) = E3
    prt%child2%momentum%p(0) = E3 - prt%child1%momentum%p(0)

    !!! found branching
    call prt%generate_ps_ini (shower%rng)
    next_brancher%p => prt
    call prt%set_simulated ()
    exit
else
    call generate_next_trial_scale (prt)

```

```

        cycle
    end if
end do
if (.not. associated (next_brancher%p)) then
    !!! no further branching found -> all partons emitted by hadron
    print *, "-all partons emitted by hadrons--"
    do i = 1, size(partons)
        call shower_replace_parent_by_hadron (shower, partons(i)%p%child1)
    end do
end if
!!! some bookkeeping
call shower%sort_partons ()
! call shower%boost_to_CMframe ()          ! really necessary?
! call shower%rotate_to_z ()              ! really necessary?
contains

subroutine generate_next_trial_scale (prt)
    type(parton_t), pointer, intent(inout) :: prt
    real(default) :: random, F
    real(default) :: zmax = 0.99_default !! ??
    call shower%rng%generate (random)
    F = one    !!! TODO
    F = alphasxpdfmax / (two * pi)
    if (prt%child1%is_quark ()) then
        F = F * (integral_over_P_gqq (prt%child1%x, zmax) + &
            integral_over_P_qqg (prt%child1%x, zmax))
    else if (prt%child1%is_gluon ()) then
        F = F * (integral_over_P_ggg (prt%child1%x, zmax) + &
            two * shower%settings%max_n_flavors * &
            integral_over_P_qqg (one - zmax, one - prt%child1%x))
    else
        call msg_bug("neither quark nor gluon in generate_next_trial_scale")
    end if
    F = F / shower%get_xpdf (prt%child1%initial%type, prt%child1%x, &
        prt%child1%t, prt%child1%type)
    prt%t = prt%t * random**(one / F)
    if (abs (prt%t) - prt%mass_squared () < &
        prt%settings%min_virtuality) then
        prt%t = prt%mass_squared ()
    end if
end subroutine generate_next_trial_scale

subroutine generate_trial_z_and_typ (prt)
    type(parton_t), pointer, intent(inout) :: prt
    real(default) :: random
    real(default) :: z, zstep, zmin, integral
    real(default) :: zmax = 0.99_default !! ??
    if (debug_on) call msg_debug (D_SHOWER, "generate_trial_z_and_typ")
    call shower%rng%generate (random)
    integral = zero
    !!! decide which branching a->bc occurs
    if (prt%child1%is_quark ()) then
        if (random < integral_over_P_qqg (prt%child1%x, zmax) / &
            (integral_over_P_qqg (prt%child1%x, zmax) + &

```



```

        integral_over_P_gqq (prt%child1%x, zmax))) then
prt%type = prt%child1%type
prt%child2%type = GLUON
integral = integral_over_P_qqg (prt%child1%x, zmax)
else
prt%type = GLUON
prt%child2%type = - prt%child1%type
integral = integral_over_P_gqq (prt%child1%x, zmax)
end if
else if (prt%child1%is_gluon ()) then
if (random < integral_over_P_ggg (prt%child1%x, zmax) / &
(integral_over_P_ggg (prt%child1%x, zmax) + two * &
shower%settings%max_n_flavors * &
integral_over_P_qqg (one - zmax, &
one - prt%child1%x))) then
prt%type = GLUON
prt%child2%type = GLUON
integral = integral_over_P_ggg (prt%child1%x, zmax)
else
call shower%rng%generate (random)
prt%type = 1 + floor(random * shower%settings%max_n_flavors)
call shower%rng%generate (random)
if (random > 0.5_default) prt%type = - prt%type
prt%child2%type = prt%type
integral = integral_over_P_qqg (one - zmax, &
one - prt%child1%x)
end if
else
call msg_bug("neither quark nor gluon in generate_next_trial_scale")
end if
!!! generate the z-value
!!! z between prt%child1%x and zmax
! prt%z = one - random * (one - prt%child1%x)      ! TODO

call shower%rng%generate (random)
zmin = prt%child1%x
zstep = max(0.1_default, 0.5_default * (zmax - zmin))
z = zmin
if (zmin > zmax) then
print *, " zmin = ", zmin, " zmax = ", zmax
call msg_fatal ("Shower: zmin greater than zmax")
end if
!!! procedure pointers would be helpful here
if (prt%is_quark () .and. prt%child1%is_quark ()) then
do
zstep = min(zstep, 0.5_default * (zmax - z))
if (abs(zstep) < 0.00001) exit
if (integral_over_P_qqg (zmin, z) < random * integral) then
if (integral_over_P_qqg (zmin, min(z + zstep, zmax)) &
< random * integral) then
z = min (z + zstep, zmax)
cycle
else
zstep = zstep * 0.5_default

```

```

        cycle
    end if
end if
end do
else if (prt%is_quark () .and. prt%child1%is_gluon ()) then
do
    zstep = min(zstep, 0.5_default * (zmax - z))
    if (abs(zstep) < 0.00001) exit
    if (integral_over_P_qqg (zmin, z) < random * integral) then
        if (integral_over_P_qqg (zmin, min(z + zstep, zmax)) &
            < random * integral) then
            z = min(z + zstep, zmax)
            cycle
        else
            zstep = zstep * 0.5_default
            cycle
        end if
    end if
end do
else if (prt%is_gluon () .and. prt%child1%is_quark ()) then
do
    zstep = min(zstep, 0.5_default * (zmax - z))
    if (abs (zstep) < 0.00001) exit
    if (integral_over_P_gqq (zmin, z) < random * integral) then
        if (integral_over_P_gqq (zmin, min(z + zstep, zmax)) &
            < random * integral) then
            z = min (z + zstep, zmax)
            cycle
        else
            zstep = zstep * 0.5_default
            cycle
        end if
    end if
end do
else if (prt%is_gluon () .and. prt%child1%is_gluon ()) then
do
    zstep = min(zstep, 0.5_default * (zmax - z))
    if (abs (zstep) < 0.00001) exit
    if (integral_over_P_ggg (zmin, z) < random * integral) then
        if (integral_over_P_ggg (zmin, min(z + zstep, zmax)) &
            < random * integral) then
            z = min(z + zstep, zmax)
            cycle
        else
            zstep = zstep * 0.5_default
            cycle
        end if
    end if
end do
else
end if
prt%z = z
prt%x = prt%child1%x / prt%z
end subroutine generate_trial_z_and_typ

```

```

end function shower_generate_next_isr_branching_veto

<Shower core: shower: TBP>+≡
  procedure :: find_recoiler => shower_find_recoiler

<Shower core: sub interfaces>+≡
  module function shower_find_recoiler (shower, prt) result(recoiler)
    class(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    type(parton_t), pointer :: recoiler
  end function shower_find_recoiler

<Shower core: procedures>+≡
  module function shower_find_recoiler (shower, prt) result(recoiler)
    class(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    type(parton_t), pointer :: recoiler
    type(parton_t), pointer :: otherprt1, otherprt2
    integer :: n_int
    otherprt1 => null()
    otherprt2 => null()
    DO_INTERACTIONS: do n_int = 1, size(shower%interactions)
      otherprt1 => shower%interactions(n_int)%i%partons(1)%p
      otherprt2 => shower%interactions(n_int)%i%partons(2)%p
      PARTON1: do
        if (associated (otherprt1%parent)) then
          if (.not. otherprt1%parent%is_proton () .and. &
              otherprt1%parent%simulated) then
            otherprt1 => otherprt1%parent
            if (associated (otherprt1, prt)) then
              exit PARTON1
            end if
          else
            exit PARTON1
          end if
        else
          exit PARTON1
        end if
      end do PARTON1
      PARTON2: do
        if (associated (otherprt2%parent)) then
          if (.not. otherprt2%parent%is_proton () .and. &
              otherprt2%parent%simulated) then
            otherprt2 => otherprt2%parent
            if (associated (otherprt2, prt)) then
              exit PARTON2
            end if
          else
            exit PARTON2
          end if
        else
          exit PARTON2
        end if
      end do PARTON2
    end do PARTON2
  end function shower_find_recoiler

```

```

        if (associated (otherprt1, prt) .or. associated (otherprt2, prt)) then
            exit DO_INTERACTIONS
        end if
        if (associated (otherprt1%parent, prt) .or. &
            associated (otherprt2%parent, prt)) then
            exit DO_INTERACTIONS
        end if
    end do DO_INTERACTIONS

    recoiler => null()
    if (associated (otherprt1%parent, prt)) then
        recoiler => otherprt2
    else if (associated (otherprt2%parent, prt)) then
        recoiler => otherprt1
    else if (associated (otherprt1, prt)) then
        recoiler => otherprt2
    else if (associated (otherprt2, prt)) then
        recoiler => otherprt1
    else
        call shower%write ()
        call prt%write ()
        call msg_error ("shower_find_recoiler: no otherparton found")
    end if
end function shower_find_recoiler

```

(Shower core: procedures)+≡

```

subroutine shower_isr_step (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), target, intent(inout) :: prt
    type(parton_t), pointer :: otherprt => null()
    real(default) :: t, tstep
    real(default), volatile :: integral
    real(default) :: random
    real(default) :: temprand1, temprand2
    otherprt => shower%find_recoiler (prt)
    ! if (.not. otherprt%child1%belongstointeraction) then
    !     otherprt => otherprt%child1
    ! end if

    if (signal_is_pending ()) return
    t = max(prt%t, prt%child1%t)
    call shower%rng%generate (random)
    ! compare Integral and log(random) instead of random and exp(-Integral)
    random = - twopi * log(random)
    integral = zero
    call shower%rng%generate (temprand1)
    call shower%rng%generate (temprand2)
    tstep = max (abs (0.02_default * t) * temprand1, &
        0.02_default * temprand2 * shower%settings%min_virtuality)
    if (t + 0.5_default * tstep > - shower%settings%min_virtuality) then
        prt%t = prt%mass_squared ()
        call prt%set_simulated ()
    else
        prt%t = t + 0.5_default * tstep
    end if
end subroutine shower_isr_step

```

```

        integral = integral + tstep * &
            integral_over_z_isr (shower, prt, otherprt, (random - integral) / tstep)
    if (integral > random) then
        prt%t = t + 0.5_default * tstep
        prt%x = prt%child1%x / prt%z
        call prt%set_simulated ()
    else
        prt%t = t + tstep
    end if
end if
end if
end subroutine shower_isr_step

```

(*Shower core: procedures*) +=

```

function integral_over_z_isr (shower, prt, otherprt, final) result (integral)
    type(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout) :: prt, otherprt
    real(default), intent(in) :: final
    !!! !!! !!! volatile argument: gfortran 7 aggressive optimization (#809)
    real(default), volatile :: integral
    real(default) :: minz, maxz, shat, s
    integer :: quark

    !!! calculate shat -> s of parton-parton system
    shat = (otherprt%momentum + prt%child1%momentum)**2
    !!! calculate s -> s of hadron-hadron system
    s = (otherprt%initial%momentum + prt%initial%momentum)**2
    integral = zero
    minz = prt%child1%x
    maxz = maxx (shat, s, shower%settings%isr_z_cutoff, &
        shower%settings%isr_minenergy)

    !!! for gluon
    if (prt%child1%is_gluon ()) then
        !!! 1: g->gg
        prt%type = GLUON
        prt%child2%type = GLUON
        prt%child2%t = abs(prt%t)
        call integral_over_z_part_isr &
            (shower, prt, otherprt, shat, minz, maxz, integral, final)
        if (integral > final) then
            return
        else
            !!! 2: q->qq
            do quark = - shower%settings%max_n_flavors, &
                shower%settings%max_n_flavors
                if (quark == 0) cycle
                prt%type = quark
                prt%child2%type = quark
                prt%child2%t = abs(prt%t)
                call integral_over_z_part_isr &
                    (shower, prt, otherprt, shat, minz, maxz, integral, final)
                if (integral > final) then
                    return
                end if
            end do
        end if
    end if
end function

```

```

        end do
    end if
    else if (prt%child1%is_quark ()) then
        !!! 1: q->qg
        prt%type = prt%child1%type
        prt%child2%type = GLUON
        prt%child2%t = abs(prt%t)
        call integral_over_z_part_isr &
            (shower, prt, otherprt, shat, minz, maxz, integral, final)
        if (integral > final) then
            return
        else
            !!! 2: g->qqbar
            prt%type = GLUON
            prt%child2%type = -prt%child1%type
            prt%child2%t = abs(prt%t)
            call integral_over_z_part_isr &
                (shower, prt, otherprt, shat, minz, maxz, integral, final)
        end if
    end if
end function integral_over_z_isr

```

(Shower core: procedures)+≡

```

subroutine integral_over_z_part_isr &
    (shower, prt, otherprt, shat, minz, maxz, retvalue, final)
type(shower_t), intent(inout) :: shower
type(parton_t), intent(inout) :: prt, otherprt
real(default), intent(in) :: shat, minz, maxz, final
real(default), intent(inout) :: retvalue
real(default) :: z, zstep
real(default) :: r1, r3, s1, s3
real(default) :: pdf_divisor
real(default) :: temprand
real(default), parameter :: zstepfactor = 0.1_default
real(default), parameter :: zstepmin = 0.0001_default
if (debug_on) call msg_debug2 (D_SHOWER, "integral_over_z_part_isr")
if (signal_is_pending ()) return
pdf_divisor = shower%get_pdf &
    (prt%initial%type, prt%child1%x, prt%t, prt%child1%type)
z = minz
s1 = shat + abs(otherprt%t) + abs(prt%child1%t)
r1 = sqrt (s1**2 - four * abs(otherprt%t * prt%child1%t))
ZLOOP: do
    if (signal_is_pending ()) return
    if (z >= maxz) then
        exit
    end if
    call shower%rng%generate (temprand)
    if (prt%child1%is_gluon ()) then
        if (prt%is_gluon ()) then
            !!! g-> gg -> divergencies at z->0 and z->1
            zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
        else
            !!! q-> gq -> divergencies at z->0

```

```

        zstep = max(zstepmin, temprand * zstepfactor * (one - z))
    end if
else
    if (prt%is_gluon ()) then
        !!! g-> qqbar -> no divergencies
        zstep = max(zstepmin, temprand * zstepfactor)
    else
        !!! q-> qg -> divergencies at z->1
        zstep = max(zstepmin, temprand * zstepfactor * (one - z))
    end if
end if
zstep = min(zstep, maxx - z)
prt%z = z + 0.5_default * zstep
s3 = shat / prt%z + abs(otherprt%t) + abs(prt%t)
r3 = sqrt (s3**2 - four * abs(otherprt%t * prt%t))
!!! TODO: WHY is this if needed?
if (abs(otherprt%t) > eps0) then
    prt%child2%t = min ((s1 * s3 - r1 * r3) / &
        (two * abs(otherprt%t)) - abs(prt%child1%t) - &
        abs(prt%t), abs(prt%child1%t))
else
    prt%child2%t = abs(prt%child1%t)
end if
do
    prt%child2%momentum%p(0) = sqrt (abs(prt%child2%t))
    if (shower%settings%isr_only_onshell_emitted_partons) then
        prt%child2%t = prt%child2%mass_squared ()
    else
        call prt%child2%next_t_ana (shower%rng)
    end if
    !!! take limits by recoiler into account
    prt%momentum%p(0) = (shat / prt%z + &
        abs(otherprt%t) - abs(prt%child1%t) - &
        prt%child2%t) / (two * sqrt(shat))
    prt%child2%momentum%p(0) = &
        prt%momentum%p(0) - prt%child1%momentum%p(0)
    !!! check if E and t of prt%child2 are consistent
    if (prt%child2%momentum%p(0)**2 < prt%child2%t &
        .and. prt%child2%t > prt%child2%mass_squared ()) then
        !!! E is too small to have  $p_T^2 = E^2 - t > 0$ 
        !!! -> cycle to find another solution
        cycle
    else
        !!! E is big enough -> exit
        exit
    end if
end do
if (thetabar (prt, otherprt, shower%settings%isr_angular_ordered) &
    .and. pdf_divisor > zero &
    .and. prt%child2%momentum%p(0) > zero) then
    retvalue = retvalue + (zstep / prt%z) * &
        (D_alpha_s_isr ((one - prt%z) * prt%t, &
            shower%settings) * &
            P_prt_to_child1 (prt) * &

```

```

        shower%get_pdf (prt%initial%type, prt%child1%x / prt%z, &
prt%t, prt%type)) / (abs(prt%t) * pdf_divisor)
    end if
    if (retvalue > final) then
        exit
    else
        z = z + zstep
    end if
end do ZLOOP
end subroutine integral_over_z_part_isr

```

This returns a pointer to the parton with the next ISR branching, again FSR branchings are ignored.

```

<Shower core: shower: TBP>+=
    procedure :: generate_next_isr_branching => &
        shower_generate_next_isr_branching

<Shower core: sub interfaces>+=
    module function shower_generate_next_isr_branching &
        (shower) result (next_brancher)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t) :: next_brancher
    end function shower_generate_next_isr_branching

<Shower core: procedures>+=
    module function shower_generate_next_isr_branching &
        (shower) result (next_brancher)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t) :: next_brancher
        integer i, index
        type(parton_t), pointer :: prt
        next_brancher%p => null()
    do
        if (signal_is_pending ()) return
        if (shower_isr_is_finished (shower)) exit
        !!! find mother with highest |t| or pt to be simulated
        index = 0
        call shower%sort_partons ()
        do i = 1,size (shower%partons)
            prt => shower%partons(i)%p
            if (.not. associated (prt)) cycle
            if (.not. shower%settings%isr_pt_ordered) then
                if (prt%belongstointeraction) cycle
            end if
            if (prt%belongstoFSR) cycle
            if (prt%is_final ()) cycle
            if (.not. prt%belongstoFSR .and. prt%simulated) cycle
            index = i
        end do
        exit
    end do
    if (debug_active (D_SHOWER)) then
        if (index == 0) then
            call msg_fatal(" no branchable partons found")
        end if
    end if
end if

```



```

prt => shower%partons(index)%p

!!! ISR simulation
if (shower%settings%isr_pt_ordered) then
  call shower_isr_step_pt (shower, prt)
else
  call shower_isr_step (shower, prt)
end if
if (prt%simulated) then
  if (prt%t < zero) then
    next_brancher%p => prt
    if (.not. shower%settings%isr_pt_ordered) &
      call prt%generate_ps_ini (shower%rng)
    exit
  else
    if (.not. shower%settings%isr_pt_ordered) then
      call shower_replace_parent_by_hadron (shower, prt%child1)
    else
      call shower_replace_parent_by_hadron (shower, prt)
    end if
  end if
end if
end do

!!! some bookkeeping
call shower%sort_partons ()
call shower%boost_to_CMframe ()      !!! really necessary?
call shower%rotate_to_z ()          !!! really necessary?
end function shower_generate_next_isr_branching

```

This is a loop which searches for all emitted and branched partons.

```

<Shower core: shower: TBP>+≡
  procedure :: generate_fsr_for_isr_partons => &
    shower_generate_fsr_for_partons_emitted_in_ISR

<Shower core: sub interfaces>+≡
  module subroutine shower_generate_fsr_for_partons_emitted_in_ISR (shower)
    class(shower_t), intent(inout) :: shower
  end subroutine shower_generate_fsr_for_partons_emitted_in_ISR

<Shower core: procedures>+≡
  module subroutine shower_generate_fsr_for_partons_emitted_in_ISR (shower)
    class(shower_t), intent(inout) :: shower
    integer :: n_int, i
    type(parton_t), pointer :: prt
    if (shower%settings%isr_only_onshell_emitted_partons) return
    if (debug_on) call msg_debug &
      (D_SHOWER, "shower_generate_fsr_for_partons_emitted_in_ISR")
    INTERACTIONS_LOOP: do n_int = 1, size (shower%interactions)
      INCOMING_PARTONS_LOOP: do i = 1, 2
        if (signal_is_pending ()) return
        prt => shower%interactions(n_int)%i%partons(i)%p
        PARENT_PARTONS_LOOP: do
          if (associated (prt%parent)) then

```

```

        if (.not. prt%parent%is_proton ()) then
            prt => prt%parent
        else
            exit
        end if
    else
        exit
    end if
    if (associated (prt%child2)) then
        if (prt%child2%is_branched ()) then
            call shower_parton_generate_fsr (shower, prt%child2)
        end if
    else
        ! call msg_fatal ("Shower: no child2 associated?")
    end if
end do PARENT_PARTONS_LOOP
end do INCOMING_PARTONS_LOOP
end do INTERACTIONS_LOOP
end subroutine shower_generate_fsr_for_partons_emitted_in_ISR

```

This executes the branching generated by `shower_generate_next_isr_branching`, that means it generates the flavors, momenta, etc.

(Shower core: shower: TBP)+≡

```

    procedure :: execute_next_isr_branching => shower_execute_next_isr_branching

```

(Shower core: sub interfaces)+≡

```

    module subroutine shower_execute_next_isr_branching (shower, prtp)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(inout) :: prtp
    end subroutine shower_execute_next_isr_branching

```

(Shower core: procedures)+≡

```

    module subroutine shower_execute_next_isr_branching (shower, prtp)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(inout) :: prtp
        type(parton_t), pointer :: prt, otherprt
        type(parton_t), pointer :: prta, prtb, prtc, prtr
        real(default) :: mbr
        real(default) :: phirand
        if (debug_on) call msg_debug (D_SHOWER, "shower_execute_next_isr_branching")
        if (.not. associated (prtp%p)) then
            call msg_fatal ("Shower: prtp not associated")
        end if

        prt => prtp%p

        if ((.not. shower%settings%isr_pt_ordered .and. &
            prt%t > - shower%settings%min_virtuality) .or. &
            (shower%settings%isr_pt_ordered .and. prt%scale < D_Min_scale)) then
            call msg_error ("Shower: no branching to be executed.")
        end if

        otherprt => shower%find_recoiler (prt)
        if (shower%settings%isr_pt_ordered) then
            !!! get the recoiler

```

```

otherprt => shower%find_recoiler (prt)
if (associated (otherprt%parent)) then
  !!! Why only for pt ordered
  if (.not. otherprt%parent%is_proton () .and. &
      shower%settings%isr_pt_ordered) otherprt => otherprt%parent
end if
if (.not. associated (prt%parent)) then
  call shower%add_parent (prt)
end if
prt%parent%belongstoFSR = .false.
if (.not. associated (prt%parent%child2)) then
  call shower%add_child (prt%parent, 2)
end if

prta => prt%parent          !!! new parton a with branching a->bc
prtb => prt                  !!! former parton
prtc => prt%parent%child2    !!! emitted parton
prtr => otherprt             !!! recoiler

mbr = (prtb%momentum + prtr%momentum)**1

!!! 1. assume you are in the restframe
!!! 2. rotate by random phi
call shower%rng%generate (phirand)
phirand = twopi * phirand
call shower_apply_lorentztrafo (shower, &
    rotation(cos(phirand), sin(phirand), vector3_canonical(3)))
!!! 3. Put the b off-shell
!!! and
!!! 4. construct the massless a
!!! and the parton (eventually emitted by a)

!!! generate the flavor of the parent (prta)
if (prtb%aux_pt /= 0) prta%type = prtb%aux_pt
if (prtb%is_quark ()) then
  if (prta%type == prtb%type) then
    !!! (anti)-quark -> (anti-)quark + gluon
    prta%type = prtb%type    ! quarks have same flavor
    prtc%type = GLUON        ! emitted gluon
  else
    !!! gluon -> quark + antiquark
    prta%type = GLUON
    prtc%type = - prtb%type
  end if
else if (prtb%is_gluon ()) then
  prta%type = GLUON
  prtc%type = GLUON
else
  ! STOP "Bug in shower_execute_next_branching: neither quark nor gluon"
end if

prta%initial => prtb%initial
prta%belongstoFSR = .false.
prta%scale = prtb%scale

```

```

prta%x = prtb%x / prtb%z

prtb%momentum = vector4_moving ((mbr**2 + prtb%t) / (two * mbr), &
    vector3_canonical(3) * &
    sign ((mbr**2 - prtb%t) / (two * mbr), &
    prtb%momentum%p(3)))
prtr%momentum = vector4_moving ((mbr**2 - prtb%t) / (two * mbr), &
    vector3_canonical(3) * &
    sign( (mbr**2 - prtb%t) / (two * mbr), &
    prtr%momentum%p(3)))

prta%momentum = vector4_moving ((0.5_default / mbr) * &
    ((mbr**2 / prtb%z) + prtb%t - prtc%mass_squared ()), &
    vector3_null)
prta%momentum = vector4_moving (prta%momentum%p(0), &
    vector3_canonical(3) * &
    (0.5_default / prtb%momentum%p(3)) * &
    ((mbr**2 / prtb%z) - two &
    * prtr%momentum%p(0) * prta%momentum%p(0) ) )
if (prta%momentum%p(0)**2 - prta%momentum%p(3)**2 - &
    prtc%mass_squared () > zero) then
    !!! This SHOULD be always fulfilled???
    prta%momentum = vector4_moving (prta%momentum%p(0), &
        vector3_moving([sqrt (prta%momentum%p(0)**2 - &
        prta%momentum%p(3)**2 - &
        prtc%mass_squared ()), zero, &
        prta%momentum%p(3)])
end if
prtc%momentum = prta%momentum - prtb%momentum

!!! 5. rotate to have a along z-axis
call shower%boost_to_CMframe ()
call shower%rotate_to_z ()
!!! 6. rotate back in phi
call shower_apply_lorentztrafo (shower, rotation &
    (cos(-phirand), sin(-phirand), vector3_canonical(3)))
else
    if (prt%child2%t > prt%child2%mass_squared ()) then
        call shower_add_children_of_emitted_timelike_parton &
            (shower, prt%child2)
        call prt%child2%set_simulated ()
    end if

    call shower%add_parent (prt)
    call shower%add_child (prt%parent, 2)

    prt%parent%momentum = prt%momentum
    prt%parent%t = prt%t
    prt%parent%x = prt%x
    prt%parent%initial => prt%initial
    prt%parent%belongstoFSR = .false.

    prta => prt
    prtb => prt%child1

```

```

    prtc => prt%child2
end if
if (signal_is_pending ()) return
if (shower%settings%isr_pt_ordered) then
    call prt%parent%generate_ps_ini (shower%rng)
else
    call prt%generate_ps_ini (shower%rng)
end if

!!! add color connections
if (prtb%is_quark ()) then

    if (prta%type == prtb%type) then
        if (prtb%type > 0) then
            !!! quark -> quark + gluon
            prtc%c2 = prtb%c1
            prtc%c1 = shower%get_next_color_nr ()
            prta%c1 = prtc%c1
        else
            !!! antiquark -> antiquark + gluon
            prtc%c1 = prtb%c2
            prtc%c2 = shower%get_next_color_nr ()
            prta%c2 = prtc%c2
        end if
    else
        !!! gluon -> quark + antiquark
        if (prtb%type > 0) then
            !!! gluon -> quark + antiquark
            prta%c1 = prtb%c1
            prtc%c1 = 0
            prtc%c2 = shower%get_next_color_nr ()
            prta%c2 = prtc%c2
        else
            !!! gluon -> antiquark + quark
            prta%c2 = prtb%c2
            prtc%c1 = shower%get_next_color_nr ()
            prtc%c2 = 0
            prta%c1 = prtc%c1
        end if
    end if
else if (prtb%is_gluon ()) then
    if (prta%is_gluon ()) then
        !!! g -> gg
        prtc%c2 = prtb%c1
        prtc%c1 = shower%get_next_color_nr ()
        prta%c1 = prtc%c1
        prta%c2 = prtb%c2
    else if (prta%is_quark ()) then
        if (prta%type > 0) then
            prta%c1 = prtb%c1
            prta%c2 = 0
            prtc%c1 = prtb%c2
            prtc%c2 = 0
        else

```

```

        prta%c1 = 0
        prta%c2 = prtb%c2
        prtc%c1 = 0
        prtc%c2 = prtb%c1
    end if
end if

call shower%sort_partons ()
call shower%boost_to_CMframe ()
call shower%rotate_to_z ()

end subroutine shower_execute_next_isr_branching

(Shower core: procedures)+≡
subroutine shower_remove_parents_and_stuff (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    type(parton_t), pointer :: actprt, nextprt
    nextprt => prt%parent
    actprt => null()
    !!! remove children of emitted timelike parton
    if (associated (prt%child2)) then
        if (associated (prt%child2%child1)) then
            call shower_remove_parton_from_partons_recursive &
                (shower, prt%child2%child1)
        end if
        prt%child2%child1 => null()
        if (associated (prt%child2%child2)) then
            call shower_remove_parton_from_partons_recursive &
                (shower, prt%child2%child2)
        end if
        prt%child2%child2 => null()
    end if
    do
        actprt => nextprt
        if (.not. associated (actprt)) then
            exit
        else if (actprt%is_proton ()) then
            !!! remove beam-remnant
            call shower_remove_parton_from_partons (shower, actprt%child2)
            exit
        end if
        if (associated (actprt%parent)) then
            nextprt => actprt%parent
        else
            nextprt => null()
        end if
        call shower_remove_parton_from_partons_recursive &
            (shower, actprt%child2)
        call shower_remove_parton_from_partons (shower, actprt)
    end do
    prt%parent=>null()
end

```

```

end subroutine shower_remove_parents_and_stuff

<Shower core: shower: TBP>+≡
  procedure :: get_ISR_scale => shower_get_ISR_scale

<Shower core: sub interfaces>+≡
  module function shower_get_ISR_scale (shower) result (scale)
    class(shower_t), intent(in) :: shower
    real(default) :: scale
  end function shower_get_ISR_scale

<Shower core: procedures>+≡
  module function shower_get_ISR_scale (shower) result (scale)
    class(shower_t), intent(in) :: shower
    real(default) :: scale
    type(parton_t), pointer :: prt1, prt2
    integer :: i
    scale = zero
    do i = 1, size (shower%interactions)
      call interaction_find_partons_nearest_to_hadron &
        (shower%interactions(i)%i, prt1, prt2, &
          shower%settings%isr_pt_ordered)
      if (.not. prt1%simulated .and. abs(prt1%scale) > scale) &
        scale = abs(prt1%scale)
      if (.not. prt1%simulated .and. abs(prt2%scale) > scale) &
        scale = abs(prt2%scale)
    end do
  end function shower_get_ISR_scale

<Shower core: shower: TBP>+≡
  procedure :: set_max_isr_scale => shower_set_max_isr_scale

<Shower core: sub interfaces>+≡
  module subroutine shower_set_max_isr_scale (shower, newscale)
    class(shower_t), intent(inout) :: shower
    real(default), intent(in) :: newscale
  end subroutine shower_set_max_isr_scale

<Shower core: procedures>+≡
  module subroutine shower_set_max_isr_scale (shower, newscale)
    class(shower_t), intent(inout) :: shower
    real(default), intent(in) :: newscale
    real(default) :: scale
    type(parton_t), pointer :: prt
    integer :: i,j
    if (debug_on) call msg_debug (D_SHOWER, "shower_set_max_isr_scale: newscale", &
      newscale)
    if (shower%settings%isr_pt_ordered) then
      scale = newscale
    else
      scale = - abs (newscale)
    end if

    INTERACTIONS: do i = 1, size (shower%interactions)

```

```

PARTONS: do j = 1, 2
  prt => shower%interactions(i)%i%partons(j)%p
  do
    if (.not. shower%settings%isr_pt_ordered) then
      if (prt%belongstointeraction) prt => prt%parent
    end if
    if (prt%t < scale) then
      if (associated (prt%parent)) then
        prt => prt%parent
      else
        exit    !!! unresolved prt found
      end if
    else
      exit    !!! prt with scale above newscale found
    end if
  end do
  if (.not. shower%settings%isr_pt_ordered) then
    if (prt%child1%belongstointeraction .or. &
      prt%is_proton ()) then
      !!! don't reset scales of "first" spacelike partons
      !!!   in virtuality ordered shower or hadrons
      cycle
    end if
  else
    if (prt%is_proton ()) then
      !!! don't reset scales of hadrons
      cycle
    end if
  end if
  if (shower%settings%isr_pt_ordered) then
    prt%scale = scale
  else
    prt%t = scale
  end if
  call prt%set_simulated (.false.)
  call shower_remove_parents_and_stuff (shower, prt)
end do PARTONS
end do INTERACTIONS
end subroutine shower_set_max_isr_scale

```

<Shower core: shower: TBP>+≡

```

  procedure :: interaction_generate_fsr_2ton => &
    shower_interaction_generate_fsr_2ton

```

<Shower core: sub interfaces>+≡

```

  module subroutine shower_interaction_generate_fsr_2ton (shower, interaction)
    class(shower_t), intent(inout) :: shower
    type(shower_interaction_t), intent(inout) :: interaction
  end subroutine shower_interaction_generate_fsr_2ton

```

<Shower core: procedures>+≡

```

  module subroutine shower_interaction_generate_fsr_2ton (shower, interaction)
    class(shower_t), intent(inout) :: shower
    type(shower_interaction_t), intent(inout) :: interaction
    type(parton_t), pointer :: prt

```



```

prt => interaction%partons(3)%p
do
  if (.not. associated (prt%parent)) exit
  prt => prt%parent
end do
call shower_parton_generate_fsr (shower, prt)
call shower_parton_update_color_connections (shower, prt)
end subroutine shower_interaction_generate_fsr_2ton

```

Perform the FSR for one parton, it is assumed, that the parton already branched. Hence, its children are to be simulated. This procedure is intended for branched FSR-partons emitted in the ISR.

(Shower core: procedures)+≡

```

subroutine shower_parton_generate_fsr (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt
  type(parton_pointer_t), dimension(:), allocatable :: partons
  logical :: single_emission = .false.
  if (debug_on) call msg_debug (D_SHOWER, "shower_parton_generate_fsr")
  if (signal_is_pending ()) return
  if (debug_active (D_SHOWER)) then
    if (.not. prt%is_branched ()) then
      call msg_error ("shower_parton_generate_fsr: parton not branched")
      return
    end if
    if (prt%child1%simulated .or. &
        prt%child2%simulated) then
      print *, "children already simulated for parton ", prt%nr
      return
    end if
  end if
  allocate (partons(1))
  partons(1)%p => prt
  if (single_emission) then
    call shower%parton_pointer_array_generate_fsr (partons, partons)
  else
    call shower%parton_pointer_array_generate_fsr_recursive (partons)
  end if
end subroutine shower_parton_generate_fsr

```

(Shower core: shower: TBP)+≡

```

procedure :: parton_pointer_array_generate_fsr_recursive => &
  shower_parton_pointer_array_generate_fsr_recursive

```

(Shower core: sub interfaces)+≡

```

recursive module subroutine shower_parton_pointer_array_generate_fsr_recursive &
  (shower, partons)
  class(shower_t), intent(inout) :: shower
  type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
    partons
end subroutine shower_parton_pointer_array_generate_fsr_recursive

```

(Shower core: procedures)+≡

```

recursive module subroutine shower_parton_pointer_array_generate_fsr_recursive &

```

```

        (shower, partons)
class(shower_t), intent(inout) :: shower
type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
    partons
type(parton_pointer_t), dimension(:), allocatable :: partons_new
if (debug_on) call msg_debug (D_SHOWER, "shower_parton_pointer_array_generate_fsr_recursive")
if (signal_is_pending ()) return
if (size (partons) == 0) return
call shower%parton_pointer_array_generate_fsr (partons, partons_new)
call shower%parton_pointer_array_generate_fsr_recursive (partons_new)
end subroutine shower_parton_pointer_array_generate_fsr_recursive

```

<Shower core: shower: TBP>+≡

```

procedure :: parton_pointer_array_generate_fsr => &
    shower_parton_pointer_array_generate_fsr

```

<Shower core: sub interfaces>+≡

```

module subroutine shower_parton_pointer_array_generate_fsr &
    (shower, partons, partons_new)
class(shower_t), intent(inout) :: shower
type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
    partons
type(parton_pointer_t), dimension(:), allocatable, intent(out) :: &
    partons_new
end subroutine shower_parton_pointer_array_generate_fsr

```

<Shower core: procedures>+≡

```

module subroutine shower_parton_pointer_array_generate_fsr &
    (shower, partons, partons_new)
class(shower_t), intent(inout) :: shower
type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
    partons
type(parton_pointer_t), dimension(:), allocatable, intent(out) :: &
    partons_new
integer :: i, size_partons, size_partons_new
if (debug_on) call msg_debug (D_SHOWER, "shower_parton_pointer_array_generate_fsr")
!!! Simulate highest/first parton
call shower_simulate_children_ana (shower, partons(1)%p)
!!! check for new daughters to be included in new_partons
size_partons = size (partons)
size_partons_new = size_partons - 1 !!! partons(1) not needed anymore
if (partons(1)%p%child1%is_branched ()) &
    size_partons_new = size_partons_new + 1
if (partons(1)%p%child2%is_branched ()) &
    size_partons_new = size_partons_new + 1

allocate (partons_new (1:size_partons_new))

if (size_partons > 1) then
    do i = 2, size_partons
        partons_new (i - 1)%p => partons(i)%p
    end do
end if
if (partons(1)%p%child1%is_branched ()) &
    partons_new (size_partons)%p => partons(1)%p%child1

```

```

if (partons(1)%p%child2%is_branched ()) then
!!! check if child1 is already included
if (size_partons_new == size_partons) then
partons_new (size_partons)%p => partons(1)%p%child2
else if (size_partons_new == size_partons + 1) then
partons_new (size_partons + 1)%p => partons(1)%p%child2
else
call msg_fatal ("Shower: wrong sizes in" &
// "shower_parton_pointer_array_generate_fsr")
end if
end if
deallocate (partons)

end subroutine shower_parton_pointer_array_generate_fsr

```

```

(Shower core: procedures)+≡
recursive subroutine shower_parton_update_color_connections &
(shower, prt)
type(shower_t), intent(inout) :: shower
type(parton_t), intent(inout) :: prt
real(default) :: temprand
if (.not. associated (prt%child1) .or. &
.not. associated (prt%child2)) return

if (signal_is_pending ()) return
if (prt%is_gluon ()) then
if (prt%child1%is_quark ()) then
!!! give the quark the colorpartner and the antiquark
!!! the anticolorpartner
if (prt%child1%type > 0) then
!!! child1 is quark, child2 is antiquark
prt%child1%c1 = prt%c1
prt%child2%c2 = prt%c2
else
!!! child1 is antiquark, child2 is quark
prt%child1%c2 = prt%c2
prt%child2%c1 = prt%c1
end if
else
!!! g -> gg splitting -> random choosing of partners
call shower%rng%generate (temprand)
if (temprand > 0.5_default) then
prt%child1%c1 = prt%c1
prt%child1%c2 = shower%get_next_color_nr ()
prt%child2%c1 = prt%child1%c2
prt%child2%c2 = prt%c2
else
prt%child1%c2 = prt%c2
prt%child2%c1 = prt%c1
prt%child2%c2 = shower%get_next_color_nr ()
prt%child1%c1 = prt%child2%c2
end if
end if
else if (prt%is_quark ()) then

```

```

    if (prt%child1%is_quark ()) then
    if (prt%child1%type > 0) then
        !!! q -> q + g
        prt%child2%c1 = prt%c1
        prt%child2%c2 = shower%get_next_color_nr ()
        prt%child1%c1 = prt%child2%c2
    else
        !!! qbar -> qbar + g
        prt%child2%c2 = prt%c2
        prt%child2%c1 = shower%get_next_color_nr ()
        prt%child1%c2 = prt%child2%c1
    end if
else
    if (prt%child2%type > 0) then
        !!! q -> g + q
        prt%child1%c1 = prt%c1
        prt%child1%c2 = shower%get_next_color_nr ()
        prt%child2%c1 = prt%child1%c2
    else
        !!! qbar -> g + qbar
        prt%child1%c2 = prt%c2
        prt%child1%c1 = shower%get_next_color_nr ()
        prt%child2%c2 = prt%child1%c1
    end if
end if
end if

    call shower_parton_update_color_connections (shower, prt%child1)
    call shower_parton_update_color_connections (shower, prt%child2)
end subroutine shower_parton_update_color_connections

```

The next two routines are for PDFs. Wrapper function to return parton densities.

```

<Shower core: shower: TBP>+≡
    procedure :: get_pdf => shower_get_pdf

<Shower core: sub interfaces>+≡
    module function shower_get_pdf (shower, mother, x, Q2, daughter) result (pdf)
        class(shower_t), intent(inout), target :: shower
        integer, intent(in) :: mother, daughter
        real(default), intent(in) :: x, Q2
        real(default) :: pdf
    end function shower_get_pdf

<Shower core: procedures>+≡
    module function shower_get_pdf (shower, mother, x, Q2, daughter) result (pdf)
        <get pdf>
        if (x > eps0) then
            pdf = pdf / x
        end if
    end function shower_get_pdf

<Shower core: shower: TBP>+≡
    procedure :: get_xpdf => shower_get_xpdf

```

```

<Shower core: sub interfaces>+≡
  module function shower_get_xpdf (shower, mother, x, Q2, daughter) result (pdf)
    class(shower_t), intent(inout), target :: shower
    integer, intent(in) :: mother, daughter
    real(default), intent(in) :: x, Q2
    real(default) :: pdf
  end function shower_get_xpdf

```

```

<Shower core: procedures>+≡
  module function shower_get_xpdf (shower, mother, x, Q2, daughter) result (pdf)
    <get pdf>
  end function shower_get_xpdf

```

```

<get pdf>≡
  class(shower_t), intent(inout), target :: shower
  integer, intent(in) :: mother, daughter
  real(default), intent(in) :: x, Q2
  real(default) :: pdf
  real(double), save :: f(-6:6) = 0._double
  real(double), save :: lastx, lastQ2 = 0._double
  pdf = zero
  if (debug_active (D_SHOWER)) then
    if (abs (mother) /= PROTON) then
      if (debug_on) call msg_debug (D_SHOWER, "mother", mother)
      call msg_fatal ("Shower: pdf only implemented for (anti-)proton")
    end if
    if (.not. (abs (daughter) >= 1 .and. abs (daughter) <= 6 .or. &
      daughter == GLUON)) then
      if (debug_on) call msg_debug (D_SHOWER, "daughter", daughter)
      call msg_fatal ("Shower: error in pdf, unknown daughter")
    end if
  end if
  if (x > zero .and. x < one) then
    if ((dble(Q2) - lastQ2) > eps0 .or. (dble(x) - lastx) > eps0) then
      call shower%pdf_data%evolve &
        (dble(x), sqrt (abs (dble(Q2))), f)
    end if
    if (abs (daughter) >= 1 .and. abs (daughter) <= 6) then
      pdf = max (f(daughter * sign (1,mother)), tiny_10)
    else
      pdf = max (f(0), tiny_10)
    end if
  end if
  lastQ2 = dble(Q2)
  lastx = dble(x)

```

Convert Whizard shower to Pythia6. Currently only works for one interaction.

```

<Shower core: shower: TBP>+≡
  procedure :: converttopythia => shower_converttopythia

```

```

<Shower core: sub interfaces>+≡
  module subroutine shower_converttopythia (shower)
    class(shower_t), intent(in) :: shower
  end subroutine shower_converttopythia

```

```

(Shower core: procedures)+≡
module subroutine shower_converttopythia (shower)
  class(shower_t), intent(in) :: shower
  <PYJETS COMMON BLOCK>
  type(parton_t), pointer :: pp, ppparent
  integer :: i
  K = 0
  do i = 1, 2
    !!! get history of the event
    pp => shower%interactions(i)%i%partons(i)%p
    !!! add these partons to the event record
    if (associated (pp%initial)) then
      !!! add hadrons
      K(i,1) = 21
      K(i,2) = pp%initial%type
      K(i,3) = 0
      P(i,1:5) = pp%initial%momentum_to_pythia6 ()
      !!! add partons emitted by the hadron
      ppparent => pp
      do while (associated (ppparent%parent))
        if (ppparent%parent%is_proton ()) then
          exit
        else
          ppparent => ppparent%parent
        end if
      end do
      K(i+2,1) = 21
      K(i+2,2) = ppparent%type
      K(i+2,3) = i
      P(i+2,1:5) = ppparent%momentum_to_pythia6 ()
      !!! add partons in the initial state of the ME
      K(i+4,1) = 21
      K(i+4,2) = pp%type
      K(i+4,3) = i
      P(i+4,1:5) = pp%momentum_to_pythia6 ()
    else
      !!! for e+e- without ISR all entries are the same
      K(i,1) = 21
      K(i,2) = pp%type
      K(i,3) = 0
      P(i,1:5) = pp%momentum_to_pythia6 ()
      P(i+2,:) = P(1,:)
      K(i+2,:) = K(1,:)
      K(i+2,3) = i
      P(i+4,:) = P(1,:)
      K(i+4,:) = K(1,:)
      K(i+4,3) = i
      P(i+4,5) = 0.
    end if
  end do
  N = 6
  !!! create intermediate (fake) Z-Boson
  !K(7,1) = 21
  !K(7,2) = 23

```

```

!K(7,3) = 0
!P(7,1:4) = P(5,1:4) + P(6,1:4)
!P(7,5) = P(7,4)**2 - P(7,3)**2 - P(7,2)**2 - P(7,1)**2
!N = 7
!!! include partons in the final state of the hard matrix element
do i = 1, size (shower%interactions(1)%i%partons) - 2
  !!! get partons that are in the final state of the hard matrix element
  pp => shower%interactions(1)%i%partons(2+i)%p
  !!! add these partons to the event record
  K(7+I,1) = 21
  K(7+I,2) = pp%type
  K(7+I,3) = 7
  P(7+I,1:5) = pp%momentum_to_pythia6 ( )
  !N = 7 + I
  N = 6 + I
end do
!!! include "Z" (again)
!N = N + 1
!K(N,1) = 11
!K(N,2) = 23
!K(N,3) = 7
!P(N,1:5) = P(7,1:5)
!nz = N
!!! include partons from the final state of the parton shower
call shower_transfer_final_partons_to_pythia (shower, 8)
!!! set "children" of "Z"
!K(nz,4) = 11
!K(nz,5) = N

!!! be sure to remove the next partons (=first obsolete partons)
!!! otherwise they might be interpreted as thrust information
K(N+1:N+3,1:3) = 0
end subroutine shower_converttopythia

```

(Shower core: procedures)+≡

```

subroutine shower_transfer_final_partons_to_pythia (shower, first)
<PYJETS COMMON BLOCK>
  type(shower_t), intent(in) :: shower
  integer, intent(in) :: first
  type(parton_t), pointer :: prt
  integer :: i, j, n_finals
  type(parton_t), dimension(:), allocatable :: final_partons
  type(parton_t) :: temp_parton
  integer :: minindex, maxindex

  prt => null()

  !!! get total number of final partons
  n_finals = 0
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    prt => shower%partons(i)%p
    if (.not. prt%belongstoFSR) cycle
    if (associated (prt%child1)) cycle

```

```

        n_finals = n_finals + 1
    end do

    allocate (final_partons(1:n_finals))
    j = 1
    do i = 1, size (shower%partons)
        if (.not. associated (shower%partons(i)%p)) cycle
        prt => shower%partons(i)%p
        if (.not. prt%belongstoFSR) cycle
        if (associated (prt%child1)) cycle
        final_partons(j) = shower%partons(i)%p
        j = j + 1
    end do

    !!! move quark to front as beginning of color string
    minindex = 1
    maxindex = size (final_partons)
    FIND_Q: do i = minindex, maxindex
        if (final_partons(i)%type >= 1 .and. final_partons(i)%type <= 6) then
            temp_parton = final_partons(minindex)
            final_partons(minindex) = final_partons(i)
            final_partons(i) = temp_parton
            exit FIND_Q
        end if
    end do FIND_Q

    !!! sort so that connected partons are next to each other, don't care about zeros
    do i = 1, size (final_partons)
        !!! ensure that final_partons begins with a color (not an anticolor)
        if (final_partons(i)%c1 > 0 .and. final_partons(i)%c2 == 0) then
            if (i == 1) then
                exit
            else
                temp_parton = final_partons(1)
                final_partons(1) = final_partons(i)
                final_partons(i) = temp_parton
                exit
            end if
        end if
    end do

    do i = 1, size (final_partons) - 1
        !!! search for color partner and move it to i + 1
        PARTNERS: do j = i + 1, size (final_partons)
            if (final_partons(j)%c2 == final_partons(i)%c1) exit PARTNERS
        end do PARTNERS
        if (j > size (final_partons)) then
            print *, "no color connected parton found" !WRONG???
            print *, "particle: ", final_partons(i)%nr, " index: ", &
                final_partons(i)%c1
            exit
        end if
        temp_parton = final_partons(i + 1)
        final_partons(i + 1) = final_partons(j)
    end do

```



```

        final_partons(j) = temp_parton
    end do

    !!! transferring partons
    do i = 1, size (final_partons)
        prt = final_partons(i)
        N = N + 1
        K(N,1) = 2
        if (prt%c1 == 0) K(N,1) = 1          !!! end of color string
        K(N,2) = prt%type
        !K(N,3) = first
        K(N,3) = 0
        K(N,4) = 0
        K(N,5) = 0
        P(N,1:5) = prt%momentum_to_pythia6()
    end do
    deallocate (final_partons)
end subroutine shower_transfer_final_partons_to_pythia

```

22.4 Interface to PYTHIA 6

```

<shower_pythia6.f90>≡
  <File header>

  module shower_pythia6

    <Use kinds with double>
    <Use strings>
    use os_interface
    use lorentz
    use shower_base
    use particles
    use model_data
    use pdf
    use tauola_interface

    <Standard module head>

    <Shower pythia6: public>

    <Shower pythia6: types>

    interface
    <Shower pythia6: sub interfaces>
    end interface

  end module shower_pythia6

<shower_pythia6_sub.f90>≡
  <File header>

```

```

submodule (shower_pythia6) shower_pythia6_s

  <Use debug>
    use constants
    use numeric_utils, only: vanishes
    use io_units
    use physics_defs
    use diagnostics
    use subevents
    use hep_common
    use helicities

    implicit none

  <Shower pythia6: variables>

  contains

  <Shower pythia6: procedures>

end submodule shower_pythia6_s

<PYJETS COMMON BLOCK>≡
  integer :: N, NPAD, K
  real(double) :: P, V
  COMMON/PYJETS/N,NPAD,K(4000,5),P(4000,5),V(4000,5)
  SAVE /PYJETS/

  <Shower pythia6: variables>≡
    integer :: N_old

```

The PYTHIA6 shower type.

```

  <Shower pythia6: public>≡
    public :: shower_pythia6_t

  <Shower pythia6: types>≡
    type, extends (shower_base_t) :: shower_pythia6_t
      integer :: initialized_for_NPRUP = 0
      logical :: warning_given = .false.
    contains
      <Shower pythia6: shower pythia6: TBP>
    end type shower_pythia6_t

```

Initialize the PYTHIA6 shower.

```

  <Shower pythia6: shower pythia6: TBP>≡
    procedure :: init => shower_pythia6_init

  <Shower pythia6: sub interfaces>≡
    module subroutine shower_pythia6_init &
      (shower, settings, taudec_settings, pdf_data, os_data)
      class(shower_pythia6_t), intent(out) :: shower
      type(shower_settings_t), intent(in) :: settings
      type(taudec_settings_t), intent(in) :: taudec_settings
      type(pdf_data_t), intent(in) :: pdf_data
    end subroutine

```

```

        type(os_data_t), intent(in) :: os_data
    end subroutine shower_pythia6_init

<Shower pythia6: procedures>+=
    module subroutine shower_pythia6_init &
        (shower, settings, taudec_settings, pdf_data, os_data)
        class(shower_pythia6_t), intent(out) :: shower
        type(shower_settings_t), intent(in) :: settings
        type(taudec_settings_t), intent(in) :: taudec_settings
        type(pdf_data_t), intent(in) :: pdf_data
        type(os_data_t), intent(in) :: os_data
        if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_init")
        shower%settings = settings
        shower%taudec_settings = taudec_settings
        shower%os_data = os_data
        call pythia6_set_verbose (settings%verbose)
        call shower%pdf_data%init (pdf_data)
        shower%name = "PYTHIA6"
        call shower%write_msg ()
    end subroutine shower_pythia6_init

<Shower pythia6: shower pythia6: TBP>+=
    procedure :: import_particle_set => shower_pythia6_import_particle_set

<Shower pythia6: sub interfaces>+=
    module subroutine shower_pythia6_import_particle_set &
        (shower, particle_set)
        class(shower_pythia6_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
    end subroutine shower_pythia6_import_particle_set

<Shower pythia6: procedures>+=
    module subroutine shower_pythia6_import_particle_set &
        (shower, particle_set)
        class(shower_pythia6_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
        type(particle_set_t) :: pset_reduced
        if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_import_particle_set")
        if (debug_active (D_SHOWER)) then
            print *, 'IDBMUP(1:2) = ', IDBMUP(1:2)
            print *, 'EBMUP, PDFGUP = ', EBMUP, PDFGUP
            print *, 'PDFSUP, IDWTUP = ', PDFSUP, IDWTUP
            print *, "NPRUP = ", NPRUP
            call particle_set%write (summary=.true., compressed=.true.)
        end if
        call particle_set%reduce (pset_reduced)
        if (debug2_active (D_SHOWER)) then
            print *, 'After particle_set%reduce: pset_reduced'
            call pset_reduced%write (summary=.true., compressed=.true.)
        end if
        call hepeup_from_particle_set (pset_reduced, tauola_convention=.true.)
        call hepeup_set_event_parameters (proc_id = 1)
        call hepeup_set_event_parameters (scale = shower%fac_scale)
    end subroutine shower_pythia6_import_particle_set

```

```

<Shower pythia6: shower pythia6: TBP>+≡
  procedure :: generate_emissions => shower_pythia6_generate_emissions

<Shower pythia6: sub interfaces>+≡
  module subroutine shower_pythia6_generate_emissions &
    (shower, valid, number_of_emissions)
    class(shower_pythia6_t), intent(inout), target :: shower
    logical, intent(out) :: valid
    integer, optional, intent(in) :: number_of_emissions
  end subroutine shower_pythia6_generate_emissions

<Shower pythia6: procedures>+≡
  module subroutine shower_pythia6_generate_emissions &
    (shower, valid, number_of_emissions)
    IMPLICIT DOUBLE PRECISION(A-H, O-Z)
    IMPLICIT INTEGER(I-N)
    COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
    SAVE/PYDAT1/
    class(shower_pythia6_t), intent(inout), target :: shower
    logical, intent(out) :: valid
    integer, optional, intent(in) :: number_of_emissions
    integer :: N, NPAD, K
    real(double) :: P, V
    common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
    COMMON/PYDAT2/KCHG(500,4),PMAS(500,4),PARF(2000),VCKM(4,4)
    COMMON/PYINT4/MWID(500),WIDS(500,5)
    save /PYJETS/,/PYDAT2/,/PYINT4/
    integer :: u_W2P
    integer :: i
    real(double) :: beta_z, pz_in, E_in
    integer, parameter :: lower = 5
    real(double), parameter :: beta_x = 0.0_double
    real(double), parameter :: beta_y = 0.0_double
    real(double), parameter :: theta = 0.0_double
    real(double), parameter :: phi = 0.0_double
    if (signal_is_pending ()) return
    call pythia6_setup_lhe_io_units (u_W2P)
    call w2p_write_lhef_event (u_W2P)
    rewind (u_W2P)
    call pythia6_set_last_treated_line(6)
    call shower%transfer_settings ()
    if (debug_active (D_SHOWER)) then
      print *, ' Before pyevnt, before boosting :'
      call pylist(2)
    end if
    if (debug_on) call msg_debug (D_SHOWER, "calling pyevnt")
    ! TODO: (bcn 2015-04-24) doesnt change anything I think
    ! P(1,1:5) = pset_reduced%prt(1)%momentum_to_pythia6 ()
    ! P(2,1:5) = pset_reduced%prt(2)%momentum_to_pythia6 ()
    call pyevnt ()
    call pyedit(12)
    do i = 1, n
      if (K(i,1) == 14 .and. abs(K(i,2)) >= 11 .and. abs(K(i,2)) <= 16) then
        if (K(i,4) > 0 .and. K(i,5) > 0 .and. K(i,4) < N .and. K(i,5) < N) then
          K(i,1) = 11

```

```

        K(i,4) = K(K(i,4),3)
        K(i,5) = K(K(i,5),3)
    end if
end if
end do
if (.not. shower%settings%hadron_collision) then
    pz_in = pup(3,1) + pup(3,2)
    E_in = pup(4,1) + pup(4,2)
    beta_z = pz_in / E_in
    call pyrobo (lower, N, theta, phi, beta_x, beta_y, beta_z)
end if
if (debug_active (D_SHOWER)) then
    print *, ' After pyevnt, after boosting :'
    call pylist(2)
    if (debug2_active (D_SHOWER)) then
        call pystat (5)
        do i = 1, 200
            print *, 'MSTJ (', i, ') = ', MSTJ(i)
            print *, 'MSTU (', i, ') = ', MSTU(i)
            print *, 'PMAS (', i, ') = ', PMAS(i,1), PMAS(i,2)
            print *, 'MWID (', i, ') = ', MWID(i)
            print *, 'PARJ (', i, ') = ', PARJ(i)
        end do
    end if
end if
close (u_W2P)
valid = pythia6_handle_errors ()
end subroutine shower_pythia6_generate_emissions

```

<Shower pythia6: shower pythia6: TBP>+≡

```
procedure :: make_particle_set => shower_pythia6_make_particle_set
```

<Shower pythia6: sub interfaces>+≡

```

module subroutine shower_pythia6_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia6_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
end subroutine shower_pythia6_make_particle_set

```

<Shower pythia6: procedures>+≡

```

module subroutine shower_pythia6_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia6_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
    call shower%combine_with_particle_set (particle_set, model, model_hadrons)
end subroutine shower_pythia6_make_particle_set

```

<Shower pythia6: shower pythia6: TBP>+≡

```
procedure :: transfer_settings => shower_pythia6_transfer_settings
```

```

<Shower pythia6: sub interfaces>+≡
  module subroutine shower_pythia6_transfer_settings (shower)
    class(shower_pythia6_t), intent(inout) :: shower
  end subroutine shower_pythia6_transfer_settings

<Shower pythia6: procedures>+≡
  module subroutine shower_pythia6_transfer_settings (shower)
    class(shower_pythia6_t), intent(inout) :: shower
    character(len=10) :: buffer
    real(default) :: rand
    logical, save :: tauola_initialized = .false.
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_transfer_settings")
    !!! We repeat these as they are overwritten by the hadronization
    call pygive ("MSTP(111)=1")      !!! Allow hadronization and decays
    call pygive ("MSTJ(1)=0")        !!! No jet fragmentation
    call pygive ("MSTJ(21)=1")      !!! Allow decays but no jet fragmentation

    if (shower%initialized_for_NPRUP >= NPRUP) then
      if (debug_on) call msg_debug (D_SHOWER, "calling upinit")
      call upinit ()
    else
      if (shower%settings%isr_active) then
        call pygive ("MSTP(61)=1")
      else
        call pygive ("MSTP(61)=0")  !!! switch off ISR
      end if
      if (shower%settings%fsr_active) then
        call pygive ("MSTP(71)=1")
      else
        call pygive ("MSTP(71)=0")  !!! switch off FSR
      end if
      call pygive ("MSTP(11)=0")    !!! Disable Pythias QED-ISR per default
      call pygive ("MSTP(171)=1")   !!! Allow variable energies

      write (buffer, "(F10.5)") sqrt (abs (shower%settings%min_virtuality))
      call pygive ("PARJ(82)=" // buffer)
      write (buffer, "(F10.5)") shower%settings%isr_tscalefactor
      call pygive ("PARP(71)=" // buffer)
      write (buffer, "(F10.5)") shower%settings%fsr_lambda
      call pygive ("PARP(72)=" // buffer)
      write (buffer, "(F10.5)") shower%settings%isr_lambda
      call pygive ("PARP(61)=" // buffer)
      write (buffer, "(I10)") shower%settings%max_n_flavors
      call pygive ("MSTJ(45)=" // buffer)
      if (shower%settings%isr_alphas_running) then
        call pygive ("MSTP(64)=2")
      else
        call pygive ("MSTP(64)=0")
      end if
      if (shower%settings%fsr_alphas_running) then
        call pygive ("MSTJ(44)=2")
      else
        call pygive ("MSTJ(44)=0")
      end if
      write (buffer, "(F10.5)") shower%settings%fixed_alpha_s

```

```

call pygive ("PARU(111)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_primordial_kt_width
call pygive ("PARP(91)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_primordial_kt_cutoff
call pygive ("PARP(93)=" // buffer)
write (buffer, "(F10.5)") 1._double - shower%settings%isr_z_cutoff
call pygive ("PARP(66)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_minenergy
call pygive ("PARP(65)=" // buffer)
if (shower%settings%isr_only_onshell_emitted_partons) then
  call pygive ("MSTP(63)=0")
else
  call pygive ("MSTP(63)=2")
end if
if (shower%settings%mlm_matching) then
  call pygive ("MSTP(62)=2")
  call pygive ("MSTP(67)=0")
end if
call pythia6_set_config (shower%settings%pythia6_pygive)
if (debug_on) call msg_debug (D_SHOWER, "calling pyinit")
call PYINIT ("USER", "", "", ODO)
call shower%rng%generate (rand)
write (buffer, "(I10)") floor (rand*900000000)
call pygive ("MRPY(1)=" // buffer)
call pygive ("MRPY(2)=0")
call pythia6_set_config (shower%settings%pythia6_pygive)
shower%initialized_for_NPRUP = NPRUP
end if
if (shower%settings%tau_dec) then
  call pygive ("MSTJ(28)=2")
end if
if (pythia6_tauola_active() .and. .not. tauola_initialized) then
  call wo_tauola_init_call (shower%taudec_settings)
  tauola_initialized = .true.
end if
end subroutine shower_pythia6_transfer_settings

```

<Shower pythia6: shower pythia6: TBP>+≡

```

procedure :: combine_with_particle_set => &
  shower_pythia6_combine_with_particle_set

```

<Shower pythia6: sub interfaces>+≡

```

module subroutine shower_pythia6_combine_with_particle_set &
  (shower, particle_set, model_in, model_hadrons)
  class(shower_pythia6_t), intent(in) :: shower
  type(particle_set_t), intent(inout) :: particle_set
  class(model_data_t), intent(in), target :: model_in
  class(model_data_t), intent(in), target :: model_hadrons
end subroutine shower_pythia6_combine_with_particle_set

```

<Shower pythia6: procedures>+≡

```

module subroutine shower_pythia6_combine_with_particle_set &
  (shower, particle_set, model_in, model_hadrons)
  class(shower_pythia6_t), intent(in) :: shower
  type(particle_set_t), intent(inout) :: particle_set

```

```

class(model_data_t), intent(in), target :: model_in
class(model_data_t), intent(in), target :: model_hadrons
call pythia6_combine_with_particle_set &
    (particle_set, model_in, model_hadrons, shower%settings)
end subroutine shower_pythia6_combine_with_particle_set

```

K(I,1) pythia status code
 1 = undecayed particle or unfragmented parton
 (single or last of parton system)
 2 = unfragmented parton
 (followed by more partons in the same color singlet)
 3 = unfragmented parton (color info in K(I,4), K(I,5))
 11 = decayed particle or fragmented parton
 12 = fragmented parton
 13 = fragmented parton that has been removed The first two
 14 = branched parton with color info like 3
 21 = documentation lines

K(I,2) PDG code

K(I,3) Parent where known else 0. Unphysical to assign
 particles partons as parents

K(I,4) Normally first daughter

K(I,5) Normally last daughter

particles are always the beams, in Pythia and Whizard. We remove all beam
 remnants (including the ISR photons) since those are added back in by Pythia.

<Shower pythia6: public>+≡

```

public :: pythia6_combine_with_particle_set

```

<Shower pythia6: sub interfaces>+≡

```

module subroutine pythia6_combine_with_particle_set (particle_set, model_in, &
    model_hadrons, settings)
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model_in
    class(model_data_t), intent(in), target :: model_hadrons
    type(shower_settings_t), intent(in) :: settings
end subroutine pythia6_combine_with_particle_set

```

<Shower pythia6: procedures>+≡

```

module subroutine pythia6_combine_with_particle_set (particle_set, model_in, &
    model_hadrons, settings)
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model_in
    class(model_data_t), intent(in), target :: model_hadrons
    type(shower_settings_t), intent(in) :: settings
    class(model_data_t), pointer :: model
    type(vector4_t) :: momentum
    type(particle_t), dimension(:), allocatable :: particles, beams
    integer :: dangling_col, dangling_anti_col, color, anti_color
    integer :: i, j, py_entries, next_color, n_tot_old, parent, real_parent
    integer :: pdg, status, child, hadro_start, i_py, i_whz
    integer, allocatable, dimension(:) :: py_index, whz_index
    logical, allocatable, dimension(:) :: valid
    real(default), parameter :: py_tiny = 1E-10_default
    integer :: N, NPAD, K

```



```

real(double) :: P, V
common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
save /PYJETS/
integer, parameter :: KSUSY1 = 1000000, KSUSY2 = 2000000

if (signal_is_pending ()) return
if (debug_active (D_SHOWER)) then
  call msg_debug (D_SHOWER, 'Combine PYTHIA6 with particle set')
  call msg_debug (D_SHOWER, 'Particle set before replacing')
  call particle_set%write (summary=.true., compressed=.true.)
  call pyplot (3)
  call msg_debug (D_SHOWER, string = "settings%hadron_collision", &
    value = settings%hadron_collision)
end if
if (settings%method == PS_PYTHIA6 .and. settings%hadron_collision) then
  call pythia6_set_last_treated_line(2)
  allocate (beams(2))
  beams = particle_set%prt(1:2)
  call particle_set%replace (beams)
  if (debug_active (D_SHOWER)) then
    call msg_debug (D_SHOWER, 'Resetting particle set to')
    call particle_set%write (summary=.true., compressed=.true.)
  end if
end if
call fill_hepevt_block_from_pythia ()
call count_valid_entries_in_pythia_record ()
call particle_set%without_hadronic_remnants &
  (particles, n_tot_old, py_entries)
if (debug_active (D_SHOWER)) then
  print *, 'n_tot_old = ', n_tot_old
  print *, 'py_entries = ', py_entries
end if
call add_particles_of_pythia ()
call particle_set%replace (particles)
if (settings%hadron_collision) then
  call set_parent_child_relations_from_K ()
  call set_parent_child_relations_of_color_strings_to_hadrons ()
  !!! call particle_set%remove_duplicates (py_tiny * 100.0_default)
else
  call set_parent_child_relations_from_hepevt ()
end if
!call fix_nonemitting_outgoings ()
if (settings%method == PS_WHIZARD) then
  call fudge_whizard_partons_in_hadro ()
end if
where ((particle_set%prt%status == PRT_OUTGOING .or. &
  particle_set%prt%status == PRT_VIRTUAL .or. &
  particle_set%prt%status == PRT_BEAM_REMNANT) .and. &
  particle_set%prt%has_children ()) &
  particle_set%prt%status = PRT_RESONANT
if (debug_active (D_SHOWER)) then
  print *, 'Particle set after replacing'
  call particle_set%write (summary=.true., compressed=.true.)
  print *, ' pythia6_set_last_treated_line will set to: ', N

```

```

end if
call pythia6_set_last_treated_line(N)

contains

<Shower pythia6: combine with particle set: procedures>

end subroutine pythia6_combine_with_particle_set

<Shower pythia6: combine with particle set: procedures>≡
subroutine count_valid_entries_in_pythia_record ()
  <HEPEVT BLOCK>
  integer :: pset_idx
  logical :: comes_from_cmshower, emitted_zero_momentum_photon, &
    direct_decendent
  integer, parameter :: cmshower = 94
  hadro_start = 0
  allocate (valid(N))
  valid = .false.
  FIND: do i_py = 5, N
    !if (K(i_py,2) >= 91 .and. K(i_py,2) <= 94) then
    if (K(i_py,2) >= 91 .and. K(i_py,2) <= 93) then
      hadro_start = i_py
      exit FIND
    end if
  end do FIND
  do i_py = N, N_old+1, -1
    status = K(i_py,1)
    if (any (P(i_py,1:4) > 1E-8_default * P(1,4)) .and. &
      (status >= 1 .and. status <= 21)) then
      pset_idx = find_pythia_particle (i_py, more_fuzzy=.false.)
      direct_decendent = IDHEP(JMOHEP(1,i_py)) == cmshower .and. &
        JMOHEP(2,i_py) == 0
      emitted_zero_momentum_photon = find_pythia_particle &
        (JMOHEP(1,i_py), more_fuzzy=.false.) == pset_idx
      comes_from_cmshower = status == 1 .and. &
        (direct_decendent .or. emitted_zero_momentum_photon)
      valid(i_py) = pset_idx == 0 .or. comes_from_cmshower
    end if
  end do
  py_entries = count (valid)
  allocate (py_index (py_entries))
  allocate (whz_index (N))
  whz_index = 0
end subroutine count_valid_entries_in_pythia_record

<Shower pythia6: combine with particle set: procedures>+≡
subroutine add_particles_of_pythia ()
  integer :: whizard_status
  integer :: pset_idx, start_in_py
  integer :: ihelicity
  type(helicity_t) :: hel
  real(default) :: lifetime

```

```

type(vector4_t) :: vertex
dangling_col = 0
dangling_anti_col = 0
next_color = 500
i_whz = 1
if (settings%method == PS_PYTHIA6 .and. settings%hadron_collision) then
    start_in_py = 3
else
    start_in_py = 7
end if
do i_py = start_in_py, N
    status = K(i_py,1)
    if (valid(i_py)) then
        call assign_colors (color, anti_color)
        momentum = real ([P(i_py,4), P(i_py,1:3)], kind=default)
        pdg = K(i_py,2)
        parent = K(i_py,3)
        call find_model (model, pdg, model_in, model_hadrons)
        if (i_py <= 4) then
            whizard_status = PRT_INCOMING
        else
            if (status <= 10) then
                whizard_status = PRT_OUTGOING
            else
                whizard_status = PRT_VIRTUAL
            end if
        end if
        call particles(n_tot_old+i_whz)%init &
            (whizard_status, pdg, model, color, anti_color, momentum)
        lifetime = V(i_py,5)
        vertex = [real (V(i_py,4), kind=default), &
            real (V(i_py,1), kind=default), &
            real (V(i_py,2), kind=default), &
            real (V(i_py,3), kind=default)]
        if (.not. vanishes(lifetime)) &
            call particles(n_tot_old+i_whz)%set_lifetime (lifetime)
        if (any (.not. vanishes(real(V(i_py,1:4), kind = default)))) &
            call particles(n_tot_old+i_whz)%set_vertex (vertex)
        !!! Set tau helicity set by TAUOLA
        if (abs (pdg) == 15) then
            call wo_tauola_get_helicity (i_py, ihelicity)
            call hel%init (ihelicity)
            call particles(n_tot_old+i_whz)%set_helicity(hel)
            call particles(n_tot_old+i_whz)%set_polarization(PRT_DEFINITE_HELICITY)
        end if
        py_index(i_whz) = i_py
        whz_index(i_py) = n_tot_old + i_whz
        i_whz = i_whz + 1
    else
        pset_idx = find_pythia_particle (i_py, more_fuzzy=.true.)
        whz_index(i_py) = pset_idx
    end if
end do
end subroutine add_particles_of_pythia

```

(Shower pythia6: combine with particle set: procedures)+=

```

subroutine assign_colors (color, anti_color)
  integer, intent(out) :: color, anti_color
  if ((K(i_py,2) == 21) .or. (abs (K(i_py,2)) <= 8) .or. &
      (abs (K(i_py,2)) >= KSUSY1+1 .and. abs (K(i_py,2)) <= KSUSY1+8) .or. &
      (abs (K(i_py,2)) >= KSUSY2+1 .and. abs (K(i_py,2)) <= KSUSY2+8) .or. &
      (abs (K(i_py,2)) >= 1000 .and. abs (K(i_py,2)) <= 9999) .and. &
      hadro_start == 0) then
    if (dangling_col == 0 .and. dangling_anti_col == 0) then
      ! new color string
      ! Gluon and gluino only color octets implemented so far
      if (K(i_py,2) == 21 .or. K(i_py,2) == 1000021) then
        color = next_color
        dangling_col = color
        next_color = next_color + 1
        anti_color = next_color
        dangling_anti_col = anti_color
        next_color = next_color + 1
      else if (K(i_py,2) > 0) then ! particles have color
        color = next_color
        dangling_col = color
        anti_color = 0
        next_color = next_color + 1
      else if (K(i_py,2) < 0) then ! antiparticles have anticolor
        anti_color = next_color
        dangling_anti_col = anti_color
        color = 0
        next_color = next_color + 1
      end if
    else if(status == 1) then
      ! end of string
      color = dangling_anti_col
      anti_color = dangling_col
      dangling_col = 0
      dangling_anti_col = 0
    else
      ! inside the string
      if(dangling_col /= 0) then
        anti_color = dangling_col
        color = next_color
        dangling_col = next_color
        next_color = next_color +1
      else if(dangling_anti_col /= 0) then
        color = dangling_anti_col
        anti_color = next_color
        dangling_anti_col = next_color
        next_color = next_color +1
      else
        call msg_bug ("Couldn't assign colors")
      end if
    end if
  else
    color = 0
  end if
end if

```

```

        anti_color = 0
    end if
end subroutine assign_colors

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine fill_hepevt_block_from_pythia ()
    integer :: first_daughter, second_mother_of_first_daughter, i_hep
    logical :: inconsistent_mother, more_than_one_points_to_first_daughter
    <HEPEVT BLOCK>
    call pyhepc(1)
    do i_hep = 1, NHEP
        first_daughter = JDAHEP(1,i_hep)
        if (first_daughter > 0) then
            more_than_one_points_to_first_daughter = &
                count (JDAHEP(1,i_hep:NHEP) == first_daughter) > 1
            if (more_than_one_points_to_first_daughter) then
                second_mother_of_first_daughter = JMOHEP(2,first_daughter)
                ! Only entries with codes 91-94 should have a second mother
                if (second_mother_of_first_daughter == 0) then
                    inconsistent_mother = JMOHEP(1,first_daughter) /= i_hep
                    if (inconsistent_mother) then
                        JMOHEP(1,first_daughter) = i_hep
                        do j = i_hep + 1, NHEP
                            if (JDAHEP(1,j) == first_daughter) then
                                JMOHEP(2,first_daughter) = j
                            end if
                        end do
                    end if
                end if
            end if
        end if
    end do
end subroutine fill_hepevt_block_from_pythia

```

<HEPEVT BLOCK>≡

```

integer, parameter :: NMXHEP = 4000
integer :: NEVHEP
integer :: NHEP
integer, dimension(NMXHEP) :: ISTHEP
integer, dimension(NMXHEP) :: IDHEP
integer, dimension(2, NMXHEP) :: JMOHEP
integer, dimension(2, NMXHEP) :: JDAHEP
double precision, dimension(5, NMXHEP) :: PHEP
double precision, dimension(4, NMXHEP) :: VHEP
common /HEPEVT/ &
    NEVHEP, NHEP, ISTHEP, IDHEP, &
    JMOHEP, JDAHEP, PHEP, VHEP
save /HEPEVT/

```

Use HEPEVT for parent-child informations

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine set_parent_child_relations_from_hepevt ()
    integer, allocatable, dimension(:) :: parents

```

```

<HEPEVT BLOCK>
integer :: parent2, parent1, npar
integer :: jsearch
if (debug_on) call msg_debug (D_SHOWER, &
    "set_parent_child_relations_from_hepevt")
if (debug_active (D_SHOWER)) then
    print *, 'NHEP, n, py_entries:', NHEP, n, py_entries
    call pylist(5)
end if
do i_whz = 1, py_entries
    parent1 = JMOHEP(1,py_index(i_whz))

    if (IDHEP(py_index(i_whz)) == 94) then
        firstmother: do jsearch = parent1-1, 1, -1
            if (JDAHEP(1,jsearch) /= py_index(i_whz)) then
                exit firstmother
            end if
            parent1 = jsearch
        end do firstmother
    end if

    parent2 = parent1
    if (JMOHEP(2,py_index(i_whz)) > 0) then
        parent2 = JMOHEP(2,py_index(i_whz))
    end if
    if (IDHEP(py_index(i_whz)) == 94) then
        lastmother: do jsearch = parent1+1, py_index(i_whz)
            if (JDAHEP(1,jsearch) /= py_index(i_whz)) then
                exit lastmother
            end if
            parent2 = jsearch
        end do lastmother
    end if

    allocate (parents(parent2-parent1+1))
    parents = 0
    child = n_tot_old + i_whz
    npar = 0
    do parent = parent1, parent2
        if (parent > 0) then
            if (parent <= 2) then
                call particle_set%parent_add_child (parent, child)
            else
                if (whz_index(parent) > 0) then
                    npar = npar + 1
                    parents(npar) = whz_index(parent)
                    call particle_set%prt(whz_index(parent))%add_child (child)
                end if
            end if
        end if
    end do
    parents = pack (parents, parents > 0)
    if (npar > 0) call particle_set%prt(child)%set_parents (parents)
    if (allocated (parents)) deallocate (parents)

```

```

end do
NHEP = 0
end subroutine set_parent_child_relations_from_hepevt

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine fix_nonemitting_outgoings ()
integer, dimension(1) :: child
integer, parameter :: cmshower = 94
do i = 1, size (particle_set%prt)
  associate (p => particle_set%prt(i))
    if (p%get_n_children () == 1) then
      child = p%get_children ()
      if (particle_set%prt(child(1))%get_pdg () == cmshower) then
        j = particle_set%reverse_find_particle (p%get_pdg (), p%p)
        if (j == i) then
          deallocate (p%child)
          p%status = PRT_OUTGOING
        end if
      end if
    end if
  end associate
end do
end subroutine fix_nonemitting_outgoings

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine set_parent_child_relations_from_K ()
do j = 1, py_entries
  parent = K(py_index(j),3)
  child = n_tot_old + j
  if (parent > 0) then
    if (parent >= 1 .and. parent <= 2) then
      call particle_set%parent_add_child (parent, child)
    else
      real_parent = whz_index (parent)
      if (real_parent > 0 .and. real_parent /= child) then
        call particle_set%parent_add_child (real_parent, child)
      end if
    end if
  end if
end do
end subroutine set_parent_child_relations_from_K

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine set_parent_child_relations_of_color_strings_to_hadrons ()
integer :: begin_string, end_string, old_start, next_start, real_child
integer, allocatable, dimension(:) :: parents
if (debug_on) call msg_debug (D_SHOWER, "set_parent_child_relations_of_color_strings_to_hadron
if (debug_on) call msg_debug (D_SHOWER, "hadro_start", hadro_start)
if (hadro_start > 0) then
  old_start = hadro_start
  do
    next_start = 0
    FIND: do i = old_start + 1, N

```

```

        if (K(i,2) >= 91 .and. K(i,2) <= 94) then
            next_start = i
            exit FIND
        end if
    end do FIND
    begin_string = K(old_start,3)
    end_string = N
    do i = begin_string, N
        if (K(i,1) == 11) then
            end_string = i
            exit
        end if
    end do
    allocate (parents (end_string - begin_string + 1))
    parents = 0
    real_child = whz_index (old_start)
    do i = begin_string, end_string
        real_parent = whz_index (i)
        if (real_parent > 0) then
            call particle_set%prt(real_parent)%add_child (real_child)
            parents (i - begin_string + 1) = real_parent
        end if
    end do
    call particle_set%prt(real_child)%set_parents (parents)
    deallocate (parents)
    if (next_start == 0) exit
    old_start = next_start
end do
end if
end subroutine set_parent_child_relations_of_color_strings_to_hadrons

```

We allow to be more_fuzzy when finding particles for parent child relations than when deciding whether we add particles or not.

(Shower pythia6: combine with particle set: procedures)+=

```

function find_pythia_particle (i_py, more_fuzzy) result (j)
    integer :: j
    integer, intent(in) :: i_py
    logical, intent(in) :: more_fuzzy
    real(default) :: rel_small
    pdg = K(i_py,2)
    momentum = real([P(i_py,4), P(i_py,1:3)], kind=default)
    if (more_fuzzy) then
        rel_small = 1E-6_default
    else
        rel_small = 1E-10_default
    end if
    j = particle_set%reverse_find_particle (pdg, momentum, &
        abs_smallness = py_tiny, &
        rel_smallness = rel_small)
end function find_pythia_particle

```

Outgoing partons after hadronization shouldn't happen and is a dirty fix to missing mother daughter relation. I suspect that it has to do with the ordering

of the color string but am not sure.

(Shower pythia6: combine with particle set: procedures)+≡

```
subroutine fudge_whizard_partons_in_hadro ()
  do i = 1, size (particle_set%prt)
    if (particle_set%prt(i)%status == PRT_OUTGOING .and. &
        (particle_set%prt(i)%flv%get_pdg () == GLUON .or. &
         particle_set%prt(i)%flv%get_pdg_abs () < 6) .or. &
         particle_set%prt(i)%status == PRT_BEAM_REMNANT) then
      particle_set%prt(i)%status = PRT_VIRTUAL
    end if
  end do
end subroutine fudge_whizard_partons_in_hadro
```

(Shower pythia6: shower pythia6: TBP)+≡

```
procedure :: get_final_colored_ME_momenta => &
  shower_pythia6_get_final_colored_ME_momenta
```

(Shower pythia6: sub interfaces)+≡

```
module subroutine shower_pythia6_get_final_colored_ME_momenta &
  (shower, momenta)
  class(shower_pythia6_t), intent(in) :: shower
  type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
end subroutine shower_pythia6_get_final_colored_ME_momenta
```

(Shower pythia6: procedures)+≡

```
module subroutine shower_pythia6_get_final_colored_ME_momenta &
  (shower, momenta)
  class(shower_pythia6_t), intent(in) :: shower
  type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
  (PYJETS COMMON BLOCK)
  integer :: i, j, n_jets
  if (signal_is_pending ()) return
```

```
  i = 7 !!! final ME partons start in 7th row of event record
  n_jets = 0
  do
    if (K(I,1) /= 21) exit
    if ((K(I,2) == 21) .or. (abs(K(I,2)) <= 6)) then
      n_jets = n_jets + 1
    end if
    i = i + 1
  end do
  if (n_jets == 0) return
  allocate (momenta(1:n_jets))
  i = 7
  j = 1
  do
    if (K(I,1) /= 21) exit
    if ((K(I,2) == 21) .or. (abs(K(I,2)) <= 6)) then
      momenta(j) = real ([P(i,4), P(i,1:3)], kind=default)
      j = j + 1
    end if
    i = i + 1
  end do
end subroutine shower_pythia6_get_final_colored_ME_momenta
```

```

<Shower pythia6: public>+≡
    public :: pythia6_setup_lhe_io_units

<Shower pythia6: sub interfaces>+≡
    module subroutine pythia6_setup_lhe_io_units (u_W2P, u_P2W)
        integer, intent(out) :: u_W2P
        integer, intent(out), optional :: u_P2W
    end subroutine pythia6_setup_lhe_io_units

<Shower pythia6: procedures>+≡
    module subroutine pythia6_setup_lhe_io_units (u_W2P, u_P2W)
        integer, intent(out) :: u_W2P
        integer, intent(out), optional :: u_P2W
        character(len=10) :: buffer
        u_W2P = free_unit ()
        if (debug_active (D_SHOWER)) then
            open (unit=u_W2P, status="replace", file="whizardout.lhe", &
                action="readwrite")
        else
            open (unit=u_W2P, status="scratch", action="readwrite")
        end if
        write (buffer, "(I10)") u_W2P
        call pygive ("MSTP(161)=" // buffer)  !!! Unit for PYUPIN (LHA)
        call pygive ("MSTP(162)=" // buffer)  !!! Unit for PYUPEV (LHA)
        if (present (u_P2W)) then
            u_P2W = free_unit ()
            write (buffer, "(I10)") u_P2W
            call pygive ("MSTP(163)=" // buffer)
            if (debug_active (D_SHOWER)) then
                open (unit=u_P2W, file="pythiaout2.lhe", status="replace", &
                    action="readwrite")
            else
                open (unit=u_P2W, status="scratch", action="readwrite")
            end if
        end if
    end subroutine pythia6_setup_lhe_io_units

<Shower pythia6: public>+≡
    public :: pythia6_set_config

<Shower pythia6: sub interfaces>+≡
    module subroutine pythia6_set_config (pygive_all)
        type(string_t), intent(in) :: pygive_all
    end subroutine pythia6_set_config

<Shower pythia6: procedures>+≡
    module subroutine pythia6_set_config (pygive_all)
        type(string_t), intent(in) :: pygive_all
        type(string_t) :: pygive_remaining, pygive_partial
        if (len (pygive_all) > 0) then
            pygive_remaining = pygive_all
            do while (len (pygive_remaining) > 0)
                call split (pygive_remaining, pygive_partial, ";")
                call pygive (char (pygive_partial))
            end do
        end if
    end subroutine pythia6_set_config

```

```

        end do
        if (pythia6_get_error() /= 0) then
            call msg_fatal &
                (" PYTHIA6 did not recognize ps_PYTHIA_PYGIVE setting.")
        end if
    end if
end subroutine pythia6_set_config

```

Exchanging error messages with PYTHIA6.

```

<Shower pythia6: public>+≡
    public :: pythia6_set_error

<Shower pythia6: sub interfaces>+≡
    module subroutine pythia6_set_error (mstu23)
        integer, intent(in) :: mstu23
    end subroutine pythia6_set_error

<Shower pythia6: procedures>+≡
    module subroutine pythia6_set_error (mstu23)
        IMPLICIT DOUBLE PRECISION(A-H, O-Z)
        IMPLICIT INTEGER(I-N)
        COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
        SAVE/PYDAT1/
        integer, intent(in) :: mstu23
        MSTU(23) = mstu23
    end subroutine pythia6_set_error

<Shower pythia6: public>+≡
    public :: pythia6_get_error

<Shower pythia6: sub interfaces>+≡
    module function pythia6_get_error () result (mstu23)
        integer :: mstu23
    end function pythia6_get_error

<Shower pythia6: procedures>+≡
    module function pythia6_get_error () result (mstu23)
        IMPLICIT DOUBLE PRECISION(A-H, O-Z)
        IMPLICIT INTEGER(I-N)
        COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
        SAVE/PYDAT1/
        integer :: mstu23
        mstu23 = MSTU(23)
    end function pythia6_get_error

<Shower pythia6: public>+≡
    public :: pythia6_tauola_active

<Shower pythia6: sub interfaces>+≡
    module function pythia6_tauola_active () result (active)
        logical :: active
    end function pythia6_tauola_active

```

```

<Shower pythia6: procedures>+≡
  module function pythia6_tauola_active () result (active)
    IMPLICIT DOUBLE PRECISION(A-H, O-Z)
    IMPLICIT INTEGER(I-N)
    COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
    SAVE/PYDAT1/
    logical :: active
    active = MSTJ(28) == 2
  end function pythia6_tauola_active

<Shower pythia6: public>+≡
  public :: pythia6_handle_errors

<Shower pythia6: sub interfaces>+≡
  module function pythia6_handle_errors () result (valid)
    logical :: valid
  end function pythia6_handle_errors

<Shower pythia6: procedures>+≡
  module function pythia6_handle_errors () result (valid)
    logical :: valid
    valid = pythia6_get_error () == 0
    if (.not. valid) then
      call pythia6_set_error (0)
    end if
  end function pythia6_handle_errors

<Shower pythia6: public>+≡
  public :: pythia6_set_verbose

<Shower pythia6: sub interfaces>+≡
  module subroutine pythia6_set_verbose (verbose)
    logical, intent(in) :: verbose
  end subroutine pythia6_set_verbose

<Shower pythia6: procedures>+≡
  module subroutine pythia6_set_verbose (verbose)
    logical, intent(in) :: verbose
    if (verbose) then
      call pygive ('MSTU(13)=1')
    else
      call pygive ('MSTU(12)=12345') !!! No title page is written
      call pygive ('MSTU(13)=0')      !!! No information is written
    end if
  end subroutine pythia6_set_verbose

<Shower pythia6: public>+≡
  public :: pythia6_set_last_treated_line

<Shower pythia6: sub interfaces>+≡
  module subroutine pythia6_set_last_treated_line (last_line)
    integer,intent(in) :: last_line
  end subroutine pythia6_set_last_treated_line

```

```

<Shower pythia6: procedures>+=
  module subroutine pythia6_set_last_treated_line (last_line)
    integer,intent(in) :: last_line
    N_old = last_line
  end subroutine pythia6_set_last_treated_line

(pythia6_up.f)=
  C...UPINIT
  C...Is supposed to fill the HEPRUP commonblock with info
  C...on incoming beams and allowed processes.

      SUBROUTINE UPINIT

  C...Double precision and integer declarations.
      IMPLICIT DOUBLE PRECISION(A-H, O-Z)
      IMPLICIT INTEGER(I-N)

  C...PYTHIA commonblock: only used to provide read unit MSTP(161).
      COMMON/PYPARS/MSTP(200),PARP(200),MSTI(200),PARI(200)
      SAVE /PYPARS/

  C...User process initialization commonblock.
      INTEGER MAXPUP
      PARAMETER (MAXPUP=100)
      INTEGER IDBMUP,PDFGUP,PDFSUP,IDWTUP,NPRUP,LPRUP
      DOUBLE PRECISION EBMUP,XSECUP,XERRUP,XMAXUP
      COMMON/HEPRUP/IDBMUP(2),EBMUP(2),PDFGUP(2),PDFSUP(2),
      &IDWTUP,NPRUP,XSECUP(MAXPUP),XERRUP(MAXPUP),XMAXUP(MAXPUP),
      &LPRUP(MAXPUP)
      SAVE /HEPRUP/

  C...Lines to read in assumed never longer than 200 characters.
      PARAMETER (MAXLEN=200)
      CHARACTER*(MAXLEN) STRING

  C...Format for reading lines.
      CHARACTER(len=6) STRFMT
      STRFMT='(A000)'
      WRITE(STRFMT(3:5),'(I3)') MAXLEN

  C...Loop until finds line beginning with "<init>" or "<init ".
      100 READ(MSTP(161),STRFMT,END=130,ERR=130) STRING
      IBEG=0
      110 IBEG=IBEG+1
  C...Allow indentation.
      IF(STRING(IBEG:IBEG).EQ.' '.AND.IBEG.LT.MAXLEN-5) GOTO 110
      IF(STRING(IBEG:IBEG+5).NE.'<init>'.AND.
      &STRING(IBEG:IBEG+5).NE.'<init ') GOTO 100

  C...Read first line of initialization info.
      READ(MSTP(161),*,END=130,ERR=130) IDBMUP(1),IDBMUP(2),EBMUP(1),
      &EBMUP(2),PDFGUP(1),PDFGUP(2),PDFSUP(1),PDFSUP(2),IDWTUP,NPRUP

  C...Read NPRUP subsequent lines with information on each process.

```

```

      DO 120 IPR=1,NPRUP
        READ(MSTP(161),*,END=130,ERR=130) XSECUP(IPR),XERRUP(IPR),
      & XMAXUP(IPR),LPRUP(IPR)
120 CONTINUE
      RETURN

C...Error exit: give up if initalization does not work.
130 WRITE(*,*) ' Failed to read LHEF initialization information.'
      WRITE(*,*) ' Event generation will be stopped.'
      CALL PYSTOP(12)

      RETURN
      END

<pythia6_up.f>+≡
C...UPEVNT
C...Dummy routine, to be replaced by a user implementing external
C...processes. Depending on cross section model chosen, it either has
C...to generate a process of the type IDPRUP requested, or pick a type
C...itself and generate this event. The event is to be stored in the
C...HEPEUP commonblock, including (often) an event weight.

C...New example: handles a standard Les Houches Events File.

      SUBROUTINE UPEVNT

C...Double precision and integer declarations.
      IMPLICIT DOUBLE PRECISION(A-H, O-Z)
      IMPLICIT INTEGER(I-N)

C...PYTHIA commonblock: only used to provide read unit MSTP(162).
      COMMON/PYPARS/MSTP(200),PARP(200),MSTI(200),PARI(200)
      SAVE /PYPARS/

C...Added by WHIZARD
      COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
      SAVE/PYDAT1/

C...User process event common block.
      INTEGER MAXNUP
      PARAMETER (MAXNUP=500)
      INTEGER NUP,IDPRUP,IDUP,ISTUP,MOTHUP,ICOLUP
      DOUBLE PRECISION XWGTUP,SCALUP,AQEDUP,AQCDUP,PUP,VTIMUP,SPINUP
      COMMON/HEPEUP/NUP,IDPRUP,XWGTUP,SCALUP,AQEDUP,AQCDUP,IDUP(MAXNUP),
      &ISTUP(MAXNUP),MOTHUP(2,MAXNUP),ICOLUP(2,MAXNUP),PUP(5,MAXNUP),
      &VTIMUP(MAXNUP),SPINUP(MAXNUP)
      SAVE /HEPEUP/

C...Lines to read in assumed never longer than 200 characters.
      PARAMETER (MAXLEN=200)
      CHARACTER*(MAXLEN) STRING

C...Format for reading lines.
      CHARACTER(len=6) STRFMT

```

```

        STRFMT='(A000)'
        WRITE(STRFMT(3:5),'(I3)') MAXLEN

C...Loop until finds line beginning with "<event>" or "<event ".
    100 READ(MSTP(162),STRFMT,END=130,ERR=130) STRING
        IBEG=0
    110 IBEG=IBEG+1
C...Allow indentation.
        IF(STRING(IBEG:IBEG).EQ.' '.AND.IBEG.LT.MAXLEN-6) GOTO 110
        IF(STRING(IBEG:IBEG+6).NE.'<event>'.AND.
&STRING(IBEG:IBEG+6).NE.'<event ') GOTO 100

C...Read first line of event info.
        READ(MSTP(162),*,END=130,ERR=130) NUP,IDPRUP,XWGTUP,SCALUP,
&AQEDUP,AQCDUP

C...Read NUP subsequent lines with information on each particle.
    DO 120 I=1,NUP
        READ(MSTP(162),*,END=130,ERR=130) IDUP(I),ISTUP(I),
& MOTHUP(1,I),MOTHUP(2,I),ICOLUP(1,I),ICOLUP(2,I),
& (PUP(J,I),J=1,5),VTIMUP(I),SPINUP(I)
    120 CONTINUE
        RETURN

C...Error exit, typically when no more events.
    130 CONTINUE
C    WRITE(*,*) ' Failed to read LHEF event information.'
C    WRITE(*,*) ' Will assume end of file has been reached.'
        NUP=0
        MSTI(51)=1
C...Added by WHIZARD, mark these failed events
        MSTU(23)=1

        RETURN
    END

(pythia6_up.f)+≡
C...UPVETO
C...Dummy routine, to be replaced by user, to veto event generation
C...on the parton level, after parton showers but before multiple
C...interactions, beam remnants and hadronization is added.
C...If resonances like W, Z, top, Higgs and SUSY particles are handed
C...undecayed from UPEVNT, or are generated by PYTHIA, they will also
C...be undecayed at this stage; if decayed their decay products will
C...have been allowed to shower.

C...All partons at the end of the shower phase are stored in the
C...HEPEVT commonblock. The interesting information is
C...NHEP = the number of such partons, in entries 1 <= i <= NHEP,
C...IDHEP(I) = the particle ID code according to PDG conventions,
C...PHEP(J,I) = the (p_x, p_y, p_z, E, m) of the particle.
C...All ISTHEP entries are 1, while the rest is zeroed.

C...The user decision is to be conveyed by the IVETO value.

```

```

C...IVETO = 0 : retain current event and generate in full;
C...      = 1 : abort generation of current event and move to next.

      SUBROUTINE UPVETO(IVETO)

C...HEPEVT commonblock.
      PARAMETER (NMXHEP=4000)
      COMMON/HEPEVT/NEVHEP,NHEP,ISTHEP(NMXHEP),IDHEP(NMXHEP),
&JMOHEP(2,NMXHEP),JDAHEP(2,NMXHEP),PHEP(5,NMXHEP),VHEP(4,NMXHEP)
      DOUBLE PRECISION PHEP,VHEP
      SAVE /HEPEVT/

C...Next few lines allow you to see what info PYVETO extracted from
C...the full event record for the first two events.
C...Delete if you don't want it.
      DATA NLIST/0/
      SAVE NLIST
      IF(NLIST.LE.2) THEN
        WRITE(*,*) ' Full event record at time of UPVETO call:'
        CALL PYLIST(1)
        WRITE(*,*) ' Part of event record made available to UPVETO:'
        CALL PYLIST(5)
        NLIST=NLIST+1
      ENDIF

C...Make decision here.
      IVETO = 0

      RETURN
      END

<ktclus.f90>≡
<File header>

module ktclus

<Use kinds>

<KTCLUS: public>

contains

<KTCLUS: procedures>

end module ktclus
<KTCLUS: procedures>≡
!C-----
!C-----
!C-----
!C      KTCLUS: written by Mike Seymour, July 1992.
!C      Last modified November 2000.
!C      Please send comments or suggestions to Mike.Seymour@rl.ac.uk
!C

```



```

!C      This is a general-purpose kt clustering package.
!C      It can handle ee, ep and pp collisions.
!C      It is loosely based on the program of Siggi Bethke.
!C
!C      The time taken (on a 10MIP machine) is (0.2microsec)*N**3
!C      where N is the number of particles.
!C      Over 90 percent of this time is used in subroutine KTPMIN, which
!C      simply finds the minimum member of a one-dimensional array.
!C      It is well worth thinking about optimization: on the SPARCstation
!C      a factor of two increase was obtained simply by increasing the
!C      optimization level from its default value.
!C
!C      The approach is to separate the different stages of analysis.
!C      KTCLUS does all the clustering and records a merging history.
!C      It returns a simple list of the y values at which each merging
!C      occurred. Then the following routines can be called to give extra
!C      information on the most recently analysed event.
!C      KTCLUR is identical but includes an R parameter, see below.
!C      KTYCUT gives the number of jets at each given YCUT value.
!C      KTYSUB gives the number of sub-jets at each given YCUT value.
!C      KTBEAM gives same info as KTCLUS but only for merges with the beam
!C      KTJOIN gives same info as KTCLUS but for merges of sub-jets.
!C      KTRECO reconstructs the jet momenta at a given value of YCUT.
!C      It also gives information on which jets at scale YCUT belong to
!C      which macro-jets at scale YMAC, for studying sub-jet properties.
!C      KTIINCL reconstructs the jet momenta according to the inclusive jet
!C      definition of Ellis and Soper.
!C      KTISUB, KTIJOI and KTIREC are like KTYSUB, KTJOIN and KTRECO,
!C      except that they only apply to one inclusive jet at a time,
!C      with the pt of that jet automatically used for ECUT.
!C      KTWICH gives a list of which particles ended up in which jets.
!C      KTWCHS gives the same thing, but only for subjets.
!C      Note that the numbering of jets used by these two routines is
!C      guaranteed to be the same as that used by KTRECO.
!C
!C      The collision type and analysis type are indicated by the first
!C      argument of KTCLUS. IMODE=<TYPE><ANGLE><MONO><RECOM> where
!C      TYPE:  1=>ee, 2=>ep with p in -z direction, 3=>pe, 4=>pp
!C      ANGLE: 1=>angular kt def., 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C              where f() $=2(\cosh(\eta)-\cos(\phi))$  is the QCD emission metric
!C      MONO:  1=>derive relative pseudoparticle angles from jets
!C              2=>monotonic definitions of relative angles
!C      RECOM: 1=>E recombination scheme, 2=>pt scheme, 3=>pt**2 scheme
!C
!C      There are also abbreviated forms for the most common combinations:
!C      IMODE=1 => E scheme in e+e-                      (=1111)
!C              2 => E scheme in ep                      (=2111)
!C              3 => E scheme in pe                      (=3111)
!C              4 => E scheme in pp                      (=4111)
!C              5 => covariant E scheme in pp            (=4211)
!C              6 => covariant pt-scheme in pp           (=4212)
!C              7 => covariant monotonic pt**2-scheme in pp (=4223)
!C
!C      KTRECO no longer needs to reconstruct the momenta according to the

```

!C same recombination scheme in which they were clustered. Its first
!C argument gives the scheme, taking the same values as RECOM above.
!C

!C Note that unlike previous versions, all variables which hold y
!C values have been named in a consistent way:
!C Y() is the output scale at which jets were merged,
!C YCUT is the input scale at which jets should be counted, and
!C jet-momenta reconstructed etc,
!C YMAC is the input macro-jet scale, used in determining whether
!C or not each jet is a sub-jet.
!C The original scheme defined in our papers is equivalent to always
!C setting YMAC=1.
!C Whenever a YCUT or YMAC variable is used, it is rounded down
!C infinitesimally, so that for example, setting YCUT=Y(2) refers
!C to the scale where the event is 2-jet, even if rounding errors
!C have shifted its value slightly.
!C

!C An R parameter can be used in hadron-hadron collisions by
!C calling KTCLUR instead of KTCLUS. This is as suggested by
!C Ellis and Soper, but implemented slightly differently,
!C as in M.H. Seymour, LU TP 94/2 (submitted to Nucl. Phys. B.).
!C R**2 multiplies the single Kt everywhere it is used.
!C Calling KTCLUR with R=1 is identical to calling KTCLUS.
!C R plays a similar role to the jet radius in a cone-type algorithm,
!C but is scaled up by about 40% (ie R=0.7 in a cone algorithm is
!C similar to this algorithm with R=1).
!C Note that R.EQ.1 must be used for the e+e- and ep versions,
!C and is strongly recommended for the hadron-hadron version.
!C However, R values smaller than 1 have been found to be useful for
!C certain applications, particularly the mass reconstruction of
!C highly-boosted colour-singlets such as high-pt hadronic Ws,
!C as in M.H. Seymour, LU TP 93/8 (to appear in Z. Phys. C.).
!C Situations in which R<1 is useful are likely to also be those in
!C which the inclusive reconstruction method is more useful.
!C

!C Also included is a set of routines for doing Lorentz boosts:
!C KTLBST finds the boost matrix to/from the cm frame of a 4-vector
!C KTRROT finds the rotation matrix from one vector to another
!C KTMUL multiplies together two matrices
!C KTMUL multiplies a vector by a matrix
!C KTINVT inverts a transformation matrix (nb NOT a general 4 by 4)
!C KTFRAM boosts a list of vectors between two arbitrary frames
!C KTBREI boosts a list of vectors between the lab and Breit frames
!C KTHADR boosts a list of vectors between the lab and hadronic cmf
!C The last two need the momenta in the +z direction of the lepton
!C and hadron beams, and the 4-momentum of the outgoing lepton.
!C

!C The main reference is:
!C S. Catani, Yu.L. Dokshitzer, M.H. Seymour and B.R. Webber,
!C Nucl.Phys.B406(1993)187.
!C The ep version was proposed in:
!C S. Catani, Yu.L. Dokshitzer and B.R. Webber,
!C Phys.Lett.285B(1992)291.
!C The inclusive reconstruction method was proposed in:

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!C      S.D. Ellis and D.E. Soper,
!C      Phys.Rev.D48(1993)3160.
!C
!C-----
!C-----
!C-----

<KTCLUS: public>≡
  public :: ktclur

<KTCLUS: procedures>+≡
  SUBROUTINE KTCLUR(IMODE,PP,NN,R,ECUT,Y,*)
    use io_units
    IMPLICIT NONE
!C--DO CLUSTER ANALYSIS OF PARTICLES IN PP
!C
!C  IMODE  = INPUT   : DESCRIBED ABOVE
!C  PP(I,J) = INPUT   : 4-MOMENTUM OF Jth PARTICLE: I=1,4 => PX,PY,PZ,E
!C  NN     = INPUT   : NUMBER OF PARTICLES
!C  R      = INPUT   : ELLIS AND SOPER'S R PARAMETER, SEE ABOVE.
!C  ECUT   = INPUT   : DENOMINATOR OF KT MEASURE. IF ZERO, ETOT IS USED
!C  Y(J)   = OUTPUT  : VALUE OF Y FOR WHICH EVENT CHANGES FROM BEING
!C                      J JET TO J-1 JET
!C  LAST ARGUMENT IS LABEL TO JUMP TO IF FOR ANY REASON THE EVENT
!C  COULD NOT BE PROCESSED (MOST LIKELY DUE TO TOO MANY PARTICLES)
!C
!C  NOTE THAT THE MOMENTA ARE DECLARED DOUBLE PRECISION,
!C  AND ALL OTHER FLOATING POINT VARIABLES ARE DECLARED DOUBLE PRECISION
!C
  INTEGER NMAX,IM,IMODE,TYPE,ANGL,MONO,RECO,N,I,J,NN, &
    IMIN,JMIN,KMIN,NUM,HIST,INJET,IABBR,NABBR
  PARAMETER (NMAX=512,NABBR=7)
  DOUBLE PRECISION PP(4,*)
  integer :: u
!CHANGE  DOUBLE PRECISION R,ECUT,Y(*),P,KT,ETOT,RSQ,KTP,KTS,KTPAIR,KTSING, &
  DOUBLE PRECISION R,ECUT,Y(*),P,KT,ETOT,RSQ,KTP,KTS, &
    KTMIN,ETSQ,KTLAST,KTMAX,KTTMP
  LOGICAL FIRST
  CHARACTER TITLE(4,4)*10
!C--KT RECORDS THE KT**2 OF EACH MERGING.
!C--KTLAST RECORDS FOR EACH MERGING, THE HIGHEST ECUT**2 FOR WHICH THE
!C  RESULT IS NOT MERGED WITH THE BEAM (COULD BE LARGER THAN THE
!C  KT**2 AT WHICH IT WAS MERGED IF THE KT VALUES ARE NOT MONOTONIC).
!C  THIS MAY SOUND POINTLESS, BUT ITS USEFUL FOR DETERMINING WHETHER
!C  SUB-JETS SURVIVED TO SCALE Y=YMAC OR NOT.
!C--HIST RECORDS MERGING HISTORY:
!C  N=>DELETED TRACK N, M*NMAX+N=>MERGED TRACKS M AND N (M<N).
  COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
    KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM
  DIMENSION INJET(NMAX),IABBR(NABBR)
  DATA FIRST,TITLE,IABBR/.TRUE., &
    'e+e-      ', 'ep      ', 'pe      ', 'pp      ', &
    'angle     ', 'DeltaR   ', 'f(DeltaR)', '*****', &
    'no        ', 'yes      ', '*****', '*****', &
    'E         ', 'Pt      ', 'Pt**2    ', '*****', &

```

```

1111,2111,3111,4111,4211,4212,4223/
!C--CHECK INPUT
IM=IMODE
IF (IM.GE.1.AND.IM.LE.NABBR) IM=IABBR(IM)
TYPE=MOD(IM/1000,10)
ANGL=MOD(IM/100,10)
MONO=MOD(IM/10,10)
RECO=MOD(IM,10)
IF (NN.GT.NMAX) CALL KTWARN('KT-MAX',100,*999)
IF (NN.LT.1) CALL KTWARN('KT-LT1',100,*999)
IF (NN.LT.2.AND.TYPE.EQ.1) CALL KTWARN('KT-LT2',100,*999)
IF (TYPE.LT.1.OR.TYPE.GT.4.OR.ANGL.LT.1.OR.ANGL.GT.4.OR. &
    MONO.LT.1.OR.MONO.GT.2.OR.RECO.LT.1.OR.RECO.GT.3) CALL KTWARN('KTCLUS',101,*999)
u = given_output_unit ()
IF (FIRST) THEN
    WRITE (u,'(/,1X,54(''*)/A)') &
        ' KTCLUS: written by Mike Seymour, July 1992.'
    WRITE (u,'(A)') &
        ' Last modified November 2000.'
    WRITE (u,'(A)') &
        ' Please send comments or suggestions to Mike.Seymour@rl.ac.uk'
    WRITE (u,'(/A,I2,2A)') &
        ' Collision type =',TYPE,' = ',TITLE(TYPE,1)
    WRITE (u,'(A,I2,2A)') &
        ' Angular variable =',ANGL,' = ',TITLE(ANGL,2)
    WRITE (u,'(A,I2,2A)') &
        ' Monotonic definition =',MONO,' = ',TITLE(MONO,3)
    WRITE (u,'(A,I2,2A)') &
        ' Recombination scheme =',RECO,' = ',TITLE(RECO,4)
    IF (R.NE.1) THEN
        WRITE (u,'(A,F5.2)') &
            ' Radius parameter =',R
        IF (TYPE.NE.4) WRITE (u,'(A)') &
            ' R.NE.1 is strongly discouraged for this collision type!'
    ENDIF
    WRITE (u,'(1X,54(''*)/A)')
    FIRST=.FALSE.
ENDIF
!C--COPY PP TO P
N=NN
NUM=NN
CALL KTCOPY(PP,N,P,(RECO.NE.1))
ETOT=0
DO I=1,N
    ETOT=ETOT+P(4,I)
END DO
IF (ETOT.EQ.0) CALL KTWARN('KTCLUS',102,*999)
IF (ECUT.EQ.0) THEN
    ETSQ=1/ETOT**2
ELSE
    ETSQ=1/ECUT**2
ENDIF
RSQ=R**2
!C--CALCULATE ALL PAIR KT's

```

```

DO I=1,N-1
  DO J=I+1,N
    KTP(J,I)=-1
    KTP(I,J)=KTPAIR(ANGL,P(1,I),P(1,J),KTP(J,I))
  END DO
END DO
!C--CALCULATE ALL SINGLE KT's
DO I=1,N
  KTS(I)=KTSING(ANGL,TYPE,P(1,I))
END DO
KTMAX=0
!C--MAIN LOOP
300 CONTINUE
!C--FIND MINIMUM MEMBER OF KTP
  CALL KTPMIN(KTP,NMAX,N,IMIN,JMIN)
!C--FIND MINIMUM MEMBER OF KTS
  CALL KTSMIN(KTS,NMAX,N,KMIN)
!C--STORE Y VALUE OF TRANSITION FROM N TO N-1 JETS
  KTMIN=KTP(IMIN,JMIN)
  KTTMP=RSQ*KTS(KMIN)
  IF ((TYPE.GE.2.AND.TYPE.LE.4).AND. &
      (KTTMP.LE.KTMIN.OR.N.EQ.1)) &
    KTMIN=KTTMP
  KT(N)=KTMIN
  Y(N)=KT(N)*ETSQ
!C--IF MONO.GT.1, SEQUENCE IS SUPPOSED TO BE MONOTONIC, IF NOT, WARN
  IF (KTMIN.LT.KTMAX.AND.MONO.GT.1) CALL KTWARN('KTCLUS',1,*999)
  IF (KTMIN.GE.KTMAX) KTMAX=KTMIN
!C--IF LOWEST KT IS TO A BEAM, THROW IT AWAY AND MOVE LAST ENTRY UP
  IF (KTMIN.EQ.KTTMP) THEN
    CALL KTMOVE(P,KTP,KTS,NMAX,N,KMIN,1)
!C--UPDATE HISTORY AND CROSS-REFERENCES
    HIST(N)=KMIN
    INJET(N)=KMIN
    DO I=N,NN
      IF (INJET(I).EQ.KMIN) THEN
        KTLAST(I)=KTMAX
        INJET(I)=0
      ELSEIF (INJET(I).EQ.N) THEN
        INJET(I)=KMIN
      ENDIF
    END DO
!C--OTHERWISE MERGE JETS IMIN AND JMIN AND MOVE LAST ENTRY UP
    ELSE
      CALL KTMERG(P,KTP,KTS,NMAX,IMIN,JMIN,N,TYPE,ANGL,MONO,RECO)
      CALL KTMOVE(P,KTP,KTS,NMAX,N,JMIN,1)
!C--UPDATE HISTORY AND CROSS-REFERENCES
      HIST(N)=IMIN*NMAX+JMIN
      INJET(N)=IMIN
      DO I=N,NN
        IF (INJET(I).EQ.JMIN) THEN
          INJET(I)=IMIN
        ELSEIF (INJET(I).EQ.N) THEN
          INJET(I)=JMIN
        ENDIF
      END DO
    END IF
  END IF

```

```

        ENDIF
      END DO
    ENDIF
!C--THATS ALL THERE IS TO IT
    N=N-1
    IF (N.GT.1 .OR. N.GT.0.AND.(TYPE.GE.2.AND.TYPE.LE.4)) GOTO 300
    IF (N.EQ.1) THEN
      KT(N)=1D20
      Y(N)=KT(N)*ETSQ
    ENDIF
    RETURN
999 RETURN 1
  END SUBROUTINE KTCLUR
!C-----
<KTCLUS: public>+=
  public :: ktreco
<KTCLUS: procedures>+=
!C-----
  SUBROUTINE KTRECO(RECO,PP,NN,ECUT,YCUT,YMAC,PJET,JET,NJET,NSUB,*)
    IMPLICIT NONE
!C--RECONSTRUCT KINEMATICS OF JET SYSTEM, WHICH HAS ALREADY BEEN
!C ANALYSED BY KTCLUS. NOTE THAT NO CONSISTENCY CHECK IS MADE: USER
!C IS TRUSTED TO USE THE SAME PP VALUES AS FOR KTCLUS
!C
!C RECO      = INPUT : RECOMBINATION SCHEME (NEED NOT BE SAME AS KTCLUS)
!C PP(I,J)   = INPUT : 4-MOMENTUM OF Jth PARTICLE: I=1,4 => PX,PY,PZ,E
!C NN        = INPUT : NUMBER OF PARTICLES
!C ECUT      = INPUT : DENOMINATOR OF KT MEASURE. IF ZERO, ETOT IS USED
!C YCUT      = INPUT : Y VALUE AT WHICH TO RECONSTRUCT JET MOMENTA
!C YMAC      = INPUT : Y VALUE USED TO DEFINE MACRO-JETS, TO DETERMINE
!C              WHICH JETS ARE SUB-JETS
!C PJET(I,J)=OUTPUT : 4-MOMENTUM OF Jth JET AT SCALE YCUT
!C JET(J)    =OUTPUT : THE MACRO-JET WHICH CONTAINS THE Jth JET,
!C              SET TO ZERO IF JET IS NOT A SUB-JET
!C NJET      =OUTPUT : THE NUMBER OF JETS
!C NSUB      =OUTPUT : THE NUMBER OF SUB-JETS (EQUAL TO THE NUMBER OF
!C              NON-ZERO ENTRIES IN JET())
!C LAST ARGUMENT IS LABEL TO JUMP TO IF FOR ANY REASON THE EVENT
!C COULD NOT BE PROCESSED
!C
!C NOTE THAT THE MOMENTA ARE DECLARED DOUBLE PRECISION,
!C AND ALL OTHER FLOATING POINT VARIABLES ARE DECLARED DOUBLE PRECISION
!C
    INTEGER NMAX,RECO,NUM,N,NN,NJET,NSUB,JET(*),HIST,IMIN,JMIN,I,J
    PARAMETER (NMAX=512)
    DOUBLE PRECISION PP(4,*),PJET(4,*)
    DOUBLE PRECISION ECUT,P,KT,KTP,KTS,ETOT,RSQ,ETSQ,YCUT,YMAC,KTLAST, &
      ROUND
    PARAMETER (ROUND=0.99999D0)
    COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
      KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM
!C--CHECK INPUT
    IF (RECO.LT.1.OR.RECO.GT.3) THEN

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```

        PRINT *, 'RECO=', RECO
        CALL KTWARN('KTRECO', 100, *999)
    ENDIF
!C--COPY PP TO P
    N=NN
    IF (NUM.NE.NN) CALL KTWARN('KTRECO', 101, *999)
    CALL KTCOPY(PP, N, P, (RECO.NE.1))
    IF (ECUT.EQ.0) THEN
        ETSQ=1/ETOT**2
    ELSE
        ETSQ=1/ECUT**2
    ENDIF
!C--KEEP MERGING UNTIL YCUT
100  IF (ETSQ*KT(N).LT.ROUND*YCUT) THEN
        IF (HIST(N).LE.NMAX) THEN
            CALL KTMOVE(P, KTP, KTS, NMAX, N, HIST(N), 0)
        ELSE
            IMIN=HIST(N)/NMAX
            JMIN=HIST(N)-IMIN*NMAX
            CALL KTMERG(P, KTP, KTS, NMAX, IMIN, JMIN, N, 0, 0, 0, RECO)
            CALL KTMOVE(P, KTP, KTS, NMAX, N, JMIN, 0)
        ENDIF
        N=N-1
        IF (N.GT.0) GOTO 100
    ENDIF
!C--IF YCUT IS TOO LARGE THERE ARE NO JETS
    NJET=N
    NSUB=N
    IF (N.EQ.0) RETURN
!C--SET UP OUTPUT MOMENTA
    DO I=1, NJET
        IF (RECO.EQ.1) THEN
            DO J=1, 4
                PJET(J, I)=P(J, I)
            END DO
        ELSE
            PJET(1, I)=P(6, I)*COS(P(8, I))
            PJET(2, I)=P(6, I)*SIN(P(8, I))
            PJET(3, I)=P(6, I)*SINH(P(7, I))
            PJET(4, I)=P(6, I)*COSH(P(7, I))
        ENDIF
        JET(I)=I
    END DO
!C--KEEP MERGING UNTIL YMAC TO FIND THE FATE OF EACH JET
300  IF (ETSQ*KT(N).LT.ROUND*YMAC) THEN
        IF (HIST(N).LE.NMAX) THEN
            IMIN=0
            JMIN=HIST(N)
            NSUB=NSUB-1
        ELSE
            IMIN=HIST(N)/NMAX
            JMIN=HIST(N)-IMIN*NMAX
            IF (ETSQ*KTLAST(N).LT.ROUND*YMAC) NSUB=NSUB-1
        ENDIF
    ENDIF

```

```

      DO I=1,NJET
        IF (JET(I).EQ.JMIN) JET(I)=IMIN
        IF (JET(I).EQ.N) JET(I)=JMIN
      END DO
      N=N-1
      IF (N.GT.0) GOTO 300
    ENDIF
    RETURN
999  RETURN 1
  END SUBROUTINE KTRECO
!C-----
<KTCLUS: procedures>+≡
!C-----
      FUNCTION KTPAIR(ANGL,P,Q,ANGLE)
      IMPLICIT NONE
!C--CALCULATE LOCAL KT OF PAIR, USING ANGULAR SCHEME:
!C  1=>ANGULAR, 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C  WHERE f(eta,phi)=2(COSH(eta)-COS(phi)) IS THE QCD EMISSION METRIC
!C--IF ANGLE<0, IT IS SET TO THE ANGULAR PART OF THE LOCAL KT ON RETURN
!C  IF ANGLE>0, IT IS USED INSTEAD OF THE ANGULAR PART OF THE LOCAL KT
      INTEGER ANGL
!  CHANGE      DOUBLE PRECISION P(9),Q(9),KTPAIR,R,KTMDPI,ANGLE,ETA,PHI,ESQ
      DOUBLE PRECISION P(9),Q(9),KTPAIR,R,ANGLE,ETA,PHI,ESQ
!C--COMPONENTS OF MOMENTA ARE PX,PY,PZ,E,1/P,PT,ETA,PHI,PT**2
      R=ANGLE
      IF (ANGL.EQ.1) THEN
        IF (R.LE.0) R=2*(1-(P(1)*Q(1)+P(2)*Q(2)+P(3)*Q(3))*(P(5)*Q(5)))
        ESQ=MIN(P(4),Q(4))**2
      ELSEIF (ANGL.EQ.2.OR.ANGL.EQ.3) THEN
        IF (R.LE.0) THEN
          ETA=P(7)-Q(7)
          PHI=KTMDPI(P(8)-Q(8))
          IF (ANGL.EQ.2) THEN
            R=ETA**2+PHI**2
          ELSE
            R=2*(COSH(ETA)-COS(PHI))
          ENDIF
        ENDIF
        ESQ=MIN(P(9),Q(9))
      ELSEIF (ANGL.EQ.4) THEN
        ESQ=(1d0/(P(5)*Q(5))-P(1)*Q(1)-P(2)*Q(2)- &
          P(3)*Q(3))*2D0/(P(5)*Q(5))/(0.0001D0+1d0/P(5)+1d0/Q(5))**2
        R=1d0
      ELSE
        CALL KTWARN('KTPAIR',200,*999)
        STOP
      ENDIF
      KTPAIR=ESQ*R
      IF (ANGLE.LT.0) ANGLE=R
999  END FUNCTION KTPAIR
!C-----
      FUNCTION KTSING(ANGL,TYPE,P)
      IMPLICIT NONE
!C--CALCULATE KT OF PARTICLE, USING ANGULAR SCHEME:

```



```

!C 1=>ANGULAR, 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C--TYPE=1 FOR E+E-, 2 FOR EP, 3 FOR PE, 4 FOR PP
!C FOR EP, PROTON DIRECTION IS DEFINED AS -Z
!C FOR PE, PROTON DIRECTION IS DEFINED AS +Z
      INTEGER ANGL,TYPE
      DOUBLE PRECISION P(9),KTSING,COSTH,R,SMALL
      DATA SMALL/1D-4/
      IF (ANGL.EQ.1.OR.ANGL.EQ.4) THEN
        COSTH=P(3)*P(5)
        IF (TYPE.EQ.2) THEN
          COSTH=-COSTH
        ELSEIF (TYPE.EQ.4) THEN
          COSTH=ABS(COSTH)
        ELSEIF (TYPE.NE.1.AND.TYPE.NE.3) THEN
          CALL KTWARN('KTSING',200,*999)
          STOP
        ENDIF
        R=2*(1-COSTH)
!C--IF CLOSE TO BEAM, USE APPROX 2*(1-COS(THETA))=SIN**2(THETA)
        IF (R.LT.SMALL) R=(P(1)**2+P(2)**2)*P(5)**2
        KTSING=P(4)**2*R
      ELSEIF (ANGL.EQ.2.OR.ANGL.EQ.3) THEN
        KTSING=P(9)
      ELSE
        CALL KTWARN('KTSING',201,*999)
        STOP
      ENDIF
999 END FUNCTION KTSING
!C-----
      SUBROUTINE KTPMIN(A,NMAX,N,IMIN,JMIN)
      IMPLICIT NONE
!C--FIND THE MINIMUM MEMBER OF A(NMAX,NMAX) WITH IMIN < JMIN <= N
      INTEGER NMAX,N,IMIN,JMIN,KMIN,I,J,K
!C--REMEMBER THAT A(X+(Y-1)*NMAX)=A(X,Y)
!C THESE LOOPING VARIABLES ARE J=Y-2, I=X+(Y-1)*NMAX
      DOUBLE PRECISION A(*),AMIN
      K=1+NMAX
      KMIN=K
      AMIN=A(KMIN)
      DO J=0,N-2
        DO I=K,K+J
          IF (A(I).LT.AMIN) THEN
            KMIN=I
            AMIN=A(KMIN)
          ENDIF
        END DO
        K=K+NMAX
      END DO
      JMIN=KMIN/NMAX+1
      IMIN=KMIN-(JMIN-1)*NMAX
      END SUBROUTINE KTPMIN
!C-----
      SUBROUTINE KTSMIN(A,NMAX,N,IMIN)
      IMPLICIT NONE

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```

!C--FIND THE MINIMUM MEMBER OF A
      INTEGER N,NMAX,IMIN,I
      DOUBLE PRECISION A(NMAX)
      IMIN=1
      DO I=1,N
        IF (A(I).LT.A(IMIN)) IMIN=I
      END DO
      END SUBROUTINE KTSMIN
!C-----
      SUBROUTINE KTCOPY(A,N,B,ONSHLL)
        IMPLICIT NONE
!C--COPY FROM A TO B. 5TH=1/(3-MTM), 6TH=PT, 7TH=ETA, 8TH=PHI, 9TH=PT**2
!C IF ONSHLL IS .TRUE. PARTICLE ENTRIES ARE PUT ON-SHELL BY SETTING E=P
        INTEGER I,N
        DOUBLE PRECISION A(4,N)
        LOGICAL ONSHLL
        DOUBLE PRECISION B(9,N),ETAMAX,SINMIN,EPS
        DATA ETAMAX,SINMIN,EPS/10,0,1D-6/
!C--SINMIN GETS CALCULATED ON FIRST CALL
        IF (SINMIN.EQ.0) SINMIN=1/COSH(ETAMAX)
        DO I=1,N
          B(1,I)=A(1,I)
          B(2,I)=A(2,I)
          B(3,I)=A(3,I)
          B(4,I)=A(4,I)
          B(5,I)=SQRT(A(1,I)**2+A(2,I)**2+A(3,I)**2)
          IF (ONSHLL) B(4,I)=B(5,I)
          IF (B(5,I).EQ.0) B(5,I)=1D-10
          B(5,I)=1/B(5,I)
          B(9,I)=A(1,I)**2+A(2,I)**2
          B(6,I)=SQRT(B(9,I))
          B(7,I)=B(6,I)*B(5,I)
          IF (B(7,I).GT.SINMIN) THEN
            B(7,I)=A(4,I)**2-A(3,I)**2
            IF (B(7,I).LE.EPS*B(4,I)**2.OR. ONSHLL) B(7,I)=B(9,I)
            B(7,I)=LOG((B(4,I)+ABS(B(3,I)))**2/B(7,I))/2
          ELSE
            B(7,I)=ETAMAX+2
          ENDIF
          B(7,I)=SIGN(B(7,I),B(3,I))
          IF (A(1,I).EQ.0 .AND. A(2,I).EQ.0) THEN
            B(8,I)=0
          ELSE
            B(8,I)=ATAN2(A(2,I),A(1,I))
          ENDIF
        END DO
      END SUBROUTINE KTCOPY
!C-----
      SUBROUTINE KTMERG(P,KTP,KTS,NMAX,I,J,N,TYPE,ANGL,MONO,RECO)
        IMPLICIT NONE
!C--MERGE THE Jth PARTICLE IN P INTO THE Ith PARTICLE
!C J IS ASSUMED GREATER THAN I. P CONTAINS N PARTICLES BEFORE MERGING.
!C--ALSO RECALCULATING THE CORRESPONDING KTP AND KTS VALUES IF MONO.GT.0
!C FROM THE RECOMBINED ANGULAR MEASURES IF MONO.GT.1

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!C--NOTE THAT IF MONO.LE.0, TYPE AND ANGL ARE NOT USED
      INTEGER ANGL,RECO,TYPE,I,J,K,N,NMAX,MONO
      DOUBLE PRECISION P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX),PT,PTT, &
! CHANGE      KTMDPI,KTUP,PI,PJ,ANG,KTPAIR,KTSING,ETAMAX,EPS
      KTUP,PI,PJ,ANG,ETAMAX,EPS
      KTUP(I,J)=KTP(MAX(I,J),MIN(I,J))
      DATA ETAMAX,EPS/10,1D-6/
      IF (J.LE.I) CALL KTWARN('KTMERG',200,*999)
!C--COMBINE ANGULAR MEASURES IF NECESSARY
      IF (MONO.GT.1) THEN
        DO K=1,N
          IF (K.NE.I.AND.K.NE.J) THEN
            IF (RECO.EQ.1) THEN
              PI=P(4,I)
              PJ=P(4,J)
            ELSEIF (RECO.EQ.2) THEN
              PI=P(6,I)
              PJ=P(6,J)
            ELSEIF (RECO.EQ.3) THEN
              PI=P(9,I)
              PJ=P(9,J)
            ELSE
              CALL KTWARN('KTMERG',201,*999)
              STOP
            ENDIF
            IF (PI.EQ.0.AND.PJ.EQ.0) THEN
              PI=1
              PJ=1
            ENDIF
            KTP(MAX(I,K),MIN(I,K))= &
              (PI*KTUP(I,K)+PJ*KTUP(J,K))/(PI+PJ)
          ENDIF
        END DO
      ENDIF
      IF (RECO.EQ.1) THEN
!C--VECTOR ADDITION
        P(1,I)=P(1,I)+P(1,J)
        P(2,I)=P(2,I)+P(2,J)
        P(3,I)=P(3,I)+P(3,J)
!c        P(4,I)=P(4,I)+P(4,J) ! JA
        P(5,I)=SQRT(P(1,I)**2+P(2,I)**2+P(3,I)**2)
        P(4,I)=P(5,I) ! JA (Massless scheme)
        IF (P(5,I).EQ.0) THEN
          P(5,I)=1
        ELSE
          P(5,I)=1/P(5,I)
        ENDIF
      ELSEIF (RECO.EQ.2) THEN
!C--PT WEIGHTED ETA-PHI ADDITION
        PT=P(6,I)+P(6,J)
        IF (PT.EQ.0) THEN
          PTT=1
        ELSE
          PTT=1/PT

```

```

ENDIF
P(7,I)=(P(6,I)*P(7,I)+P(6,J)*P(7,J))*PTT
P(8,I)=KTMDPI(P(8,I)+P(6,J)*PTT*KTMDPI(P(8,J)-P(8,I)))
P(6,I)=PT
P(9,I)=PT**2
ELSEIF (RECO.EQ.3) THEN
!C--PT**2 WEIGHTED ETA-PHI ADDITION
PT=P(9,I)+P(9,J)
IF (PT.EQ.0) THEN
PTT=1
ELSE
PTT=1/PT
ENDIF
P(7,I)=(P(9,I)*P(7,I)+P(9,J)*P(7,J))*PTT
P(8,I)=KTMDPI(P(8,I)+P(9,J)*PTT*KTMDPI(P(8,J)-P(8,I)))
P(6,I)=P(6,I)+P(6,J)
P(9,I)=P(6,I)**2
ELSE
CALL KTWARN('KTMERG',202,*999)
STOP
ENDIF
!C--IF MONO.GT.0 CALCULATE NEW KT MEASURES. IF MONO.GT.1 USE ANGULAR ONES.
IF (MONO.LE.0) RETURN
!C--CONVERTING BETWEEN 4-MTM AND PT,ETA,PHI IF NECESSARY
IF (ANGL.NE.1.AND.RECO.EQ.1) THEN
P(9,I)=P(1,I)**2+P(2,I)**2
P(7,I)=P(4,I)**2-P(3,I)**2
IF (P(7,I).LE.EPS*P(4,I)**2) P(7,I)=P(9,I)
IF (P(7,I).GT.0) THEN
P(7,I)=LOG((P(4,I)+ABS(P(3,I)))*2/P(7,I))/2
IF (P(7,I).GT.ETAMAX) P(7,I)=ETAMAX+2
ELSE
P(7,I)=ETAMAX+2
ENDIF
P(7,I)=SIGN(P(7,I),P(3,I))
IF (P(1,I).NE.0.AND.P(2,I).NE.0) THEN
P(8,I)=ATAN2(P(2,I),P(1,I))
ELSE
P(8,I)=0
ENDIF
ELSEIF (ANGL.EQ.1.AND.RECO.NE.1) THEN
P(1,I)=P(6,I)*COS(P(8,I))
P(2,I)=P(6,I)*SIN(P(8,I))
P(3,I)=P(6,I)*SINH(P(7,I))
P(4,I)=P(6,I)*COSH(P(7,I))
IF (P(4,I).NE.0) THEN
P(5,I)=1/P(4,I)
ELSE
P(5,I)=1
ENDIF
ENDIF
ANG=0
DO K=1,N
IF (K.NE.I.AND.K.NE.J) THEN

```

```

        IF (MONO.GT.1) ANG=KTUP(I,K)
        KTP(MIN(I,K),MAX(I,K))= &
            KTPAIR(ANGL,P(1,I),P(1,K),ANG)
    ENDIF
END DO
KTS(I)=KTSING(ANGL,TYPE,P(1,I))
999 END SUBROUTINE KTMERG
!C-----
    SUBROUTINE KTMOVE(P,KTP,KTS,NMAX,N,J,IOPT)
    IMPLICIT NONE
!C--MOVE THE Nth PARTICLE IN P TO THE Jth POSITION
!C--ALSO MOVING KTP AND KTS IF IOPT.GT.0
    INTEGER I,J,N,NMAX,IOPT
    DOUBLE PRECISION P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX)
    DO I=1,9
        P(I,J)=P(I,N)
    END DO
    IF (IOPT.LE.0) RETURN
    DO I=1,J-1
        KTP(I,J)=KTP(I,N)
        KTP(J,I)=KTP(N,I)
    END DO
    DO I=J+1,N-1
        KTP(J,I)=KTP(I,N)
        KTP(I,J)=KTP(N,I)
    END DO
    KTS(J)=KTS(N)
END SUBROUTINE KTMOVE
!C-----
<KTCLUS: procedures>+≡
    FUNCTION KTMDPI(PHI)
    IMPLICIT NONE
!C--RETURNS PHI, MOVED ONTO THE RANGE [-PI,PI)
    DOUBLE PRECISION KTMDPI,PHI,PI,TWOPI,THRPI,EPS
    PARAMETER (PI=3.14159265358979324D0,TWOPI=6.28318530717958648D0, &
        THRPI=9.42477796076937972D0)
    PARAMETER (EPS=1D-15)
    KTMDPI=PHI
    IF (KTMDPI.LE.PI) THEN
        IF (KTMDPI.GT.-PI) THEN
            GOTO 100
        ELSEIF (KTMDPI.GT.-THRPI) THEN
            KTMDPI=KTMDPI+TWOPI
        ELSE
            KTMDPI=-MOD(PI-KTMDPI,TWOPI)+PI
        ENDIF
    ELSEIF (KTMDPI.LE.THRPI) THEN
        KTMDPI=KTMDPI-TWOPI
    ELSE
        KTMDPI=MOD(PI+KTMDPI,TWOPI)-PI
    ENDIF
100 IF (ABS(KTMDPI).LT.EPS) KTMDPI=0
END FUNCTION KTMDPI
!C-----

```

```

      SUBROUTINE KTWARN(SUBRTN,ICODE,*)
!C      DEALS WITH ERRORS DURING EXECUTION
!C      SUBRTN = NAME OF CALLING SUBROUTINE
!C      ICODE = ERROR CODE:      - 99 PRINT WARNING & CONTINUE
!C                               100-199 PRINT WARNING & JUMP
!C                               200-   PRINT WARNING & STOP DEAD
!C-----
      INTEGER ICODE
      CHARACTER(len=6) SUBRTN
      WRITE (6,10) SUBRTN,ICODE
10    FORMAT(/' KTWARN CALLED FROM SUBPROGRAM ',A6,': CODE =',I4/)
      IF (ICODE.LT.100) RETURN
      IF (ICODE.LT.200) RETURN 1
      STOP
      END SUBROUTINE KTWARN
!C-----
!C-----
!C-----

```

22.5 Interface to PYTHIA 8

(shower_pythia8.f90)≡
⟨File header⟩

module shower_pythia8

⟨Use kinds with double⟩

⟨Use strings⟩

use os_interface

use lorentz

use shower_base

use particles

use model_data

use pdf

use whizard_lha

use pythia8

use tauola_interface, only: taudec_settings_t

⟨Standard module head⟩

⟨Shower pythia8: public⟩

⟨Shower pythia8: variables⟩

⟨Shower pythia8: types⟩

interface

⟨Shower pythia8: sub interfaces⟩

end interface

end module shower_pythia8

```

<shower_pythia8_sub.f90>≡
  <File header>

  submodule (shower_pythia8) shower_pythia8_s

    <Use debug>
    use constants
    use numeric_utils, only: vanishes
    use io_units
    use physics_defs
    use diagnostics
    use helicities
    use subevents

    implicit none

  contains

    <Shower pythia8: procedures>

  end submodule shower_pythia8_s

<Shower pythia8: public>≡
  public :: shower_pythia8_t

<Shower pythia8: types>≡
  type, extends(shower_base_t) :: shower_pythia8_t
    private
    type(pythia8_t) :: pythia
    type(whizard_lha_t) :: lhaup
    logical :: user_process_set = .false.
    logical :: pythia_initialized = .false., &
      lhaup_initialized = .false.
  contains
    <Shower pythia8: shower pythia8: TBP>
  end type shower_pythia8_t

<Shower pythia8: shower pythia8: TBP>≡
  procedure :: init => shower_pythia8_init

<Shower pythia8: sub interfaces>≡
  module subroutine shower_pythia8_init &
    (shower, settings, taudec_settings, pdf_data, os_data)
    class(shower_pythia8_t), intent(out) :: shower
    type(shower_settings_t), intent(in) :: settings
    type(taudec_settings_t), intent(in) :: taudec_settings
    type(pdf_data_t), intent(in) :: pdf_data
    type(os_data_t), intent(in) :: os_data
  end subroutine shower_pythia8_init

<Shower pythia8: procedures>≡
  module subroutine shower_pythia8_init &
    (shower, settings, taudec_settings, pdf_data, os_data)
    class(shower_pythia8_t), intent(out) :: shower
    type(shower_settings_t), intent(in) :: settings

```

```

type(taudec_settings_t), intent(in) :: taudec_settings
type(pdf_data_t), intent(in) :: pdf_data
type(os_data_t), intent(in) :: os_data
if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_init")
shower%settings = settings
shower%taudec_settings = taudec_settings
shower%os_data = os_data
call shower%pdf_data%init (pdf_data)
shower%name = "PYTHIA8"
call shower%write_msg ()
call shower%pythia%init (verbose = settings%verbose)
call shower%lhaup%init ()
end subroutine shower_pythia8_init

```

Setup the user process for the LHA interface.

We fill the user process with the correct information on the beams, and set the strategy of the user process to weighted events. `process_id` and `n_processes` are not used by LHA user process for weighted (or unweighted) events, but required by the LHA user process interface. Therefore, we choose arbitrary defaults.

```

<Shower pythia8: shower pythia8: TBP>+≡
  procedure, private :: set_user_process => shower_pythia8_set_user_process

<Shower pythia8: sub interfaces>+≡
  module subroutine shower_pythia8_set_user_process (shower, pset)
    class(shower_pythia8_t), intent(inout) :: shower
    type(particle_set_t), intent(in) :: pset
  end subroutine shower_pythia8_set_user_process

<Shower pythia8: procedures>+≡
  module subroutine shower_pythia8_set_user_process (shower, pset)
    class(shower_pythia8_t), intent(inout) :: shower
    type(particle_set_t), intent(in) :: pset
    integer, dimension(2) :: beam_pdg
    real(default), dimension(2) :: beam_energy
    integer, parameter :: process_id = 1, n_processes = 1
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_set_user_process")
    ! TODO sbrass find correct beam entries, fallback would be first two entries
    beam_pdg = [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()]
    beam_energy = [energy(pset%prt(1)%p), energy(pset%prt(2)%p)]
    call shower%lhaup%set_init (beam_pdg, beam_energy, &
      n_processes, unweighted = .false., negative_weights = .false.)
    call shower%lhaup%set_process_parameters (process_id = process_id, &
      cross_section = one, error = one)
  end subroutine shower_pythia8_set_user_process

```

Import a particle set and make it accessible for PYTHIA8 as an user process. We check whether the LHA object needs to be initialized and do the appropriate steps.

```

<Shower pythia8: shower pythia8: TBP>+≡
  procedure :: import_particle_set => shower_pythia8_import_particle_set

<Shower pythia8: sub interfaces>+≡
  module subroutine shower_pythia8_import_particle_set &
    (shower, particle_set)

```



```

        class(shower_pythia8_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
    end subroutine shower_pythia8_import_particle_set

<Shower pythia8: procedures>+≡
    module subroutine shower_pythia8_import_particle_set &
        (shower, particle_set)
        class(shower_pythia8_t), target, intent(inout) :: shower
        type(particle_set_t), intent(in) :: particle_set
        type(particle_set_t) :: pset_reduced
        integer, parameter :: PROCESS_ID = 1
        logical :: keep_beams
        if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_import_particle_set")
        if (.not. shower%user_process_set) then
            call shower%set_user_process (particle_set)
            shower%user_process_set = .true.
        end if
        if (debug_active (D_SHOWER)) then
            call particle_set%write (summary=.true., compressed=.true.)
        end if
        call shower%lhaup%set_event_process (process_id = PROCESS_ID, scale = shower%fac_scale, &
            alpha_qcd = shower%alpha_s, alpha_qed = -one, weight = -one)
        call shower%lhaup%set_event (process_id = PROCESS_ID, particle_set = particle_set, &
            keep_beams = .false., keep_remnants = .true., polarization = .true.)
        if (debug_active (D_SHOWER)) then
            call shower%lhaup%list_init ()
            call shower%lhaup%list_event ()
        end if
    end subroutine shower_pythia8_import_particle_set

<Shower pythia8: shower pythia8: TBP>+≡
    procedure :: generate_emissions => shower_pythia8_generate_emissions

<Shower pythia8: sub interfaces>+≡
    module subroutine shower_pythia8_generate_emissions &
        (shower, valid, number_of_emissions)
        class(shower_pythia8_t), intent(inout), target :: shower
        logical, intent(out) :: valid
        integer, optional, intent(in) :: number_of_emissions
    end subroutine shower_pythia8_generate_emissions

<Shower pythia8: procedures>+≡
    module subroutine shower_pythia8_generate_emissions &
        (shower, valid, number_of_emissions)
        class(shower_pythia8_t), intent(inout), target :: shower
        logical, intent(out) :: valid
        integer, optional, intent(in) :: number_of_emissions
        if (signal_is_pending ()) return
        call shower%transfer_settings ()
        call shower%pythia%next (valid)
    end subroutine shower_pythia8_generate_emissions

<Shower pythia8: shower pythia8: TBP>+≡
    procedure :: make_particle_set => shower_pythia8_make_particle_set

```

```

<Shower pythia8: sub interfaces>+≡
  module subroutine shower_pythia8_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia8_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
  end subroutine shower_pythia8_make_particle_set

<Shower pythia8: procedures>+≡
  module subroutine shower_pythia8_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia8_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
    type(particle_t), dimension(:), allocatable :: beam
    integer :: n_whizard, n_tot_pythia
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_make_particle_set")
    if (signal_is_pending ()) return
    associate (settings => shower%settings)
      if (debug_active (D_SHOWER)) then
        call msg_debug (D_SHOWER, 'Combine PYTHIA8 with particle set')
        call msg_debug (D_SHOWER, 'Particle set before replacing')
        call particle_set%write (summary=.true., compressed=.true.)
        call shower%pythia%list_event ()
        call msg_debug (D_SHOWER, string = "settings%hadron_collision", &
          value = settings%hadron_collision)
      end if
    end associate
    call shower%pythia%get_shower_particles (&
      model, model_hadrons, particle_set, &
      helicity = PRT_DEFINITE_HELICITY, &
      recover_beams = shower%settings%hadron_collision)
    if (debug_active (D_SHOWER)) then
      print *, 'Particle set after replacing'
      call particle_set%write (summary=.true., compressed=.true.)
    end if
  end subroutine shower_pythia8_make_particle_set

```

Transfer WHIZARD shower settings to Pythia8. Import a pointer to shower%rng and initialize Pythia itself, at once.

```

<Shower pythia8: shower pythia8: TBP>+≡
  procedure, private :: transfer_settings => shower_pythia8_transfer_settings

<Shower pythia8: sub interfaces>+≡
  module subroutine shower_pythia8_transfer_settings (shower)
    class(shower_pythia8_t), intent(inout), target :: shower
  end subroutine shower_pythia8_transfer_settings

<Shower pythia8: procedures>+≡
  module subroutine shower_pythia8_transfer_settings (shower)
    class(shower_pythia8_t), intent(inout), target :: shower
    if (debug_on) call msg_debug &
      (D_SHOWER, "shower_pythia8_transfer_settings")

```

```

if (debug_on) call msg_debug2 &
    (D_SHOWER, "pythia_initialized", shower%pythia_initialized)
if (shower%pythia_initialized) return
associate (pythia => shower%pythia)
    call pythia%set_lhaup_ptr (shower%lhaup)
    call pythia%import_rng (shower%rng)
    call shower%pythia%parse_and_set_config (shower%settings%pythia8_config)
    if (len (shower%settings%pythia8_config_file) > 0) &
        call pythia%read_file (shower%settings%pythia8_config_file)
    call pythia%read_string (var_str ("Beams:frameType = 5"))
    ! call pythia%read_string (var_str ("ParticleDecays:allowPhotonRadiation = off"))
    call pythia%read_string (var_str ("HadronLevel:all = off"))
    if (.not. shower%settings%verbose) then
        call pythia%read_string (var_str ("Print:quiet = on"))
    end if
    if (.not. shower%settings%isr_active) then
        call pythia%read_string (var_str ("PartonLevel:ISR = off"))
    else
        call pythia%read_string (var_str ("PartonLevel:ISR = on"))
    end if
    if (.not. shower%settings%fsr_active) then
        call pythia%read_string (var_str ("PartonLevel:FSR = off"))
    else
        call pythia%read_string (var_str ("PartonLevel:FSR = on"))
    end if
    call pythia%init_pythia ()
end associate
shower%pythia_initialized = .true.
end subroutine shower_pythia8_transfer_settings

```

<Shower pythia8: shower pythia8: TBP>+≡

```

procedure :: get_final_colored_ME_momenta => &
    shower_pythia8_get_final_colored_ME_momenta

```

<Shower pythia8: sub interfaces>+≡

```

module subroutine shower_pythia8_get_final_colored_ME_momenta &
    (shower, momenta)
    class(shower_pythia8_t), intent(in) :: shower
    type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
end subroutine shower_pythia8_get_final_colored_ME_momenta

```

<Shower pythia8: procedures>+≡

```

module subroutine shower_pythia8_get_final_colored_ME_momenta &
    (shower, momenta)
    class(shower_pythia8_t), intent(in) :: shower
    type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
    if (debug_on) call msg_debug &
        (D_MATCHING, "shower_pythia8_get_final_colored_ME_momenta")
    call shower%pythia%get_final_colored_ME_momenta (momenta)
end subroutine shower_pythia8_get_final_colored_ME_momenta

```

Chapter 23

Multiple Interactions (MPI) Code

23.1 The Multiple Interactions main module

This file contains the module `muli` which is the multiple parton interactions interface module to `WHIZARD`. `muli` is supposed to run together with initial state radiation. Both share a momentum evolution variable and compete for beam momentum, so the generation of this scale variable must be fully transparent to `WHIZARD`. This here is a stub as long as there is no working `WHIZARD` implementation for multiple interactions. It gives an interface for the necessary routines.

```
<muli.f90>≡  
  <File header>  
  
  module muli  
    use, intrinsic :: iso_fortran_env  
    <Use kinds>
```

No internal dependencies

Figure 23.1: Module dependencies in `src/muli`.

⟨Standard module head⟩

⟨Muli: variables⟩

⟨Muli: public⟩

⟨Muli: types⟩

contains

⟨Muli: procedures⟩

end module muli

23.1.1 The main Multiple Interactions type

⟨Muli: public⟩≡

public :: muli_t

⟨Muli: types⟩≡

type :: muli_t

real(default) :: GeV2_scale_cutoff

logical :: initialized = .false.

integer, dimension(4) :: flow

contains

⟨Muli: muli: TBP⟩

end type muli_t

⟨Muli: muli: TBP⟩≡

generic :: initialize => muli_initialize

procedure :: muli_initialize

⟨Muli: procedures⟩≡

**subroutine muli_initialize (this, GeV2_scale_cutoff, gev2_s, &
mul_dir, random_seed)**

class(muli_t), intent(out) :: this

real(kind=default), intent(in) :: gev2_s, GeV2_scale_cutoff

character(*), intent(in) :: mul_dir

integer, intent(in), optional :: random_seed

this%initialized = .true.

end subroutine muli_initialize

⟨Muli: muli: TBP⟩+≡

procedure :: apply_initial_interaction => muli_apply_initial_interaction

⟨Muli: procedures⟩+≡

**subroutine muli_apply_initial_interaction (this, GeV2_s, &
x1, x2, pdg_f1, pdg_f2, n1, n2)**

class(muli_t), intent(inout) :: this

real(default), intent(in) :: GeV2_s, x1, x2

integer, intent(in):: pdg_f1, pdg_f2, n1, n2

end subroutine muli_apply_initial_interaction

```

<Muli: muli: TBP>+≡
  procedure :: restart => muli_restart

<Muli: procedures>+≡
  subroutine muli_restart (this)
    class(muli_t), intent(inout) :: this
  end subroutine muli_restart

<Muli: muli: TBP>+≡
  procedure :: is_initialized => muli_is_initialized

<Muli: procedures>+≡
  elemental function muli_is_initialized (this) result (res)
    logical :: res
    class(muli_t), intent(in) :: this
    res = this%initialized
  end function muli_is_initialized

<Muli: muli: TBP>+≡
  procedure :: generate_gev2_pt2 => muli_generate_gev2_pt2

<Muli: procedures>+≡
  subroutine muli_generate_gev2_pt2 (this, gev2_start_scale, gev2_new_scale)
    class(muli_t), intent(inout) :: this
    real(kind=default), intent(in) :: gev2_start_scale
    real(kind=default), intent(out) :: gev2_new_scale
    call this%generate_next_scale ()
    gev2_new_scale = 1
  end subroutine muli_generate_gev2_pt2

<Muli: muli: TBP>+≡
  procedure :: generate_partons => muli_generate_partons

<Muli: procedures>+≡
  subroutine muli_generate_partons (this, n1, n2, x_proton_1, x_proton_2, &
    pdg_f1, pdg_f2, pdg_f3, pdg_f4)
    class(muli_t), intent(inout) :: this
    integer, intent(in) :: n1, n2
    real(kind=default), intent(out) :: x_proton_1, x_proton_2
    integer, intent(out) :: pdg_f1, pdg_f2, pdg_f3, pdg_f4
    integer, dimension(4) :: pdg_f
    call this%generate_color_flows ()
    pdg_f = 0
    pdg_f1 = 0
    pdg_f2 = 0
    pdg_f3 = 0
    pdg_f4 = 0
  end subroutine muli_generate_partons

<Muli: muli: TBP>+≡
  procedure :: generate_color_flows => muli_generate_color_flows

```

```

<Muli: procedures>+≡
  subroutine multi_generate_color_flows (this)
    class(muli_t), intent(inout) :: this
    integer, dimension(4) :: flow
  end subroutine multi_generate_color_flows

<Muli: muli: TBP>+≡
  procedure :: get_color_flow => multi_get_color_flow

<Muli: procedures>+≡
  pure function multi_get_color_flow (this) result (flow)
    class(muli_t), intent(in) :: this
    integer, dimension(4) :: flow
    flow = this%flow
  end function multi_get_color_flow

<Muli: muli: TBP>+≡
  procedure :: get_color_correlations => multi_get_color_correlations

<Muli: procedures>+≡
  subroutine multi_get_color_correlations &
    (this, start_index, final_index, flow)
    class(muli_t), intent(in) :: this
    integer, intent(in) :: start_index
    integer, intent(out) :: final_index
    integer, dimension(2,4), intent(out) :: flow
    integer :: pos, f_end, f_beginning
    final_index = start_index
    flow = reshape([0,0,0,0,0,0,0,0],[2,4])
  end subroutine multi_get_color_correlations

<Muli: muli: TBP>+≡
  procedure :: replace_parton => multi_replace_parton

<Muli: procedures>+≡
  subroutine multi_replace_parton &
    (this, proton_id, old_id, new_id, pdg_f, x_proton, gev_scale)
    class(muli_t), intent(inout) :: this
    integer, intent(in) :: proton_id, old_id, new_id, pdg_f
    real(kind=default), intent(in) :: x_proton, gev_scale
  end subroutine multi_replace_parton

<Muli: muli: TBP>+≡
  procedure :: generate_next_scale => multi_generate_next_scale

<Muli: procedures>+≡
  subroutine multi_generate_next_scale (this, integrand_kind)
    class(muli_t), intent(inout) :: this
    integer, intent(in), optional :: integrand_kind
  end subroutine multi_generate_next_scale

```

Chapter 24

BLHA Interface

The code in this chapter implements support for the BLHA record that communicates data for NLO processes.

These are the modules:

blha_config

blha_olp_interfaces

The module is split into a configuration interface which manages configuration and handles the request and contract files, a module which interfaces the OLP matrix elements and a driver.

```
(blha_config.f90)≡  
  <File header>  
  
  module blha_config  
  
    use kinds  
    <Use strings>  
    use variables, only: var_list_t  
    use model_data  
    use beam_structures, only: beam_structure_t  
  
    <Standard module head>  
  
    <BLHA config: public>  
  
    <BLHA config: parameters>  
  
    <BLHA config: types>  
  
    <BLHA config: variables>  
  
    <BLHA config: interfaces>  
  
    interface  
    <BLHA config: sub interfaces>  
    end interface
```

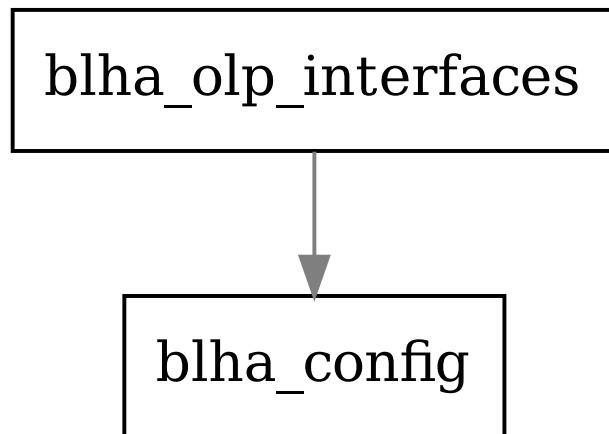



Figure 24.1: Module dependencies in `src/blha`.

```

end module blha_config

⟨blha_config_sub.f90⟩≡
  ⟨File header⟩

submodule (blha_config) blha_config_s

  ⟨Use mpi f08⟩
  use io_units
  use constants
  use string_utils
  use physics_defs, only: PHOTON, PHOTON_OFFSHELL
  use diagnostics
  use flavors
  use pdg_arrays

  implicit none

contains

  ⟨BLHA config: procedures⟩

end submodule blha_config_s

```

24.1 Configuration

Parameters to enumerate the different options in the order.

```

⟨BLHA config: parameters⟩≡
  integer, public, parameter :: &
    BLHA_CT_QCD = 1, BLHA_CT_EW = 2, BLHA_CT_OTHER = 3
  integer, public, parameter :: &
    BLHA_IRREG_CDR = 1, BLHA_IRREG_DRED = 2, BLHA_IRREG_THV = 3, &
    BLHA_IRREG_MREG = 4, BLHA_IRREG_OTHER = 5
  integer, public, parameter :: &
    BLHA_MPS_ONSHELL = 1, BLHA_MPS_OTHER = 2
  integer, public, parameter :: &
    BLHA_MODE_GOSAM = 1, BLHA_MODE_FEYNARTS = 2, BLHA_MODE_GENERIC = 3, &
    BLHA_MODE_OPENLOOPS = 4
  integer, public, parameter :: &
    BLHA_VERSION_1 = 1, BLHA_VERSION_2 = 2
  integer, public, parameter :: &
    BLHA_AMP_LOOP = 1, BLHA_AMP_COLOR_C = 2, BLHA_AMP_SPIN_C = 3, &
    BLHA_AMP_TREE = 4, BLHA_AMP_LOOPINDUCED = 5
  integer, public, parameter :: &
    BLHA_EW_INTERNAL = 0, &
    BLHA_EW_GF = 1, BLHA_EW_MZ = 2, BLHA_EW_MSBAR = 3, &
    BLHA_EW_0 = 4, BLHA_EW_RUN = 5
  integer, public, parameter :: &
    BLHA_WIDTH_COMPLEX = 1, BLHA_WIDTH_FIXED = 2, &
    BLHA_WIDTH_RUNNING = 3, BLHA_WIDTH_POLE = 4, &
    BLHA_WIDTH_DEFAULT = 5

```

Those are the default pdg codes for massive particles in BLHA programs

```
<BLHA config: parameters>+=
  integer, parameter, public :: OLP_N_MASSIVE_PARTICLES = 12
  integer, dimension(OLP_N_MASSIVE_PARTICLES), public :: &
    OLP_MASSIVE_PARTICLES = [5, -5, 6, -6, 13, -13, 15, -15, 23, 24, -24, 25]
  integer, parameter :: OLP_HEL_UNPOLARIZED = 0
```

The user might provide an extra command string for OpenLoops to apply special libraries instead of the default ones, such as signal-only amplitudes for off-shell top production. We check in this subroutine that the provided string is valid and print out the possible options to ease the user's memory.

```
<BLHA config: parameters>+=
  integer, parameter :: N_KNOWN_SPECIAL_OL_METHODS = 3

<BLHA config: procedures>=
  subroutine check_extra_cmd (extra_cmd)
    type(string_t), intent(in) :: extra_cmd
    type(string_t), dimension(N_KNOWN_SPECIAL_OL_METHODS) :: known_methods
    integer :: i
    logical :: found
    known_methods(1) = 'top'
    known_methods(2) = 'not'
    known_methods(3) = 'stop'
    if (extra_cmd == var_str("")) return
    found = .false.
    do i = 1, N_KNOWN_SPECIAL_OL_METHODS
      found = found .or. &
        (extra_cmd == var_str ('extra approx ')) // known_methods(i))
    end do
    if (.not. found) &
      call msg_fatal ("The given extra OpenLoops method is not kown ", &
        [var_str ("Available commands are: "), &
        var_str ("extra approx top (only WbWb signal),"), &
        var_str ("extra approx stop (only WbWb singletop),"), &
        var_str ("extra approx not (no top in WbWb).")])
    end subroutine check_extra_cmd
```

This type contains the pdg code of the particle to be written in the process specification string and an optional additional information about the polarization of the particles. Note that the output can only be processed by OpenLoops.

```
<BLHA config: types>=
  type :: blha_particle_string_element_t
    integer :: pdg = 0
    integer :: hel = OLP_HEL_UNPOLARIZED
    logical :: polarized = .false.
  contains
    <BLHA config: blha particle string element: TBP>
  end type blha_particle_string_element_t
```

```
<BLHA config: blha particle string element: TBP>=
  generic :: init => init_default
```

```

generic :: init => init_polarized
procedure :: init_default => blha_particle_string_element_init_default
procedure :: init_polarized => blha_particle_string_element_init_polarized

<BLHA config: sub interfaces>≡
  module subroutine blha_particle_string_element_init_default (blha_p, id)
    class(blha_particle_string_element_t), intent(out) :: blha_p
    integer, intent(in) :: id
  end subroutine blha_particle_string_element_init_default
  module subroutine blha_particle_string_element_init_polarized (blha_p, id, hel)
    class(blha_particle_string_element_t), intent(out) :: blha_p
    integer, intent(in) :: id, hel
  end subroutine blha_particle_string_element_init_polarized

<BLHA config: procedures>+≡
  module subroutine blha_particle_string_element_init_default (blha_p, id)
    class(blha_particle_string_element_t), intent(out) :: blha_p
    integer, intent(in) :: id
    blha_p%pdg = id
  end subroutine blha_particle_string_element_init_default

  module subroutine blha_particle_string_element_init_polarized (blha_p, id, hel)
    class(blha_particle_string_element_t), intent(out) :: blha_p
    integer, intent(in) :: id, hel
    blha_p%polarized = .true.
    blha_p%pdg = id
    blha_p%hel = hel
  end subroutine blha_particle_string_element_init_polarized

<BLHA config: blha particle string element: TBP>+≡
  generic :: write_pdg => write_pdg_unit
  generic :: write_pdg => write_pdg_character
  procedure :: write_pdg_unit => blha_particle_string_element_write_pdg_unit
  procedure :: write_pdg_character &
    => blha_particle_string_element_write_pdg_character

<BLHA config: sub interfaces>+≡
  module subroutine blha_particle_string_element_write_pdg_unit (blha_p, unit)
    class(blha_particle_string_element_t), intent(in) :: blha_p
    integer, intent(in), optional :: unit
  end subroutine blha_particle_string_element_write_pdg_unit
  module subroutine blha_particle_string_element_write_pdg_character (blha_p, c)
    class(blha_particle_string_element_t), intent(in) :: blha_p
    character(3), intent(inout) :: c
  end subroutine blha_particle_string_element_write_pdg_character

<BLHA config: procedures>+≡
  module subroutine blha_particle_string_element_write_pdg_unit (blha_p, unit)
    class(blha_particle_string_element_t), intent(in) :: blha_p
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, '(I3)') blha_p%pdg
  end subroutine blha_particle_string_element_write_pdg_unit

```

```

<BLHA config: procedures>+≡
module subroutine blha_particle_string_element_write_pdg_character (blha_p, c)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  character(3), intent(inout) :: c
  write (c, '(I3)') blha_p%pdg
end subroutine blha_particle_string_element_write_pdg_character

<BLHA config: blha particle string element: TBP>+≡
generic :: write_helicity => write_helicity_unit
generic :: write_helicity => write_helicity_character
procedure :: write_helicity_unit &
  => blha_particle_string_element_write_helicity_unit
procedure :: write_helicity_character &
  => blha_particle_string_element_write_helicity_character

<BLHA config: sub interfaces>+≡
module subroutine blha_particle_string_element_write_helicity_unit (blha_p, unit)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  integer, intent(in), optional :: unit
end subroutine blha_particle_string_element_write_helicity_unit
module subroutine blha_particle_string_element_write_helicity_character (blha_p, c)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  character(4), intent(inout) :: c
end subroutine blha_particle_string_element_write_helicity_character

<BLHA config: procedures>+≡
module subroutine blha_particle_string_element_write_helicity_unit (blha_p, unit)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, '(A1,I0,A1)') '(', blha_p%hel, ')'
end subroutine blha_particle_string_element_write_helicity_unit

<BLHA config: procedures>+≡
module subroutine blha_particle_string_element_write_helicity_character (blha_p, c)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  character(4), intent(inout) :: c
  write (c, '(A1,I0,A1)') '(', blha_p%hel, ')'
end subroutine blha_particle_string_element_write_helicity_character

```

This type encapsulates a BLHA request.

```

<BLHA config: public>≡
public :: blha_configuration_t
public :: blha_cfg_process_node_t

<BLHA config: types>+≡
type :: blha_cfg_process_node_t
  type(blha_particle_string_element_t), dimension(:), allocatable :: pdg_in, pdg_out
  integer, dimension(:), allocatable :: fingerprint
  integer :: nsub
  integer, dimension(:), allocatable :: ids
  integer :: amplitude_type
  type(blha_cfg_process_node_t), pointer :: next => null ()

```

```

end type blha_cfg_process_node_t

type :: blha_configuration_t
  type(string_t) :: name
  class(model_data_t), pointer :: model => null ()
  type(string_t) :: md5
  integer :: version = 2
  logical :: dirty = .false.
  integer :: n_proc = 0
  real(default) :: accuracy_target
  logical :: debug_unstable = .false.
  integer :: mode = BLHA_MODE_GENERIC
  logical :: polarized = .false.
  type(blha_cfg_process_node_t), pointer :: processes => null ()
  !integer, dimension(2) :: matrix_element_square_type = BLHA_MEST_SUM
  integer :: correction_type
  type(string_t) :: correction_type_other
  integer :: irreg = BLHA_IRREG_THV
  type(string_t) :: irreg_other
  integer :: massive_particle_scheme = BLHA_MPS_ONSHELL
  type(string_t) :: massive_particle_scheme_other
  type(string_t) :: model_file
  logical :: subdivide_subprocesses = .false.
  integer :: alphas_power = -1, alpha_power = -1
  integer :: ew_scheme = BLHA_EW_GF
  integer :: width_scheme = BLHA_WIDTH_DEFAULT
  logical :: openloops_use_cms = .false.
  integer :: openloops_phs_tolerance = 0
  type(string_t) :: openloops_extra_cmd
  type(string_t) :: openloops_allowed_libs
  integer :: openloops_stability_log = 0
  integer :: n_off_photons_is = 0
  integer :: n_off_photons_fs = 0
end type blha_configuration_t

```

Translate the SINDARIN input string to the corresponding named integer.

```

<BLHA config: public>+≡
  public :: ew_scheme_string_to_int

<BLHA config: sub interfaces>+≡
  module function ew_scheme_string_to_int (ew_scheme_str) result (ew_scheme_int)
    integer :: ew_scheme_int
    type(string_t), intent(in) :: ew_scheme_str
  end function ew_scheme_string_to_int

<BLHA config: procedures>+≡
  module function ew_scheme_string_to_int (ew_scheme_str) result (ew_scheme_int)
    integer :: ew_scheme_int
    type(string_t), intent(in) :: ew_scheme_str
    select case (char(ew_scheme_str))
    case ('GF', 'Gmu')
      ew_scheme_int = BLHA_EW_GF
    case ('alpha_qed', 'alpha_internal')
      ew_scheme_int = BLHA_EW_INTERNAL
    case ('alpha_mz')

```

```

        ew_scheme_int = BLHA_EW_MZ
    case ('alpha_0', 'alpha_thompson')
        ew_scheme_int = BLHA_EW_0
    case default
        call msg_fatal ("ew_scheme: " // char (ew_scheme_str) // &
            " not supported. Try 'Gmu', 'alpha_internal', 'alpha_mz' or 'alpha_0'.")
    end select
end function ew_scheme_string_to_int

```

Translate the SINDARIN input string to the corresponding named integer denoting the type of NLO correction.

```

<BLHA config: public>+≡
    public :: correction_type_string_to_int

<BLHA config: sub interfaces>+≡
    module function correction_type_string_to_int &
        (correction_type_str) result (correction_type_int)
        integer :: correction_type_int
        type(string_t), intent(in) :: correction_type_str
    end function correction_type_string_to_int

<BLHA config: procedures>+≡
    module function correction_type_string_to_int &
        (correction_type_str) result (correction_type_int)
        integer :: correction_type_int
        type(string_t), intent(in) :: correction_type_str
        select case (char (correction_type_str))
        case ('QCD')
            correction_type_int = BLHA_CT_QCD
        case ('EW')
            correction_type_int = BLHA_CT_EW
        case default
            call msg_warning ("nlo_correction_type: " // char (correction_type_str) // &
                " not supported. Try setting it to 'QCD', 'EW'.")
        end select
    end function correction_type_string_to_int

```

This types control the creation of BLHA-interface files

```

<BLHA config: public>+≡
    public :: blha_flv_state_t
    public :: blha_master_t

<BLHA config: types>+≡
    type :: blha_flv_state_t
        integer, dimension(:), allocatable :: flavors
        integer :: flv_mult
        logical :: flv_real = .false.
    end type blha_flv_state_t

    type :: blha_master_t
        integer, dimension(5) :: blha_mode = BLHA_MODE_GENERIC
        logical :: compute_borns = .false.
        logical :: compute_real_trees = .false.
        logical :: compute_loops = .true.

```

```

logical :: compute_correlations = .false.
logical :: compute_dglap = .false.
integer :: ew_scheme
type(string_t), dimension(:), allocatable :: suffix
type(blha_configuration_t), dimension(:), allocatable :: blha_cfg
integer :: n_files = 0
integer, dimension(:), allocatable :: i_file_to_nlo_index
contains
<BLHA config: blha master: TBP>
end type blha_master_t

```

Master-Routines

```

<BLHA config: blha master: TBP>≡
  procedure :: set_methods => blha_master_set_methods

<BLHA config: sub interfaces>+≡
  module subroutine blha_master_set_methods (master, is_nlo, var_list)
    class(blha_master_t), intent(inout) :: master
    logical, intent(in) :: is_nlo
    type(var_list_t), intent(in) :: var_list
  end subroutine blha_master_set_methods

<BLHA config: procedures>+≡
  module subroutine blha_master_set_methods (master, is_nlo, var_list)
    class(blha_master_t), intent(inout) :: master
    logical, intent(in) :: is_nlo
    type(var_list_t), intent(in) :: var_list
    type(string_t) :: method, born_me_method, real_tree_me_method
    type(string_t) :: loop_me_method, correlation_me_method
    type(string_t) :: dglap_me_method
    type(string_t) :: default_method
    logical :: cmp_born, cmp_real
    logical :: cmp_loop, cmp_corr
    logical :: cmp_dglap
    if (is_nlo) then
      method = var_list%get_sval (var_str ("method"))
      born_me_method = var_list%get_sval (var_str ("born_me_method"))
      if (born_me_method == "") born_me_method = method
      real_tree_me_method = var_list%get_sval (var_str ("real_tree_me_method"))
      if (real_tree_me_method == "") real_tree_me_method = method
      loop_me_method = var_list%get_sval (var_str ("loop_me_method"))
      if (loop_me_method == "") loop_me_method = method
      correlation_me_method = var_list%get_sval (var_str ("correlation_me_method"))
      if (correlation_me_method == "") correlation_me_method = method
      dglap_me_method = var_list%get_sval (var_str ("dglap_me_method"))
      if (dglap_me_method == "") dglap_me_method = method
      cmp_born = born_me_method /= 'omega'
      cmp_real = is_nlo .and. (real_tree_me_method /= 'omega')
      cmp_loop = is_nlo .and. (loop_me_method /= 'omega')
      cmp_corr = is_nlo .and. (correlation_me_method /= 'omega')
      cmp_dglap = is_nlo .and. (dglap_me_method /= 'omega')
      call set_me_method (1, loop_me_method)
      call set_me_method (2, correlation_me_method)
      call set_me_method (3, real_tree_me_method)
      call set_me_method (4, born_me_method)
    end if
  end subroutine blha_master_set_methods

```



```

        call set_me_method (5, dglap_me_method)
    else
        default_method = var_list%get_sval (var_str (" $method"))
        cmp_born = default_method /= 'omega'
        cmp_real = .false.; cmp_loop = .false.; cmp_corr = .false.
        call set_me_method (4, default_method)
    end if
    master%n_files = count ([cmp_born, cmp_real, cmp_loop, cmp_corr, cmp_dglap])
    call set_nlo_indices ()
    master%compute_borns = cmp_born
    master%compute_real_trees = cmp_real
    master%compute_loops = cmp_loop
    master%compute_correlations = cmp_corr
    master%compute_dglap = cmp_dglap
contains
    subroutine set_nlo_indices ()
        integer :: i_file
        allocate (master%i_file_to_nlo_index (master%n_files))
        master%i_file_to_nlo_index = 0
        i_file = 0
        if (cmp_loop) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 1
        end if
        if (cmp_corr) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 2
        end if
        if (cmp_real) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 3
        end if
        if (cmp_born) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 4
        end if
        if (cmp_dglap) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 5
        end if
    end subroutine set_nlo_indices

    subroutine set_me_method (i, me_method)
        integer, intent(in) :: i
        type(string_t) :: me_method
        select case (char (me_method))
        case ('gosam')
            call master%set_gosam (i)
        case ('openloops')
            call master%set_openloops (i)
        end select
    end subroutine set_me_method
end subroutine blha_master_set_methods

```

```

<BLHA config: blha master: TBP>+≡
    procedure :: allocate_config_files => blha_master_allocate_config_files

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_allocate_config_files (master)
        class(blha_master_t), intent(inout) :: master
    end subroutine blha_master_allocate_config_files

<BLHA config: procedures>+≡
    module subroutine blha_master_allocate_config_files (master)
        class(blha_master_t), intent(inout) :: master
        allocate (master%blha_cfg (master%n_files))
        allocate (master%suffix (master%n_files))
    end subroutine blha_master_allocate_config_files

<BLHA config: blha master: TBP>+≡
    procedure :: set_ew_scheme => blha_master_set_ew_scheme

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_ew_scheme (master, ew_scheme)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: ew_scheme
    end subroutine blha_master_set_ew_scheme

<BLHA config: procedures>+≡
    module subroutine blha_master_set_ew_scheme (master, ew_scheme)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: ew_scheme
        master%ew_scheme = ew_scheme_string_to_int (ew_scheme)
    end subroutine blha_master_set_ew_scheme

<BLHA config: blha master: TBP>+≡
    procedure :: set_correction_type => blha_master_set_correction_type

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_correction_type (master, correction_type_str)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: correction_type_str
    end subroutine blha_master_set_correction_type

<BLHA config: procedures>+≡
    module subroutine blha_master_set_correction_type (master, correction_type_str)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: correction_type_str
        master%blha_cfg(:)%correction_type = &
            correction_type_string_to_int (correction_type_str)
    end subroutine blha_master_set_correction_type

<BLHA config: blha master: TBP>+≡
    procedure :: set_photon_characteristics => blha_master_set_photon_characteristics

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_photon_characteristics (master, flv_born, n_in)
        class(blha_master_t), intent(inout) :: master
        integer, dimension(:,:), intent(in) :: flv_born
        integer, intent(in) :: n_in
    end subroutine blha_master_set_photon_characteristics

```

<BLHA config: procedures>+≡

```

module subroutine blha_master_set_photon_characteristics (master, flv_born, n_in)
  class(blha_master_t), intent(inout) :: master
  integer, dimension(:,:), intent(in) :: flv_born
  integer, intent(in) :: n_in
  integer :: i_file, i, i_flv
  integer :: noff_is, noff_fs, noff_is_max, noff_fs_max
  do i_file = 1, master%n_files
    noff_is_max = 0; noff_fs_max = 0
    do i_flv = 1, size (flv_born, 2)
      noff_is = 0; noff_fs = 0
      do i = 1, n_in
        if (flv_born (i, i_flv) == PHOTON) noff_is = noff_is + 1
      end do
      noff_is_max = max (noff_is, noff_is_max)
      do i = n_in + 1, size (flv_born(:, i_flv))
        if (flv_born (i, i_flv) == PHOTON) noff_fs = noff_fs + 1
      end do
      noff_fs_max = max (noff_fs, noff_fs_max)
    end do
    if (master%blha_cfg(i_file)%correction_type == BLHA_CT_EW &
      .and. master%ew_scheme == BLHA_EW_0 &
      .and. (noff_is_max > 0 .or. noff_fs_max > 0)) then
      call msg_fatal ("For NLO EW/mixed corrections, 'alpha_0'/" &
        // "'alpha_thompson' are ", [ var_str ("inconsistent EW input " &
        // "schemes. Please use 'alpha_mz' or 'Gmu'")])
    end if
    master%blha_cfg(i_file)%n_off_photons_is = noff_is_max
    master%blha_cfg(i_file)%n_off_photons_fs = noff_fs_max
  end do
end subroutine blha_master_set_photon_characteristics

```

<BLHA config: blha master: TBP>+≡

```

procedure :: generate => blha_master_generate

```

<BLHA config: sub interfaces>+≡

```

module subroutine blha_master_generate (master, basename, model, &
  n_in, alpha_power, alphas_power, flv_born, flv_real)
  class(blha_master_t), intent(inout) :: master
  type(string_t), intent(in) :: basename
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_in
  integer, intent(in) :: alpha_power, alphas_power
  integer, intent(in), dimension(:,:), allocatable :: flv_born, flv_real
end subroutine blha_master_generate

```

<BLHA config: procedures>+≡

```

module subroutine blha_master_generate (master, basename, model, &
  n_in, alpha_power, alphas_power, flv_born, flv_real)
  class(blha_master_t), intent(inout) :: master
  type(string_t), intent(in) :: basename
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_in
  integer, intent(in) :: alpha_power, alphas_power
  integer, intent(in), dimension(:,:), allocatable :: flv_born, flv_real

```

```

integer :: i_file
if (master%n_files < 1) &
    call msg_fatal ("Attempting to generate OLP-files, but none are specified!")
i_file = 1
call master%generate_loop (basename, model, n_in, alpha_power, &
    alphas_power, flv_born, i_file)
call master%generate_correlation (basename, model, n_in, alpha_power, &
    alphas_power, flv_born, i_file)
call master%generate_real_tree (basename, model, n_in, alpha_power, &
    alphas_power, flv_real, i_file)
call master%generate_born (basename, model, n_in, alpha_power, &
    alphas_power, flv_born, i_file)
call master%generate_dglap (basename, model, n_in, alpha_power, &
    alphas_power, flv_born, i_file)
end subroutine blha_master_generate

```

(BLHA config: blha master: TBP)+≡

```

procedure :: generate_loop => blha_master_generate_loop

```

(BLHA config: sub interfaces)+≡

```

module subroutine blha_master_generate_loop (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_born, i_file)
class(blha_master_t), intent(inout) :: master
type(string_t), intent(in) :: basename
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in
integer, intent(in) :: alpha_power, alphas_power
integer, dimension(:,:), allocatable, intent(in) :: flv_born
integer, intent(inout) :: i_file
end subroutine blha_master_generate_loop

```

(BLHA config: procedures)+≡

```

module subroutine blha_master_generate_loop (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_born, i_file)
class(blha_master_t), intent(inout) :: master
type(string_t), intent(in) :: basename
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in
integer, intent(in) :: alpha_power, alphas_power
integer, dimension(:,:), allocatable, intent(in) :: flv_born
integer, intent(inout) :: i_file
type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
integer :: i_flv
if (master%compute_loops) then
    if (allocated (flv_born)) then
        allocate (blha_flavor (size (flv_born, 2)))
        do i_flv = 1, size (flv_born, 2)
            allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
            blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
            blha_flavor(i_flv)%flv_mult = 2
        end do
        master%suffix(i_file) = blha_get_additional_suffix (var_str ("_LOOP"))
        call blha_init_virtual (master%blha_cfg(i_file), blha_flavor, &
            n_in, alpha_power, alphas_power, master%ew_scheme, &
            basename, model, master%blha_mode(1), master%suffix(i_file))
    end if
end if

```

```

        i_file = i_file + 1
    else
        call msg_fatal ("BLHA Loops requested but " &
            // "Born flavor not existing")
    end if
end if
end if
end subroutine blha_master_generate_loop

```

(BLHA config: blha master: TBP)+≡

```

    procedure :: generate_correlation => blha_master_generate_correlation

```

(BLHA config: sub interfaces)+≡

```

    module subroutine blha_master_generate_correlation (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
    end subroutine blha_master_generate_correlation

```

(BLHA config: procedures)+≡

```

    module subroutine blha_master_generate_correlation (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
        type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
        integer :: i_flv
        if (master%compute_correlations) then
            if (allocated (flv_born)) then
                allocate (blha_flavor (size (flv_born, 2)))
                do i_flv = 1, size (flv_born, 2)
                    allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
                    blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
                    blha_flavor(i_flv)%flv_mult = 3
                end do
                master%suffix(i_file) = blha_get_additional_suffix (var_str ("_SUB"))
                call blha_init_subtraction (master%blha_cfg(i_file), blha_flavor, &
                    n_in, alpha_power, alphas_power, master%ew_scheme, &
                    basename, model, master%blha_mode(2), master%suffix(i_file))
                i_file = i_file + 1
            else
                call msg_fatal ("BLHA Correlations requested but "&
                    // "Born flavor not existing")
            end if
        end if
    end subroutine blha_master_generate_correlation

```

<BLHA config: blha master: TBP>+≡

```
procedure :: generate_real_tree => blha_master_generate_real_tree
```

<BLHA config: sub interfaces>+≡

```
module subroutine blha_master_generate_real_tree (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_real, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in
    integer, intent(in) :: alpha_power, alphas_power
    integer, dimension(:,:), allocatable, intent(in) :: flv_real
    integer, intent(inout) :: i_file
end subroutine blha_master_generate_real_tree
```

<BLHA config: procedures>+≡

```
module subroutine blha_master_generate_real_tree (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_real, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in
    integer, intent(in) :: alpha_power, alphas_power
    integer, dimension(:,:), allocatable, intent(in) :: flv_real
    integer, intent(inout) :: i_file
    type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
    integer :: i_flv
    if (master%compute_real_trees) then
        if (allocated (flv_real)) then
            allocate (blha_flavor (size (flv_real, 2)))
            do i_flv = 1, size (flv_real, 2)
                allocate (blha_flavor(i_flv)%flavors (size (flv_real(:,i_flv))))
                blha_flavor(i_flv)%flavors = flv_real(:,i_flv)
                blha_flavor(i_flv)%flv_mult = 1
            end do
            master%suffix(i_file) = blha_get_additional_suffix (var_str ("_REAL"))
            call blha_init_real (master%blha_cfg(i_file), blha_flavor, &
                n_in, alpha_power, alphas_power, master%ew_scheme, &
                basename, model, master%blha_mode(3), master%suffix(i_file))
            i_file = i_file + 1
        else
            call msg_fatal ("BLHA Trees requested but "&
                // "Real flavor not existing")
        end if
    end if
end subroutine blha_master_generate_real_tree
```

<BLHA config: blha master: TBP>+≡

```
procedure :: generate_born => blha_master_generate_born
```

<BLHA config: sub interfaces>+≡

```
module subroutine blha_master_generate_born (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_born, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
```

```

        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
    end subroutine blha_master_generate_born

<BLHA config: procedures>+≡
    module subroutine blha_master_generate_born (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
        type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
        integer :: i_flv
        if (master%compute_borns) then
            if (allocated (flv_born)) then
                allocate (blha_flavor (size (flv_born, 2)))
                do i_flv = 1, size (flv_born, 2)
                    allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
                    blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
                    blha_flavor(i_flv)%flv_mult = 1
                end do
                master%suffix(i_file) = blha_get_additional_suffix (var_str ("_BORN"))
                call blha_init_born (master%blha_cfg(i_file), blha_flavor, &
                    n_in, alpha_power, alphas_power, master%ew_scheme, &
                    basename, model, master%blha_mode(4), master%suffix(i_file))
                i_file = i_file + 1
            end if
        end if
    end subroutine blha_master_generate_born

<BLHA config: blha master: TBP>+≡
    procedure :: generate_dglap => blha_master_generate_dglap

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_generate_dglap (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
    end subroutine blha_master_generate_dglap

<BLHA config: procedures>+≡
    module subroutine blha_master_generate_dglap (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master

```

```

type(string_t), intent(in) :: basename
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in
integer, intent(in) :: alpha_power, alphas_power
integer, dimension(:,:), allocatable, intent(in) :: flv_born
integer, intent(inout) :: i_file
type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
integer :: i_flv
if (master%compute_dglap) then
  if (allocated (flv_born)) then
    allocate (blha_flavor (size (flv_born, 2)))
    do i_flv = 1, size (flv_born, 2)
      allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
      blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
      blha_flavor(i_flv)%flv_mult = 2
    end do
    master%suffix(i_file) = blha_get_additional_suffix (var_str ("_DGLAP"))
    call blha_init_dglap (master%blha_cfg(i_file), blha_flavor, &
      n_in, alpha_power, alphas_power, master%ew_scheme, &
      basename, model, master%blha_mode(5), master%suffix(i_file))
    i_file = i_file + 1
  end if
end if
end subroutine blha_master_generate_dglap

```

(BLHA config: blha master: TBP)+≡

```

procedure :: setup_additional_features => blha_master_setup_additional_features

```

(BLHA config: sub interfaces)+≡

```

module subroutine blha_master_setup_additional_features (master, &
  pbs_tolerance, use_cms, stability_log, extra_cmd, &
  allowed_libs, beam_structure)
class(blha_master_t), intent(inout) :: master
integer, intent(in) :: pbs_tolerance
logical, intent(in) :: use_cms
type(string_t), intent(in), optional :: extra_cmd, allowed_libs
integer, intent(in) :: stability_log
type(beam_structure_t), intent(in), optional :: beam_structure
end subroutine blha_master_setup_additional_features

```

(BLHA config: procedures)+≡

```

module subroutine blha_master_setup_additional_features (master, &
  pbs_tolerance, use_cms, stability_log, extra_cmd, &
  allowed_libs, beam_structure)
class(blha_master_t), intent(inout) :: master
integer, intent(in) :: pbs_tolerance
logical, intent(in) :: use_cms
type(string_t), intent(in), optional :: extra_cmd, allowed_libs
integer, intent(in) :: stability_log
type(beam_structure_t), intent(in), optional :: beam_structure
integer :: i_file
logical :: polarized, throw_warning

polarized = .false.
if (present (beam_structure)) polarized = beam_structure%has_polarized_beams ()

```



```

throw_warning = .false.
if (use_cms) then
  throw_warning = throw_warning .or. (master%compute_loops &
    .and. master%blha_mode(1) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_correlations &
    .and. master%blha_mode(2) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_real_trees &
    .and. master%blha_mode(3) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_borns &
    .and. master%blha_mode(4) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_dglap &
    .and. master%blha_mode(5) /= BLHA_MODE_OPENLOOPS)
  if (throw_warning) call cms_warning ()
end if

do i_file = 1, master%n_files
  if (phs_tolerance > 0) then
    select case (master%blha_mode (master%i_file_to_nlo_index(i_file)))
    case (BLHA_MODE_GOSAM)
      if (polarized) call gosam_error_message ()
    case (BLHA_MODE_OPENLOOPS)
      master%blha_cfg(i_file)%openloops_use_cms = use_cms
      master%blha_cfg(i_file)%openloops_phs_tolerance = phs_tolerance
      master%blha_cfg(i_file)%polarized = polarized
      if (present (extra_cmd)) then
        master%blha_cfg(i_file)%openloops_extra_cmd = extra_cmd
      else
        master%blha_cfg(i_file)%openloops_extra_cmd = var_str ('')
      end if
      if (present (allowed_libs)) then
        master%blha_cfg(i_file)%openloops_allowed_libs = allowed_libs
      else
        master%blha_cfg(i_file)%openloops_allowed_libs = var_str ('')
      end if
      master%blha_cfg(i_file)%openloops_stability_log = stability_log
    end select
  end if
end do
contains
subroutine cms_warning ()
  call msg_warning ("You have set ?openloops_use_cms = true, but not all active matrix ", &
    [var_str ("element methods are set to OpenLoops. Note that other "), &
    var_str ("methods might not necessarily support the complex mass "), &
    var_str ("scheme. This can yield inconsistencies in your NLO results!")])
end subroutine cms_warning

subroutine gosam_error_message ()
  call msg_fatal ("You are trying to evaluate a process at NLO ", &
    [var_str ("which involves polarized beams using GoSam. "), &
    var_str ("This feature is not supported yet. "), &
    var_str ("Please use OpenLoops instead")])
end subroutine gosam_error_message
end subroutine blha_master_setup_additional_features

```

```

<BLHA config: blha master: TBP>+≡
    procedure :: set_gosam => blha_master_set_gosam

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_gosam (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
    end subroutine blha_master_set_gosam

<BLHA config: procedures>+≡
    module subroutine blha_master_set_gosam (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_mode(i) = BLHA_MODE_GOSAM
    end subroutine blha_master_set_gosam

<BLHA config: blha master: TBP>+≡
    procedure :: set_openloops => blha_master_set_openloops

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_openloops (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
    end subroutine blha_master_set_openloops

<BLHA config: procedures>+≡
    module subroutine blha_master_set_openloops (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_mode(i) = BLHA_MODE_OPENLOOPS
    end subroutine blha_master_set_openloops

<BLHA config: blha master: TBP>+≡
    procedure :: set_polarization => blha_master_set_polarization

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_set_polarization (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
    end subroutine blha_master_set_polarization

<BLHA config: procedures>+≡
    module subroutine blha_master_set_polarization (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_cfg(i)%polarized = .true.
    end subroutine blha_master_set_polarization

<BLHA config: procedures>+≡
    subroutine blha_init_born (blha_cfg, blha_flavor, n_in, &
        ap, asp, ew_scheme, basename, model, blha_mode, suffix)
        type(blha_configuration_t), intent(inout) :: blha_cfg
        type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
        integer, intent(in) :: n_in

```

```

integer, intent(in) :: ap, asp
integer, intent(in) :: ew_scheme
type(string_t), intent(in) :: basename
type(model_data_t), intent(in), target :: model
integer, intent(in) :: blha_mode
type(string_t), intent(in) :: suffix
integer, dimension(:), allocatable :: amp_type
integer :: i, n_cp_loopind

allocate (amp_type (size (blha_flavor)))
n_cp_loopind = 0
n_cp_loopind = size (blha_flavor(1)%flavors)
if ((ap + asp) == n_cp_loopind) then
  do i = 1, size (blha_flavor)
    amp_type(i) = BLHA_AMP_LOOPINDUCED
  end do
else
  do i = 1, size (blha_flavor)
    amp_type(i) = BLHA_AMP_TREE
  end do
end if
call blha_configuration_init (blha_cfg, basename // suffix , &
  model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
  blha_flavor, amp_type)
call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
  irreg = BLHA_IRREG_CDR, alphas_power = asp, &
  alpha_power = ap, ew_scheme = ew_scheme, &
  debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_born

subroutine blha_init_virtual (blha_cfg, blha_flavor, n_in, &
  ap, asp, ew_scheme, basename, model, blha_mode, suffix)
type(blha_configuration_t), intent(inout) :: blha_cfg
type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
integer, intent(in) :: n_in
integer, intent(in) :: ap, asp
integer, intent(in) :: ew_scheme
type(string_t), intent(in) :: basename
type(model_data_t), intent(in), target :: model
integer, intent(in) :: blha_mode
type(string_t), intent(in) :: suffix
integer, dimension(:), allocatable :: amp_type
integer :: i

allocate (amp_type (size (blha_flavor) * 2))
do i = 1, size (blha_flavor)
  amp_type(2 * i - 1) = BLHA_AMP_LOOP
  amp_type(2 * i) = BLHA_AMP_COLOR_C
end do
call blha_configuration_init (blha_cfg, basename // suffix , &
  model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
  blha_flavor, amp_type)

```

```

call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, &
    alphas_power = asp, &
    alpha_power = ap, &
    ew_scheme = ew_scheme, &
    debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_virtual

subroutine blha_init_dglap (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
    type(blha_configuration_t), intent(inout) :: blha_cfg
    type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
    integer, intent(in) :: n_in
    integer, intent(in) :: ap, asp
    integer, intent(in) :: ew_scheme
    type(string_t), intent(in) :: basename
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: blha_mode
    type(string_t), intent(in) :: suffix
    integer, dimension(:), allocatable :: amp_type
    integer :: i

    allocate (amp_type (size (blha_flavor) * 2))
    do i = 1, size (blha_flavor)
        amp_type(2 * i - 1) = BLHA_AMP_TREE
        amp_type(2 * i) = BLHA_AMP_COLOR_C
    end do
    call blha_configuration_init (blha_cfg, basename // suffix, &
        model, blha_mode)
    call blha_configuration_append_processes (blha_cfg, n_in, &
        blha_flavor, amp_type)
    call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
        irreg = BLHA_IRREG_CDR, &
        alphas_power = asp, &
        alpha_power = ap, &
        ew_scheme = ew_scheme, &
        debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_dglap

subroutine blha_init_subtraction (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
    type(blha_configuration_t), intent(inout) :: blha_cfg
    type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
    integer, intent(in) :: n_in
    integer, intent(in) :: ap, asp
    integer, intent(in) :: ew_scheme
    type(string_t), intent(in) :: basename
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: blha_mode
    type(string_t), intent(in) :: suffix
    integer, dimension(:), allocatable :: amp_type
    integer :: i

    allocate (amp_type (size (blha_flavor) * 3))

```

```

do i = 1, size (blha_flavor)
  amp_type(3 * i - 2) = BLHA_AMP_TREE
  amp_type(3 * i - 1) = BLHA_AMP_COLOR_C
  amp_type(3 * i) = BLHA_AMP_SPIN_C
end do
call blha_configuration_init (blha_cfg, basename // suffix , &
  model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
  blha_flavor, amp_type)
call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
  irreg = BLHA_IRREG_CDR, &
  alphas_power = asp, &
  alpha_power = ap, &
  ew_scheme = ew_scheme, &
  debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_subtraction

subroutine blha_init_real (blha_cfg, blha_flavor, n_in, &
  ap, asp, ew_scheme, basename, model, blha_mode, suffix)
  type(blha_configuration_t), intent(inout) :: blha_cfg
  type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
  integer, intent(in) :: n_in
  integer, intent(in) :: ap, asp
  integer :: ap_ew, ap_qcd
  integer, intent(in) :: ew_scheme
  type(string_t), intent(in) :: basename
  type(model_data_t), intent(in), target :: model
  integer, intent(in) :: blha_mode
  type(string_t), intent(in) :: suffix
  integer, dimension(:), allocatable :: amp_type
  integer :: i

  allocate (amp_type (size (blha_flavor)))
  do i = 1, size (blha_flavor)
    amp_type(i) = BLHA_AMP_TREE
  end do
  select case (blha_cfg%correction_type)
  case (BLHA_CT_QCD)
    ap_ew = ap
    ap_qcd = asp + 1
  case (BLHA_CT_EW)
    ap_ew = ap + 1
    ap_qcd = asp
  end select
  call blha_configuration_init (blha_cfg, basename // suffix , &
    model, blha_mode)
  call blha_configuration_append_processes (blha_cfg, n_in, &
    blha_flavor, amp_type)

  call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, &
    alphas_power = ap_qcd, &
    alpha_power = ap_ew, &
    ew_scheme = ew_scheme, &

```

```

        debug = blha_mode == BLHA_MODE_GOSAM)
    end subroutine blha_init_real

<BLHA config: public>+≡
    public :: blha_get_additional_suffix

<BLHA config: sub interfaces>+≡
    module function blha_get_additional_suffix (base_suffix) result (suffix)
        type(string_t) :: suffix
        type(string_t), intent(in) :: base_suffix
    end function blha_get_additional_suffix

<BLHA config: procedures>+≡
    module function blha_get_additional_suffix (base_suffix) result (suffix)
        type(string_t) :: suffix
        type(string_t), intent(in) :: base_suffix
    <blha master: blha master extend suffixes: variables>
        suffix = base_suffix
    <blha master: blha master extend suffixes: procedure>
    end function blha_get_additional_suffix

<MPI: blha master: blha master extend suffixes: variables>≡
    integer :: n_size, rank

<MPI: blha master: blha master extend suffixes: procedure>≡
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    if (n_size > 1) then
        suffix = suffix // var_str ("-") // str (rank)
    end if

<BLHA config: blha master: TBP>+≡
    procedure :: write_olp => blha_master_write_olp

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_write_olp (master, basename)
        class(blha_master_t), intent(in) :: master
        type(string_t), intent(in) :: basename
    end subroutine blha_master_write_olp

<BLHA config: procedures>+≡
    module subroutine blha_master_write_olp (master, basename)
        class(blha_master_t), intent(in) :: master
        type(string_t), intent(in) :: basename
        integer :: unit
        type(string_t) :: filename
        integer :: i_file
        do i_file = 1, master%n_files
            filename = basename // master%suffix(i_file) // ".olp"
            unit = free_unit ()
            open (unit, file = char (filename), status = 'replace', action = 'write')
            call blha_configuration_write &
                (master%blha_cfg(i_file), master%suffix(i_file), unit)
            close (unit)
        end do
    end subroutine blha_master_write_olp

```

```

<BLHA config: blha master: TBP>+≡
    procedure :: final => blha_master_final

<BLHA config: sub interfaces>+≡
    module subroutine blha_master_final (master)
        class(blha_master_t), intent(inout) :: master
    end subroutine blha_master_final

<BLHA config: procedures>+≡
    module subroutine blha_master_final (master)
        class(blha_master_t), intent(inout) :: master
        master%n_files = 0
        deallocate (master%suffix)
        deallocate (master%blha_cfg)
        deallocate (master%i_file_to_nlo_index)
    end subroutine blha_master_final

<BLHA config: public>+≡
    public :: blha_configuration_init

<BLHA config: sub interfaces>+≡
    module subroutine blha_configuration_init (cfg, name, model, mode)
        type(blha_configuration_t), intent(inout) :: cfg
        type(string_t), intent(in) :: name
        class(model_data_t), target, intent(in) :: model
        integer, intent(in), optional :: mode
    end subroutine blha_configuration_init

<BLHA config: procedures>+≡
    module subroutine blha_configuration_init (cfg, name, model, mode)
        type(blha_configuration_t), intent(inout) :: cfg
        type(string_t), intent(in) :: name
        class(model_data_t), target, intent(in) :: model
        integer, intent(in), optional :: mode
        if (.not. associated (cfg%model)) then
            cfg%name = name
            cfg%model => model
        end if
        if (present (mode)) cfg%mode = mode
    end subroutine blha_configuration_init

```

Create an array of massive particle indices, to be used by the "MassiveParticle"-statement of the order file.

```

<BLHA config: procedures>+≡
    subroutine blha_configuration_get_massive_particles &
        (cfg, massive, i_massive)
        type(blha_configuration_t), intent(in) :: cfg
        logical, intent(out) :: massive
        integer, intent(out), dimension(:), allocatable :: i_massive
        integer, parameter :: max_particles = 10
        integer, dimension(max_particles) :: i_massive_tmp
        integer, dimension(max_particles) :: checked
        type(blha_cfg_process_node_t), pointer :: current_process
        integer :: k
        integer :: n_massive

```

```

n_massive = 0; k = 1
checked = 0
if (associated (cfg%processes)) then
    current_process => cfg%processes
else
    call msg_fatal ("BLHA, massive particles: " // &
        "No processes allocated!")
end if
do
    call check_pdg_list (current_process%pdg_in%pdg)
    call check_pdg_list (current_process%pdg_out%pdg)
    if (k > max_particles) &
        call msg_fatal ("BLHA, massive particles: " // &
            "Max. number of particles exceeded!")
    if (associated (current_process%next)) then
        current_process => current_process%next
    else
        exit
    end if
end do
if (n_massive > 0) then
    allocate (i_massive (n_massive))
    i_massive = i_massive_tmp (1:n_massive)
    massive = .true.
else
    massive = .false.
end if
contains
subroutine check_pdg_list (pdg_list)
    integer, dimension(:), intent(in) :: pdg_list
    integer :: i, i_pdg
    type(flavor_t) :: flv
    do i = 1, size (pdg_list)
        i_pdg = abs (pdg_list(i))
        call flv%init (i_pdg, cfg%model)
        if (flv%get_mass () > 0._default) then
            !!! Avoid duplicates in output
            if (.not. any (checked == i_pdg)) then
                i_massive_tmp(k) = i_pdg
                checked(k) = i_pdg
                k = k + 1
                n_massive = n_massive + 1
            end if
        end if
    end do
end subroutine check_pdg_list
end subroutine blha_configuration_get_massive_particles

```

<BLHA config: public>+≡

public :: blha_configuration_append_processes

<BLHA config: sub interfaces>+≡

module subroutine blha_configuration_append_processes (cfg, n_in, flavor, amp_type)
 type(blha_configuration_t), intent(inout) :: cfg


```

integer, intent(in) :: n_in
type(blha_flv_state_t), dimension(:), intent(in) :: flavor
integer, dimension(:), intent(in), optional :: amp_type
end subroutine blha_configuration_append_processes

<BLHA config: procedures>+≡
module subroutine blha_configuration_append_processes (cfg, n_in, flavor, amp_type)
type(blha_configuration_t), intent(inout) :: cfg
integer, intent(in) :: n_in
type(blha_flv_state_t), dimension(:), intent(in) :: flavor
integer, dimension(:), intent(in), optional :: amp_type
integer :: n_tot
type(blha_cfg_process_node_t), pointer :: current_node
integer :: i_process, i_flv
integer, dimension(:), allocatable :: pdg_in, pdg_out
integer, dimension(:), allocatable :: flavor_state
integer :: proc_offset, n_proc_tot
proc_offset = 0; n_proc_tot = 0
do i_flv = 1, size (flavor)
    n_proc_tot = n_proc_tot + flavor(i_flv)%flv_mult
end do
if (.not. associated (cfg%processes)) &
    allocate (cfg%processes)
current_node => cfg%processes
do i_flv = 1, size (flavor)
    n_tot = size (flavor(i_flv)%flavors)
    allocate (pdg_in (n_in), pdg_out (n_tot - n_in))
    allocate (flavor_state (n_tot))
    flavor_state = flavor(i_flv)%flavors
    do i_process = 1, flavor(i_flv)%flv_mult
        pdg_in = flavor_state (1 : n_in)
        pdg_out = flavor_state (n_in + 1 : )
        if (cfg%polarized) then
            select case (cfg%mode)
            case (BLHA_MODE_OPENLOOPS)
                call allocate_and_init_pdg_and_helicities (current_node, &
                    pdg_in, pdg_out, amp_type (proc_offset + i_process))
            case (BLHA_MODE_GOSAM)
                !!! Nothing special for GoSam yet. This exception is already caught
                !!! in blha_master_setup_additional_features
            end select
        else
            call allocate_and_init_pdg (current_node, pdg_in, pdg_out, &
                amp_type (proc_offset + i_process))
        end if
        if (proc_offset + i_process /= n_proc_tot) then
            allocate (current_node%next)
            current_node => current_node%next
        end if
        if (i_process == flavor(i_flv)%flv_mult) &
            proc_offset = proc_offset + flavor(i_flv)%flv_mult
    end do
    deallocate (pdg_in, pdg_out)
    deallocate (flavor_state)
end do

```

contains

```

subroutine allocate_and_init_pdg (node, pdg_in, pdg_out, amp_type)
  type(blha_cfg_process_node_t), intent(inout), pointer :: node
  integer, intent(in), dimension(:), allocatable :: pdg_in, pdg_out
  integer, intent(in) :: amp_type
  allocate (node%pdg_in (size (pdg_in)))
  allocate (node%pdg_out (size (pdg_out)))
  node%pdg_in%pdg = pdg_in
  node%pdg_out%pdg = pdg_out
  node%amplitude_type = amp_type
end subroutine allocate_and_init_pdg

subroutine allocate_and_init_pdg_and_helicities (node, pdg_in, pdg_out, amp_type)
  type(blha_cfg_process_node_t), intent(inout), pointer :: node
  integer, intent(in), dimension(:), allocatable :: pdg_in, pdg_out
  integer, intent(in) :: amp_type
  integer :: h1, h2
  if (size (pdg_in) == 2) then
    do h1 = -1, 1, 2
      do h2 = -1, 1, 2
        call allocate_and_init_pdg (current_node, pdg_in, pdg_out, amp_type)
        current_node%pdg_in(1)%polarized = .true.
        current_node%pdg_in(2)%polarized = .true.
        current_node%pdg_in(1)%hel = h1
        current_node%pdg_in(2)%hel = h2
        if (h1 + h2 /= 2) then !!! not end of loop
          allocate (current_node%next)
          current_node => current_node%next
        end if
      end do
    end do
  else
    do h1 = -1, 1, 2
      call allocate_and_init_pdg (current_node, pdg_in, pdg_out, amp_type)
      current_node%pdg_in(1)%polarized = .true.
      current_node%pdg_in(1)%hel = h1
      if (h1 /= 1) then !!! not end of loop
        allocate (current_node%next)
        current_node => current_node%next
      end if
    end do
  end if
end subroutine allocate_and_init_pdg_and_helicities

end subroutine blha_configuration_append_processes

```

Change parameter(s).

(BLHA config: public)+≡

public :: blha_configuration_set

(BLHA config: sub interfaces)+≡

module subroutine blha_configuration_set (cfg, &

```

        version, irreg, massive_particle_scheme, &
        model_file, alphas_power, alpha_power, ew_scheme, width_scheme, &
        accuracy, debug)
type(blha_configuration_t), intent(inout) :: cfg
integer, optional, intent(in) :: version
integer, optional, intent(in) :: irreg
integer, optional, intent(in) :: massive_particle_scheme
type(string_t), optional, intent(in) :: model_file
integer, optional, intent(in) :: alphas_power, alpha_power
integer, optional, intent(in) :: ew_scheme
integer, optional, intent(in) :: width_scheme
real(default), optional, intent(in) :: accuracy
logical, optional, intent(in) :: debug
end subroutine blha_configuration_set

```

(BLHA config: procedures)+≡

```

module subroutine blha_configuration_set (cfg, &
        version, irreg, massive_particle_scheme, &
        model_file, alphas_power, alpha_power, ew_scheme, width_scheme, &
        accuracy, debug)
type(blha_configuration_t), intent(inout) :: cfg
integer, optional, intent(in) :: version
integer, optional, intent(in) :: irreg
integer, optional, intent(in) :: massive_particle_scheme
type(string_t), optional, intent(in) :: model_file
integer, optional, intent(in) :: alphas_power, alpha_power
integer, optional, intent(in) :: ew_scheme
integer, optional, intent(in) :: width_scheme
real(default), optional, intent(in) :: accuracy
logical, optional, intent(in) :: debug
if (present (version)) &
    cfg%version = version
if (present (irreg)) &
    cfg%irreg = irreg
if (present (massive_particle_scheme)) &
    cfg%massive_particle_scheme = massive_particle_scheme
if (present (model_file)) &
    cfg%model_file = model_file
if (present (alphas_power)) &
    cfg%alphas_power = alphas_power
if (present (alpha_power)) &
    cfg%alpha_power = alpha_power
if (present (ew_scheme)) &
    cfg%ew_scheme = ew_scheme
if (present (width_scheme)) &
    cfg%width_scheme = width_scheme
if (present (accuracy)) &
    cfg%accuracy_target = accuracy
if (present (debug)) &
    cfg%debug_unstable = debug
cfg%dirty = .false.
end subroutine blha_configuration_set

```

(BLHA config: public)+≡

```

public :: blha_configuration_get_n_proc
<BLHA config: sub interfaces>+=
  module function blha_configuration_get_n_proc (cfg) result (n_proc)
    type(blha_configuration_t), intent(in) :: cfg
    integer :: n_proc
  end function blha_configuration_get_n_proc
<BLHA config: procedures>+=
  module function blha_configuration_get_n_proc (cfg) result (n_proc)
    type(blha_configuration_t), intent(in) :: cfg
    integer :: n_proc
    n_proc = cfg%n_proc
  end function blha_configuration_get_n_proc

```

Write the BLHA file. Internal mode is intended for md5summing only.

Special cases of external photons in `OpenLoops`:

For electroweak corrections the particle ID (PID) of photons is a crucial input for the computation of matrix elements by `OpenLoops`. According to "arXiv: 1907.13071", section 3.2, external photons are classified by the following types:

- PID = -2002: off-shell photons, that undergo $\gamma \rightarrow f\bar{f}$ splittings at NLO EW, or initial state photons from QED PDFs
- PID = 2002: on-shell photons, that do not undergo $\gamma \rightarrow f\bar{f}$ splittings at NLO EW, or initial state photons for example at photon colliders
- PID = 22: unresolved photons, representing radiated photons at NLO EW, absent at LO

For the first two types scattering amplitudes for processes with external photons at NLO EW get renormalisation factors containing photon-coupling and wave function counterterms. Logarithmic mass singularities arising due to the renormalisation of off-shell external photon wave functions are cancelled by collinear singularities of photon PDF counterterms or analogous terms in virtual contributions originating from $\gamma \rightarrow f\bar{f}$ splittings of final state photons.

The finite remainders of the renormalisation factors are thus dictated by the specific photon PID stated above. As consequence, we have to adjust the input PIDs written into the BLHA file which will be read by `OpenLoops`.

Concretely, for the case of electroweak corrections initial state photons associated with photon PDFs and final state photons (if existent at LO) are labeled as off-shell photons with PID "-2002". On-shell photons with PID "2002" are neglected for now since to include them for processes at NLO EW is non-trivial from the phenomenological point of view. Processes at NLO EW typically are studied at high energy scales for which photon-induced sub-processes in most cases can not be neglected. However, on-shell, e. g. tagged, photons are defined at low energy scales and thus the process has to be described with external photon fields and couplings at two different scales.

Another issue which has to be addressed if various photon PIDs are taken into account is that real and virtual amplitudes have to be computed at the same order in α at a specific scale for the subtraction scheme to be consistent. The complication comes by the fact that the EW coupling α of each external photon in the amplitudes will automatically be rescaled by `OpenLoops` corresponding

to the specific photon type. Following eq. (3.30) of "arXiv: 1907.13071", by default the coupling of an on-shell photon will be changed to $\alpha(0)$ and that of an off-shell photon to α_{G_μ} if not chosen already at a high scale, e. g. $\alpha(M_Z)$. In order to not spoil the IR cancellation `OpenLoops` supplies to register unresolved photons with PID "22" describing a radiated photon at NLO EW for which the photon-coupling α is left unchanged at the value which is computed with the electroweak input scheme chosen by the user. This is adopted here by labeling each emitted photon as unresolved with PID "22" if no photons are present at LO.

For EW corrections the freedom to choose an electroweak input scheme is restricted, however, since the number of external photons present at LO is not conserved for the corresponding real flavor structures due to possible $\gamma \rightarrow f\bar{f}$ splittings. This forbids to choose $\alpha = \alpha(0)$ since otherwise the order in $\alpha(0)$ is not conserved in the real amplitudes corresponding to the factorizing Born process. Consequently, for FKS the NLO components are not of the same order in $\alpha(0)$. The option `$blha_ew_scheme = "alpha_0"` is thus refused for the case if EW corrections are activated and photons are present at LO.

```

<BLHA config: public>+≡
    public :: blha_configuration_write

<BLHA config: sub interfaces>+≡
    module subroutine blha_configuration_write (cfg, suffix, unit, internal, no_version)
        type(blha_configuration_t), intent(in) :: cfg
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: internal, no_version
        type(string_t), intent(in) :: suffix
    end subroutine blha_configuration_write

<BLHA config: procedures>+≡
    module subroutine blha_configuration_write (cfg, suffix, unit, internal, no_version)
        type(blha_configuration_t), intent(in) :: cfg
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: internal, no_version
        type(string_t), intent(in) :: suffix
        integer, dimension(:), allocatable :: pdg_flv
        integer :: u
        logical :: full, nlo3
        type(string_t) :: buf
        type(blha_cfg_process_node_t), pointer :: node
        integer :: i
        character(3) :: pdg_char
        character(5) :: pdg_char_extra
        character(4) :: hel_char
        character(6) :: suffix_char
        character(len=25), parameter :: pad = ""
        logical :: write_process, no_v, loop_ind
        no_v = .false. ; if (present (no_version)) no_v = no_version
        u = given_output_unit (unit); if (u < 0) return
        full = .true.; if (present (internal)) full = .not. internal
        loop_ind = .false.
        if (full .and. cfg%dirty) call msg_bug ( &
            "BUG: attempted to write out a dirty BLHA configuration")
        if (full) then
            if (no_v) then

```

```

        write (u, "(A)") "# BLHA order written by WHIZARD [version]"
    else
        write (u, "(A)") "# BLHA order written by WHIZARD <Version>"
    end if
    write (u, "(A)")
end if
select case (cfg%mode)
    case (BLHA_MODE_GOSAM); buf = "GoSam"
    case (BLHA_MODE_OPENLOOPS); buf = "OpenLoops"
    case default; buf = "vanilla"
end select
write (u, "(A)") "# BLHA interface mode: " // char (buf)
write (u, "(A)") "# process: " // char (cfg%name)
write (u, "(A)") "# model: " // char (cfg%model%get_name ())
select case (cfg%version)
    case (1); buf = "BLHA1"
    case (2); buf = "BLHA2"
end select
write (u, '(A25,A)') "InterfaceVersion " // pad, char (buf)
node => cfg%processes
do while (associated (node))
    loop_ind = node%amplitude_type == BLHA_AMP_LOOPINDUCED
    node => node%next
end do
if (.not. loop_ind) then
    select case (cfg%correction_type)
        case (BLHA_CT_QCD); buf = "QCD"
        case (BLHA_CT_EW); buf = "EW"
        case default; buf = cfg%correction_type_other
    end select
    write (u, '(A25,A)') "CorrectionType" // pad, char (buf)
end if

select case (cfg%mode)
case (BLHA_MODE_OPENLOOPS)
    buf = cfg%name // '.olc'
    write (u, '(A25,A)') "Extra AnswerFile" // pad, char (buf)
end select

select case (cfg%irreg)
    case (BLHA_IRREG_CDR); buf = "CDR"
    case (BLHA_IRREG_DRED); buf = "DRED"
    case (BLHA_IRREG_THV); buf = "tHV"
    case (BLHA_IRREG_MREG); buf = "MassReg"
    case default; buf = cfg%irreg_other
end select
write (u, '(A25,A)') "IRregularisation" // pad, char (buf)
select case (cfg%massive_particle_scheme)
    case (BLHA_MPS_ONSHELL); buf = "OnShell"
    case default; buf = cfg%massive_particle_scheme_other
end select
if (cfg%mode == BLHA_MODE_GOSAM) &
    write (u, '(A25,A)') "MassiveParticleScheme" // pad, char (buf)
select case (cfg%version)

```

```

case (1)
  if (cfg%alphas_power >= 0) write (u,'(A25,A)') &
    "AlphasPower" // pad, int2char (cfg%alphas_power)
  if (cfg%alpha_power >= 0) write (u,'(A25,A)') &
    "AlphaPower " // pad, int2char (cfg%alpha_power)
case (2)
  if (cfg%alphas_power >= 0) write (u,'(A25,A)') &
    "CouplingPower QCD " // pad, int2char (cfg%alphas_power)
  if (cfg%alpha_power >= 0) write (u,'(A25,A)') &
    "CouplingPower QED " // pad, int2char (cfg%alpha_power)
end select
select case (cfg%mode)
case (BLHA_MODE_GOSAM)
  select case (cfg%ew_scheme)
    case (BLHA_EW_GF, BLHA_EW_INTERNAL); buf = "alphaGF"
    case (BLHA_EW_MZ); buf = "alphaMZ"
    case (BLHA_EW_MSBAR); buf = "alphaMSbar"
    case (BLHA_EW_0); buf = "alpha0"
    case (BLHA_EW_RUN); buf = "alphaRUN"
  end select
  write (u,'(A25, A)') "EWScheme " // pad, char (buf)
case (BLHA_MODE_OPENLOOPS)
  select case (cfg%ew_scheme)
    case (BLHA_EW_0); buf = "alpha0"
    case (BLHA_EW_GF); buf = "Gmu"
    case (BLHA_EW_MZ, BLHA_EW_INTERNAL); buf = "alphaMZ"
    case default
      call msg_fatal ("OpenLoops input: Only supported EW schemes &
        & are 'alpha0', 'Gmu', and 'alphaMZ'")
    end select
  write (u,'(A25, A)') "ewscheme " // pad, char (buf)
end select
select case (cfg%mode)
case (BLHA_MODE_GOSAM)
  write (u,'(A25)', advance='no') "MassiveParticles " // pad
  do i = 1, size (OLP_MASSIVE_PARTICLES)
    if (OLP_MASSIVE_PARTICLES(i) > 0) &
      write (u,'(I2,I1)', advance='no') OLP_MASSIVE_PARTICLES(i)
  end do
  write (u,*)
case (BLHA_MODE_OPENLOOPS)
  if (cfg%openloops_use_cms) then
    write (u,'(A25,I1)') "extra use_cms " // pad, 1
  else
    write (u,'(A25,I1)') "extra use_cms " // pad, 0
  end if
  write (u,'(A25,I1)') "extra me_cache " // pad, 0
  !!! Turn off calculation of 1/eps & 1/eps^2 poles in one-loop calculation
  !!! Not needed in FKS (or any numerical NLO subtraction scheme)
  write (u,'(A25,I1)') "extra IR_on " // pad, 0
  if (cfg%openloops_phs_tolerance > 0) then
    write (u,'(A25,A4,I0)') "extra psp_tolerance " // pad, "10e-", &
      cfg%openloops_phs_tolerance
  end if

```

```

call check_extra_cmd (cfg%openloops_extra_cmd)
write (u, '(A)') char (cfg%openloops_extra_cmd)
if (cfg%openloops_allowed_libs /= '') then
  write (u, '(A25,A)') "extra allowed_libs" // pad, &
    char (cfg%openloops_allowed_libs)
end if
if (cfg%openloops_stability_log > 0) &
  write (u, '(A25,I1)') "extra stability_log " // pad, &
    cfg%openloops_stability_log
end select
if (full) then
  write (u, "(A)")
  write (u, "(A)") "# Process definitions"
  write (u, "(A)")
end if
if (cfg%debug_unstable) &
  write (u, '(A25,A)') "DebugUnstable " // pad, "True"
write (u, *)
node => cfg%processes
do while (associated (node))
  write_process = .true.
  allocate (pdg_flv (size (node%pdg_in) + size (node%pdg_out)))
  do i = 1, size (node%pdg_in)
    pdg_flv (i) = node%pdg_in(i)%pdg
  end do
  do i = 1, size (node%pdg_out)
    pdg_flv (i + size (node%pdg_in)) = node%pdg_out(i)%pdg
  end do
  suffix_char = char (suffix)
  if (cfg%correction_type == BLHA_CT_EW .and. cfg%alphas_power > 0) then
    if ((suffix_char (1:5) == "_BORN" .and. .not. query_coupling_powers &
      (pdg_flv, cfg%alpha_power, cfg%alphas_power)) .or. &
      ((suffix_char (1:4) == "_SUB" .or. suffix_char (1:5) == "_LOOP" .or. &
      suffix_char (1:6) == "_DGLAP") .and. (.not. (query_coupling_powers &
      (pdg_flv, cfg%alpha_power, cfg%alphas_power) .or. query_coupling_powers &
      (pdg_flv, cfg%alpha_power + 1, cfg%alphas_power - 1)) .or. &
      all (is_gluon (pdg_flv)))))) then
      deallocate (pdg_flv)
      node => node%next
      cycle
    end if
  end if
  select case (node%amplitude_type)
    case (BLHA_AMP_LOOP); buf = "Loop"
    case (BLHA_AMP_COLOR_C); buf = "ccTree"
    case (BLHA_AMP_SPIN_C)
      if (cfg%mode == BLHA_MODE_OPENLOOPS) then
        buf = "sctree_polvect"
      else
        buf = "scTree"
      end if
    case (BLHA_AMP_TREE); buf = "Tree"
    case (BLHA_AMP_LOOPINDUCED); buf = "LoopInduced"
  end select
end select

```



```

nlo3 = qcd_ew_interferences (pdg_flg) .and. &
  (node%amplitude_type == BLHA_AMP_COLOR_C .or. &
   node%amplitude_type == BLHA_AMP_SPIN_C) .and. &
  .not. query_coupling_powers (pdg_flg, cfg%alpha_power+2, cfg%alphas_power-2)
if (write_process) then
  write (u, '(A25, A)') "AmplitudeType " // pad, char (buf)
  buf = ""
  if (cfg%correction_type == BLHA_CT_EW .and. cfg%alphas_power > 0 .and. &
      (suffix_char (1:4) == "_SUB" .or. suffix_char (1:5) == "_LOOP" &
       .or. suffix_char (1:6) == "_DGLAP")) then
    if (query_coupling_powers (pdg_flg, cfg%alpha_power, cfg%alphas_power) &
        .and. .not. nlo3) then
      write (u, '(A25,A)') "CorrectionType" // pad, "EW"
      select case (cfg%version)
        case (1)
          if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
            "AlphasPower" // pad, int2char (cfg%alphas_power)
          if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
            "AlphaPower " // pad, int2char (cfg%alpha_power)
        case (2)
          if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
            "CouplingPower QCD " // pad, int2char (cfg%alphas_power)
          if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
            "CouplingPower QED " // pad, int2char (cfg%alpha_power)
      end select
    else if (query_coupling_powers &
              (pdg_flg, cfg%alpha_power + 1, cfg%alphas_power - 1)) then
      write (u, '(A25,A)') "CorrectionType" // pad, "QCD"
      select case (cfg%version)
        case (1)
          if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
            "AlphasPower" // pad, int2char (cfg%alphas_power - 1)
          if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
            "AlphaPower " // pad, int2char (cfg%alpha_power + 1)
        case (2)
          if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
            "CouplingPower QCD " // pad, int2char (cfg%alphas_power - 1)
          if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
            "CouplingPower QED " // pad, int2char (cfg%alpha_power + 1)
      end select
    end if
  end if
do i = 1, size (node%pdg_in)
  if (cfg%correction_type == BLHA_CT_EW .and. node%pdg_in(i)%pdg == PHOTON &
      .and. cfg%n_off_photons_is > 0) then
    if (cfg%ew_scheme == BLHA_EW_0) then
      call msg_fatal ("ew_scheme: 'alpha_0' or 'alpha_thompson' " &
                     // "in combination", [ var_str ("with off-shell external photons " &
                     // "is not consistent with FKS.")])
    end if
    write (pdg_char_extra, '(I5)') PHOTON_OFFSHELL
    buf = (buf // pdg_char_extra) // " "
  else
    call node%pdg_in(i)%write_pdg (pdg_char)
  end if
end do

```

```

        if (node%pdg_in(i)%polarized) then
            call node%pdg_in(i)%write_helicity (hel_char)
            buf = (buf // pdg_char // hel_char) // " "
        else
            buf = (buf // pdg_char) // " "
        end if
    end if
end do
buf = buf // "-> "
do i = 1, size (node%pdg_out)
    if (cfg%correction_type == BLHA_CT_EW .and. node%pdg_out(i)%pdg == PHOTON &
        .and. cfg%n_off_photons_fs > 0) then
        if (cfg%ew_scheme == BLHA_EW_0) then
            call msg_fatal ("ew_scheme: 'alpha_0' or 'alpha_thompson' " &
                // "in combination with off-shell external photons " &
                // "is not consistent with FKS. Try a different one.")
        end if
        write (pdg_char_extra, '(I5)') PHOTON_OFFSHELL
        buf = (buf // pdg_char_extra) // " "
    else
        call node%pdg_out(i)%write_pdg (pdg_char)
        buf = (buf // pdg_char) // " "
    end if
end do
write (u, "(A)") char (trim (buf))
write (u, *)
end if
deallocate (pdg_flv)
node => node%next
end do
end subroutine blha_configuration_write

```

24.2 Module definition

These modules implement the communication with one loop matrix element providers according to the Binoth LesHouches Accord Interface. The actual matrix element(s) are loaded as a dynamic library.

This module defines the common OLP-interfaces defined through the Binoth Les-Houches accord.

`<blha_olp_interfaces.f90>`≡
<File header>

```

module blha_olp_interfaces

    use, intrinsic :: iso_c_binding !NODEP!
    use, intrinsic :: iso_fortran_env

    use kinds
    <Use strings>
    use os_interface
    use lorentz

```

```

    use interactions
    use model_data

    use prclib_interfaces
    use process_libraries
    use prc_core_def
    use prc_core
    use prc_external
    use blha_config

    <Standard module head>

    <BLHA OLP interfaces: public>

    <BLHA OLP interfaces: public parameters>

    <BLHA OLP interfaces: types>

    <BLHA OLP interfaces: interfaces>

    interface
    <BLHA OLP interfaces: sub interfaces>
    end interface

end module blha_olp_interfaces

<blha_olp_interfaces_sub.f90>≡
<File header>

submodule (blha_olp_interfaces) blha_olp_interfaces_s

    <Use debug>
    use constants
    use numeric_utils, only: vanishes
    use numeric_utils, only: extend_integer_array, crop_integer_array
    use io_units
    use string_utils
    use physics_defs
    use diagnostics
    use sm_qcd
    use flavors
    use pdg_arrays, only: is_gluon, is_quark, qcd_ew_interferences

    implicit none

    <BLHA OLP interfaces: parameters>

contains

    <BLHA OLP interfaces: procedures>

end submodule blha_olp_interfaces_s

```

```

<BLHA OLP interfaces: public>≡
  public :: blha_template_t

<BLHA OLP interfaces: types>≡
  type :: blha_template_t
    integer :: I_BORN = 0
    integer :: I_REAL = 1
    integer :: I_LOOP = 2
    integer :: I_SUB = 3
    integer :: I_DGLAP = 4
    logical, dimension(0:4) :: compute_component
    logical :: include_polarizations = .false.
    logical :: switch_off_muon_yukawas = .false.
    logical :: use_internal_color_correlations = .true.
    real(default) :: external_top_yukawa = -1._default
    integer :: ew_scheme
    integer :: loop_method = BLHA_MODE_GENERIC
  contains
    <BLHA OLP interfaces: blha template: TBP>
  end type blha_template_t

<BLHA OLP interfaces: blha template: TBP>≡
  procedure :: write => blha_template_write

<BLHA OLP interfaces: sub interfaces>≡
  module subroutine blha_template_write (blha_template, unit)
    class(blha_template_t), intent(in) :: blha_template
    integer, intent(in), optional :: unit
  end subroutine blha_template_write

<BLHA OLP interfaces: procedures>≡
  module subroutine blha_template_write (blha_template, unit)
    class(blha_template_t), intent(in) :: blha_template
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(A,4(L1))") "Compute components: ", &
      blha_template%compute_component
    write (u,"(A,L1)") "Include polarizations: ", &
      blha_template%include_polarizations
    write (u,"(A,L1)") "Switch off muon yukawas: ", &
      blha_template%switch_off_muon_yukawas
    write (u,"(A,L1)") "Use internal color correlations: ", &
      blha_template%use_internal_color_correlations
  end subroutine blha_template_write

```

Compute the total number of used helicity states for the given particle PDG codes, given a model. Applies only if polarization is supported. This yields the `n_hel` value as required below.

```

<BLHA OLP interfaces: blha template: TBP>+≡
  procedure :: get_n_hel => blha_template_get_n_hel

<BLHA OLP interfaces: sub interfaces>+≡
  module function blha_template_get_n_hel (blha_template, pdg, model) result (n_hel)
    class(blha_template_t), intent(in) :: blha_template

```

```

        integer, dimension(:), intent(in) :: pdg
        class(model_data_t), intent(in), target :: model
        integer :: n_hel
    end function blha_template_get_n_hel

<BLHA OLP interfaces: procedures>+≡
module function blha_template_get_n_hel (blha_template, pdg, model) result (n_hel)
    class(blha_template_t), intent(in) :: blha_template
    integer, dimension(:), intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
    integer :: n_hel
    type(flavor_t) :: flv
    integer :: f
    n_hel = 1
    if (blha_template%include_polarizations) then
        do f = 1, size (pdg)
            call flv%init (pdg(f), model)
            n_hel = n_hel * flv%get_multiplicity ()
        end do
    end if
end function blha_template_get_n_hel

<BLHA OLP interfaces: parameters>≡
integer, parameter :: I_ALPHA_0 = 1
integer, parameter :: I_GF = 2
integer, parameter :: I_ALPHA_MZ = 3
integer, parameter :: I_ALPHA_INTERNAL = 4
integer, parameter :: I_SW2 = 5

<BLHA OLP interfaces: public>+≡
public :: prc_blha_t

<BLHA OLP interfaces: types>+≡
type, abstract, extends (prc_external_t) :: prc_blha_t
    integer :: n_particles
    integer :: n_hel
    integer :: n_proc
    integer, dimension(:, :), allocatable :: i_tree, i_spin_c, i_color_c
    integer, dimension(:, :), allocatable :: i_virt
    integer, dimension(:, :), allocatable :: i_hel
    logical, dimension(5) :: ew_parameter_mask
    integer :: sqme_tree_pos
contains
    <BLHA OLP interfaces: prc blha: TBP>
end type prc_blha_t

```

Obviously, this process-core type uses the BLHA interface.

```

<BLHA OLP interfaces: prc blha: TBP>≡
    procedure, nopass :: uses_blha => prc_blha_uses_blha

<BLHA OLP interfaces: sub interfaces>+≡
    module function prc_blha_uses_blha () result (flag)
        logical :: flag
    end function prc_blha_uses_blha

```

```

<BLHA OLP interfaces: procedures>+≡
  module function prc_blha_uses_blha () result (flag)
    logical :: flag
    flag = .true.
  end function prc_blha_uses_blha

<BLHA OLP interfaces: public>+≡
  public :: blha_driver_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_driver_t) :: blha_driver_t
    type(string_t) :: contract_file
    type(string_t) :: nlo_suffix
    logical :: include_polarizations = .false.
    logical :: switch_off_muon_yukawas = .false.
    real(default) :: external_top_yukawa = -1.0
    procedure(olp_start), nopass, pointer :: &
      blha_olp_start => null ()
    procedure(olp_eval), nopass, pointer :: &
      blha_olp_eval => null ()
    procedure(olp_info), nopass, pointer :: &
      blha_olp_info => null ()
    procedure(olp_set_parameter), nopass, pointer :: &
      blha_olp_set_parameter => null ()
    procedure(olp_eval2), nopass, pointer :: &
      blha_olp_eval2 => null ()
    procedure(olp_option), nopass, pointer :: &
      blha_olp_option => null ()
    procedure(olp_polvec), nopass, pointer :: &
      blha_olp_polvec => null ()
    procedure(olp_finalize), nopass, pointer :: &
      blha_olp_finalize => null ()
    procedure(olp_print_parameter), nopass, pointer :: &
      blha_olp_print_parameter => null ()
  contains
    <BLHA OLP interfaces: blha driver: TBP>
  end type blha_driver_t

<BLHA OLP interfaces: public>+≡
  public :: prc_blha_writer_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_writer_t) :: prc_blha_writer_t
    type(blha_configuration_t) :: blha_cfg
  contains
    <BLHA OLP interfaces: blha writer: TBP>
  end type prc_blha_writer_t

<BLHA OLP interfaces: public>+≡
  public :: blha_def_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_def_t) :: blha_def_t
    type(string_t) :: suffix

```

```

contains
  <BLHA OLP interfaces: blha def: TBP>
end type blha_def_t

<BLHA OLP interfaces: public>+≡
  public :: blha_state_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_state_t) :: blha_state_t
  contains
    <BLHA OLP interfaces: blha state: TBP>
  end type blha_state_t

<BLHA OLP interfaces: blha state: TBP>≡
  procedure :: reset_new_kinematics => blha_state_reset_new_kinematics

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine blha_state_reset_new_kinematics (object)
    class(blha_state_t), intent(inout) :: object
  end subroutine blha_state_reset_new_kinematics

<BLHA OLP interfaces: procedures>+≡
  module subroutine blha_state_reset_new_kinematics (object)
    class(blha_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine blha_state_reset_new_kinematics

<BLHA OLP interfaces: public parameters>≡
  integer, parameter, public :: OLP_PARAMETER_LIMIT = 10
  integer, parameter, public :: OLP_MOMENTUM_LIMIT = 50
  integer, parameter, public :: OLP_RESULTS_LIMIT = 60

<BLHA OLP interfaces: public>+≡
  public :: olp_start

<BLHA OLP interfaces: interfaces>≡
  interface
    subroutine olp_start (contract_file_name, ierr) bind (C,name = "OLP_Start")
      import
      character(kind = c_char, len = 1), intent(in) :: contract_file_name
      integer(kind = c_int), intent(out) :: ierr
    end subroutine olp_start
  end interface

<BLHA OLP interfaces: public>+≡
  public :: olp_eval

<BLHA OLP interfaces: interfaces>+≡
  interface
    subroutine olp_eval (label, momenta, mu, parameters, res) &
      bind (C, name = "OLP_EvalSubProcess")
      import
      integer(kind = c_int), value, intent(in) :: label
      real(kind = c_double), value, intent(in) :: mu

```

```

        real(kind = c_double), dimension(OLP_MOMENTUM_LIMIT), intent(in) :: &
            momenta
        real(kind = c_double), dimension(OLP_PARAMETER_LIMIT), intent(in) :: &
            parameters
        real(kind = c_double), dimension(OLP_RESULTS_LIMIT), intent(out) :: res
    end subroutine olp_eval
end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_info

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_info (olp_file, olp_version, message) bind(C)
            import
            character(kind = c_char), intent(inout), dimension(15) :: olp_file
            character(kind = c_char), intent(inout), dimension(15) :: olp_version
            character(kind = c_char), intent(inout), dimension(255) :: message
        end subroutine olp_info
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_set_parameter

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_set_parameter &
            (variable_name, real_part, complex_part, success) bind(C)
            import
            character(kind = c_char, len = 1), intent(in) :: variable_name
            real(kind = c_double), intent(in) :: real_part, complex_part
            integer(kind = c_int), intent(out) :: success
        end subroutine olp_set_parameter
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_eval2

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_eval2 (label, momenta, mu, res, acc) bind(C)
            import
            integer(kind = c_int), intent(in) :: label
            real(kind = c_double), intent(in) :: mu
            real(kind = c_double), dimension(OLP_MOMENTUM_LIMIT), intent(in) :: momenta
            real(kind = c_double), dimension(OLP_RESULTS_LIMIT), intent(out) :: res
            real(kind = c_double), intent(out) :: acc
        end subroutine olp_eval2
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_option

```



```

<BLHA OLP interfaces: interfaces>+≡
  interface
    subroutine olp_option (line, stat) bind(C)
      import
      character(kind = c_char, len=1), intent(in) :: line
      integer(kind = c_int), intent(out) :: stat
    end subroutine
  end interface

<BLHA OLP interfaces: public>+≡
  public :: olp_polvec

<BLHA OLP interfaces: interfaces>+≡
  interface
    subroutine olp_polvec (p, q, eps) bind(C)
      import
      real(kind = c_double), dimension(0:3), intent(in) :: p, q
      real(kind = c_double), dimension(0:7), intent(out) :: eps
    end subroutine
  end interface

<BLHA OLP interfaces: public>+≡
  public :: olp_finalize

<BLHA OLP interfaces: interfaces>+≡
  interface
    subroutine olp_finalize () bind(C)
      import
    end subroutine olp_finalize
  end interface

<BLHA OLP interfaces: public>+≡
  public :: olp_print_parameter

<BLHA OLP interfaces: interfaces>+≡
  interface
    subroutine olp_print_parameter (filename) bind(C)
      import
      character(kind = c_char, len = 1), intent(in) :: filename
    end subroutine olp_print_parameter
  end interface

<BLHA OLP interfaces: public>+≡
  public :: blha_result_array_size

<BLHA OLP interfaces: sub interfaces>+≡
  pure module function blha_result_array_size &
    (n_part, amp_type) result (rsize)
    integer, intent(in) :: n_part, amp_type
    integer :: rsize
  end function blha_result_array_size

```

```

<BLHA OLP interfaces: procedures>+=
  pure module function blha_result_array_size &
    (n_part, amp_type) result (rsize)
    integer, intent(in) :: n_part, amp_type
    integer :: rsize
    select case (amp_type)
      case (BLHA_AMP_TREE)
        rsize = 1
      case (BLHA_AMP_LOOP)
        rsize = 4
      case (BLHA_AMP_COLOR_C)
        rsize = n_part * (n_part - 1) / 2
      case (BLHA_AMP_SPIN_C)
        rsize = 2 * n_part**2
      case (BLHA_AMP_LOOPINDUCED)
        rsize = 1
      case default
        rsize = 0
    end select
  end function blha_result_array_size

<BLHA OLP interfaces: prc blha: TBP>+=
  procedure :: create_momentum_array => prc_blha_create_momentum_array

<BLHA OLP interfaces: sub interfaces>+=
  module function prc_blha_create_momentum_array (object, p) result (mom)
    class(prc_blha_t), intent(in) :: object
    type(vector4_t), intent(in), dimension(:) :: p
    real(double), dimension(5*object%n_particles) :: mom
  end function prc_blha_create_momentum_array

<BLHA OLP interfaces: procedures>+=
  module function prc_blha_create_momentum_array (object, p) result (mom)
    class(prc_blha_t), intent(in) :: object
    type(vector4_t), intent(in), dimension(:) :: p
    real(double), dimension(5*object%n_particles) :: mom
    integer :: n, i, k

    n = size (p)
    if (n > 10) call msg_fatal ("Number of external particles exceeds" &
      // "size of BLHA-internal momentum array")

    mom = zero
    k = 1
    do i = 1, n
      mom(k : k + 3) = vector4_get_components (p(i))
      mom(k + 4) = invariant_mass (p(i))
      k = k + 5
    end do
  end function prc_blha_create_momentum_array

<BLHA OLP interfaces: blha template: TBP>+=
  procedure :: init => blha_template_init

```

```

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine blha_template_init (template, requires_polarizations, &
    switch_off_muon_yukawas, external_top_yukawa, ew_scheme)
    class(blha_template_t), intent(inout) :: template
    logical, intent(in) :: requires_polarizations, switch_off_muon_yukawas
    real(default), intent(in) :: external_top_yukawa
    type(string_t), intent(in) :: ew_scheme
  end subroutine blha_template_init

<BLHA OLP interfaces: procedures>+≡
  module subroutine blha_template_init (template, requires_polarizations, &
    switch_off_muon_yukawas, external_top_yukawa, ew_scheme)
    class(blha_template_t), intent(inout) :: template
    logical, intent(in) :: requires_polarizations, switch_off_muon_yukawas
    real(default), intent(in) :: external_top_yukawa
    type(string_t), intent(in) :: ew_scheme
    template%compute_component = .false.
    template%include_polarizations = requires_polarizations
    template%switch_off_muon_yukawas = switch_off_muon_yukawas
    template%external_top_yukawa = external_top_yukawa
    template%ew_scheme = ew_scheme_string_to_int (ew_scheme)
  end subroutine blha_template_init

<BLHA OLP interfaces: blha template: TBP>+≡
  procedure :: set_born => blha_template_set_born
  procedure :: set_real_trees => blha_template_set_real_trees
  procedure :: set_loop => blha_template_set_loop
  procedure :: set_subtraction => blha_template_set_subtraction
  procedure :: set_dglap => blha_template_set_dglap

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine blha_template_set_born (template)
    class(blha_template_t), intent(inout) :: template
  end subroutine blha_template_set_born
  module subroutine blha_template_set_real_trees (template)
    class(blha_template_t), intent(inout) :: template
  end subroutine blha_template_set_real_trees
  module subroutine blha_template_set_loop (template)
    class(blha_template_t), intent(inout) :: template
  end subroutine blha_template_set_loop
  module subroutine blha_template_set_subtraction (template)
    class(blha_template_t), intent(inout) :: template
  end subroutine blha_template_set_subtraction
  module subroutine blha_template_set_dglap (template)
    class(blha_template_t), intent(inout) :: template
  end subroutine blha_template_set_dglap

<BLHA OLP interfaces: procedures>+≡
  module subroutine blha_template_set_born (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component (template%I_BORN) = .true.
  end subroutine blha_template_set_born

  module subroutine blha_template_set_real_trees (template)
    class(blha_template_t), intent(inout) :: template

```

```

        template%compute_component (template%I_REAL) = .true.
    end subroutine blha_template_set_real_trees

    module subroutine blha_template_set_loop (template)
        class(blha_template_t), intent(inout) :: template
        template%compute_component(template%I_LOOP) = .true.
    end subroutine blha_template_set_loop

    module subroutine blha_template_set_subtraction (template)
        class(blha_template_t), intent(inout) :: template
        template%compute_component (template%I_SUB) = .true.
    end subroutine blha_template_set_subtraction

    module subroutine blha_template_set_dglap (template)
        class(blha_template_t), intent(inout) :: template
        template%compute_component (template%I_DGLAP) = .true.
    end subroutine blha_template_set_dglap

    <BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: set_internal_color_correlations &
        => blha_template_set_internal_color_correlations

    <BLHA OLP interfaces: sub interfaces>+≡
    module subroutine blha_template_set_internal_color_correlations (template)
        class(blha_template_t), intent(inout) :: template
    end subroutine blha_template_set_internal_color_correlations

    <BLHA OLP interfaces: procedures>+≡
    module subroutine blha_template_set_internal_color_correlations (template)
        class(blha_template_t), intent(inout) :: template
        template%use_internal_color_correlations = .true.
    end subroutine blha_template_set_internal_color_correlations

    <BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: get_internal_color_correlations &
        => blha_template_get_internal_color_correlations

    <BLHA OLP interfaces: sub interfaces>+≡
    pure module function blha_template_get_internal_color_correlations &
        (template) result (val)
        logical :: val
        class(blha_template_t), intent(in) :: template
    end function blha_template_get_internal_color_correlations

    <BLHA OLP interfaces: procedures>+≡
    pure module function blha_template_get_internal_color_correlations &
        (template) result (val)
        logical :: val
        class(blha_template_t), intent(in) :: template
        val = template%use_internal_color_correlations
    end function blha_template_get_internal_color_correlations

    <BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: compute_born => blha_template_compute_born

```

```

procedure :: compute_real_trees => blha_template_compute_real_trees
procedure :: compute_loop => blha_template_compute_loop
procedure :: compute_subtraction => blha_template_compute_subtraction
procedure :: compute_dglap => blha_template_compute_dglap

<BLHA OLP interfaces: sub interfaces>+=
  pure module function blha_template_compute_born (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
  end function blha_template_compute_born
  pure module function blha_template_compute_real_trees (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
  end function blha_template_compute_real_trees
  pure module function blha_template_compute_loop (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
  end function blha_template_compute_loop
  pure module function blha_template_compute_subtraction (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
  end function blha_template_compute_subtraction
  pure module function blha_template_compute_dglap (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
  end function blha_template_compute_dglap

<BLHA OLP interfaces: procedures>+=
  pure module function blha_template_compute_born (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
    val = template%compute_component (template%I_BORN)
  end function blha_template_compute_born

  pure module function blha_template_compute_real_trees (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
    val = template%compute_component (template%I_REAL)
  end function blha_template_compute_real_trees

  pure module function blha_template_compute_loop (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
    val = template%compute_component (template%I_LOOP)
  end function blha_template_compute_loop

  pure module function blha_template_compute_subtraction (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val
    val = template%compute_component (template%I_SUB)
  end function blha_template_compute_subtraction

  pure module function blha_template_compute_dglap (template) result (val)
    class(blha_template_t), intent(in) :: template
    logical :: val

```

```

        val = template%compute_component (template%I_DGLAP)
    end function blha_template_compute_dglap

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: set_loop_method => blha_template_set_loop_method

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine blha_template_set_loop_method (template, master)
        class(blha_template_t), intent(inout) :: template
        class(blha_master_t), intent(in) :: master
    end subroutine blha_template_set_loop_method

<BLHA OLP interfaces: procedures>+≡
    module subroutine blha_template_set_loop_method (template, master)
        class(blha_template_t), intent(inout) :: template
        class(blha_master_t), intent(in) :: master
        template%loop_method = master%blha_mode(1)
    end subroutine blha_template_set_loop_method

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: check => blha_template_check

<BLHA OLP interfaces: sub interfaces>+≡
    module function blha_template_check (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
    end function blha_template_check

<BLHA OLP interfaces: procedures>+≡
    module function blha_template_check (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = count (template%compute_component) == 1
    end function blha_template_check

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: reset => blha_template_reset

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine blha_template_reset (template)
        class(blha_template_t), intent(inout) :: template
    end subroutine blha_template_reset

<BLHA OLP interfaces: procedures>+≡
    module subroutine blha_template_reset (template)
        class(blha_template_t), intent(inout) :: template
        template%compute_component = .false.
    end subroutine blha_template_reset

<BLHA OLP interfaces: blha writer: TBP>≡
    procedure :: write => prc_blha_writer_write

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine prc_blha_writer_write (writer, unit)
        class(prc_blha_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
    end subroutine prc_blha_writer_write

```

```

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_writer_write (writer, unit)
    class(prc_blha_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    write (unit, "(ix,A)") char (writer%get_process_string ())
  end subroutine prc_blha_writer_write

<BLHA OLP interfaces: blha writer: TBP>+≡
  procedure :: get_process_string => prc_blha_writer_get_process_string

<BLHA OLP interfaces: sub interfaces>+≡
  module function prc_blha_writer_get_process_string (writer) result (s_proc)
    class(prc_blha_writer_t), intent(in) :: writer
    type(string_t) :: s_proc
  end function prc_blha_writer_get_process_string

<BLHA OLP interfaces: procedures>+≡
  module function prc_blha_writer_get_process_string (writer) result (s_proc)
    class(prc_blha_writer_t), intent(in) :: writer
    type(string_t) :: s_proc
    s_proc = var_str ("")
  end function prc_blha_writer_get_process_string

<BLHA OLP interfaces: blha writer: TBP>+≡
  procedure :: get_n_proc => prc_blha_writer_get_n_proc

<BLHA OLP interfaces: sub interfaces>+≡
  module function prc_blha_writer_get_n_proc (writer) result (n_proc)
    class(prc_blha_writer_t), intent(in) :: writer
    integer :: n_proc
  end function prc_blha_writer_get_n_proc

<BLHA OLP interfaces: procedures>+≡
  module function prc_blha_writer_get_n_proc (writer) result (n_proc)
    class(prc_blha_writer_t), intent(in) :: writer
    integer :: n_proc
    n_proc = blha_configuration_get_n_proc (writer%blha_cfg)
  end function prc_blha_writer_get_n_proc

<BLHA OLP interfaces: blha driver: TBP>≡
  procedure(blha_driver_set_GF), deferred :: &
    set_GF

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine blha_driver_set_GF (driver, GF)
      import
      class(blha_driver_t), intent(inout) :: driver
      real(default), intent(in) :: GF
    end subroutine blha_driver_set_GF
  end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
  procedure(blha_driver_set_alpha_s), deferred :: &
    set_alpha_s

```

```

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine blha_driver_set_alpha_s (driver, alpha_s)
      import
      class(blha_driver_t), intent(in) :: driver
      real(default), intent(in) :: alpha_s
    end subroutine blha_driver_set_alpha_s
  end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
  procedure(blha_driver_set_weinberg_angle), deferred :: &
    set_weinberg_angle

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine blha_driver_set_weinberg_angle (driver, sw2)
      import
      class(blha_driver_t), intent(inout) :: driver
      real(default), intent(in) :: sw2
    end subroutine blha_driver_set_weinberg_angle
  end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
  procedure(blha_driver_set_alpha_qed), deferred :: set_alpha_qed

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine blha_driver_set_alpha_qed (driver, alpha)
      import
      class(blha_driver_t), intent(inout) :: driver
      real(default), intent(in) :: alpha
    end subroutine blha_driver_set_alpha_qed
  end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
  procedure(blha_driver_print_alpha_s), deferred :: &
    print_alpha_s

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine blha_driver_print_alpha_s (object)
      import
      class(blha_driver_t), intent(in) :: object
    end subroutine blha_driver_print_alpha_s
  end interface

<BLHA OLP interfaces: public>+≡
  public :: parameter_error_message

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine parameter_error_message (par, subr)
    type(string_t), intent(in) :: par, subr
  end subroutine parameter_error_message

```



```

<BLHA OLP interfaces: procedures>+=
  module subroutine parameter_error_message (par, subr)
    type(string_t), intent(in) :: par, subr
    type(string_t) :: message
    message = "Setting of parameter " // par &
              // "failed in " // subr // "!"
    call msg_fatal (char (message))
  end subroutine parameter_error_message

<BLHA OLP interfaces: public>+=
  public :: ew_parameter_error_message

<BLHA OLP interfaces: sub interfaces>+=
  module subroutine ew_parameter_error_message (par)
    type(string_t), intent(in) :: par
  end subroutine ew_parameter_error_message

<BLHA OLP interfaces: procedures>+=
  module subroutine ew_parameter_error_message (par)
    type(string_t), intent(in) :: par
    type(string_t) :: message
    message = "Setting of parameter " // par &
              // "failed. This happens because the chosen " &
              // "EWScheme in the BLHA file does not fit " &
              // "your parameter choice"
    call msg_fatal (char (message))
  end subroutine ew_parameter_error_message

<BLHA OLP interfaces: blha driver: TBP>+=
  procedure :: set_mass_and_width => blha_driver_set_mass_and_width

<BLHA OLP interfaces: sub interfaces>+=
  module subroutine blha_driver_set_mass_and_width &
    (driver, i_pdg, mass, width)
    class(blha_driver_t), intent(inout) :: driver
    integer, intent(in) :: i_pdg
    real(default), intent(in), optional :: mass
    real(default), intent(in), optional :: width
  end subroutine blha_driver_set_mass_and_width

<BLHA OLP interfaces: procedures>+=
  module subroutine blha_driver_set_mass_and_width &
    (driver, i_pdg, mass, width)
    class(blha_driver_t), intent(inout) :: driver
    integer, intent(in) :: i_pdg
    real(default), intent(in), optional :: mass
    real(default), intent(in), optional :: width
    type(string_t) :: buf
    character(kind=c_char,len=20) :: c_string
    integer :: ierr
    if (present (mass)) then
      buf = 'mass(' // str (abs(i_pdg)) // ')'
      c_string = char(buf) // c_null_char
      call driver%blha_olp_set_parameter &
        (c_string, dble(mass), 0._double, ierr)
    end if
  end subroutine blha_driver_set_mass_and_width

```

```

        if (ierr == 0) then
            buf = "BLHA driver: Attempt to set mass of particle " // &
                str (abs(i_pdg)) // "failed"
            call msg_fatal (char(buf))
        end if
    end if
end if
if (present (width)) then
    buf = 'width(' // str (abs(i_pdg)) // ')'
    c_string = char(buf)//c_null_char
    call driver%blha_olp_set_parameter &
        (c_string, dble(width), 0._double, ierr)
    if (ierr == 0) then
        buf = "BLHA driver: Attempt to set width of particle " // &
            str (abs(i_pdg)) // "failed"
        call msg_fatal (char(buf))
    end if
end if
end if
end subroutine blha_driver_set_mass_and_width

```

<BLHA OLP interfaces: blha driver: TBP>+≡

```

    procedure (blha_driver_init_dlaccess_to_library), deferred :: &
        init_dlaccess_to_library

```

<BLHA OLP interfaces: interfaces>+≡

```

    abstract interface
        subroutine blha_driver_init_dlaccess_to_library &
            (object, os_data, dlaccess, success)
        import
        class(blha_driver_t), intent(in) :: object
        type(os_data_t), intent(in) :: os_data
        type(dlaccess_t), intent(out) :: dlaccess
        logical, intent(out) :: success
    end subroutine blha_driver_init_dlaccess_to_library
end interface

```

<BLHA OLP interfaces: blha driver: TBP>+≡

```

    procedure :: load => blha_driver_load

```

<BLHA OLP interfaces: sub interfaces>+≡

```

    module subroutine blha_driver_load (object, os_data, success)
        class(blha_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical, intent(out) :: success
    end subroutine blha_driver_load

```

<BLHA OLP interfaces: procedures>+≡

```

    module subroutine blha_driver_load (object, os_data, success)
        class(blha_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical, intent(out) :: success
        type(dlaccess_t) :: dlaccess
        type(c_funptr) :: c_funptr
        logical :: init_success

        call object%init_dlaccess_to_library (os_data, dlaccess, init_success)
    end subroutine blha_driver_load

```

```

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Start"))
call c_f_procpointer (c_fptr, object%blha_olp_start)
call check_for_error (var_str ("OLP_Start"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_EvalSubProcess"))
call c_f_procpointer (c_fptr, object%blha_olp_eval)
call check_for_error (var_str ("OLP_EvalSubProcess"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Info"))
call c_f_procpointer (c_fptr, object%blha_olp_info)
call check_for_error (var_str ("OLP_Info"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_SetParameter"))
call c_f_procpointer (c_fptr, object%blha_olp_set_parameter)
call check_for_error (var_str ("OLP_SetParameter"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_EvalSubProcess2"))
call c_f_procpointer (c_fptr, object%blha_olp_eval2)
call check_for_error (var_str ("OLP_EvalSubProcess2"))

!!! The following three functions are not implemented in OpenLoops.
!!! In another BLHA provider, they need to be implemented separately.

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Option"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_option)
!!! call check_for_error (var_str ("OLP_Option"))

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Polvec"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_polvec)
!!! call check_for_error (var_str ("OLP_Polvec"))

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Finalize"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_finalize)
!!! call check_for_error (var_str ("OLP_Finalize"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_PrintParameter"))
call c_f_procpointer (c_fptr, object%blha_olp_print_parameter)
call check_for_error (var_str ("OLP_PrintParameter"))

success = .true.
contains
  subroutine check_for_error (function_name)
    type(string_t), intent(in) :: function_name
    if (dlaccess_has_error (dlaccess)) &
      call msg_fatal (char ("Loading of " // function_name // " failed!"))
  end subroutine check_for_error
end subroutine blha_driver_load

```

```

<BLHA OLP interfaces: parameters>+≡
  integer, parameter :: LEN_MAX_FLAVOR_STRING = 100
  integer, parameter :: N_MAX_FLAVORS = 100
<BLHA OLP interfaces: blha driver: TBP>+≡

```

```

    procedure :: read_contract_file => blha_driver_read_contract_file
<BLHA OLP interfaces: sub interfaces>+=
    module subroutine blha_driver_read_contract_file (driver, flavors, &
        amp_type, flv_index, hel_index, label, helicities)
        class(blha_driver_t), intent(inout) :: driver
        integer, intent(in), dimension(:, :) :: flavors
        integer, intent(out), dimension(:), allocatable :: amp_type, &
            flv_index, hel_index, label
        integer, intent(out), dimension(:, :) :: helicities
    end subroutine blha_driver_read_contract_file
<BLHA OLP interfaces: procedures>+=
    module subroutine blha_driver_read_contract_file (driver, flavors, &
        amp_type, flv_index, hel_index, label, helicities)
        class(blha_driver_t), intent(inout) :: driver
        integer, intent(in), dimension(:, :) :: flavors
        integer, intent(out), dimension(:), allocatable :: amp_type, &
            flv_index, hel_index, label
        integer, intent(out), dimension(:, :) :: helicities
        integer :: unit, filestat
        character(len=LEN_MAX_FLAVOR_STRING) :: rd_line
        logical :: read_flavor, give_warning
        integer :: label_count, i_flv, i
        integer :: i_hel, n_in
        integer :: i_next, n_entries
        integer, dimension(size(flavors, 1) + 2) :: i_array
        integer, dimension(size(flavors, 1) + 2) :: hel_array
        integer, dimension(size(flavors, 1)) :: flv_array
        integer, parameter :: NO_NUMBER = -1000
        integer, parameter :: PROC_NOT_FOUND = -1001
        integer, parameter :: list_incr = 50
        integer :: n_found
        allocate (amp_type (N_MAX_FLAVORS), flv_index (N_MAX_FLAVORS), &
            hel_index (N_MAX_FLAVORS), label (N_MAX_FLAVORS))
        amp_type = -1; flv_index = -1; hel_index = -1; label = -1
        helicities = 0
        n_in = size (helicities, dim = 2)
        n_entries = size (flavors, 1) + 2
        unit = free_unit ()
        open (unit, file = char (driver%contract_file), status="old")
        read_flavor = .false.
        label_count = 1
        i_hel = 1
        n_found = 0
        give_warning = .false.
        do
            read (unit, "(A)", iostat = filestat) rd_line
            if (filestat == iostat_end) then
                exit
            else
                if (rd_line(1:13) == 'AmplitudeType') then
                    if (i_hel > 2 * n_in) i_hel = 1
                    i_next = find_next_word_index (rd_line, 13)
                    if (label_count > size (amp_type)) &

```

```

        call extend_integer_array (amp_type, list_incr)
    if (rd_line(i_next : i_next + 11) == 'LoopInduced') then
        amp_type(label_count) = BLHA_AMP_LOOPINDUCED
    else if (rd_line(i_next : i_next + 4) == 'Loop') then
        amp_type(label_count) = BLHA_AMP_LOOP
    else if (rd_line(i_next : i_next + 4) == 'Tree') then
        amp_type(label_count) = BLHA_AMP_TREE
    else if (rd_line(i_next : i_next + 6) == 'ccTree') then
        amp_type(label_count) = BLHA_AMP_COLOR_C
    else if (rd_line(i_next : i_next + 6) == 'scTree' .or. &
        rd_line(i_next : i_next + 14) == 'sctree_polvect') then
        amp_type(label_count) = BLHA_AMP_SPIN_C
    else
        call msg_fatal ("AmplitudeType present but AmpType not known!")
    end if
    read_flavor = .true.
else if (read_flavor .and. .not. (rd_line(1:13) == 'CouplingPower' &
    .or. rd_line(1:14) == 'CorrectionType')) then
    i_array = create_flavor_string (rd_line, n_entries)
    if (driver%include_polarizations) then
        hel_array = create_helicity_string (rd_line, n_entries)
        call check_helicity_array (hel_array, n_entries, n_in)
    else
        hel_array = 0
    end if
    if (.not. all (i_array == PROC_NOT_FOUND)) then
        do i_flv = 1, size (flavors, 2)
            flv_array = 0
            do i = 1, size (flv_array)
                if (i_array (i) == PHOTON_OFFSHELL .and. &
                    flavors (i, i_flv) == PHOTON) then
                    flv_array (i) = i_array (i)
                else
                    flv_array (i) = flavors (i, i_flv)
                end if
            end do
        end do
        if (all (i_array (1 : n_entries - 2) == flv_array (:))) then
            if (label_count > size (label)) &
                call extend_integer_array (label, list_incr)
            label(label_count) = i_array (n_entries)
            if (label_count > size (flv_index)) &
                call extend_integer_array (flv_index, list_incr)
            flv_index (label_count) = i_flv
            if (label_count > size (hel_index)) &
                call extend_integer_array (hel_index, list_incr)
            hel_index (label_count) = i_hel
            if (driver%include_polarizations) then
                helicities (label(label_count), :) = hel_array (1:n_in)
                i_hel = i_hel + 1
            end if
            n_found = n_found + 1
            label_count = label_count + 1
            exit
        end if
    end if
end if

```

```

        end do
        give_warning = .false.
    else
        give_warning = .true.
    end if
    read_flavor = .false.
end if
end if
end do
call crop_integer_array (amp_type, label_count-1)
if (n_found == 0) then
    call msg_fatal ("The desired process has not been found ", &
        [var_str ("by the OLP-Provider. Maybe the value of alpha_power "), &
        var_str ("or alphas_power does not correspond to the process. "), &
        var_str ("If you are using OpenLoops, you can set the option "), &
        var_str ("openloops_verbosity to a value larger than 1 to obtain "), &
        var_str ("more information")])
else if (give_warning) then
    call msg_warning ("Some processes have not been found in the OLC file.", &
        [var_str ("This is because these processes do not fit the required "), &
        var_str ("coupling alpha_power and alphas_power. Be aware that the "), &
        var_str ("results of this calculation are not necessarily an accurate "), &
        var_str ("description of the physics of interest.")])
end if
close(unit)
contains

function create_flavor_string (s, n_entries) result (i_array)
    character(len=LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(in) :: n_entries
    integer, dimension(n_entries) :: i_array
    integer :: k, current_position
    integer :: i_entry
    k = 1; current_position = 1
    do
        if (current_position > LEN_MAX_FLAVOR_STRING) &
            call msg_fatal ("Read OLC File: Current position exceeds maximum value")
        if (s(current_position:current_position) /= " ") then
            call create_flavor (s, i_entry, current_position)
            if (i_entry /= NO_NUMBER .and. i_entry /= PROC_NOT_FOUND) then
                i_array(k) = i_entry
                k = k + 1
                if (k > n_entries) then
                    return
                else
                    call increment_current_position (s, current_position)
                end if
            else if (i_entry == PROC_NOT_FOUND) then
                i_array = PROC_NOT_FOUND
                return
            else
                call increment_current_position (s, current_position)
            end if
        end if
    end do
end function

```

```

        else
            call increment_current_position (s, current_position)
        end if
    end do
end function create_flavor_string

function create_helicity_string (s, n_entries) result (hel_array)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(in) :: n_entries
    integer, dimension(n_entries) :: hel_array
    integer :: k, current_position
    integer :: hel
    k = 1; current_position = 1
    do
        if (current_position > LEN_MAX_FLAVOR_STRING) &
            call msg_fatal ("Read OLC File: Current position exceeds maximum value")
        if (s(current_position:current_position) /= " ") then
            call create_helicity (s, hel, current_position)
            if (hel >= -1 .and. hel <= 1) then
                hel_array(k) = hel
                k = k + 1
                if (k > n_entries) then
                    return
                else
                    call increment_current_position (s, current_position)
                end if
            else
                call increment_current_position (s, current_position)
            end if
        else
            call increment_current_position (s, current_position)
        end if
    end do
end function create_helicity_string

subroutine increment_current_position (s, current_position)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(inout) :: current_position
    current_position = find_next_word_index (s, current_position)
end subroutine increment_current_position

subroutine get_next_buffer (s, current_position, buf, last_buffer_index)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(inout) :: current_position
    character(len = 10), intent(out) :: buf
    integer, intent(out) :: last_buffer_index
    integer :: i
    i = 1; buf = ""
    do
        if (s(current_position:current_position) /= " ") then
            buf(i:i) = s(current_position:current_position)
            i = i + 1; current_position = current_position + 1
        else
            exit
        end if
    end do

```

```

        end if
    end do
    last_buffer_index = i
end subroutine get_next_buffer

function is_particle_buffer (buf, i) result (valid)
    logical :: valid
    character(len = 10), intent(in) :: buf
    integer, intent(in) :: i
    valid = (buf(1 : i - 1) /= "->" .and. buf(1 : i - 1) /= "|" &
        .and. buf(1 : i - 1) /= "Process")
end function is_particle_buffer

subroutine create_flavor (s, i_particle, current_position)
    character(len=LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(out) :: i_particle
    integer, intent(inout) :: current_position
    character(len=10) :: buf
    integer :: i, last_buffer_index
    call get_next_buffer (s, current_position, buf, last_buffer_index)
    i = last_buffer_index
    if (is_particle_buffer (buf, i)) then
        call strip_helicity (buf, i)
        i_particle = read_ival (var_str (buf(1 : i - 1)))
    else if (buf(1 : i - 1) == "Process") then
        i_particle = PROC_NOT_FOUND
    else
        i_particle = NO_NUMBER
    end if
end subroutine create_flavor

subroutine create_helicity (s, helicity, current_position)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(out) :: helicity
    integer, intent(inout) :: current_position
    character(len = 10) :: buf
    integer :: i, last_buffer_index
    logical :: success
    call get_next_buffer (s, current_position, buf, last_buffer_index)
    i = last_buffer_index
    if (is_particle_buffer (buf, i)) then
        call strip_flavor (buf, i, helicity, success)
    else
        helicity = 0
    end if
end subroutine create_helicity

subroutine strip_helicity (buf, i)
    character(len = 10), intent(in) :: buf
    integer, intent(inout) :: i
    integer :: i_last
    i_last = i - 1
    if (i_last < 4) return
    if (buf(i_last - 2 : i_last) == "(1)") then

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```

        i = i - 3
    else if (buf(i_last - 3 : i_last) == "(-1)") then
        i = i - 4
    end if
end subroutine strip_helicity

subroutine strip_flavor (buf, i, helicity, success)
    character(len = 10), intent(in) :: buf
    integer, intent(in) :: i
    integer, intent(out) :: helicity
    logical, intent(out) :: success
    integer :: i_last
    i_last = i - 1
    helicity = 0
    if (i_last < 4) return
    if (buf(i_last - 2 : i_last) == "(1)") then
        helicity = 1
        success = .true.
    else if (buf(i_last - 3 : i_last) == "(-1)") then
        helicity = -1
        success = .true.
    else
        success = .false.
    end if
end subroutine strip_flavor

function find_next_word_index (word, i_start) result (i_next)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: word
    integer, intent(in) :: i_start
    integer :: i_next
    i_next = i_start + 1
    do
        if (word(i_next : i_next) /= " ") then
            exit
        else
            i_next = i_next + 1
        end if
        if (i_next > LEN_MAX_FLAVOR_STRING) &
            call msg_fatal ("Find next word: line limit exceeded")
    end do
end function find_next_word_index

subroutine check_helicity_array (hel_array, n_entries, n_in)
    integer, intent(in), dimension(:) :: hel_array
    integer, intent(in) :: n_entries, n_in
    integer :: n_particles, i
    logical :: valid
    n_particles = n_entries - 2
    !!! only allow polarisations for incoming fermions for now
    valid = all (hel_array (n_in + 1 : n_particles) == 0)
    do i = 1, n_in
        valid = valid .and. (hel_array(i) == 1 .or. hel_array(i) == -1)
    end do
    if (.not. valid) &

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        call msg_fatal ("Invalid helicities encountered!")
    end subroutine check_helicity_array

end subroutine blha_driver_read_contract_file

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: set_alpha_qed => prc_blha_set_alpha_qed

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine prc_blha_set_alpha_qed (object, model)
        class(prc_blha_t), intent(inout) :: object
        type(model_data_t), intent(in), target :: model
    end subroutine prc_blha_set_alpha_qed

<BLHA OLP interfaces: procedures>+≡
    module subroutine prc_blha_set_alpha_qed (object, model)
        class(prc_blha_t), intent(inout) :: object
        type(model_data_t), intent(in), target :: model
        real(default) :: alpha

        alpha = one / model%get_real (var_str ('alpha_em_i'))

        select type (driver => object%driver)
            class is (blha_driver_t)
                call driver%set_alpha_qed (alpha)
            end select
    end subroutine prc_blha_set_alpha_qed

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: set_GF => prc_blha_set_GF

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine prc_blha_set_GF (object, model)
        class(prc_blha_t), intent(inout) :: object
        type(model_data_t), intent(in), target :: model
    end subroutine prc_blha_set_GF

<BLHA OLP interfaces: procedures>+≡
    module subroutine prc_blha_set_GF (object, model)
        class(prc_blha_t), intent(inout) :: object
        type(model_data_t), intent(in), target :: model
        real(default) :: GF

        GF = model%get_real (var_str ('GF'))
        select type (driver => object%driver)
            class is (blha_driver_t)
                call driver%set_GF (GF)
            end select
    end subroutine prc_blha_set_GF

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: set_weinberg_angle => prc_blha_set_weinberg_angle

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<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_set_weinberg_angle (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
  end subroutine prc_blha_set_weinberg_angle

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_set_weinberg_angle (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
    real(default) :: sw2

    sw2 = model%get_real (var_str ('sw2'))
    select type (driver => object%driver)
    class is (blha_driver_t)
      call driver%set_weinberg_angle (sw2)
    end select
  end subroutine prc_blha_set_weinberg_angle

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: set_electroweak_parameters => &
    prc_blha_set_electroweak_parameters

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_set_electroweak_parameters (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
  end subroutine prc_blha_set_electroweak_parameters

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_set_electroweak_parameters (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
    if (count (object%ew_parameter_mask) == 0) then
      call msg_fatal ("Cannot decide EW parameter setting: No scheme set!")
    else if (count (object%ew_parameter_mask) > 1) then
      call msg_fatal ("Cannot decide EW parameter setting: More than one scheme set!")
    end if
    if (object%ew_parameter_mask (I_ALPHA_INTERNAL)) call object%set_alpha_qed (model)
    if (object%ew_parameter_mask (I_GF)) call object%set_GF (model)
    if (object%ew_parameter_mask (I_SW2)) call object%set_weinberg_angle (model)
  end subroutine prc_blha_set_electroweak_parameters

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: read_contract_file => prc_blha_read_contract_file

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_read_contract_file (object, flavors)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in), dimension(:, :) :: flavors
  end subroutine prc_blha_read_contract_file

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_read_contract_file (object, flavors)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in), dimension(:, :) :: flavors

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integer, dimension(:), allocatable :: amp_type, flv_index, hel_index, label
integer, dimension(:,:), allocatable :: helicities
integer :: i_proc, i_hel
allocate (helicities (N_MAX_FLAVORS, object%data%n_in))
select type (driver => object%driver)
class is (blha_driver_t)
    call driver%read_contract_file (flavors, amp_type, flv_index, &
        hel_index, label, helicities)
end select
object%n_proc = count (amp_type >= 0)
do i_proc = 1, object%n_proc
    if (amp_type (i_proc) < 0) exit
    if (hel_index(i_proc) < 0 .and. object%includes_polarization ()) &
        call msg_bug ("Object includes polarization, but helicity index is undefined.")
    i_hel = hel_index (i_proc)
    select case (amp_type (i_proc))
    case (BLHA_AMP_TREE)
        if (allocated (object%i_tree)) then
            object%i_tree(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Tree matrix element present, &
                &but neither Born nor real indices are allocated!")
        end if
    case (BLHA_AMP_COLOR_C)
        if (allocated (object%i_color_c)) then
            object%i_color_c(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Color-correlated matrix element present, &
                &but cc-indices are not allocated!")
        end if
    case (BLHA_AMP_SPIN_C)
        if (allocated (object%i_spin_c)) then
            object%i_spin_c(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Spin-correlated matrix element present, &
                &but sc-indices are not allocated!")
        end if
    case (BLHA_AMP_LOOP)
        if (allocated (object%i_virt)) then
            object%i_virt(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Loop matrix element present, &
                &but virt-indices are not allocated!")
        end if
    case (BLHA_AMP_LOOPINDUCED)
        if (allocated (object%i_tree)) then
            object%i_tree(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Loop matrix element present, &
                &but neither Born nor real indices are allocated!")
        end if
    case default
        call msg_fatal ("Undefined amplitude type")
    end select
end select

```

```

        if (allocated (object%i_hel)) &
            object%i_hel (i_proc, :) = helicities (label(i_proc), :)
    end do
end subroutine prc_blha_read_contract_file

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: print_parameter_file => prc_blha_print_parameter_file

<BLHA OLP interfaces: sub interfaces>+≡
    module subroutine prc_blha_print_parameter_file (object, i_component)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: i_component
    end subroutine prc_blha_print_parameter_file

<BLHA OLP interfaces: procedures>+≡
    module subroutine prc_blha_print_parameter_file (object, i_component)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: i_component
        type(string_t) :: filename

        select type (def => object%def)
        class is (blha_def_t)
            filename = def%basename // '_' // str (i_component) // '.olp_parameters'
        end select
        select type (driver => object%driver)
        class is (blha_driver_t)
            call driver%blha_olp_print_parameter (char(filename)//c_null_char)
        end select
    end subroutine prc_blha_print_parameter_file

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: compute_amplitude => prc_blha_compute_amplitude

<BLHA OLP interfaces: sub interfaces>+≡
    module function prc_blha_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
         core_state) result (amp)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: j
        type(vector4_t), dimension(:), intent(in) :: p
        integer, intent(in) :: f, h, c
        real(default), intent(in) :: fac_scale, ren_scale
        real(default), intent(in), allocatable :: alpha_qcd_forced
        class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
        complex(default) :: amp
    end function prc_blha_compute_amplitude

<BLHA OLP interfaces: procedures>+≡
    module function prc_blha_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
         core_state) result (amp)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: j
        type(vector4_t), dimension(:), intent(in) :: p
        integer, intent(in) :: f, h, c

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real(default), intent(in) :: fac_scale, ren_scale
real(default), intent(in), allocatable :: alpha_qcd_forced
class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
complex(default) :: amp
select type (core_state)
class is (blha_state_t)
    core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)
end select
amp = zero
end function prc_blha_compute_amplitude

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<BLHA OLP interfaces: prc blha: TBP>+≡

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procedure :: init_blha => prc_blha_init_blha

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<BLHA OLP interfaces: sub interfaces>+≡

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module subroutine prc_blha_init_blha (object, blha_template, n_in, &
    n_particles, n_flv, n_hel)
    class(prc_blha_t), intent(inout) :: object
    type(blha_template_t), intent(in) :: blha_template
    integer, intent(in) :: n_in, n_particles, n_flv, n_hel
end subroutine prc_blha_init_blha

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<BLHA OLP interfaces: procedures>+≡

```

module subroutine prc_blha_init_blha (object, blha_template, n_in, &
    n_particles, n_flv, n_hel)
    class(prc_blha_t), intent(inout) :: object
    type(blha_template_t), intent(in) :: blha_template
    integer, intent(in) :: n_in, n_particles, n_flv, n_hel
    object%n_particles = n_particles
    object%n_flv = n_flv
    object%n_hel = n_hel
    if (blha_template%compute_loop ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_virt (n_flv, n_hel), &
                object%i_color_c (n_flv, n_hel))
            if (blha_template%use_internal_color_correlations) then
                allocate (object%i_hel (n_flv * n_in * n_hel * 2, n_in))
            else
                allocate (object%i_hel (n_flv * n_in * n_hel, n_in))
            end if
        else
            allocate (object%i_virt (n_flv, 1), object%i_color_c (n_flv, 1))
        end if
        object%i_virt = -1
        object%i_color_c = -1
    else if (blha_template%compute_subtraction ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel), &
                object%i_color_c (n_flv, n_hel), &
                object%i_spin_c (n_flv, n_hel), &
                object%i_hel (3 * (n_flv * n_hel * n_in), n_in))
            object%i_hel = 0
        else
            allocate (object%i_tree (n_flv, 1), object%i_color_c (n_flv, 1) , &
                object%i_spin_c (n_flv, 1))
        end if
    end if
end subroutine prc_blha_init_blha

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        end if
        object%i_tree = -1
        object%i_color_c = -1
        object%i_spin_c = -1
    else if (blha_template%compute_dglap ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel), &
                    object%i_color_c (n_flv, n_hel), &
                    object%i_hel (3 * (n_flv * n_hel * n_in), n_in))
            object%i_hel = 0
        else
            allocate (object%i_tree (n_flv, 1), object%i_color_c (n_flv, 1))
        end if
        object%i_tree = -1
        object%i_color_c = -1
    else if (blha_template%compute_real_trees () .or. blha_template%compute_born ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel))
            allocate (object%i_hel (n_flv * n_hel * n_in, n_in))
            object%i_hel = 0
        else
            allocate (object%i_tree (n_flv, 1))
        end if
        object%i_tree = -1
    end if

    call object%init_ew_parameters (blha_template%ew_scheme)

    select type (driver => object%driver)
    class is (blha_driver_t)
        driver%include_polarizations = blha_template%include_polarizations
        driver%switch_off_muon_yukawas = blha_template%switch_off_muon_yukawas
        driver%external_top_yukawa = blha_template%external_top_yukawa
    end select
end subroutine prc_blha_init_blha

```

(BLHA OLP interfaces: prc blha: TBP)+≡

```

    procedure :: set_mass_and_width => prc_blha_set_mass_and_width

```

(BLHA OLP interfaces: sub interfaces)+≡

```

    module subroutine prc_blha_set_mass_and_width (object, i_pdg, mass, width)
        class(prc_blha_t), intent(inout) :: object
        integer, intent(in) :: i_pdg
        real(default), intent(in) :: mass, width
    end subroutine prc_blha_set_mass_and_width

```

(BLHA OLP interfaces: procedures)+≡

```

    module subroutine prc_blha_set_mass_and_width (object, i_pdg, mass, width)
        class(prc_blha_t), intent(inout) :: object
        integer, intent(in) :: i_pdg
        real(default), intent(in) :: mass, width
        select type (driver => object%driver)
        class is (blha_driver_t)
            call driver%set_mass_and_width (i_pdg, mass, width)
        end select
    end subroutine

```

```

end subroutine prc_blha_set_mass_and_width

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: set_particle_properties => prc_blha_set_particle_properties

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_set_particle_properties (object, model)
    class(prc_blha_t), intent(inout) :: object
    class(model_data_t), intent(in), target :: model
  end subroutine prc_blha_set_particle_properties

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_set_particle_properties (object, model)
    class(prc_blha_t), intent(inout) :: object
    class(model_data_t), intent(in), target :: model
    integer :: i, i_pdg
    type(flavor_t) :: flv
    real(default) :: mass, width
    integer :: ierr
    real(default) :: top_yukawa
    do i = 1, OLP_N_MASSIVE_PARTICLES
      i_pdg = OLP_MASSIVE_PARTICLES(i)
      if (i_pdg < 0) cycle
      call flv%init (i_pdg, model)
      mass = flv%get_mass (); width = flv%get_width ()
      select type (driver => object%driver)
        class is (blha_driver_t)
          call driver%set_mass_and_width (i_pdg, mass = mass, width = width)
          if (i_pdg == 5) call driver%blha_olp_set_parameter &
            ('yuk(5)'//c_null_char, dble(mass), 0._double, ierr)
          if (i_pdg == 6) then
            if (driver%external_top_yukawa > 0._default) then
              top_yukawa = driver%external_top_yukawa
            else
              top_yukawa = mass
            end if
            call driver%blha_olp_set_parameter &
              ('yuk(6)'//c_null_char, dble(top_yukawa), 0._double, ierr)
          end if
          if (driver%switch_off_muon_yukawas) then
            if (i_pdg == 13) call driver%blha_olp_set_parameter &
              ('yuk(13)'//c_null_char, 0._double, 0._double, ierr)
          end if
        end select
      end do
    end subroutine prc_blha_set_particle_properties

```

This mask adapts which electroweak parameters are supposed to set according to the chosen BLHA EWScheme. This is only implemented for the default OLP method so far.

```

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: init_ew_parameters => prc_blha_init_ew_parameters

```



```

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_init_ew_parameters (object, ew_scheme)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in) :: ew_scheme
  end subroutine prc_blha_init_ew_parameters

```

```

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_init_ew_parameters (object, ew_scheme)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in) :: ew_scheme
    object%ew_parameter_mask = .false.
    select case (ew_scheme)
    case (BLHA_EW_0)
      object%ew_parameter_mask (I_ALPHA_0) = .true.
    case (BLHA_EW_GF)
      object%ew_parameter_mask (I_GF) = .true.
    case (BLHA_EW_MZ)
      object%ew_parameter_mask (I_ALPHA_MZ) = .true.
    case (BLHA_EW_INTERNAL)
      object%ew_parameter_mask (I_ALPHA_INTERNAL) = .true.
    end select
  end subroutine prc_blha_init_ew_parameters

```

Computes a virtual matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of `dimension(4)`, corresponding to the ϵ^2 -, ϵ^1 - and ϵ^0 -poles of the virtual matrix element at position `r(1:3)` and the Born matrix element at position `r(4)`. The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

```

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: compute_sqme_virt => prc_blha_compute_sqme_virt

```

```

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_compute_sqme_virt (object, &
    i_flv, i_hel, p, ren_scale, es_scale, loop_method, sqme, bad_point)
    class(prc_blha_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale, es_scale
    integer, intent(in) :: loop_method
    real(default), dimension(4), intent(out) :: sqme
    logical, intent(out) :: bad_point
  end subroutine prc_blha_compute_sqme_virt

```

```

<BLHA OLP interfaces: procedures>+≡
  module subroutine prc_blha_compute_sqme_virt (object, &
    i_flv, i_hel, p, ren_scale, es_scale, loop_method, sqme, bad_point)
    class(prc_blha_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale, es_scale
    integer, intent(in) :: loop_method
    real(default), dimension(4), intent(out) :: sqme

```

```

logical, intent(out) :: bad_point
real(double), dimension(5 * object%n_particles) :: mom
real(double), dimension(:), allocatable :: r
real(double) :: mu_dble, es_dble
real(double) :: acc_dble
real(default) :: acc
real(default) :: alpha_s
integer :: ierr
if (object%i_virt(i_flv, i_hel) >= 0) then
  allocate (r (blha_result_array_size (object%n_particles, BLHA_AMP_LOOP)))
  if (debug_on) call msg_debug2 (D_VIRTUAL, "prc_blha_compute_sqme_virt")
  if (debug_on) call msg_debug2 (D_VIRTUAL, "i_flv", i_flv)
  if (debug_on) call msg_debug2 (D_VIRTUAL, "object%i_virt(i_flv, i_hel)", object%i_virt(i_flv, i_hel))
  if (debug2_active (D_VIRTUAL)) then
    call msg_debug2 (D_VIRTUAL, "use momenta: ")
    call vector4_write_set (p, show_mass = .true., &
      check_conservation = .true.)
  end if
  mom = object%create_momentum_array (p)
  if (vanishes (ren_scale)) &
    call msg_fatal ("prc_blha_compute_sqme_virt: ren_scale vanishes")
  mu_dble = dble (ren_scale)
  es_dble = dble (es_scale)
  alpha_s = object%qcd%alpha%get (ren_scale)
  select type (driver => object%driver)
  class is (blha_driver_t)
    if (loop_method == BLHA_MODE_OPENLOOPS) then
      call driver%blha_olp_set_parameter ('mureg'//c_null_char, es_dble, 0._double, ierr)
      if (ierr == 0) call parameter_error_message (var_str ('mureg'), &
        var_str ('prc_blha_compute_sqme_virt'))
    end if
    call driver%set_alpha_s (alpha_s)
    call driver%blha_olp_eval2 (object%i_virt(i_flv, i_hel), mom, mu_dble, r, acc_dble)
  end select
  acc = acc_dble
  sqme = r(1:4)
  bad_point = acc > object%maximum_accuracy
  if (object%includes_polarization ()) sqme = object%n_hel * sqme
else
  sqme = zero
end if
end subroutine prc_blha_compute_sqme_virt

```

Computes a tree-level matrix element from an interface to an external one-loop provider. The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

<BLHA OLP interfaces: prc blha: TBP>+≡

procedure :: compute_sqme => prc_blha_compute_sqme

<BLHA OLP interfaces: sub interfaces>+≡

module subroutine prc_blha_compute_sqme (object, i_flv, i_hel, p, &
ren_scale, sqme, bad_point)

```

class(prc_blha_t), intent(in) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(out) :: sqme
logical, intent(out) :: bad_point
end subroutine prc_blha_compute_sqme
<BLHA OLP interfaces: procedures>+≡
module subroutine prc_blha_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
class(prc_blha_t), intent(in) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(out) :: sqme
logical, intent(out) :: bad_point
real(double), dimension(5*object%n_particles) :: mom
real(double), dimension(OLP_RESULTS_LIMIT) :: r
real(double) :: mu_dble, acc_dble
real(default) :: acc, alpha_s
if (object%i_tree(i_flv, i_hel) >= 0) then
    if (debug_on) call msg_debug2 (D_REAL, "prc_blha_compute_sqme")
    if (debug_on) call msg_debug2 (D_REAL, "i_flv", i_flv)
    if (debug2_active (D_REAL)) then
        call msg_debug2 (D_REAL, "use momenta: ")
        call vector4_write_set (p, show_mass = .true., &
            check_conservation = .true.)
    end if
    mom = object%create_momentum_array (p)
    if (vanishes (ren_scale)) &
        call msg_fatal ("prc_blha_compute_sqme: ren_scale vanishes")
    mu_dble = dble(ren_scale)
    alpha_s = object%qcd%alpha%get (ren_scale)
    select type (driver => object%driver)
    class is (blha_driver_t)
        call driver%set_alpha_s (alpha_s)
        call driver%blha_olp_eval2 (object%i_tree(i_flv, i_hel), mom, &
            mu_dble, r, acc_dble)
        sqme = r(object%sqme_tree_pos)
    end select
    acc = acc_dble
    bad_point = acc > object%maximum_accuracy
    if (object%includes_polarization ()) sqme = object%n_hel * sqme
else
    sqme = zero
end if
end subroutine prc_blha_compute_sqme

```

For the color correlated matrix the standard is to compute the diagonal entries from the born amplitudes and corresponding casimirs. However, if EW corrections are activated, the thus derived entries can be computed with born amplitudes of wrong coupling powers if the flavor structure potentially induces QCD-EW interference amplitudes. For this purpose a second possibility, to

compute the diagonal from the off-diagonal elements is implemented as a special case.

```

<BLHA OLP interfaces: public>+=
  public :: blha_color_c_fill_diag

<BLHA OLP interfaces: sub interfaces>+=
  module subroutine blha_color_c_fill_diag &
    (sqme_born, flavors, sqme_color_c, special_case)
    real(default), intent(in) :: sqme_born
    integer, intent(in), dimension(:) :: flavors
    logical, intent(in), optional :: special_case
    real(default), intent(inout), dimension(:, :) :: sqme_color_c
  end subroutine blha_color_c_fill_diag

<BLHA OLP interfaces: procedures>+=
  module subroutine blha_color_c_fill_diag &
    (sqme_born, flavors, sqme_color_c, special_case)
    real(default), intent(in) :: sqme_born
    integer, intent(in), dimension(:) :: flavors
    logical, intent(in), optional :: special_case
    real(default), intent(inout), dimension(:, :) :: sqme_color_c
    real(default) :: sqme_line_off
    integer :: i, j
    logical :: special_c
    special_c = .false.
    if (present (special_case)) &
      special_c = special_case .and. qcd_ew_interferences (flavors)
    do i = 1, size (flavors)
      if (is_quark (flavors(i))) then
        sqme_line_off = zero
        do j = 1, size (flavors)
          if (j /= i) sqme_line_off = sqme_line_off + sqme_color_c (i, j)
        end do
        if (special_c) then
          sqme_color_c (i, i) = - sqme_line_off
        else
          sqme_color_c (i, i) = -cf * sqme_born
        end if
      else if (is_gluon (flavors(i))) then
        sqme_line_off = zero
        do j = 1, size (flavors)
          if (j /= i) sqme_line_off = sqme_line_off + sqme_color_c (i, j)
        end do
        if (special_c) then
          sqme_color_c (i, i) = - sqme_line_off
        else
          sqme_color_c (i, i) = -ca * sqme_born
        end if
      else
        sqme_color_c (i, i) = zero
      end if
    end do
  end subroutine blha_color_c_fill_diag

<BLHA OLP interfaces: public>+=

```

```

public :: blha_color_c_fill_offdiag
<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine blha_color_c_fill_offdiag &
    (n, r, sqme_color_c, offset, n_flv)
    integer, intent(in) :: n
    real(default), intent(in), dimension(:) :: r
    real(default), intent(inout), dimension(:,:) :: sqme_color_c
    integer, intent(in), optional :: offset, n_flv
  end subroutine blha_color_c_fill_offdiag

<BLHA OLP interfaces: procedures>+≡
  module subroutine blha_color_c_fill_offdiag &
    (n, r, sqme_color_c, offset, n_flv)
    integer, intent(in) :: n
    real(default), intent(in), dimension(:) :: r
    real(default), intent(inout), dimension(:,:) :: sqme_color_c
    integer, intent(in), optional :: offset, n_flv
    integer :: i, j, pos, incr
    if (present (offset)) then
      incr = offset
    else
      incr = 0
    end if
    pos = 0
    do j = 1, n
      do i = 1, j
        if (i /= j) then
          pos = (j - 1) * (j - 2) / 2 + i
          if (present (n_flv)) incr = incr + n_flv - 1
          if (present (offset)) pos = pos + incr
          sqme_color_c (i, j) = -r (pos)
          sqme_color_c (j, i) = sqme_color_c (i, j)
        end if
      end do
    end do
  end subroutine blha_color_c_fill_offdiag

```

Computes a color-correlated matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of dimension($n * (n - 1) / 2$). The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{hel}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

```

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: compute_sqme_color_c_raw => prc_blha_compute_sqme_color_c_raw

<BLHA OLP interfaces: sub interfaces>+≡
  module subroutine prc_blha_compute_sqme_color_c_raw &
    (object, i_flv, i_hel, p, ren_scale, rr, bad_point)
    class(prc_blha_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out), dimension(:) :: rr
  end subroutine prc_blha_compute_sqme_color_c_raw

```

```

        logical, intent(out) :: bad_point
    end subroutine prc_blha_compute_sqme_color_c_raw

<BLHA OLP interfaces: procedures>+≡
module subroutine prc_blha_compute_sqme_color_c_raw &
    (object, i_flv, i_hel, p, ren_scale, rr, bad_point)
    class(prc_blha_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out), dimension(:) :: rr
    logical, intent(out) :: bad_point
    real(double), dimension(5 * object%n_particles) :: mom
    real(double), dimension(size(rr)) :: r
    real(default) :: alpha_s, acc
    real(double) :: mu_dble, acc_dble
    if (debug2_active (D_REAL)) then
        call msg_debug2 (D_REAL, "use momenta: ")
        call vector4_write_set (p, show_mass = .true., &
            check_conservation = .true.)
    end if
    if (object%i_color_c(i_flv, i_hel) >= 0) then
        mom = object%create_momentum_array (p)
        if (vanishes (ren_scale)) &
            call msg_fatal ("prc_blha_compute_sqme_color_c: ren_scale vanishes")
        mu_dble = dble(ren_scale)
        alpha_s = object%qcd%alpha%get (ren_scale)

        select type (driver => object%driver)
        class is (blha_driver_t)
            call driver%set_alpha_s (alpha_s)
            call driver%blha_olp_eval2 (object%i_color_c(i_flv, i_hel), &
                mom, mu_dble, r, acc_dble)
        end select
        rr = r
        acc = acc_dble
        bad_point = acc > object%maximum_accuracy
        if (object%includes_polarization ()) rr = object%n_hel * rr
    else
        rr = zero
    end if
end subroutine prc_blha_compute_sqme_color_c_raw

<BLHA OLP interfaces: prc blha: TBP>+≡
procedure :: compute_sqme_color_c => prc_blha_compute_sqme_color_c

<BLHA OLP interfaces: sub interfaces>+≡
module subroutine prc_blha_compute_sqme_color_c &
    (object, i_flv, i_hel, p, ren_scale, born_color_c, bad_point, born_out)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(inout), dimension(:, :) :: born_color_c
    real(default), intent(out), optional :: born_out

```

```

        logical, intent(out) :: bad_point
    end subroutine prc_blha_compute_sqme_color_c
<BLHA OLP interfaces: procedures>+≡
module subroutine prc_blha_compute_sqme_color_c &
    (object, i_flv, i_hel, p, ren_scale, born_color_c, bad_point, born_out)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(inout), dimension(:,:) :: born_color_c
    real(default), intent(out), optional :: born_out
    logical, intent(out) :: bad_point
    real(default), dimension(:), allocatable :: r
    logical :: bad_point2
    real(default) :: born
    integer, dimension(:), allocatable :: flavors
    if (debug2_active (D_REAL)) then
        call msg_debug2 (D_REAL, "use momenta: ")
        call vector4_write_set (p, show_mass = .true., &
            check_conservation = .true.)
    end if
    allocate (r (blha_result_array_size &
        (size(born_color_c, dim=1), BLHA_AMP_COLOR_C)))
    call object%compute_sqme_color_c_raw (i_flv, i_hel, p, ren_scale, r, bad_point)

    select type (driver => object%driver)
    class is (blha_driver_t)
        if (allocated (object%i_tree)) then
            call object%compute_sqme (i_flv, i_hel, p, ren_scale, born, bad_point2)
        else
            born = zero
        end if
        if (present (born_out)) born_out = born
    end select
    call blha_color_c_fill_offdiag (object%n_particles, r, born_color_c)
    flavors = object%get_flv_state (i_flv)
    call blha_color_c_fill_diag (born, flavors, born_color_c)

    bad_point = bad_point .or. bad_point2
end subroutine prc_blha_compute_sqme_color_c

<BLHA OLP interfaces: prc blha: TBP>+≡
generic :: get_beam_helicities => get_beam_helicities_single
generic :: get_beam_helicities => get_beam_helicities_array
procedure :: get_beam_helicities_single => prc_blha_get_beam_helicities_single
procedure :: get_beam_helicities_array => prc_blha_get_beam_helicities_array
<BLHA OLP interfaces: sub interfaces>+≡
module function prc_blha_get_beam_helicities_single &
    (object, i, invert_second) result (hel)
    integer, dimension(:), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
    integer, intent(in) :: i

```

```

end function prc_blha_get_beam_helicities_single
module function prc_blha_get_beam_helicities_array &
    (object, invert_second) result (hel)
    integer, dimension(:,:), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
end function prc_blha_get_beam_helicities_array

<BLHA OLP interfaces: procedures>+≡
module function prc_blha_get_beam_helicities_single &
    (object, i, invert_second) result (hel)
    integer, dimension(:), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
    integer, intent(in) :: i
    logical :: inv
    inv = .false.; if (present (invert_second)) inv = invert_second
    allocate (hel (object%data%n_in))
    hel = object%i_hel (i, :)
    if (inv .and. object%data%n_in == 2) hel(2) = -hel(2)
end function prc_blha_get_beam_helicities_single

<BLHA OLP interfaces: procedures>+≡
module function prc_blha_get_beam_helicities_array &
    (object, invert_second) result (hel)
    integer, dimension(:,:), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
    integer :: i
    allocate (hel (object%n_proc, object%data%n_in))
    do i = 1, object%n_proc
        hel(i,:) = object%get_beam_helicities (i, invert_second)
    end do
end function prc_blha_get_beam_helicities_array

<BLHA OLP interfaces: prc blha: TBP>+≡
procedure :: includes_polarization => prc_blha_includes_polarization

<BLHA OLP interfaces: sub interfaces>+≡
module function prc_blha_includes_polarization (object) result (polarized)
    logical :: polarized
    class(prc_blha_t), intent(in) :: object
end function prc_blha_includes_polarization

<BLHA OLP interfaces: procedures>+≡
module function prc_blha_includes_polarization (object) result (polarized)
    logical :: polarized
    class(prc_blha_t), intent(in) :: object
    select type (driver => object%driver)
    class is (blha_driver_t)
        polarized = driver%include_polarizations
    end select
end function prc_blha_includes_polarization

```


Setup an index mapping for flavor structures and helicities that give the same matrix element. The index mapping is according to the order of flavor structures known to the `prc_core` class. Overrides `prc_core_set_equivalent_flv_hel_indices`.

(BLHA OLP interfaces: prc blha: TBP)+≡

```
procedure :: set_equivalent_flv_hel_indices => prc_blha_set_equivalent_flv_hel_indices
```

(BLHA OLP interfaces: sub interfaces)+≡

```
module subroutine prc_blha_set_equivalent_flv_hel_indices (object)
  class(prc_blha_t), intent(inout) :: object
end subroutine prc_blha_set_equivalent_flv_hel_indices
```

(BLHA OLP interfaces: procedures)+≡

```
module subroutine prc_blha_set_equivalent_flv_hel_indices (object)
  class(prc_blha_t), intent(inout) :: object
  integer :: n_flv, n_hel
  integer :: i_flv1, i_flv2, i_hel1, i_hel2
  integer, dimension(:,,:), allocatable :: amp_id, amp_id_color
  if (allocated (object%i_virt)) then
    amp_id = object%i_virt
  else
    amp_id = object%i_tree
  end if
  if (allocated (object%i_color_c)) then
    amp_id_color = object%i_color_c
  end if
  n_flv = size (amp_id, dim=1)
  n_hel = size (amp_id, dim=2)
  if (.not. allocated (object%data%eqv_flv_index)) &
    allocate (object%data%eqv_flv_index(n_flv))
  if (.not. allocated (object%data%eqv_hel_index)) &
    allocate (object%data%eqv_hel_index(n_hel))
  if (size (object%data%eqv_flv_index) /= n_flv) &
    call msg_bug ("BLHA Core: Size mismatch between eqv_flv_index and number of flavors.")
  if (size (object%data%eqv_hel_index) /= n_hel) &
    call msg_bug ("BLHA Core: Size mismatch between eqv_hel_index and number of helicities.")
  do i_flv1 = 1, n_flv
    do i_hel1 = 1, n_hel
      FLV_LOOP: do i_flv2 = 1, i_flv1
        do i_hel2 = 1, i_hel1
          if (amp_id(i_flv2, i_hel2) == amp_id(i_flv1, i_hel1)) then
            if (.not. allocated (amp_id_color)) then
              object%data%eqv_flv_index(i_flv1) = i_flv2
              object%data%eqv_hel_index(i_hel1) = i_hel2
              exit FLV_LOOP
            else if (amp_id_color(i_flv2, i_hel2) == &
              amp_id_color(i_flv1, i_hel1)) then
              object%data%eqv_flv_index(i_flv1) = i_flv2
              object%data%eqv_hel_index(i_hel1) = i_hel2
              exit FLV_LOOP
            end if
          end if
        end do
      end do
    end do FLV_LOOP
  end do
end do
```

```

end subroutine prc_blha_set_equivalent_flv_hel_indices

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure(prc_blha_init_driver), deferred :: &
    init_driver

<BLHA OLP interfaces: interfaces>+≡
  abstract interface
    subroutine prc_blha_init_driver (object, os_data)
      import
      class(prc_blha_t), intent(inout) :: object
      type(os_data_t), intent(in) :: os_data
    end subroutine prc_blha_init_driver
  end interface

```

In general, the BLHA consists of a virtual matrix element and n_{sub} subtraction terms. The subtraction terms can be pure Born matrix elements (to be used in collinear subtraction or in internal color-correlation), color-correlated matrix elements or spin-correlated matrix elements. The numbers should be ordered in such a way that \mathcal{V}_{fin} is first, followed by the pure Born, the color-correlated and the spin-correlated matrix elements. This repeats n_{flv} times. Let ν_i be the position of the i th virtual matrix element. The next \mathcal{V}_{fin} is at position $\nu_i = \nu_{i-1} + n_{\text{sub}} + 1$. Obviously, $\nu_1 = 1$. This allows us to determine the virtual matrix element positions using the recursive function implemented below.

```

<BLHA OLP interfaces: public>+≡
  public :: blha_loop_positions

<BLHA OLP interfaces: sub interfaces>+≡
  recursive module function blha_loop_positions (i_flv, n_sub) result (index)
    integer :: index
    integer, intent(in) :: i_flv, n_sub
  end function blha_loop_positions

<BLHA OLP interfaces: procedures>+≡
  recursive module function blha_loop_positions (i_flv, n_sub) result (index)
    integer :: index
    integer, intent(in) :: i_flv, n_sub
    index = 0
    if (i_flv == 1) then
      index = 1
    else
      index = blha_loop_positions (i_flv - 1, n_sub) + n_sub + 1
    end if
  end function blha_loop_positions

```

24.2.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<blha_ut.f90>≡
  <File header>

  module blha_ut

```

```

        use unit_tests
        use blha_util

        <Standard module head>

        <BLHA: public tests>

contains

        <BLHA: test driver>

end module blha_util

```

<blha_util.f90>≡
 <File header>

```

module blha_util

  <Use strings>
  use format_utils, only: write_separator
  use variables, only: var_list_t
  use os_interface
  use models
  use blha_config

```

```

  <Standard module head>

  <BLHA: test declarations>

contains

  <BLHA: test procedures>

  <BLHA: tests>

end module blha_util

```

API: driver for the unit tests below.

<BLHA: public tests>≡
 public :: blha_test

```

<BLHA: test driver>≡
  subroutine blha_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    call test(blha_1, "blha_1", "Test the creation of BLHA-OLP files", u, results)
    call test(blha_2, "blha_2", "Test the creation of BLHA-OLP files for "&
      &"multiple flavor structures", u, results)
    call test(blha_3, "blha_3", "Test helicity-information in OpenLoops OLP files", &
      u, results)
  end subroutine blha_test

```

(BLHA: test procedures)≡

```

subroutine setup_and_write_blha_configuration (u, single, polarized)
  integer, intent(in) :: u
  logical, intent(in), optional :: single
  logical, intent(in), optional :: polarized
  logical :: polrzd, singl
  type(blha_master_t) :: blha_master
  integer :: i
  integer :: n_in, n_out
  integer :: alpha_power, alphas_power
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(string_t) :: proc_id, method, correction_type
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(var_list_t) :: var_list
  type(model_t), pointer :: model => null ()
  integer :: openloops_phs_tolerance

  polrzd = .false.; if (present (polarized)) polrzd = polarized
  singl = .true.; if (present (single)) singl = single

  if (singl) then
    write (u, "(A)") "* Process: e+ e- -> W+ W- b b~"
    n_in = 2; n_out = 4
    alpha_power = 4; alphas_power = 0
    allocate (flv_born (n_in + n_out, 1))
    allocate (flv_real (n_in + n_out + 1, 1))
    flv_born(1,1) = 11; flv_born(2,1) = -11
    flv_born(3,1) = 24; flv_born(4,1) = -24
    flv_born(5,1) = 5; flv_born(6,1) = -5
    flv_real(1:6,1) = flv_born(:,1)
    flv_real(7,1) = 21
  else
    write (u, "(A)") "* Process: e+ e- -> u:d:s U:D:S"
    n_in = 2; n_out = 2
    alpha_power = 2; alphas_power = 0
    allocate (flv_born (n_in + n_out, 3))
    allocate (flv_real (n_in + n_out + 1, 3))
    flv_born(1,:) = 11; flv_born(2,:) = -11
    flv_born(3,1) = 1; flv_born(4,1) = -1
    flv_born(3,2) = 2; flv_born(4,2) = -2
    flv_born(3,3) = 3; flv_born(4,3) = -3
    flv_real(1:4,:) = flv_born
    flv_real(5,:) = 21
  end if
  proc_id = var_str ("BLHA_Test")

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), os_data, model)

  write (u, "(A)") "* BLHA matrix elements assumed for all process components"
  write (u, "(A)") "* Mode: GoSam"

```

```

method = var_str ("gosam")
correction_type = var_str ("QCD")
call var_list%append_string (var_str ("$born_me_method"), method)
call var_list%append_string (var_str ("$real_tree_me_method"), method)
call var_list%append_string (var_str ("$loop_me_method"), method)
call var_list%append_string (var_str ("$correlation_me_method"), method)
call blha_master%set_ew_scheme (var_str ("GF"))
call blha_master%set_methods (.true., var_list)
call blha_master%allocate_config_files ()
call blha_master%set_correction_type (correction_type)
call blha_master%generate (proc_id, model, n_in, &
    alpha_power, alphas_power, flv_born, flv_real)

call test_output (u)

call blha_master%final ()
call var_list%final ()
write (u, "(A)") "* Switch to OpenLoops"
openloops_phs_tolerance = 7

method = var_str ("openloops")
correction_type = var_str ("QCD")
call var_list%append_string (var_str ("$born_me_method"), method)
call var_list%append_string (var_str ("$real_tree_me_method"), method)
call var_list%append_string (var_str ("$loop_me_method"), method)
call var_list%append_string (var_str ("$correlation_me_method"), method)
call blha_master%set_methods (.true., var_list)
call blha_master%allocate_config_files ()
call blha_master%set_correction_type (correction_type)
call blha_master%generate (proc_id, model, n_in, &
    alpha_power, alphas_power, flv_born, flv_real)

if (polrzd) then
    do i = 1, 4
        call blha_master%set_polarization (i)
    end do
end if
call blha_master%setup_additional_features &
    (openloops_phs_tolerance, .false., 0)

call test_output (u)

contains

subroutine test_output (u)
    integer, intent(in) :: u
    do i = 1, 4
        call write_separator (u)
        call write_component_type (i, u)
        call write_separator (u)
        call blha_configuration_write &
            (blha_master%blha_cfg(i), blha_master%suffix(i), u, no_version = .true.)
    end do

```

```

end subroutine test_output

subroutine write_component_type (i, u)
  integer, intent(in) :: i, u
  type(string_t) :: message, component_type
  message = var_str ("OLP-File content for ")
  select case (i)
  case (1)
    component_type = var_str ("loop")
  case (2)
    component_type = var_str ("subtraction")
  case (3)
    component_type = var_str ("real")
  case (4)
    component_type = var_str ("born")
  end select
  message = message // component_type // " matrix elements"
  write (u, "(A)") char (message)
end subroutine write_component_type

end subroutine setup_and_write_blha_configuration

<BLHA: test declarations>≡
public :: blha_1

<BLHA: tests>≡
subroutine blha_1 (u)
  integer, intent(in) :: u
  write (u, "(A)") "* Test output: blha_1"
  write (u, "(A)") "* Purpose: Test the creation of olp-files for single "&
    &"and unpolarized flavor structures"
  write (u, "(A)")
  call setup_and_write_blha_configuration (u, single = .true., polarized = .false.)
end subroutine blha_1

<BLHA: test declarations>+≡
public :: blha_2

<BLHA: tests>+≡
subroutine blha_2 (u)
  integer, intent(in) :: u
  write (u, "(A)") "* Test output: blha_2"
  write (u, "(A)") "* Purpose: Test the creation of olp-files for multiple "&
    &"and unpolarized flavor structures"
  write (u, "(A)")
  call setup_and_write_blha_configuration (u, single = .false., polarized = .false.)
end subroutine blha_2

<BLHA: test declarations>+≡
public :: blha_3

<BLHA: tests>+≡
subroutine blha_3 (u)
  integer, intent(in) :: u

```

```
write (u, "(A)") "* Test output: blha_3"
write (u, "(A)") "* Purpose: Test the creation of olp-files for single "&
      &"and polarized flavor structures"
write (u, "(A)")
      call setup_and_write_blha_configuration (u, single = .true., polarized = .true.)
end subroutine blha_3
```

Chapter 25

GoSam Interface

The code in this chapter makes amplitudes accessible to **WHIZARD** that are generated and computed by the GoSam package.

These are the modules:

loop_archive Provide some useful extra functionality.

prc_gosam The actual interface, following the **WHIZARD** conventions for matrix-element generator methods.



No internal dependencies

Figure 25.1: Module dependencies in `src/gosam`.

25.1 Gosam Interface

```
<prc_gosam.f90>≡  
  <File header>  
  
  module prc_gosam  
  
    use, intrinsic :: iso_c_binding !NODEP!  
    use, intrinsic :: iso_fortran_env  
  
    use kinds  
    <Use strings>  
    use physics_defs  
    use os_interface  
    use lorentz  
    use interactions  
    use model_data  
    use variables  
    use prc_core_def  
    use prc_core  
    use blha_config  
    use blha_olp_interfaces  
  
    <Standard module head>  
  
    <Prc gosam: constants>  
  
    <Prc gosam: public>  
  
    <Prc gosam: types>  
  
    <Prc gosam: interfaces>  
  
    interface  
    <Prc gosam: sub interfaces>  
    end interface  
  
    contains  
  
    <Prc gosam: main procedures>  
  
  end module prc_gosam  
  
<prc_gosam_sub.f90>≡  
  <File header>  
  
  submodule (prc_gosam) prc_gosam_s  
  
    use io_units  
    use constants  
    use numeric_utils  
    use system_defs, only: TAB  
    use system_dependencies  
    use file_utils
```

```

    use string_utils
    use diagnostics
    use sm_qcd
    use flavors
    use pdg_arrays
    use process_constants
    use prclib_interfaces
    use process_libraries

    implicit none

contains

  <Prc gosam: procedures>

  end submodule prc_gosam_s

  <Prc gosam: types>≡
    type, extends (prc_blha_writer_t) :: gosam_writer_t
      type(string_t) :: gosam_dir
      type(string_t) :: golem_dir
      type(string_t) :: samurai_dir
      type(string_t) :: ninja_dir
      type(string_t) :: form_dir
      type(string_t) :: qgraf_dir
      type(string_t) :: filter_lo, filter_nlo
      type(string_t) :: symmetries
      integer :: form_threads
      integer :: form_workspace
      type(string_t) :: fc
    contains
      <Prc gosam: gosam writer: TBP>
    end type gosam_writer_t

  <Prc gosam: public>≡
    public :: gosam_def_t

  <Prc gosam: types>+≡
    type, extends (blha_def_t) :: gosam_def_t
      logical :: execute_olp = .true.
    contains
      <Prc gosam: gosam def: TBP>
    end type gosam_def_t

  <Prc gosam: types>+≡
    type, extends (blha_driver_t) :: gosam_driver_t
      type(string_t) :: gosam_dir
      type(string_t) :: olp_file
      type(string_t) :: olc_file
      type(string_t) :: olp_dir
      type(string_t) :: olp_lib
    contains
      <Prc gosam: gosam driver: TBP>

```

```

end type gosam_driver_t

<Prc gosam: public>+≡
  public :: prc_gosam_t

<Prc gosam: types>+≡
  type, extends (prc_blha_t) :: prc_gosam_t
    logical :: initialized = .false.
  contains
    <Prc gosam: prc gosam: TBP>
  end type prc_gosam_t

<Prc gosam: types>+≡
  type, extends (blha_state_t) :: gosam_state_t
  contains
    <Prc gosam: gosam state: TBP>
  end type gosam_state_t

Gfortran 7/8/9 bug: has to remain in main module.

<Prc gosam: gosam def: TBP>≡
  procedure :: init => gosam_def_init

<Prc gosam: main procedures>≡
  subroutine gosam_def_init (object, basename, model_name, &
    prt_in, prt_out, nlo_type, restrictions, var_list)
    class(gosam_def_t), intent(inout) :: object
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    integer, intent(in) :: nlo_type
    type(string_t), intent(in), optional :: restrictions
    type(var_list_t), intent(in) :: var_list
    object%basename = basename
    allocate (gosam_writer_t :: object%writer)
    select case (nlo_type)
    case (BORN)
      object%suffix = '_BORN'
    case (NLO_REAL)
      object%suffix = '_REAL'
    case (NLO_VIRTUAL)
      object%suffix = '_LOOP'
    case (NLO_SUBTRACTION)
      object%suffix = '_SUB'
    end select
    select type (writer => object%writer)
    type is (gosam_writer_t)
      call writer%init (model_name, prt_in, prt_out, restrictions)
      writer%filter_lo = var_list%get_sval (var_str ("gosam_filter_lo"))
      writer%filter_nlo = var_list%get_sval (var_str ("gosam_filter_nlo"))
      writer%symmetries = &
        var_list%get_sval (var_str ("gosam_symmetries"))
      writer%form_threads = &
        var_list%get_ival (var_str ("form_threads"))

```

```

        writer%form_workspace = &
            var_list%get_ival (var_str ("form_workspace"))
        writer%fc = &
            var_list%get_sval (var_str ("gosam_fc"))
    end select
end subroutine gosam_def_init

<Prc gosam: gosam writer: TBP>≡
    procedure :: write_config => gosam_writer_write_config

<Prc gosam: sub interfaces>≡
    module subroutine gosam_writer_write_config (gosam_writer)
        class(gosam_writer_t), intent(in) :: gosam_writer
    end subroutine gosam_writer_write_config

<Prc gosam: procedures>≡
    module subroutine gosam_writer_write_config (gosam_writer)
        class(gosam_writer_t), intent(in) :: gosam_writer
        integer :: unit
        unit = free_unit ()
        open (unit, file = "golem.in", status = "replace", action = "write")
        call gosam_writer%generate_configuration_file (unit)
        close(unit)
    end subroutine gosam_writer_write_config

<Prc gosam: gosam def: TBP>+≡
    procedure, nopass :: type_string => gosam_def_type_string

<Prc gosam: sub interfaces>+≡
    module function gosam_def_type_string () result (string)
        type(string_t) :: string
    end function gosam_def_type_string

<Prc gosam: procedures>+≡
    module function gosam_def_type_string () result (string)
        type(string_t) :: string
        string = "gosam"
    end function gosam_def_type_string

<Prc gosam: gosam def: TBP>+≡
    procedure :: write => gosam_def_write

<Prc gosam: sub interfaces>+≡
    module subroutine gosam_def_write (object, unit)
        class(gosam_def_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine gosam_def_write

<Prc gosam: procedures>+≡
    module subroutine gosam_def_write (object, unit)
        class(gosam_def_t), intent(in) :: object
        integer, intent(in) :: unit
        select type (writer => object%writer)
        type is (gosam_writer_t)
            call writer%write (unit)
        end select

```

```

        end subroutine gosam_def_write

<Prc gosam: gosam def: TBP>+≡
    procedure :: read => gosam_def_read

<Prc gosam: sub interfaces>+≡
    module subroutine gosam_def_read (object, unit)
        class(gosam_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine gosam_def_read

<Prc gosam: procedures>+≡
    module subroutine gosam_def_read (object, unit)
        class(gosam_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine gosam_def_read

Gfortran 7/8/9 bug: has to remain in main module.

<Prc gosam: gosam def: TBP>+≡
    procedure :: allocate_driver => gosam_def_allocate_driver

<Prc gosam: main procedures>+≡
    subroutine gosam_def_allocate_driver (object, driver, basename)
        class(gosam_def_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        if (.not. allocated (driver)) allocate (gosam_driver_t :: driver)
    end subroutine gosam_def_allocate_driver

<Prc gosam: gosam writer: TBP>+≡
    procedure, nopass :: type_name => gosam_writer_type_name

<Prc gosam: sub interfaces>+≡
    module function gosam_writer_type_name () result (string)
        type(string_t) :: string
    end function gosam_writer_type_name

<Prc gosam: procedures>+≡
    module function gosam_writer_type_name () result (string)
        type(string_t) :: string
        string = "gosam"
    end function gosam_writer_type_name

<Prc gosam: gosam writer: TBP>+≡
    procedure :: init => gosam_writer_init

<Prc gosam: sub interfaces>+≡
    pure module subroutine gosam_writer_init &
        (writer, model_name, prt_in, prt_out, restrictions)
        class(gosam_writer_t), intent(inout) :: writer
        type(string_t), intent(in) :: model_name
        type(string_t), dimension(:), intent(in) :: prt_in, prt_out
        type(string_t), intent(in), optional :: restrictions
    end subroutine gosam_writer_init

```

```

<Prc gosam: procedures>+=
  pure module subroutine gosam_writer_init &
    (writer, model_name, prt_in, prt_out, restrictions)
    class(gosam_writer_t), intent(inout) :: writer
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    type(string_t), intent(in), optional :: restrictions
    writer%gosam_dir = GOSAM_DIR
    writer%golem_dir = GOLEM_DIR
    writer%samurai_dir = SAMURAI_DIR
    writer%ninja_dir = NINJA_DIR
    writer%form_dir = FORM_DIR
    writer%qgraf_dir = QGRAF_DIR
    call writer%base_init (model_name, prt_in, prt_out)
  end subroutine gosam_writer_init

<Prc gosam: gosam driver: TBP>=
  procedure, nopass :: type_name => gosam_driver_type_name

<Prc gosam: sub interfaces>+=
  module function gosam_driver_type_name () result (string)
    type(string_t) :: string
  end function gosam_driver_type_name

<Prc gosam: procedures>+=
  module function gosam_driver_type_name () result (string)
    type(string_t) :: string
    string = "gosam"
  end function gosam_driver_type_name

<Prc gosam: gosam driver: TBP>+=
  procedure :: init_gosam => gosam_driver_init_gosam

<Prc gosam: sub interfaces>+=
  module subroutine gosam_driver_init_gosam (object, os_data, olp_file, &
    olc_file, olp_dir, olp_lib)
    class(gosam_driver_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: olp_file, olc_file, olp_dir, olp_lib
  end subroutine gosam_driver_init_gosam

<Prc gosam: procedures>+=
  module subroutine gosam_driver_init_gosam (object, os_data, olp_file, &
    olc_file, olp_dir, olp_lib)
    class(gosam_driver_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: olp_file, olc_file, olp_dir, olp_lib
    object%gosam_dir = GOSAM_DIR
    object%olp_file = olp_file
    object%contract_file = olc_file
    object%olp_dir = olp_dir
    object%olp_lib = olp_lib
  end subroutine gosam_driver_init_gosam

```

```

(Prc gosam: gosam driver: TBP)+≡
    procedure :: init_dlaccess_to_library => gosam_driver_init_dlaccess_to_library

(Prc gosam: sub interfaces)+≡
    module subroutine gosam_driver_init_dlaccess_to_library &
        (object, os_data, dlaccess, success)
        class(gosam_driver_t), intent(in) :: object
        type(os_data_t), intent(in) :: os_data
        type(dlaccess_t), intent(out) :: dlaccess
        logical, intent(out) :: success
    end subroutine gosam_driver_init_dlaccess_to_library

(Prc gosam: procedures)+≡
    module subroutine gosam_driver_init_dlaccess_to_library &
        (object, os_data, dlaccess, success)
        class(gosam_driver_t), intent(in) :: object
        type(os_data_t), intent(in) :: os_data
        type(dlaccess_t), intent(out) :: dlaccess
        logical, intent(out) :: success
        type(string_t) :: libname, msg_buffer
        libname = object%olp_dir // '/.libs/libgolem_olp.' // &
            os_data%shrllib_ext
        msg_buffer = "One-Loop-Provider: Using Gosam"
        call msg_message (char(msg_buffer))
        msg_buffer = "Loading library: " // libname
        call msg_message (char(msg_buffer))
        call dlaccess_init (dlaccess, var_str("."), libname, os_data)
        success = .not. dlaccess_has_error (dlaccess)
    end subroutine gosam_driver_init_dlaccess_to_library

(Prc gosam: gosam writer: TBP)+≡
    procedure :: generate_configuration_file => &
        gosam_writer_generate_configuration_file

(Prc gosam: sub interfaces)+≡
    module subroutine gosam_writer_generate_configuration_file &
        (object, unit)
        class(gosam_writer_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine gosam_writer_generate_configuration_file

(Prc gosam: procedures)+≡
    module subroutine gosam_writer_generate_configuration_file &
        (object, unit)
        class(gosam_writer_t), intent(in) :: object
        integer, intent(in) :: unit
        type(string_t) :: fc_bin
        type(string_t) :: form_bin, qgraf_bin, haggies_bin
        type(string_t) :: fcflags_golem, ldflags_golem
        type(string_t) :: fcflags_samurai, ldflags_samurai
        type(string_t) :: fcflags_ninja, ldflags_ninja
        type(string_t) :: ldflags_avh_olo, ldflags_qcdloop
        fc_bin = DEFAULT_FC
        form_bin = object%form_dir // '/bin/tform'
        qgraf_bin = object%qgraf_dir // '/bin/qgraf'
        if (object%gosam_dir /= "") then

```

```

        haggies_bin = '/usr/bin/java -jar ' // object%gosam_dir // &
        '/share/golem/haggies/haggies.jar'
    else
        call msg_fatal ("generate_configuration_file: At least " // &
            "the GoSam Directory has to be specified!")
    end if
    if (object%golem_dir /= "") then
        fcflags_golem = "-I" // object%golem_dir // "/include/golem95"
        ldflags_golem = "-L" // object%golem_dir // "/lib -lgolem"
    end if
    if (object%samurai_dir /= "") then
        fcflags_samurai = "-I" // object%samurai_dir // "/include/samurai"
        ldflags_samurai = "-L" // object%samurai_dir // "/lib -lsamurai"
        ldflags_avh_olo = "-L" // object%samurai_dir // "/lib -lavh_olo"
        ldflags_qcdloop = "-L" // object%samurai_dir // "/lib -lqcdloop"
    end if
    if (object%ninja_dir /= "") then
        fcflags_ninja = "-I" // object%ninja_dir // "/include/ninja " &
            // "-I" // object%ninja_dir // "/include"
        ldflags_ninja = "-L" // object%ninja_dir // "/lib -lninja"
    end if
    write (unit, "(A)") "#+avh_olo.ldflags=" &
        // char (ldflags_avh_olo)
    write (unit, "(A)") "reduction_programs=golem95, samurai, ninja"
    write (unit, "(A)") "extensions=autotools"
    write (unit, "(A)") "#+qcdloop.ldflags=" &
        // char (ldflags_qcdloop)
    write (unit, "(A)") "#+zzz.extensions=qcdloop, avh_olo"
    write (unit, "(A)") "#fc.bin=" // char (fc_bin)
    write (unit, "(A)") "form.bin=" // char (form_bin)
    write (unit, "(A)") "qgraf.bin=" // char (qgraf_bin)
    write (unit, "(A)") "#golem95.fcflags=" // char (fcflags_golem)
    write (unit, "(A)") "#golem95.ldflags=" // char (ldflags_golem)
    write (unit, "(A)") "haggies.bin=" // char (haggies_bin)
    write (unit, "(A)") "#samurai.fcflags=" // char (fcflags_samurai)
    write (unit, "(A)") "#samurai.ldflags=" // char (ldflags_samurai)
    write (unit, "(A)") "#ninja.fcflags=" // char (fcflags_ninja)
    write (unit, "(A)") "#ninja.ldflags=" // char (ldflags_ninja)
    !!! This might collide with the mass-setup in the order-file
    !!! write (unit, "(A)") "zero=mU,mD,mC,mS,mB"
    !!! This is covered by the BLHA2 interface
    write (unit, "(A)") "PSP_check=False"
    if (char (object%filter_lo) /= "") &
        write (unit, "(A)") "filter.lo=" // char (object%filter_lo)
    if (char (object%filter_nlo) /= "") &
        write (unit, "(A)") "filter.nlo=" // char (object%filter_nlo)
    if (char (object%symmetries) /= "") &
        write (unit, "(A)") "symmetries=" // char (object%symmetries)
    write (unit, "(A,IO)") "form.threads=", object%form_threads
    write (unit, "(A,IO)") "form.workspace=", object%form_workspace
    if (char (object%fc) /= "") &
        write (unit, "(A)") "fc.bin=" // char (object%fc)
    end subroutine gosam_writer_generate_configuration_file

```


We have to assure that all files necessary for the configure process in the GoSam code are ready. This is done with a stamp mechanism.

```

<Prc gosam: gosam driver: TBP>+=
    procedure :: write_makefile => gosam_driver_write_makefile

<Prc gosam: sub interfaces>+=
    module subroutine gosam_driver_write_makefile (object, unit, libname)
        class(gosam_driver_t), intent(in) :: object
        integer, intent(in) :: unit
        type(string_t), intent(in) :: libname
    end subroutine gosam_driver_write_makefile

<Prc gosam: procedures>+=
    module subroutine gosam_driver_write_makefile (object, unit, libname)
        class(gosam_driver_t), intent(in) :: object
        integer, intent(in) :: unit
        type(string_t), intent(in) :: libname
        write (unit, "(2A)") "OLP_FILE = ", char (object%olp_file)
        write (unit, "(2A)") "OLP_DIR = ", char (object%olp_dir)
        write (unit, "(A)")
        write (unit, "(A)") "all: $(OLP_DIR)/config.log"
        write (unit, "(2A)") TAB, "make -C $(OLP_DIR) install"
        write (unit, "(A)")
        write (unit, "(3A)") "$(OLP_DIR)/config.log: "
        write (unit, "(4A)") TAB, char (object%gosam_dir // "/bin/gosam.py "), &
            "-olp $(OLP_FILE) -destination=$(OLP_DIR)", &
            "-f -z"
        write (unit, "(3A)") TAB, "cd $(OLP_DIR); ./autogen.sh -prefix=", &
            "$(dir $(abspath $(lastword $(MAKEFILE_LIST))))"
    end subroutine gosam_driver_write_makefile

<Prc gosam: gosam driver: TBP>+=
    procedure :: set_alpha_s => gosam_driver_set_alpha_s

<Prc gosam: sub interfaces>+=
    module subroutine gosam_driver_set_alpha_s (driver, alpha_s)
        class(gosam_driver_t), intent(in) :: driver
        real(default), intent(in) :: alpha_s
    end subroutine gosam_driver_set_alpha_s

<Prc gosam: procedures>+=
    module subroutine gosam_driver_set_alpha_s (driver, alpha_s)
        class(gosam_driver_t), intent(in) :: driver
        real(default), intent(in) :: alpha_s
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'alphaS'//c_null_char, &
             dble (alpha_s), 0._double, ierr)
    end subroutine gosam_driver_set_alpha_s

<Prc gosam: gosam driver: TBP>+=
    procedure :: set_alpha_qed => gosam_driver_set_alpha_qed

<Prc gosam: sub interfaces>+=
    module subroutine gosam_driver_set_alpha_qed (driver, alpha)
        class(gosam_driver_t), intent(inout) :: driver

```

```

        real(default), intent(in) :: alpha
    end subroutine gosam_driver_set_alpha_qed

<Prc gosam: procedures>+=
    module subroutine gosam_driver_set_alpha_qed (driver, alpha)
        class(gosam_driver_t), intent(inout) :: driver
        real(default), intent(in) :: alpha
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'alpha'//c_null_char, &
             dble (alpha), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('alpha'))
    end subroutine gosam_driver_set_alpha_qed

<Prc gosam: gosam driver: TBP>+=
    procedure :: set_GF => gosam_driver_set_GF

<Prc gosam: sub interfaces>+=
    module subroutine gosam_driver_set_GF (driver, GF)
        class(gosam_driver_t), intent(inout) :: driver
        real(default), intent(in) :: GF
    end subroutine gosam_driver_set_GF

<Prc gosam: procedures>+=
    module subroutine gosam_driver_set_GF (driver, GF)
        class(gosam_driver_t), intent(inout) :: driver
        real(default), intent(in) :: GF
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'GF'//c_null_char, &
             dble(GF), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('GF'))
    end subroutine gosam_driver_set_GF

<Prc gosam: gosam driver: TBP>+=
    procedure :: set_weinberg_angle => gosam_driver_set_weinberg_angle

<Prc gosam: sub interfaces>+=
    module subroutine gosam_driver_set_weinberg_angle (driver, sw2)
        class(gosam_driver_t), intent(inout) :: driver
        real(default), intent(in) :: sw2
    end subroutine gosam_driver_set_weinberg_angle

<Prc gosam: procedures>+=
    module subroutine gosam_driver_set_weinberg_angle (driver, sw2)
        class(gosam_driver_t), intent(inout) :: driver
        real(default), intent(in) :: sw2
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'sw2'//c_null_char, &
             dble(sw2), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('sw2'))
    end subroutine gosam_driver_set_weinberg_angle

<Prc gosam: gosam driver: TBP>+=
    procedure :: print_alpha_s => gosam_driver_print_alpha_s

```

```

<Prc gosam: sub interfaces>+≡
    module subroutine gosam_driver_print_alpha_s (object)
        class(gosam_driver_t), intent(in) :: object
        end subroutine gosam_driver_print_alpha_s
<Prc gosam: procedures>+≡
    module subroutine gosam_driver_print_alpha_s (object)
        class(gosam_driver_t), intent(in) :: object
        call object%blha_olp_print_parameter (c_char_'alphaS'//c_null_char)
    end subroutine gosam_driver_print_alpha_s

<Prc gosam: prc gosam: TBP>≡
    procedure :: prepare_library => prc_gosam_prepare_library

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_prepare_library (object, os_data, libname)
        class(prc_gosam_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
    end subroutine prc_gosam_prepare_library

<Prc gosam: procedures>+≡
    module subroutine prc_gosam_prepare_library (object, os_data, libname)
        class(prc_gosam_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        select type (writer => object%def%writer)
            type is (gosam_writer_t)
                call writer%write_config ()
            end select
        call object%create_olp_library (libname)
        call object%load_driver (os_data)
    end subroutine prc_gosam_prepare_library

<Prc gosam: prc gosam: TBP>+≡
    procedure :: prepare_external_code => &
        prc_gosam_prepare_external_code

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_gosam_t), intent(inout) :: core
        integer, intent(in), dimension(:,,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
    end subroutine prc_gosam_prepare_external_code

<Prc gosam: procedures>+≡
    module subroutine prc_gosam_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_gosam_t), intent(inout) :: core
        integer, intent(in), dimension(:,,:), allocatable :: flv_states

```

```

type(var_list_t), intent(in) :: var_list
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in) :: libname
type(model_data_t), intent(in), target :: model
integer, intent(in) :: i_core
logical, intent(in) :: is_nlo
core%sqme_tree_pos = 4
call core%prepare_library (os_data, libname)
call core%start ()
call core%read_contract_file (flv_states)
call core%set_particle_properties (model)
call core%set_electroweak_parameters (model)
call core%print_parameter_file (i_core)
end subroutine prc_gosam_prepare_external_code

```

<Prc gosam: prc gosam: TBP>+≡

```

procedure :: write_makefile => prc_gosam_write_makefile

```

<Prc gosam: sub interfaces>+≡

```

module subroutine prc_gosam_write_makefile (object, unit, libname)
  class(prc_gosam_t), intent(in) :: object
  integer, intent(in) :: unit
  type(string_t), intent(in) :: libname
end subroutine prc_gosam_write_makefile

```

<Prc gosam: procedures>+≡

```

module subroutine prc_gosam_write_makefile (object, unit, libname)
  class(prc_gosam_t), intent(in) :: object
  integer, intent(in) :: unit
  type(string_t), intent(in) :: libname
  select type (driver => object%driver)
    type is (gosam_driver_t)
      call driver%write_makefile (unit, libname)
  end select
end subroutine prc_gosam_write_makefile

```

<Prc gosam: prc gosam: TBP>+≡

```

procedure :: execute_makefile => prc_gosam_execute_makefile

```

<Prc gosam: sub interfaces>+≡

```

module subroutine prc_gosam_execute_makefile (object, libname)
  class(prc_gosam_t), intent(in) :: object
  type(string_t), intent(in) :: libname
end subroutine prc_gosam_execute_makefile

```

<Prc gosam: procedures>+≡

```

module subroutine prc_gosam_execute_makefile (object, libname)
  class(prc_gosam_t), intent(in) :: object
  type(string_t), intent(in) :: libname
  select type (driver => object%driver)
    type is (gosam_driver_t)
      call os_system_call ("make -f " // &
        libname // "_gosam.makefile")
  end select
end subroutine prc_gosam_execute_makefile

```

```

<Prc gosam: prc gosam: TBP>+≡
    procedure :: create_olp_library => prc_gosam_create_olp_library

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_create_olp_library (object, libname)
        class(prc_gosam_t), intent(inout) :: object
        type(string_t), intent(in) :: libname
    end subroutine prc_gosam_create_olp_library

<Prc gosam: procedures>+≡
    module subroutine prc_gosam_create_olp_library (object, libname)
        class(prc_gosam_t), intent(inout) :: object
        type(string_t), intent(in) :: libname
        integer :: unit
        select type (driver => object%driver)
        type is (gosam_driver_t)
            unit = free_unit ()
            open (unit, file = char (libname // "_gosam.makefile"), &
                status = "replace", action= "write")
            call object%write_makefile (unit, libname)
            close (unit)
            call object%execute_makefile (libname)
        end select
    end subroutine prc_gosam_create_olp_library

<Prc gosam: prc gosam: TBP>+≡
    procedure :: load_driver => prc_gosam_load_driver

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_load_driver (object, os_data)
        class(prc_gosam_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
    end subroutine prc_gosam_load_driver

<Prc gosam: procedures>+≡
    module subroutine prc_gosam_load_driver (object, os_data)
        class(prc_gosam_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical :: dl_success

        select type (driver => object%driver)
        type is (gosam_driver_t)
            call driver%load (os_data, dl_success)
            if (.not. dl_success) &
                call msg_fatal ("GoSam Libraries could not be loaded")
        end select
    end subroutine prc_gosam_load_driver

<Prc gosam: prc gosam: TBP>+≡
    procedure :: start => prc_gosam_start

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_start (object)
        class(prc_gosam_t), intent(inout) :: object
    end subroutine prc_gosam_start

```

```

<Prc gosam: procedures>+≡
  module subroutine prc_gosam_start (object)
    class(prc_gosam_t), intent(inout) :: object
    integer :: ierr
    if (object%includes_polarization()) &
      call msg_fatal ('GoSam does not support polarized beams!')
    select type (driver => object%driver)
    type is (gosam_driver_t)
      call driver%blha_olp_start (string_f2c (driver%contract_file), ierr)
    end select
  end subroutine prc_gosam_start

<Prc gosam: prc gosam: TBP>+≡
  procedure :: write => prc_gosam_write

<Prc gosam: sub interfaces>+≡
  module subroutine prc_gosam_write (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine prc_gosam_write

<Prc gosam: procedures>+≡
  module subroutine prc_gosam_write (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
    call msg_message (unit = unit, string = "GOSAM")
  end subroutine prc_gosam_write

<Prc gosam: prc gosam: TBP>+≡
  procedure :: write_name => prc_gosam_write_name

<Prc gosam: sub interfaces>+≡
  module subroutine prc_gosam_write_name (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine prc_gosam_write_name

<Prc gosam: procedures>+≡
  module subroutine prc_gosam_write_name (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(1x,A)") "Core: GoSam"
  end subroutine prc_gosam_write_name

<Prc gosam: prc gosam: TBP>+≡
  procedure :: init_driver => prc_gosam_init_driver

<Prc gosam: sub interfaces>+≡
  module subroutine prc_gosam_init_driver (object, os_data)
    class(prc_gosam_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
  end subroutine prc_gosam_init_driver

```

```

<Prc gosam: procedures>+=
module subroutine prc_gosam_init_driver (object, os_data)
  class(prc_gosam_t), intent(inout) :: object
  type(os_data_t), intent(in) :: os_data
  type(string_t) :: olp_file, olc_file, olp_dir
  type(string_t) :: suffix

  select type (def => object%def)
  type is (gosam_def_t)
    suffix = def%suffix
    olp_file = def%basename // suffix // '.olp'
    olc_file = def%basename // suffix // '.olc'
    olp_dir = def%basename // suffix // '_olp_modules'
  class default
    call msg_bug ("prc_gosam_init_driver: core_def should be of gosam-type")
  end select

  select type(driver => object%driver)
  type is (gosam_driver_t)
    driver%nlo_suffix = suffix
    call driver%init_gosam (os_data, olp_file, olc_file, olp_dir, &
      var_str ("libgolem_olp"))
  end select
end subroutine prc_gosam_init_driver

<Prc gosam: prc gosam: TBP>+=
procedure :: set_initialized => prc_gosam_set_initialized

<Prc gosam: sub interfaces>+=
module subroutine prc_gosam_set_initialized (prc_gosam)
  class(prc_gosam_t), intent(inout) :: prc_gosam
end subroutine prc_gosam_set_initialized

<Prc gosam: procedures>+=
module subroutine prc_gosam_set_initialized (prc_gosam)
  class(prc_gosam_t), intent(inout) :: prc_gosam
  prc_gosam%initialized = .true.
end subroutine prc_gosam_set_initialized

```

The BLHA-interface conventions require the quantity $S_{ij} = \langle M_{i,+} | T_i T_j | M_{i,-} \rangle$ to be produced, where i is the position of the splitting gluon. However, $\bar{M} = \langle M_{i,-} | M_{i,+} \rangle$ is needed. This can be obtained using color conservation, $\sum_j T_j |M\rangle = 0$, so that

$$\sum_{j \neq i} S_{ij} = -\langle M_{i,+} | T_i^2 | M_{i,-} \rangle = -C_A \langle M_{i,+} | M_{i,-} \rangle = -C_A \bar{M}^*$$

According to BLHA conventions, the real part of S_{ij} is located at positions $2i + 2nj$ in the output array, where n denotes the number of external particles and the enumeration of particles starts at zero. The subsequent position, i.e. $2i + 2nj + 1$ is designated to the imaginary part of S_{ij} . Note that, since the first array position is 1, the implemented position association deviates from the above one in the addition of 1.

```

<Prc gosam: procedures>+=

```

```

(Prc gosam: prc gosam: TBP)+≡
  procedure :: compute_sqme_spin_c => prc_gosam_compute_sqme_spin_c

(Prc gosam: sub interfaces)+≡
  module subroutine prc_gosam_compute_sqme_spin_c (object, &
    i_flv, i_hel, em, p, ren_scale, me_sc, bad_point)
    class(prc_gosam_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    integer, intent(in) :: em
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    complex(default), intent(out) :: me_sc
    logical, intent(out) :: bad_point
  end subroutine prc_gosam_compute_sqme_spin_c

(Prc gosam: procedures)+≡
  module subroutine prc_gosam_compute_sqme_spin_c (object, &
    i_flv, i_hel, em, p, ren_scale, me_sc, bad_point)
    class(prc_gosam_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    integer, intent(in) :: em
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    complex(default), intent(out) :: me_sc
    logical, intent(out) :: bad_point
    real(double), dimension(5*object%n_particles) :: mom
    real(double), dimension(OLP_RESULTS_LIMIT) :: r
    real(double) :: ren_scale_dble
    integer :: i, igm1, n
    integer :: pos_real, pos_imag
    real(double) :: acc_dble
    real(default) :: acc, alpha_s
    if (object%i_spin_c(i_flv, i_hel) >= 0) then
      me_sc = cmplx (zero ,zero, kind=default)
      mom = object%create_momentum_array (p)
      if (vanishes (ren_scale)) &
        call msg_fatal ("prc_gosam_compute_sqme_spin_c: ren_scale vanishes")
      alpha_s = object%qcd%alpha%get (ren_scale)
      ren_scale_dble = dble (ren_scale)
      select type (driver => object%driver)
      type is (gosam_driver_t)
        call driver%set_alpha_s (alpha_s)
        call driver%blha_olp_eval2 (object%i_spin_c(i_flv, i_hel), &
          mom, ren_scale_dble, r, acc_dble)
      end select
      igm1 = em - 1
      n = size(p)
      do i = 0, n - 1
        pos_real = 2 * igm1 + 2 * n * i + 1
        pos_imag = pos_real + 1
        me_sc = me_sc + cmplx (r(pos_real), r(pos_imag), default)
      end do

      me_sc = - conjg(me_sc) / CA

```



```

        acc = acc_dble
        if (acc > object%maximum_accuracy) bad_point = .true.
    else
        r = 0._double
    end if
end subroutine prc_gosam_compute_sqme_spin_c

```

Gfortran 7/8/9 bug, has to remain in main module.

```

<Prc gosam: prc gosam: TBP>+≡
    procedure :: allocate_workspace => prc_gosam_allocate_workspace

<Prc gosam: main procedures>+≡
    subroutine prc_gosam_allocate_workspace (object, core_state)
        class(prc_gosam_t), intent(in) :: object
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        allocate (gosam_state_t :: core_state)
    end subroutine prc_gosam_allocate_workspace

<Prc gosam: gosam state: TBP>≡
    procedure :: write => gosam_state_write

<Prc gosam: sub interfaces>+≡
    module subroutine gosam_state_write (object, unit)
        class(gosam_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine gosam_state_write

<Prc gosam: procedures>+≡
    module subroutine gosam_state_write (object, unit)
        class(gosam_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call msg_warning (unit = unit, string = "gosam_state_write: What to write?")
    end subroutine gosam_state_write

<Prc gosam: prc gosam: TBP>+≡
    procedure :: set_particle_properties => prc_gosam_set_particle_properties

<Prc gosam: sub interfaces>+≡
    module subroutine prc_gosam_set_particle_properties (object, model)
        class(prc_gosam_t), intent(inout) :: object
        class(model_data_t), intent(in), target :: model
    end subroutine prc_gosam_set_particle_properties

<Prc gosam: procedures>+≡
    module subroutine prc_gosam_set_particle_properties (object, model)
        class(prc_gosam_t), intent(inout) :: object
        class(model_data_t), intent(in), target :: model
        integer :: i, i_pdg
        type(flavor_t) :: flv
        real(default) :: mass, width
        integer :: ierr
        real(default) :: top_yukawa
        do i = 1, OLP_N_MASSIVE_PARTICLES
            i_pdg = OLP_MASSIVE_PARTICLES(i)
            if (i_pdg < 0) cycle

```

```

call flv%init (i_pdg, model)
mass = flv%get_mass (); width = flv%get_width ()
select type (driver => object%driver)
class is (blha_driver_t)
  if (i_pdg == 13) then
    call driver%set_mass_and_width (i_pdg, mass = mass)
  else
    call driver%set_mass_and_width (i_pdg, mass = mass, width = width)
  end if
  if (i_pdg == 5) call driver%blha_olp_set_parameter &
    ('yuk(5)'//c_null_char, dble(mass), 0._double, ierr)
  if (i_pdg == 6) then
    if (driver%external_top_yukawa > 0._default) then
      top_yukawa = driver%external_top_yukawa
    else
      top_yukawa = mass
    end if
    call driver%blha_olp_set_parameter &
      ('yuk(6)'//c_null_char, dble(top_yukawa), 0._double, ierr)
  end if
  if (driver%switch_off_muon_yukawas) then
    if (i_pdg == 13) call driver%blha_olp_set_parameter &
      ('yuk(13)' //c_null_char, 0._double, 0._double, ierr)
  end if
end select
end do
end subroutine prc_gosam_set_particle_properties

```

Chapter 26

OpenLoops Interface

The interface to OpenLoops.

No internal dependencies

Figure 26.1: Module dependencies in `src/openloops`.

```

<prc_openloops.f90>≡
  <File header>

  module prc_openloops

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use string_utils, only: str
    use physics_defs
    use variables
    use os_interface
    use lorentz
    use interactions
    use model_data
    use prc_core_def
    use prc_core

    use blha_config
    use blha_olp_interfaces

    <Use mpi f08>

    <Standard module head>

    <Prc openloops: public>

    <Prc openloops: main parameters>

    <Prc openloops: types>

    <Prc openloops: interfaces>

    interface
    <Prc openloops: sub interfaces>
    end interface

    contains

    <Prc openloops: main procedures>

  end module prc_openloops
<prc_openloops_sub.f90>≡
  <File header>

  submodule (prc_openloops) prc_openloops_s

  <Use debug>
  use io_units
  use constants
  use numeric_utils
  use diagnostics
  use system_dependencies

```

```

use sm_physics, only: top_width_sm_lo, top_width_sm_qcd_nlo_jk
use sm_qcd
use prclib_interfaces

implicit none

<Prc openloops: parameters>

contains

<Prc openloops: procedures>

end submodule prc_openloops_s

<Prc openloops: parameters>≡
  real(default), parameter :: openloops_default_bmass = 0._default
  real(default), parameter :: openloops_default_topmass = 172._default
  real(default), parameter :: openloops_default_topwidth = 0._default
  real(default), parameter :: openloops_default_wmass = 80.399_default
  real(default), parameter :: openloops_default_wwidth = 0._default
  real(default), parameter :: openloops_default_zmass = 91.1876_default
  real(default), parameter :: openloops_default_zwidth = 0._default
  real(default), parameter :: openloops_default_higgsmass = 125._default
  real(default), parameter :: openloops_default_higgswidth = 0._default

<Prc openloops: main parameters>≡
  integer :: N_EXTERNAL = 0

<Prc openloops: interfaces>≡
  abstract interface
    subroutine ol_evaluate_scpowheg (id, pp, emitter, res, resmunu) bind(C)
      import
      integer(kind = c_int), value :: id, emitter
      real(kind = c_double), intent(in) :: pp(5 * N_EXTERNAL)
      real(kind = c_double), intent(out) :: res, resmunu(16)
    end subroutine ol_evaluate_scpowheg
  end interface

<Prc openloops: interfaces>+≡
  abstract interface
    subroutine ol_getparameter_double (variable_name, value) bind(C)
      import
      character(kind = c_char, len = 1), intent(in) :: variable_name
      real(kind = c_double), intent(out) :: value
    end subroutine ol_getparameter_double
  end interface

<Prc openloops: types>≡
  type, extends (prc_blha_writer_t) :: openloops_writer_t
  contains
  <Prc openloops: openloops writer: TBP>

```

```

end type openloops_writer_t

<Prc openloops: public>≡
  public :: openloops_def_t

<Prc openloops: types>+≡
  type, extends (blha_def_t) :: openloops_def_t
    integer :: verbosity
  contains
    <Prc openloops: openloops def: TBP>
  end type openloops_def_t

<Prc openloops: types>+≡
  type, extends (blha_driver_t) :: openloops_driver_t
    integer :: n_external = 0
    type(string_t) :: olp_file
    procedure(ol_evaluate_scpowheg), nopass, pointer :: &
      evaluate_spin_correlations_powheg => null ()
    procedure(ol_getparameter_double), nopass, pointer :: &
      get_parameter_double => null ()
  contains
    <Prc openloops: openloops driver: TBP>
  end type openloops_driver_t

<Prc openloops: types>+≡
  type :: openloops_threshold_data_t
    logical :: nlo = .true.
    real(default) :: alpha_ew
    real(default) :: sinthw
    real(default) :: m_b, m_W
    real(default) :: vtb
  contains
    <Prc openloops: openloops threshold data: TBP>
  end type openloops_threshold_data_t

<Prc openloops: openloops threshold data: TBP>≡
  procedure :: compute_top_width => &
    openloops_threshold_data_compute_top_width

<Prc openloops: sub interfaces>≡
  module function openloops_threshold_data_compute_top_width &
    (data, mtop, alpha_s) result (wtop)
    real(default) :: wtop
    class(openloops_threshold_data_t), intent(in) :: data
    real(default), intent(in) :: mtop, alpha_s
  end function openloops_threshold_data_compute_top_width

<Prc openloops: procedures>≡
  module function openloops_threshold_data_compute_top_width &
    (data, mtop, alpha_s) result (wtop)
    real(default) :: wtop
    class(openloops_threshold_data_t), intent(in) :: data
    real(default), intent(in) :: mtop, alpha_s
    if (data%nlo) then

```

```

        wtop = top_width_sm_qcd_nlo_jk (data%alpha_ew, data%sinthw, &
            data%vtb, mtop, data%m_W, data%m_b, alpha_s)
    else
        wtop = top_width_sm_lo (data%alpha_ew, data%sinthw, data%vtb, &
            mtop, data%m_W, data%m_b)
    end if
end function openloops_threshold_data_compute_top_width

<Prc openloops: public>+≡
    public :: openloops_state_t

<Prc openloops: types>+≡
    type, extends (blha_state_t) :: openloops_state_t
        type(openloops_threshold_data_t), allocatable :: threshold_data
    contains
        <Prc openloops: openloops state: TBP>
    end type openloops_state_t

<Prc openloops: openloops state: TBP>≡
    procedure :: init_threshold => openloops_state_init_threshold

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_state_init_threshold (object, model)
        class(openloops_state_t), intent(inout) :: object
        type(model_data_t), intent(in) :: model
    end subroutine openloops_state_init_threshold

<Prc openloops: procedures>+≡
    module subroutine openloops_state_init_threshold (object, model)
        class(openloops_state_t), intent(inout) :: object
        type(model_data_t), intent(in) :: model
        if (model%get_name () == "SM_tt_threshold") then
            allocate (object%threshold_data)
            associate (data => object%threshold_data)
                data%nlo = btest (int (model%get_real (var_str ('offshell_strategy'))), 0)
                data%alpha_ew = one / model%get_real (var_str ('alpha_em_i'))
                data%sinthw = model%get_real (var_str ('sw'))
                data%m_b = model%get_real (var_str ('mb'))
                data%m_W = model%get_real (var_str ('mW'))
                data%vtb = model%get_real (var_str ('Vtb'))
            end associate
        end if
    end subroutine openloops_state_init_threshold

<Prc openloops: public>+≡
    public :: prc_openloops_t

<Prc openloops: types>+≡
    type, extends (prc_blha_t) :: prc_openloops_t
    contains
        <Prc openloops: prc openloops: TBP>
    end type prc_openloops_t

```

```

<Prc openloops: openloops writer: TBP>≡
  procedure, nopass :: type_name => openloops_writer_type_name

<Prc openloops: sub interfaces>+≡
  module function openloops_writer_type_name () result (string)
    type(string_t) :: string
  end function openloops_writer_type_name

<Prc openloops: procedures>+≡
  module function openloops_writer_type_name () result (string)
    type(string_t) :: string
    string = "openloops"
  end function openloops_writer_type_name

```

Gfortran 7/8/9 bug: has to remain in the main module.

```

<Prc openloops: openloops def: TBP>≡
  procedure :: init => openloops_def_init

<Prc openloops: main procedures>≡
  subroutine openloops_def_init (object, basename, model_name, &
    prt_in, prt_out, nlo_type, restrictions, var_list)
    class(openloops_def_t), intent(inout) :: object
    type(string_t), intent(in) :: basename, model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    integer, intent(in) :: nlo_type
    type(string_t), intent(in), optional :: restrictions
    type(var_list_t), intent(in) :: var_list
  <Prc openloops: openloops def init: variables>
    object%basename = basename
    allocate (openloops_writer_t :: object%writer)
    select case (nlo_type)
    case (BORN)
      object%suffix = '_BORN'
    case (NLO_REAL)
      object%suffix = '_REAL'
    case (NLO_VIRTUAL)
      object%suffix = '_LOOP'
    case (NLO_SUBTRACTION, NLO_MISMATCH)
      object%suffix = '_SUB'
    case (NLO_DGLAP)
      object%suffix = '_DGLAP'
    end select
  <Prc openloops: openloops def init: suffix>
    select type (writer => object%writer)
    class is (prc_blha_writer_t)
      call writer%init (model_name, prt_in, prt_out, restrictions)
    end select
    object%verbosity = var_list%get_ival (var_str ("openloops_verbosity"))
  end subroutine openloops_def_init

```

Add additional suffix for each rank of the communicator, such that the filenames do not clash.

```

<MPI: Prc openloops: openloops def init: variables>≡
  integer :: n_size, rank

```



```

<MPI: Prc openloops: openloops def init: suffix>≡
  call MPI_comm_rank (MPI_COMM_WORLD, rank)
  call MPI_Comm_size (MPI_COMM_WORLD, n_size)
  if (n_size > 1) then
    object%suffix = object%suffix // var_str ("_") // str (rank)
  end if

<Prc openloops: openloops def: TBP>+≡
  procedure, nopass :: type_string => openloops_def_type_string

<Prc openloops: sub interfaces>+≡
  module function openloops_def_type_string () result (string)
    type(string_t) :: string
  end function openloops_def_type_string

<Prc openloops: procedures>+≡
  module function openloops_def_type_string () result (string)
    type(string_t) :: string
    string = "openloops"
  end function openloops_def_type_string

<Prc openloops: openloops def: TBP>+≡
  procedure :: write => openloops_def_write

<Prc openloops: sub interfaces>+≡
  module subroutine openloops_def_write (object, unit)
    class(openloops_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine openloops_def_write

<Prc openloops: procedures>+≡
  module subroutine openloops_def_write (object, unit)
    class(openloops_def_t), intent(in) :: object
    integer, intent(in) :: unit
    select type (writer => object%writer)
      type is (openloops_writer_t)
        call writer%write (unit)
      end select
  end subroutine openloops_def_write

<Prc openloops: openloops driver: TBP>≡
  procedure :: init_dlaccess_to_library => &
    openloops_driver_init_dlaccess_to_library

<Prc openloops: sub interfaces>+≡
  module subroutine openloops_driver_init_dlaccess_to_library &
    (object, os_data, dlaccess, success)
    class(openloops_driver_t), intent(in) :: object
    type(os_data_t), intent(in) :: os_data
    type(dlaccess_t), intent(out) :: dlaccess
    logical, intent(out) :: success
  end subroutine openloops_driver_init_dlaccess_to_library

<Prc openloops: procedures>+≡
  module subroutine openloops_driver_init_dlaccess_to_library &
    (object, os_data, dlaccess, success)
    class(openloops_driver_t), intent(in) :: object

```

```

type(os_data_t), intent(in) :: os_data
type(dlaccess_t), intent(out) :: dlaccess
logical, intent(out) :: success
type(string_t) :: ol_library, msg_buffer
ol_library = OPENLOOPS_DIR // '/lib/libopenloops.' // &
    os_data%shrlib_ext
msg_buffer = "One-Loop-Provider: Using OpenLoops"
call msg_message (char(msg_buffer))
msg_buffer = "Loading library: " // ol_library
call msg_message (char(msg_buffer))
if (os_file_exist (ol_library)) then
    call dlaccess_init (dlaccess, var_str (""), ol_library, os_data)
else
    call msg_fatal ("Link OpenLoops: library not found")
end if
success = .not. dlaccess_has_error (dlaccess)
end subroutine openloops_driver_init_dlaccess_to_library

```

<Prc openloops: openloops driver: TBP>+≡

```

procedure :: set_alpha_s => openloops_driver_set_alpha_s

```

<Prc openloops: sub interfaces>+≡

```

module subroutine openloops_driver_set_alpha_s (driver, alpha_s)
    class(openloops_driver_t), intent(in) :: driver
    real(default), intent(in) :: alpha_s
end subroutine openloops_driver_set_alpha_s

```

<Prc openloops: procedures>+≡

```

module subroutine openloops_driver_set_alpha_s (driver, alpha_s)
    class(openloops_driver_t), intent(in) :: driver
    real(default), intent(in) :: alpha_s
    integer :: ierr
    if (associated (driver%blha_olp_set_parameter)) then
        call driver%blha_olp_set_parameter &
            (c_char_'alphas'//c_null_char, &
             dble (alpha_s), 0._double, ierr)
    else
        call msg_fatal ("blha_olp_set_parameter not associated!")
    end if
    if (ierr == 0) call parameter_error_message (var_str ('alphas'), &
        var_str ('openloops_driver_set_alpha_s'))
end subroutine openloops_driver_set_alpha_s

```

<Prc openloops: openloops driver: TBP>+≡

```

procedure :: set_alpha_qed => openloops_driver_set_alpha_qed

```

<Prc openloops: sub interfaces>+≡

```

module subroutine openloops_driver_set_alpha_qed (driver, alpha)
    class(openloops_driver_t), intent(inout) :: driver
    real(default), intent(in) :: alpha
end subroutine openloops_driver_set_alpha_qed

```

<Prc openloops: procedures>+≡

```

module subroutine openloops_driver_set_alpha_qed (driver, alpha)
    class(openloops_driver_t), intent(inout) :: driver

```

```

    real(default), intent(in) :: alpha
    integer :: ierr
    call driver%blha_olp_set_parameter &
        (c_char_'alpha_qed'//c_null_char, &
         dble(alpha), 0._double, ierr)
    if (ierr == 0) call ew_parameter_error_message (var_str ('alpha_qed'))
end subroutine openloops_driver_set_alpha_qed

<Prc openloops: openloops driver: TBP>+≡
    procedure :: set_GF => openloops_driver_set_GF

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_driver_set_GF (driver, GF)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: GF
    end subroutine openloops_driver_set_GF

<Prc openloops: procedures>+≡
    module subroutine openloops_driver_set_GF (driver, GF)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: GF
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'Gmu'//c_null_char, &
             dble(GF), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('Gmu'))
    end subroutine openloops_driver_set_GF

<Prc openloops: openloops driver: TBP>+≡
    procedure :: set_weinberg_angle => openloops_driver_set_weinberg_angle

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_driver_set_weinberg_angle (driver, sw2)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: sw2
    end subroutine openloops_driver_set_weinberg_angle

<Prc openloops: procedures>+≡
    module subroutine openloops_driver_set_weinberg_angle (driver, sw2)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: sw2
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'sw2'//c_null_char, &
             dble(sw2), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('sw2'))
    end subroutine openloops_driver_set_weinberg_angle

<Prc openloops: openloops driver: TBP>+≡
    procedure :: print_alpha_s => openloops_driver_print_alpha_s

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_driver_print_alpha_s (object)
        class(openloops_driver_t), intent(in) :: object
    end subroutine openloops_driver_print_alpha_s

```

```

<Prc openloops: procedures>+≡
    module subroutine openloops_driver_print_alpha_s (object)
        class(openloops_driver_t), intent(in) :: object
        call object%blha_olp_print_parameter (c_char_'alphas'//c_null_char)
    end subroutine openloops_driver_print_alpha_s

<Prc openloops: openloops driver: TBP>+≡
    procedure, nopass :: type_name => openloops_driver_type_name

<Prc openloops: sub interfaces>+≡
    module function openloops_driver_type_name () result (type)
        type(string_t) :: type
    end function openloops_driver_type_name

<Prc openloops: procedures>+≡
    module function openloops_driver_type_name () result (type)
        type(string_t) :: type
        type = "OpenLoops"
    end function openloops_driver_type_name

<Prc openloops: openloops driver: TBP>+≡
    procedure :: load_procedures => openloops_driver_load_procedures

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_driver_load_procedures &
        (object, os_data, success)
        class(openloops_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical, intent(out) :: success
    end subroutine openloops_driver_load_procedures

<Prc openloops: procedures>+≡
    module subroutine openloops_driver_load_procedures &
        (object, os_data, success)
        class(openloops_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical, intent(out) :: success
        type(dlaccess_t) :: dlaccess
        type(c_funptr) :: c_funptr
        logical :: init_success

        call object%init_dlaccess_to_library (os_data, dlaccess, init_success)

        c_funptr = dlaccess_get_c_funptr (dlaccess, var_str ("ol_evaluate_scpowheg"))
        call c_f_procpointer (c_funptr, object%evaluate_spin_correlations_powheg)
        call check_for_error (var_str ("ol_evaluate_scpowheg"))
        c_funptr = dlaccess_get_c_funptr (dlaccess, var_str ("ol_getparameter_double"))
        call c_f_procpointer (c_funptr, object%get_parameter_double)
        call check_for_error (var_str ("ol_getparameter_double"))
        success = .true.

    contains
        subroutine check_for_error (function_name)
            type(string_t), intent(in) :: function_name
            if (dlaccess_has_error (dlaccess)) &

```

```

        call msg_fatal (char ("Loading of " // function_name // " failed!"))
    end subroutine check_for_error
end subroutine openloops_driver_load_procedures

<Prc openloops: openloops def: TBP>+≡
    procedure :: read => openloops_def_read

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_def_read (object, unit)
        class(openloops_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine openloops_def_read

<Prc openloops: procedures>+≡
    module subroutine openloops_def_read (object, unit)
        class(openloops_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine openloops_def_read

Gfortran 7/8/9 bug: has to remain in the main module.

<Prc openloops: openloops def: TBP>+≡
    procedure :: allocate_driver => openloops_def_allocate_driver

<Prc openloops: main procedures>+≡
    subroutine openloops_def_allocate_driver (object, driver, basename)
        class(openloops_def_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        if (.not. allocated (driver)) allocate (openloops_driver_t :: driver)
    end subroutine openloops_def_allocate_driver

<Prc openloops: openloops state: TBP>+≡
    procedure :: write => openloops_state_write

<Prc openloops: sub interfaces>+≡
    module subroutine openloops_state_write (object, unit)
        class(openloops_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine openloops_state_write

<Prc openloops: procedures>+≡
    module subroutine openloops_state_write (object, unit)
        class(openloops_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine openloops_state_write

Gfortran 7/8/9 bug: has to remain in the main module.

<Prc openloops: prc openloops: TBP>≡
    procedure :: allocate_workspace => prc_openloops_allocate_workspace

<Prc openloops: main procedures>+≡
    subroutine prc_openloops_allocate_workspace (object, core_state)
        class(prc_openloops_t), intent(in) :: object
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        allocate (openloops_state_t :: core_state)

```

```

end subroutine prc_openloops_allocate_workspace

<Prc openloops: prc openloops: TBP>+≡
  procedure :: init_driver => prc_openloops_init_driver

<Prc openloops: sub interfaces>+≡
  module subroutine prc_openloops_init_driver (object, os_data)
    class(prc_openloops_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
  end subroutine prc_openloops_init_driver

<Prc openloops: procedures>+≡
  module subroutine prc_openloops_init_driver (object, os_data)
    class(prc_openloops_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: olp_file, olc_file
    type(string_t) :: suffix

    select type (def => object%def)
    type is (openloops_def_t)
      suffix = def%suffix
      olp_file = def%basename // suffix // '.olp'
      olc_file = def%basename // suffix // '.olc'
    class default
      call msg_bug ("prc_openloops_init_driver: core_def should be openloops-type")
    end select

    select type (driver => object%driver)
    type is (openloops_driver_t)
      driver%olp_file = olp_file
      driver%contract_file = olc_file
      driver%nlo_suffix = suffix
    end select
  end subroutine prc_openloops_init_driver

<Prc openloops: prc openloops: TBP>+≡
  procedure :: write => prc_openloops_write

<Prc openloops: sub interfaces>+≡
  module subroutine prc_openloops_write (object, unit)
    class(prc_openloops_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine prc_openloops_write

<Prc openloops: procedures>+≡
  module subroutine prc_openloops_write (object, unit)
    class(prc_openloops_t), intent(in) :: object
    integer, intent(in), optional :: unit
    call msg_message (unit = unit, string = "OpenLoops")
  end subroutine prc_openloops_write

<Prc openloops: prc openloops: TBP>+≡
  procedure :: write_name => prc_openloops_write_name

```

```

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_write_name (object, unit)
        class(prc_openloops_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_openloops_write_name

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_write_name (object, unit)
        class(prc_openloops_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u,"(1x,A)") "Core: OpenLoops"
    end subroutine prc_openloops_write_name

<Prc openloops: prc openloops: TBP>+≡
    procedure :: prepare_library => prc_openloops_prepare_library

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_prepare_library (object, os_data, model)
        class(prc_openloops_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(model_data_t), intent(in), target :: model
    end subroutine prc_openloops_prepare_library

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_prepare_library (object, os_data, model)
        class(prc_openloops_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(model_data_t), intent(in), target :: model
        call object%load_driver (os_data)
        call object%reset_parameters ()
        call object%set_particle_properties (model)
        select type(def => object%def)
            type is (openloops_def_t)
                call object%set_verbosity (def%verbosity)
        end select
    end subroutine prc_openloops_prepare_library

<Prc openloops: prc openloops: TBP>+≡
    procedure :: load_driver => prc_openloops_load_driver

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_load_driver (object, os_data)
        class(prc_openloops_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
    end subroutine prc_openloops_load_driver

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_load_driver (object, os_data)
        class(prc_openloops_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical :: success
        select type (driver => object%driver)
            type is (openloops_driver_t)

```

```

        call driver%load (os_data, success)
        call driver%load_procedures (os_data, success)
    end select
end subroutine prc_openloops_load_driver

<Prc openloops: prc openloops: TBP>+≡
    procedure :: start => prc_openloops_start

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_start (object)
        class(prc_openloops_t), intent(inout) :: object
    end subroutine prc_openloops_start

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_start (object)
        class(prc_openloops_t), intent(inout) :: object
        integer :: ierr
        select type (driver => object%driver)
        type is (openloops_driver_t)
            call driver%blha_olp_start (char (driver%olp_file)//c_null_char, ierr)
        end select
    end subroutine prc_openloops_start

<Prc openloops: prc openloops: TBP>+≡
    procedure :: set_n_external => prc_openloops_set_n_external

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_set_n_external (object, n)
        class(prc_openloops_t), intent(inout) :: object
        integer, intent(in) :: n
    end subroutine prc_openloops_set_n_external

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_set_n_external (object, n)
        class(prc_openloops_t), intent(inout) :: object
        integer, intent(in) :: n
        N_EXTERNAL = n
    end subroutine prc_openloops_set_n_external

<Prc openloops: prc openloops: TBP>+≡
    procedure :: reset_parameters => prc_openloops_reset_parameters

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_reset_parameters (object)
        class(prc_openloops_t), intent(inout) :: object
    end subroutine prc_openloops_reset_parameters

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_reset_parameters (object)
        class(prc_openloops_t), intent(inout) :: object
        integer :: ierr
        select type (driver => object%driver)
        type is (openloops_driver_t)
            call driver%blha_olp_set_parameter ('mass(5)//c_null_char, &
                dble(openloops_default_bmass), 0._double, ierr)
            call driver%blha_olp_set_parameter ('mass(6)//c_null_char, &

```



```

        dble(openloops_default_topmass), 0._double, ierr)
    call driver%blha_olp_set_parameter ('width(6)'/c_null_char, &
        dble(openloops_default_topwidth), 0._double, ierr)
    call driver%blha_olp_set_parameter ('mass(23)'/c_null_char, &
        dble(openloops_default_zmass), 0._double, ierr)
    call driver%blha_olp_set_parameter ('width(23)'/c_null_char, &
        dble(openloops_default_zwidth), 0._double, ierr)
    call driver%blha_olp_set_parameter ('mass(24)'/c_null_char, &
        dble(openloops_default_wmass), 0._double, ierr)
    call driver%blha_olp_set_parameter ('width(24)'/c_null_char, &
        dble(openloops_default_wwidth), 0._double, ierr)
    call driver%blha_olp_set_parameter ('mass(25)'/c_null_char, &
        dble(openloops_default_higsmass), 0._double, ierr)
    call driver%blha_olp_set_parameter ('width(25)'/c_null_char, &
        dble(openloops_default_higswidth), 0._double, ierr)
end select
end subroutine prc_openloops_reset_parameters

```

Set the verbosity level for openloops. The different levels are as follows:

- 0 minimal output (startup message et.al.)
- 1 show which libraries are loaded
- 2 show debug information of the library loader, but not during run time
- 3 show debug information during run time
- 4 output for each call of `set_parameters`.

```

<Prc openloops: prc openloops: TBP>+≡
    procedure :: set_verbosity => prc_openloops_set_verbosity

<Prc openloops: sub interfaces>+≡
    module subroutine prc_openloops_set_verbosity (object, verbose)
        class(prc_openloops_t), intent(inout) :: object
        integer, intent(in) :: verbose
    end subroutine prc_openloops_set_verbosity

<Prc openloops: procedures>+≡
    module subroutine prc_openloops_set_verbosity (object, verbose)
        class(prc_openloops_t), intent(inout) :: object
        integer, intent(in) :: verbose
        integer :: ierr
        select type (driver => object%driver)
        type is (openloops_driver_t)
            call driver%blha_olp_set_parameter ('verbose'/c_null_char, &
                dble(verbose), 0._double, ierr)
        end select
    end subroutine prc_openloops_set_verbosity

<Prc openloops: prc openloops: TBP>+≡
    procedure :: prepare_external_code => &
        prc_openloops_prepare_external_code

```

<Prc openloops: sub interfaces>+≡

```

module subroutine prc_openloops_prepare_external_code &
  (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
  class(prc_openloops_t), intent(inout) :: core
  integer, intent(in), dimension(:,:), allocatable :: flv_states
  type(var_list_t), intent(in) :: var_list
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in) :: libname
  type(model_data_t), intent(in), target :: model
  integer, intent(in) :: i_core
  logical, intent(in) :: is_nlo
end subroutine prc_openloops_prepare_external_code

```

<Prc openloops: procedures>+≡

```

module subroutine prc_openloops_prepare_external_code &
  (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
  class(prc_openloops_t), intent(inout) :: core
  integer, intent(in), dimension(:,:), allocatable :: flv_states
  type(var_list_t), intent(in) :: var_list
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in) :: libname
  type(model_data_t), intent(in), target :: model
  integer, intent(in) :: i_core
  logical, intent(in) :: is_nlo
  integer :: ierr
  core%sqme_tree_pos = 1
  call core%set_n_external (core%data%get_n_tot ())
  call core%prepare_library (os_data, model)
  call core%start ()
  call core%set_electroweak_parameters (model)
  select type (driver => core%driver)
  type is (openloops_driver_t)
    !!! We have to set the external vector boson wavefunction to the MadGraph convention
    !!! in order to be consistent with our calculation of the spin correlated contributions.
    call driver%blha_olp_set_parameter ('wf_v_select'//c_null_char, &
      3._double, 0._double, ierr)
    if (ierr == 0) call parameter_error_message (var_str ('wf_v_select'), &
      var_str ('prc_openloops_prepare_external_code'))
  end select
  call core%read_contract_file (flv_states)
  call core%print_parameter_file (i_core)
end subroutine prc_openloops_prepare_external_code

```

Computes a spin-correlated matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of dimension(16). The current interface does not give out an accuracy, so that `bad_point` is always `.false..` OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested.

<Prc openloops: prc openloops: TBP>+≡

```

procedure :: compute_sqme_spin_c => prc_openloops_compute_sqme_spin_c

```

<Prc openloops: sub interfaces>+≡

```

module subroutine prc_openloops_compute_sqme_spin_c (object, &
  i_flv, i_hel, em, p, ren_scale, sqme_spin_c, bad_point)

```

```

class(prc_openloops_t), intent(inout) :: object
integer, intent(in) :: i_flv, i_hel
integer, intent(in) :: em
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(out), dimension(6) :: sqme_spin_c
logical, intent(out) :: bad_point
end subroutine prc_openloops_compute_sqme_spin_c

(Prc openloops: procedures) +=
module subroutine prc_openloops_compute_sqme_spin_c (object, &
    i_flv, i_hel, em, p, ren_scale, sqme_spin_c, bad_point)
class(prc_openloops_t), intent(inout) :: object
integer, intent(in) :: i_flv, i_hel
integer, intent(in) :: em
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(out), dimension(6) :: sqme_spin_c
logical, intent(out) :: bad_point
real(default), dimension(16) :: sqme_spin_c_tmp
real(double), dimension(5*N_EXTERNAL) :: mom
real(double) :: res
real(double), dimension(16) :: res_munu
real(default) :: alpha_s
if (object%i_spin_c(i_flv, i_hel) >= 0) then
    mom = object%create_momentum_array (p)
    if (vanishes (ren_scale)) call msg_fatal &
        ("prc_openloops_compute_sqme_spin_c: ren_scale vanishes")
    alpha_s = object%qcd%alpha%get (ren_scale)
    select type (driver => object%driver)
    type is (openloops_driver_t)
        call driver%set_alpha_s (alpha_s)
        call driver%evaluate_spin_correlations_powheg &
            (object%i_spin_c(i_flv, i_hel), mom, em, res, res_munu)
    end select
    sqme_spin_c_tmp = res_munu
    bad_point = .false.
    if (object%includes_polarization ()) &
        sqme_spin_c_tmp = object%n_hel * sqme_spin_c_tmp
    if (debug_on) then
        if (sum(sqme_spin_c_tmp) == 0) then
            call msg_debug(D_SUBTRACTION, 'Spin-correlated matrix elements provided by OpenLoops a
        end if
    end if
else
    sqme_spin_c_tmp = zero
end if
!!! Using symmetry of the 4x4 matrix of spin correlated squared Born MEs and
!!! the fact that we multiply only with vectors with E=0. We thus store the
!!! upper triangle of the lower 3x3 matrix as columns in a 1-dim array
sqme_spin_c(1:2) = sqme_spin_c_tmp(6:7)
sqme_spin_c(3) = sqme_spin_c_tmp(11)
sqme_spin_c(4) = sqme_spin_c_tmp(8)
sqme_spin_c(5) = sqme_spin_c_tmp(12)
sqme_spin_c(6) = sqme_spin_c_tmp(16)

```

```

end subroutine prc_openloops_compute_sqme_spin_c

<Prc openloops: prc openloops: TBP>+≡
  procedure :: get_alpha_qed => prc_openloops_get_alpha_qed

<Prc openloops: sub interfaces>+≡
  module function prc_openloops_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_openloops_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qed
  end function prc_openloops_get_alpha_qed

<Prc openloops: procedures>+≡
  module function prc_openloops_get_alpha_qed &
    (object, core_state) result (alpha_qed)
    class(prc_openloops_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(double) :: value
    real(default) :: alpha_qed
    select type (driver => object%driver)
    type is (openloops_driver_t)
      call driver%get_parameter_double ('alpha_qed'//c_null_char, value)
      alpha_qed = value
    return
  end select
  call msg_fatal ("prc_openloops_get_alpha_qed: " // &
    "called by wrong driver, only supported for OpenLoops!")
end function prc_openloops_get_alpha_qed

```

Chapter 27

FKS Subtraction Scheme

The code in this chapter implements the FKS subtraction scheme for use with WHIZARD.

These are the modules:

fks_regions Given a process definition, identify singular regions in the associated phase space.

virtual Handle the virtual correction matrix element.

real_subtraction Handle the real-subtraction matrix element.

nlo_data Manage the subtraction objects.

dglap_remnant Handle the DGLAP Remnant matrix element.

This chapter deals with next-to-leading order contributions to cross sections. Basically, there are three major issues to be addressed: The creation of the $N + 1$ -particle flavor structure, the construction of the $N + 1$ -particle phase space and the actual calculation of the real- and virtual-subtracted matrix elements. The first is dealt with using the **auto_components** class, and it will be shown that the second and third issue are connected in FKS subtraction.

27.1 Brief outline of FKS subtraction

In the current state, this discussion is only concerned with lepton collisions. For hadron collisions, renormalization of parton distributions has to be taken into account. Further, for QCD corrections, initial-state radiation is necessarily present.

The aim is to calculate the next-to-leading order cross section according to

$$d\sigma_{\text{NLO}} = \mathcal{B} + \mathcal{V} + \mathcal{R}d\Phi_{\text{rad}}.$$

Analytically, the divergences, in terms of poles in the complex quantity $\varepsilon = 2 - d/2$, cancel. However, this is in general only valid in an arbitrary, complex number of dimensions. This is, roughly, the content of the KLN-theorem. WHIZARD, as any other numerical program, is confined to four dimensions. We

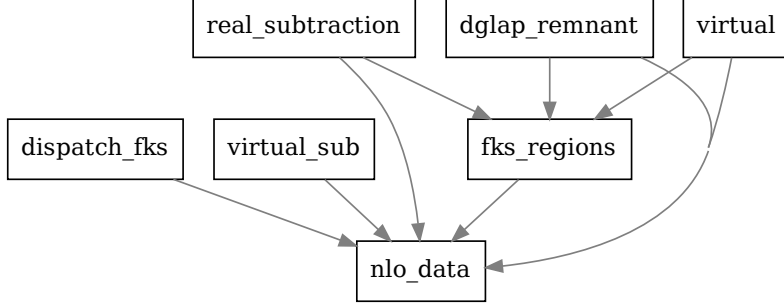


Figure 27.1: Module dependencies in `src/fks`.

will assume that the KLN-theorem is valid and that there exist subtraction terms \mathcal{C} such that

$$d\sigma_{\text{NLO}} = \mathcal{B} + \underbrace{\mathcal{V} + \mathcal{C}}_{\text{finite}} + \underbrace{\mathcal{R} - \mathcal{C}}_{\text{finite}},$$

i.e. the subtraction terms correspond to the divergent limits of the real and virtual matrix element.

Because \mathcal{C} subtracts the divergences of \mathcal{R} as well as those of \mathcal{V} , it suffices to consider one of them, so we focus on \mathcal{R} . For this purpose, \mathcal{R} is rewritten as

$$\mathcal{R} = \frac{1}{\xi^2} \frac{1}{1-y} (\xi^2(1-y)\mathcal{R}) = \frac{1}{\xi^2} \frac{1}{1-y} \tilde{\mathcal{R}},$$

with $\xi = (2k_{\text{rad}}^0)/\sqrt{s}$ and $y = \cos\theta$, where k_{rad}^0 denotes the energy of the radiated parton and θ is the angle between emitter and radiated parton. $\tilde{\mathcal{R}}$ is finite, therefore the whole singularity structure is contained in the prefactor $\xi^{-2}(1-y)^{-1}$. Combined with the d -dimensional phase space element,

$$\frac{d^{d-1}k}{2k^0(2\pi)^{d-1}} = \frac{s^{1-\varepsilon}}{(4\pi)^{d-1}} \xi^{1-2\varepsilon} (1-y^2)^{-\varepsilon} d\xi dy d\Omega^{d-2},$$

this yields

$$d\Phi_{\text{rad}} \mathcal{R} = dy(1-y)^{-1-\varepsilon} d\xi \xi^{-1-2\varepsilon} \tilde{\mathcal{R}}.$$

This can further be rewritten in terms of plus-distributions,

$$\begin{aligned} \xi^{-1-2\varepsilon} &= -\frac{1}{2\varepsilon} \delta(\xi) + \left(\frac{1}{\xi}\right)_+ - 2\varepsilon \left(\frac{\log \xi}{\xi}\right)_+ + \mathcal{O}(\varepsilon^2), \\ (1-y)^{-1-\varepsilon} &= -\frac{2^{-\varepsilon}}{\varepsilon} \delta(1-y) + \left(\frac{1}{1-y}\right)_+ - \varepsilon \left(\frac{1}{1-y}\right)_+ \log(1-y) + \mathcal{O}(\varepsilon^2), \end{aligned}$$

(imagine that all this is written inside of integrals, which are spared for ease of

notation) such that

$$d\Phi_{\text{rad}}\mathcal{R} = -\frac{1}{2\varepsilon}dy(1-y)^{-1-\varepsilon}\tilde{R}(0,y) - d\xi \left[\frac{2^{-\varepsilon}}{\varepsilon} \left(\frac{1}{\xi} \right)_+ - 2 \left(\frac{\log \xi}{\xi} \right)_+ \right] \tilde{R}(\xi,1) \\ + dyd\xi \left(\frac{1}{\xi} \right)_+ \left(\frac{1}{1-y} \right)_+ \tilde{R}(\xi,y) + \mathcal{O}(\varepsilon).$$

The summand in the second line is of order $\mathcal{O}(1)$ and is the only one to reproduce $\mathcal{R}(\xi,y)$. It thus constitutes the sum of the real matrix element and the corresponding counterterms. The first summand consequently consists of the subtraction terms to the virtual matrix elements. Above formula thus allows to calculate all quantities to render the matrix elements finite.

alr	flst_alr	emitter	ftuple_list
1	[-11,11,2,-2,21,21]	3	(3,5), (3,6), (4,5), (4,6), (5,6)
2	[-11,11,2,-2,21,21]	4	(3,5), (3,6), (4,5), (4,6), (5,6)
3	[-11,11,2,-2,21,21]	5	(3,5), (3,6), (4,5), (4,6), (5,6)
4	[-11,11,2,-2,2,-2]	5	(3,4), (3,6), (4,5), (5,6)

Table 27.1: List of singular regions. The particles are represented by their PDG codes. The third column contains the emitter for the specific singular region. For the process involving an additional gluon, the gluon can either be emitted from one of the quarks or from the first gluon. Each emitter yields the same list of fundamental tuples, five in total. The last singular region corresponds to the process where the gluon splits up into two quarks. As the matrix element for this process has no information on which quarks originate from a gluon splitting, there are ftuples for all the quark pairs and not just those involving the emitter.

27.2 Identifying singular regions

In the FKS subtraction scheme, the phase space is decomposed into disjoint singular regions, such that

$$\sum_i \mathcal{S}_i + \sum_{ij} \mathcal{S}_{ij} = 1. \quad (27.1)$$

The quantities \mathcal{S}_i and \mathcal{S}_{ij} are functions of phase space corresponding to a pair of particles indices which can make up a divergent phase space region. We call such an index pair a fundamental tuple. For example, the process $e^+ e^- \rightarrow u \bar{u} g$ has two singular regions, (3, 5) and (4, 5), indicating that the gluon can be soft or collinear with respect to either the quark or the anti-quark. Therefore, the functions \mathcal{S}_{ij} have to be chosen in such a way that their contribution makes up most of (27.1) in phase-space configurations where (final-state) particle j is collinear to particle i or/and particle j is soft. The functions \mathcal{S}_i is the corresponding quantity for initial-state divergences.

As a singular region we understand the collection of real flavor structures associated with an emitter and a list of all possible fundamental tuples. As an example, consider the process $e^+ e^- \rightarrow u \bar{u} g$. At next-to-leading order, processes with an additionally radiated particle have to be considered. In this case, these are $e^+ e^- \rightarrow u \bar{u}, g g$, and $e^+ e^- \rightarrow u \bar{u} u \bar{u}$ (or the same process with any other quark). Table 27.1 sums up all possible singular regions for this problem.

Thus, during the preparation of a NLO-calculation, the possible singular regions have to be identified. `fk_regions.f90` deals with this issue.

alr	ftuple	emitter	flst_alr
1	(3, 5)	5	[-11,11,-2,21,2,21]
2	(4, 5)	5	[-11,11,2,21,-2,21]
3	(3, 6)	5	[-11,11,-2,21,2,21]
4	(4, 6)	5	[-11,11,2,21,-2,21]
5	(5, 6)	5	[-11,11,2,-2,21,21]
6	(5, 6)	5	[-11,11,2,-2,2,-2]

Table 27.2: Initial list of singular regions

27.3 FKS Regions

```
<fks_regions.f90>≡  
  <File header>  
  
  module fks_regions  
  
    <Use kinds>  
    <Use strings>  
    use diagnostics  
    use os_interface  
    use constants  
    use process_constants  
    use lorentz  
    use models  
    use resonances, only: resonance_contributors_t, resonance_history_t  
    use phs_fks, only: phs_identifier_t, check_for_phs_identifier  
  
    use nlo_data  
  
    <Standard module head>  
  
    <FKS regions: public>  
  
    <FKS regions: parameters>  
  
    <FKS regions: types>  
  
    <FKS regions: interfaces>  
  
    interface  
    <FKS regions: sub interfaces>  
    end interface  
  
    contains  
  
    <FKS regions: main procedures>  
  
  end module fks_regions  
  
<fks_regions_sub.f90>≡  
  <File header>  
  
  submodule (fks_regions) fks_regions_s  
  
    <Use debug>  
    use format_utils, only: write_separator  
    use numeric_utils  
    use string_utils, only: str  
    use io_units  
    use permutations  
    use physics_defs  
    use flavors  
    use pdg_arrays
```

```

implicit none

contains

<FKS regions: procedures>

end submodule fks_regions_s

```

There are three fundamental splitting types: $q \rightarrow qg$, $g \rightarrow gg$ and $g \rightarrow qq$ for FSR and additionally $q \rightarrow gq$ for ISR which is different from $q \rightarrow qq$ by which particle enters the hard process.

```

<FKS regions: parameters>≡
integer, parameter :: UNDEFINED_SPLITTING = 0
integer, parameter :: F_TO_FV = 1
integer, parameter :: V_TO_VV = 2
integer, parameter :: V_TO_FF = 3
integer, parameter :: F_TO_VF = 4

```

We group the indices of the emitting and the radiated particle in the `ftuple`-object.

```

<FKS regions: public>≡
public :: ftuple_t

<FKS regions: types>≡
type :: ftuple_t
integer, dimension(2) :: ireg = [-1,-1]
integer :: i_res = 0
integer :: splitting_type
logical :: pseudo_isr = .false.
logical :: qcd_split = .false.
contains
<FKS regions: ftuple: TBP>
end type ftuple_t

```

```

<FKS regions: interfaces>≡
interface assignment(=)
module procedure ftuple_assign
end interface

interface operator(==)
module procedure ftuple_equal
end interface

interface operator(>)
module procedure ftuple_greater
end interface

interface operator(<)
module procedure ftuple_less
end interface

```

```

(FKS regions: sub interfaces)≡
    pure module subroutine ftuple_assign (ftuple_out, ftuple_in)
        type(ftuple_t), intent(out) :: ftuple_out
        type(ftuple_t), intent(in) :: ftuple_in
    end subroutine ftuple_assign

(FKS regions: procedures)≡
    pure module subroutine ftuple_assign (ftuple_out, ftuple_in)
        type(ftuple_t), intent(out) :: ftuple_out
        type(ftuple_t), intent(in) :: ftuple_in
        ftuple_out%ireg = ftuple_in%ireg
        ftuple_out%i_res = ftuple_in%i_res
        ftuple_out%splitting_type = ftuple_in%splitting_type
        ftuple_out%pseudo_isr = ftuple_in%pseudo_isr
        ftuple_out%qcd_split = ftuple_in%qcd_split
    end subroutine ftuple_assign

(FKS regions: sub interfaces)+≡
    elemental module function ftuple_equal (f1, f2) result (value)
        logical :: value
        type(ftuple_t), intent(in) :: f1, f2
    end function ftuple_equal

(FKS regions: procedures)+≡
    elemental module function ftuple_equal (f1, f2) result (value)
        logical :: value
        type(ftuple_t), intent(in) :: f1, f2
        value = all (f1%ireg == f2%ireg) .and. f1%i_res == f2%i_res &
            .and. f1%splitting_type == f2%splitting_type &
            .and. (f1%pseudo_isr .eqv. f2%pseudo_isr) &
            .and. (f1%qcd_split .eqv. f2%qcd_split)
    end function ftuple_equal

(FKS regions: procedures)+≡
    elemental function ftuple_equal_ireg (f1, f2) result (value)
        logical :: value
        type(ftuple_t), intent(in) :: f1, f2
        value = all (f1%ireg == f2%ireg)
    end function ftuple_equal_ireg

(FKS regions: sub interfaces)+≡
    elemental module function ftuple_greater (f1, f2) result (greater)
        logical :: greater
        type(ftuple_t), intent(in) :: f1, f2
    end function ftuple_greater

(FKS regions: procedures)+≡
    elemental module function ftuple_greater (f1, f2) result (greater)
        logical :: greater
        type(ftuple_t), intent(in) :: f1, f2
        if (f1%ireg(1) == f2%ireg(1)) then
            greater = f1%ireg(2) > f2%ireg(2)
        else
            greater = f1%ireg(1) > f2%ireg(1)
        end if
    end function ftuple_greater

```

```

        end if
    end function ftuple_greater

<FKS regions: sub interfaces>+≡
    elemental module function ftuple_less (f1, f2) result (less)
        logical :: less
        type(ftuple_t), intent(in) :: f1, f2
    end function ftuple_less

<FKS regions: procedures>+≡
    elemental module function ftuple_less (f1, f2) result (less)
        logical :: less
        type(ftuple_t), intent(in) :: f1, f2
        if (f1%ireg(1) == f2%ireg(1)) then
            less = f1%ireg(2) < f2%ireg(2)
        else
            less = f1%ireg(1) < f2%ireg(1)
        end if
    end function ftuple_less

<FKS regions: procedures>+≡
    subroutine ftuple_sort_array (ftuple_array, equivalences)
        type(ftuple_t), intent(inout), dimension(:), allocatable :: ftuple_array
        logical, intent(inout), dimension(:,:), allocatable :: equivalences
        type(ftuple_t) :: ftuple_tmp
        logical, dimension(:), allocatable :: eq_tmp
        integer :: i1, i2, n
        n = size (ftuple_array)
        allocate (eq_tmp (n))
        do i1 = 2, n
            i2 = i1
            do while (ftuple_array(i2 - 1) > ftuple_array(i2))
                ftuple_tmp = ftuple_array(i2 - 1)
                eq_tmp = equivalences(i2, :)
                ftuple_array(i2 - 1) = ftuple_array(i2)
                ftuple_array(i2) = ftuple_tmp
                equivalences(i2 - 1, :) = equivalences(i2, :)
                equivalences(i2, :) = eq_tmp
                i2 = i2 - 1
            end do
            if (i2 == 1) exit
        end do
    end subroutine ftuple_sort_array

<FKS regions: ftuple: TBP>≡
    procedure :: write => ftuple_write

<FKS regions: sub interfaces>+≡
    module subroutine ftuple_write (ftuple, unit, newline)
        class(ftuple_t), intent(in) :: ftuple
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: newline
    end subroutine ftuple_write

```

(FKS regions: procedures)+≡

```

module subroutine ftuple_write (ftuple, unit, newline)
  class(ftuple_t), intent(in) :: ftuple
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: newline
  integer :: u
  logical :: nl
  u = given_output_unit (unit); if (u < 0) return
  nl = .true.; if (present(newline)) nl = newline
  if (all (ftuple%ireg > -1)) then
    if (ftuple%i_res > 0) then
      if (nl) then
        write (u, "(A1,I1,A1,I1,A1,I1,A1)") &
          '(', ftuple%ireg(1), ',', ftuple%ireg(2), ';', ftuple%i_res, ')'
      else
        write (u, "(A1,I1,A1,I1,A1,I1,A1)", advance = "no") &
          '(', ftuple%ireg(1), ',', ftuple%ireg(2), ';', ftuple%i_res, ')'
      end if
    else
      if (nl) then
        write (u, "(A1,I1,A1,I1,A1)") &
          '(', ftuple%ireg(1), ',', ftuple%ireg(2), ')'
      else
        write (u, "(A1,I1,A1,I1,A1)", advance = "no") &
          '(', ftuple%ireg(1), ',', ftuple%ireg(2), ')'
      end if
    end if
  else
    write (u, "(A)") "(Empty)"
  end if
end subroutine ftuple_write

```

(FKS regions: procedures)+≡

```

function ftuple_string (ftuples, latex)
  type(string_t) :: ftuple_string
  type(ftuple_t), intent(in), dimension(:) :: ftuples
  logical, intent(in) :: latex
  integer :: i, nreg
  if (latex) then
    ftuple_string = var_str ("$\left\{" )
  else
    ftuple_string = var_str ("{" )
  end if
  nreg = size(ftuples)
  do i = 1, nreg
    if (ftuples(i)%i_res == 0) then
      ftuple_string = ftuple_string // var_str "(" // &
        str (ftuples(i)%ireg(1)) // var_str "," // &
        str (ftuples(i)%ireg(2)) // var_str ")"
    else
      ftuple_string = ftuple_string // var_str "(" // &
        str (ftuples(i)%ireg(1)) // var_str "," // &
        str (ftuples(i)%ireg(2)) // var_str ";" // &
        str (ftuples(i)%i_res) // var_str ")"
    end if
  end do
end function ftuple_string

```

```

        end if
        if (ftuples(i)%pseudo_isr) ftuple_string = ftuple_string // var_str ("*")
        if (i < nreg) ftuple_string = ftuple_string // var_str (",")
    end do
    if (latex) then
        ftuple_string = ftuple_string // var_str ("\right\}$")
    else
        ftuple_string = ftuple_string // var_str ("}")
    end if
end function ftuple_string

```

<FKS regions: ftuple: TBP>+≡

```

procedure :: get => ftuple_get

```

<FKS regions: sub interfaces>+≡

```

module subroutine ftuple_get (ftuple, pos1, pos2)
    class(ftuple_t), intent(in) :: ftuple
    integer, intent(out) :: pos1, pos2
end subroutine ftuple_get

```

<FKS regions: procedures>+≡

```

module subroutine ftuple_get (ftuple, pos1, pos2)
    class(ftuple_t), intent(in) :: ftuple
    integer, intent(out) :: pos1, pos2
    pos1 = ftuple%ireg(1)
    pos2 = ftuple%ireg(2)
end subroutine ftuple_get

```

<FKS regions: ftuple: TBP>+≡

```

procedure :: set => ftuple_set

```

<FKS regions: sub interfaces>+≡

```

module subroutine ftuple_set (ftuple, pos1, pos2)
    class(ftuple_t), intent(inout) :: ftuple
    integer, intent(in) :: pos1, pos2
end subroutine ftuple_set

```

<FKS regions: procedures>+≡

```

module subroutine ftuple_set (ftuple, pos1, pos2)
    class(ftuple_t), intent(inout) :: ftuple
    integer, intent(in) :: pos1, pos2
    ftuple%ireg(1) = pos1
    ftuple%ireg(2) = pos2
end subroutine ftuple_set

```

Determines the splitting type for FSR. There are three different types of splittings relevant here: $g \rightarrow gg$ tagged V_T0_VV, $g \rightarrow qq$ tagged V_T0_FF and $q \rightarrow qq$ tagged F_T0_FV. For FSR, there is no need to differentiate between $q \rightarrow qq$ and $q \rightarrow gq$ splittings.

<FKS regions: ftuple: TBP>+≡

```

procedure :: determine_splitting_type_fsr => &
    ftuple_determine_splitting_type_fsr

```

```

(FKS regions: sub interfaces)+≡
  module subroutine ftuple_determine_splitting_type_fsr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
  end subroutine ftuple_determine_splitting_type_fsr

(FKS regions: procedures)+≡
  module subroutine ftuple_determine_splitting_type_fsr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
    associate (flst => flv%flst)
      if (is_vector (flst(i)) .and. is_vector (flst(j))) then
        ftuple%splitting_type = V_TO_VV
      else if (flst(i)+flst(j) == 0 &
        .and. is_fermion (flst(i))) then
        ftuple%splitting_type = V_TO_FF
      else if (is_fermion(flst(i)) .and. is_massless_vector (flst(j)) &
        .or. is_fermion(flst(j)) .and. is_massless_vector (flst(i))) then
        ftuple%splitting_type = F_TO_FV
      else
        ftuple%splitting_type = UNDEFINED_SPLITTING
      end if
    end associate
  end subroutine ftuple_determine_splitting_type_fsr

```

Determines the splitting type for ISR. There are four different types of splittings relevant here: $g \rightarrow gg$ tagged V_TO_VV, $g \rightarrow qq$ tagged V_TO_FF, $q \rightarrow qq$ tagged F_TO_FV and $q \rightarrow gq$ tagged F_TO_VF. The latter two need to be considered separately for ISR as they differ with respect to which particle enters the hard process. A splitting F_TO_FV may lead to soft divergences while F_TO_VF does not.

We also want to emphasize that the splitting type naming convention for ISR names the splittings considering backwards evolution. So in the splitting V_TO_FF, it is the *gluon* that enters the hard process.

Special treatment here is required if emitter 0 is assigned. This is the case only when a gluon was radiated from any of the IS particles. In this case, both splittings are soft divergent so we can equivalently choose 1 or 2 as the emitter here even if both have different flavors.

```

(FKS regions: ftuple: TBP)+≡
  procedure :: determine_splitting_type_isr => &
    ftuple_determine_splitting_type_isr

(FKS regions: sub interfaces)+≡
  module subroutine ftuple_determine_splitting_type_isr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
  end subroutine ftuple_determine_splitting_type_isr

(FKS regions: procedures)+≡
  module subroutine ftuple_determine_splitting_type_isr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple

```



```

type(flv_structure_t), intent(in) :: flv
integer, intent(in) :: i, j
integer :: em
em = i; if (i == 0) em = 1
associate (flst => flv%flst)
  if (is_vector (flst(em)) .and. is_vector (flst(j))) then
    ftuple%splitting_type = V_TO_VV
  else if (is_massless_vector(flst(em)) .and. is_fermion(flst(j))) then
    ftuple%splitting_type = F_TO_VF
  else if (is_fermion(flst(em)) .and. is_massless_vector(flst(j))) then
    ftuple%splitting_type = F_TO_FV
  else if (is_fermion(flst(em)) .and. is_fermion(flst(j))) then
    ftuple%splitting_type = V_TO_FF
  else
    ftuple%splitting_type = UNDEFINED_SPLITTING
  end if
end associate
end subroutine ftuple_determine_splitting_type_isr

```

(FKS regions: ftuple: TBP)+≡

```

procedure :: determine_sub_correction_type => &
  ftuple_determine_sub_correction_type

```

(FKS regions: sub interfaces)+≡

```

module subroutine ftuple_determine_sub_correction_type &
  (ftuple, flv_born, flv_real, i, j)
  class(ftuple_t), intent(inout) :: ftuple
  type(flv_structure_t), intent(in) :: flv_born, flv_real
  integer, intent(in) :: i, j
end subroutine ftuple_determine_sub_correction_type

```

(FKS regions: procedures)+≡

```

module subroutine ftuple_determine_sub_correction_type &
  (ftuple, flv_born, flv_real, i, j)
  class(ftuple_t), intent(inout) :: ftuple
  type(flv_structure_t), intent(in) :: flv_born, flv_real
  integer, intent(in) :: i, j
  type(flv_structure_t) :: flv_test_qcd
  integer :: em
  em = i; if (i == 0) em = 1
  select case (ftuple%splitting_type)
  case (V_TO_VV)
    ftuple%qcd_split = is_gluon (flv_real%flst(em)) .and. is_gluon (flv_real%flst(j))
  case (F_TO_VF)
    ftuple%qcd_split = is_gluon (flv_real%flst(em))
  case (F_TO_FV)
    if (i == 0) then
      ftuple%qcd_split = is_gluon (flv_real%flst(j))
    else
      ftuple%qcd_split = is_gluon (flv_real%flst(i)) .or. is_gluon (flv_real%flst(j))
    end if
  case (V_TO_FF)
    if (any ([i, j] <= flv_real%n_in)) then
      flv_test_qcd = flv_real%insert_particle_isr (i, j, GLUON)
    else

```

```

        flv_test_qcd = flv_real%insert_particle_fsr (i, j, GLUON)
    end if
    ftuple%qcd_split = flv_test_qcd .equiv. flv_born
    case (UNDEFINED_SPLITTING)
        ftuple%qcd_split = .false.
    end select
end subroutine ftuple_determine_sub_correction_type

```

Two debug functions to check the consistency of ftuples

```

<FKS regions: ftuple: TBP>+≡
    procedure :: has_negative_elements => ftuple_has_negative_elements
    procedure :: has_identical_elements => ftuple_has_identical_elements

<FKS regions: sub interfaces>+≡
    elemental module function ftuple_has_negative_elements &
        (ftuple) result (value)
        logical :: value
        class(ftuple_t), intent(in) :: ftuple
    end function ftuple_has_negative_elements
    elemental module function ftuple_has_identical_elements &
        (ftuple) result (value)
        logical :: value
        class(ftuple_t), intent(in) :: ftuple
    end function ftuple_has_identical_elements

<FKS regions: procedures>+≡
    elemental module function ftuple_has_negative_elements &
        (ftuple) result (value)
        logical :: value
        class(ftuple_t), intent(in) :: ftuple
        value = any (ftuple%ireg < 0)
    end function ftuple_has_negative_elements

    elemental module function ftuple_has_identical_elements &
        (ftuple) result (value)
        logical :: value
        class(ftuple_t), intent(in) :: ftuple
        value = ftuple%ireg(1) == ftuple%ireg(2)
    end function ftuple_has_identical_elements

```

Each singular region can have a different number of emitter-radiation pairs. This is coped with using the linked list `ftuple_list`.

```

<FKS regions: types>+≡
    type :: ftuple_list_t
        integer :: index = 0
        type(ftuple_t) :: ftuple
        type(ftuple_list_t), pointer :: next => null ()
        type(ftuple_list_t), pointer :: prev => null ()
        type(ftuple_list_t), pointer :: equiv => null ()
    contains
        <FKS regions: ftuple list: TBP>
    end type ftuple_list_t

```

```

<FKS regions: ftuple list: TBP>≡
    procedure :: write => ftuple_list_write

<FKS regions: sub interfaces>+≡
    module subroutine ftuple_list_write (list, unit, verbose)
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine ftuple_list_write

<FKS regions: procedures>+≡
    module subroutine ftuple_list_write (list, unit, verbose)
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        type(ftuple_list_t), pointer :: current
        logical :: verb
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        verb = .false.; if (present (verbose)) verb = verbose
        select type (list)
        type is (ftuple_list_t)
            current => list
            do
                call current%ftuple%write (unit = u, newline = .false.)
                if (verb .and. associated (current%equiv)) &
                    write (u, '(A)', advance = "no") ""
                if (associated (current%next)) then
                    current => current%next
                else
                    exit
                end if
            end do
            write (u, *) ""
        end select
    end subroutine ftuple_list_write

<FKS regions: ftuple list: TBP>+≡
    procedure :: append => ftuple_list_append

<FKS regions: sub interfaces>+≡
    module subroutine ftuple_list_append (list, ftuple)
        class(ftuple_list_t), intent(inout), target :: list
        type(ftuple_t), intent(in) :: ftuple
    end subroutine ftuple_list_append

<FKS regions: procedures>+≡
    module subroutine ftuple_list_append (list, ftuple)
        class(ftuple_list_t), intent(inout), target :: list
        type(ftuple_t), intent(in) :: ftuple
        type(ftuple_list_t), pointer :: current

        select type (list)
        type is (ftuple_list_t)
            if (list%index == 0) then
                nullify (list%next)

```

```

        list%index = 1
        list%ftuple = ftuple
    else
        current => list
        do
            if (associated (current%next)) then
                current => current%next
            else
                allocate (current%next)
                nullify (current%next%next)
                nullify (current%next%equiv)
                current%next%prev => current
                current%next%index = current%index + 1
                current%next%ftuple = ftuple
                exit
            end if
        end do
    end if
end select
end subroutine ftuple_list_append

```

(FKS regions: ftuple list: TBP)+≡

```

    procedure :: get_n_tuples => ftuple_list_get_n_tuples

```

(FKS regions: sub interfaces)+≡

```

    impure elemental module function ftuple_list_get_n_tuples &
        (list) result(n_tuples)
        integer :: n_tuples
        class(ftuple_list_t), intent(in), target :: list
    end function ftuple_list_get_n_tuples

```

(FKS regions: procedures)+≡

```

    impure elemental module function ftuple_list_get_n_tuples &
        (list) result(n_tuples)
        integer :: n_tuples
        class(ftuple_list_t), intent(in), target :: list
        type(ftuple_list_t), pointer :: current
        n_tuples = 0
        select type (list)
        type is (ftuple_list_t)
            current => list
            if (current%index > 0) then
                n_tuples = 1
                do
                    if (associated (current%next)) then
                        current => current%next
                        n_tuples = n_tuples + 1
                    else
                        exit
                    end if
                end do
            end if
        end select
    end function ftuple_list_get_n_tuples

```

```

<FKS regions: ftuple list: TBP>+≡
    procedure :: get_entry => ftuple_list_get_entry

<FKS regions: sub interfaces>+≡
    module function ftuple_list_get_entry (list, index) result (entry)
        type(ftuple_list_t), pointer :: entry
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in) :: index
    end function ftuple_list_get_entry

<FKS regions: procedures>+≡
    module function ftuple_list_get_entry (list, index) result (entry)
        type(ftuple_list_t), pointer :: entry
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in) :: index
        type(ftuple_list_t), pointer :: current
        integer :: i
        entry => null()
        select type (list)
        type is (ftuple_list_t)
            current => list
            if (index == 1) then
                entry => current
            else
                do i = 1, index - 1
                    current => current%next
                end do
                entry => current
            end if
        end select
    end function ftuple_list_get_entry

<FKS regions: ftuple list: TBP>+≡
    procedure :: get_ftuple => ftuple_list_get_ftuple

<FKS regions: sub interfaces>+≡
    module function ftuple_list_get_ftuple (list, index) result (ftuple)
        type(ftuple_t) :: ftuple
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in) :: index
    end function ftuple_list_get_ftuple

<FKS regions: procedures>+≡
    module function ftuple_list_get_ftuple (list, index) result (ftuple)
        type(ftuple_t) :: ftuple
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in) :: index
        type(ftuple_list_t), pointer :: entry
        entry => list%get_entry (index)
        ftuple = entry%ftuple
    end function ftuple_list_get_ftuple

<FKS regions: ftuple list: TBP>+≡
    procedure :: set_equiv => ftuple_list_set_equiv

```

<FKS regions: sub interfaces>+≡

```
module subroutine ftuple_list_set_equiv (list, i1, i2)
  class(ftuple_list_t), intent(in) :: list
  integer, intent(in) :: i1, i2
end subroutine ftuple_list_set_equiv
```

<FKS regions: procedures>+≡

```
module subroutine ftuple_list_set_equiv (list, i1, i2)
  class(ftuple_list_t), intent(in) :: list
  integer, intent(in) :: i1, i2
  type(ftuple_list_t), pointer :: list1, list2 => null ()
  select type (list)
  type is (ftuple_list_t)
    if (list%get_ftuple (i1) > list%get_ftuple (i2)) then
      list1 => list%get_entry (i2)
      list2 => list%get_entry (i1)
    else
      list1 => list%get_entry (i1)
      list2 => list%get_entry (i2)
    end if
  end do
  if (associated (list1%equiv)) then
    list1 => list1%equiv
  else
    exit
  end if
end do
list1%equiv => list2
end select
end subroutine ftuple_list_set_equiv
```

<FKS regions: ftuple list: TBP>+≡

```
procedure :: check_equiv => ftuple_list_check_equiv
```

<FKS regions: sub interfaces>+≡

```
module function ftuple_list_check_equiv(list, i1, i2) result (eq)
  class(ftuple_list_t), intent(in) :: list
  integer, intent(in) :: i1, i2
  logical :: eq
end function ftuple_list_check_equiv
```

<FKS regions: procedures>+≡

```
module function ftuple_list_check_equiv(list, i1, i2) result (eq)
  class(ftuple_list_t), intent(in) :: list
  integer, intent(in) :: i1, i2
  logical :: eq
  type(ftuple_list_t), pointer :: current
  eq = .false.
  select type (list)
  type is (ftuple_list_t)
    current => list%get_entry (i1)
  do
    if (associated (current%equiv)) then
      current => current%equiv
      if (current%index == i2) then
```

```

        eq = .true.
        exit
    end if
else
    exit
end if
end do
end select
end function ftuple_list_check_equiv

```

(FKS regions: ftuple list: TBP)+≡

```

    procedure :: to_array => ftuple_list_to_array

```

(FKS regions: sub interfaces)+≡

```

    module subroutine ftuple_list_to_array &
        (ftuple_list, ftuple_array, equivalences, ordered)
        class(ftuple_list_t), intent(in), target :: ftuple_list
        type(ftuple_t), intent(out), dimension(:), allocatable :: ftuple_array
        logical, intent(out), dimension(:,:), allocatable :: equivalences
        logical, intent(in) :: ordered
    end subroutine ftuple_list_to_array

```

(FKS regions: procedures)+≡

```

    module subroutine ftuple_list_to_array &
        (ftuple_list, ftuple_array, equivalences, ordered)
        class(ftuple_list_t), intent(in), target :: ftuple_list
        type(ftuple_t), intent(out), dimension(:), allocatable :: ftuple_array
        logical, intent(out), dimension(:,:), allocatable :: equivalences
        logical, intent(in) :: ordered
        integer :: i_tuple, n
        type(ftuple_list_t), pointer :: current => null ()
        integer :: i1, i2
        type(ftuple_t) :: ftuple_tmp
        logical, dimension(:), allocatable :: eq_tmp
        n = ftuple_list%get_n_tuples ()
        allocate (ftuple_array (n), equivalences (n, n))
        equivalences = .false.
        select type (ftuple_list)
        type is (ftuple_list_t)
            current => ftuple_list
            i_tuple = 1
            do
                ftuple_array(i_tuple) = current%ftuple
                if (associated (current%equiv)) then
                    i1 = current%index
                    i2 = current%equiv%index
                    equivalences (i1, i2) = .true.
                end if
                if (associated (current%next)) then
                    current => current%next
                    i_tuple = i_tuple + 1
                else
                    exit
                end if
            end do
        end select
    end subroutine

```

```

end select
if (ordered) call ftuple_sort_array (ftuple_array, equivalences)
end subroutine ftuple_list_to_array

```

<FKS regions: procedures>+≡

```

subroutine print_equivalence_matrix (ftuple_array, equivalences)
  type(ftuple_t), intent(in), dimension(:) :: ftuple_array
  logical, intent(in), dimension(:, :) :: equivalences
  integer :: i, i1, i2
  print *, 'Equivalence matrix: '
  do i = 1, size (ftuple_array)
    call ftuple_array(i)%get(i1,i2)
    print *, 'i: ', i, '(', i1, i2, '): ', equivalences(i,:)
  end do
end subroutine print_equivalence_matrix

```

Class for working with the flavor specification arrays.

<FKS regions: public>+≡

```

public :: flv_structure_t

```

<FKS regions: types>+≡

```

type :: flv_structure_t
  integer, dimension(:), allocatable :: flst
  integer, dimension(:), allocatable :: tag
  integer :: nlegs = 0
  integer :: n_in = 0
  logical, dimension(:), allocatable :: massive
  logical, dimension(:), allocatable :: colored
  real(default), dimension(:), allocatable :: charge
  real(default) :: prt_symm_fs = 1._default
  integer :: eqv_index = 0
contains
<FKS regions: flv structure: TBP>
end type flv_structure_t

```

Returns **true** if the two particles at position *i* and *j* in the flavor array can originate from the same splitting. For this purpose, the function first checks whether the splitting is allowed at all. If this is the case, the emitter is removed from the flavor array. If the resulting array is equivalent to the Born flavor structure **flv_born**, the pair is accepted as a valid splitting.

We first check whether the splitting is possible. The array **flv_orig** contains all particles which share a vertex with the particles at position *i* and *j*. If any of these particles belongs to the initial state, a PDG-ID flip is necessary to correctly recognize the vertex. If its size is equal to zero, no splitting is possible and the subroutine is exited. Otherwise, we loop over all possible underlying Born flavor structures and check if any of them equals the actual underlying Born flavor structure. For a quark emitting a gluon, **flv_orig** contains the PDG code of the anti-quark. To be on the safe side, a second array is created, which contains both the positively and negatively signed PDG codes. Then, the original tuple (*i, j*) is removed from the real flavor structure and the particles in **flv_orig2** are inserted. If the resulting Born configuration is equal to the

underlying Born configuration, up to a permutation of final-state particles, the tuple (i, j) is accepted as valid.

```

(FKS regions: flv structure: TBP)≡
  procedure :: valid_pair => flv_structure_valid_pair

(FKS regions: sub interfaces)+≡
  module function flv_structure_valid_pair &
    (flv, i, j, flv_ref, model) result (valid)
    logical :: valid
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i,j
    type(flv_structure_t), intent(in) :: flv_ref
    type(model_t), intent(in) :: model
  end function flv_structure_valid_pair

(FKS regions: procedures)+≡
  module function flv_structure_valid_pair &
    (flv, i, j, flv_ref, model) result (valid)
    logical :: valid
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i,j
    type(flv_structure_t), intent(in) :: flv_ref
    type(model_t), intent(in) :: model
    integer :: k, n_orig
    type(flv_structure_t) :: flv_test
    integer, dimension(:), allocatable :: flv_orig
    valid = .false.
    if (all ([i, j] <= flv%n_in)) return
    if (i <= flv%n_in .and. is_fermion(flv%flst(i))) then
      call model%match_vertex (-flv%flst(i), flv%flst(j), flv_orig)
    else if (j <= flv%n_in .and. is_fermion(flv%flst(j))) then
      call model%match_vertex (flv%flst(i), -flv%flst(j), flv_orig)
    else
      call model%match_vertex (flv%flst(i), flv%flst(j), flv_orig)
    end if
    n_orig = size (flv_orig)
    if (n_orig == 0) then
      return
    else
      do k = 1, n_orig
        if (any ([i, j] <= flv%n_in)) then
          flv_test = flv%insert_particle_isr (i, j, flv_orig(k))
        else
          flv_test = flv%insert_particle_fsr (i, j, flv_orig(k))
        end if
        valid = flv_ref .equiv. flv_test
        call flv_test%final ()
        if (valid) return
      end do
    end if
    deallocate (flv_orig)
  end function flv_structure_valid_pair

```

This function checks whether two flavor arrays are the same up to a permutation

of the final-state particles

(FKS regions: procedures)+≡

```
function flv_structure_equivalent (flv1, flv2, with_tag) result (equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  logical, intent(in) :: with_tag
  type(flv_perm_t) :: perm
  integer :: n
  n = size (flv1%flst)
  equiv = .true.
  if (n /= size (flv2%flst)) then
    call msg_fatal &
      ('flv_structure_equivalent: flavor arrays do not have equal lengths')
  else if (flv1%n_in /= flv2%n_in) then
    call msg_fatal &
      ('flv_structure_equivalent: flavor arrays do not have equal n_in')
  else
    call perm%init (flv1, flv2, flv1%n_in, flv1%nlegs, with_tag)
    equiv = perm%eqv (flv2, flv1, with_tag)
    call perm%final ()
  end if
end function flv_structure_equivalent
```

(FKS regions: sub interfaces)+≡

```
module function flv_structure_equivalent_no_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
end function flv_structure_equivalent_no_tag
module function flv_structure_equivalent_with_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
endfunction flv_structure_equivalent_with_tag
```

(FKS regions: procedures)+≡

```
module function flv_structure_equivalent_no_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  equiv = flv_structure_equivalent (flv1, flv2, .false.)
end function flv_structure_equivalent_no_tag

module function flv_structure_equivalent_with_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  equiv = flv_structure_equivalent (flv1, flv2, .true.)
end function flv_structure_equivalent_with_tag
```

(FKS regions: sub interfaces)+≡

```
pure module subroutine flv_structure_assign_flv (flv_out, flv_in)
  type(flv_structure_t), intent(out) :: flv_out
  type(flv_structure_t), intent(in) :: flv_in
end subroutine flv_structure_assign_flv
```

<FKS regions: procedures>+≡

```

pure module subroutine flv_structure_assign_flv (flv_out, flv_in)
  type(flv_structure_t), intent(out) :: flv_out
  type(flv_structure_t), intent(in) :: flv_in
  flv_out%nlegs = flv_in%nlegs
  flv_out%n_in = flv_in%n_in
  flv_out%prt_symm_fs = flv_in%prt_symm_fs
  if (allocated (flv_in%flst)) then
    allocate (flv_out%flst (size (flv_in%flst)))
    flv_out%flst = flv_in%flst
  end if
  if (allocated (flv_in%tag)) then
    allocate (flv_out%tag (size (flv_in%tag)))
    flv_out%tag = flv_in%tag
  end if
  if (allocated (flv_in%massive)) then
    allocate (flv_out%massive (size (flv_in%massive)))
    flv_out%massive = flv_in%massive
  end if
  if (allocated (flv_in%colored)) then
    allocate (flv_out%colored (size (flv_in%colored)))
    flv_out%colored = flv_in%colored
  end if
end subroutine flv_structure_assign_flv

```

<FKS regions: sub interfaces>+≡

```

pure module subroutine flv_structure_assign_integer (flv_out, iarray)
  type(flv_structure_t), intent(out) :: flv_out
  integer, intent(in), dimension(:) :: iarray
end subroutine flv_structure_assign_integer

```

<FKS regions: procedures>+≡

```

pure module subroutine flv_structure_assign_integer (flv_out, iarray)
  type(flv_structure_t), intent(out) :: flv_out
  integer, intent(in), dimension(:) :: iarray
  integer :: i
  flv_out%nlegs = size (iarray)
  allocate (flv_out%flst (flv_out%nlegs))
  allocate (flv_out%tag (flv_out%nlegs))
  flv_out%flst = iarray
  flv_out%tag = [(i, i = 1, flv_out%nlegs)]
end subroutine flv_structure_assign_integer

```

Returns a new flavor array with the particle at position *index* removed.

<FKS regions: flv structure: TBP>+≡

```

procedure :: remove_particle => flv_structure_remove_particle

```

<FKS regions: sub interfaces>+≡

```

module function flv_structure_remove_particle (flv, index) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: index
end function flv_structure_remove_particle

```

<FKS regions: procedures>+≡

```

module function flv_structure_remove_particle (flv, index) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: index
  integer :: n1, n2
  integer :: i, removed_tag
  n1 = size (flv%flst); n2 = n1 - 1
  allocate (flv_new%flst (n2), flv_new%tag (n2))
  flv_new%nlegs = n2
  flv_new%n_in = flv%n_in
  removed_tag = flv%tag(index)
  if (index == 1) then
    flv_new%flst(1 : n2) = flv%flst(2 : n1)
    flv_new%tag(1 : n2) = flv%tag(2 : n1)
  else if (index == n1) then
    flv_new%flst(1 : n2) = flv%flst(1 : n2)
    flv_new%tag(1 : n2) = flv%tag(1 : n2)
  else
    flv_new%flst(1 : index - 1) = flv%flst(1 : index - 1)
    flv_new%flst(index : n2) = flv%flst(index + 1 : n1)
    flv_new%tag(1 : index - 1) = flv%tag(1 : index - 1)
    flv_new%tag(index : n2) = flv%tag(index + 1 : n1)
  end if
  do i = 1, n2
    if (flv_new%tag(i) > removed_tag) &
      flv_new%tag(i) = flv_new%tag(i) - 1
  end do
  call flv_new%compute_prt_symm_fs (flv_new%n_in)
end function flv_structure_remove_particle

```

Removes the particles at position i1 and i2 and inserts a new particle of matching flavor at position i1.

<FKS regions: flv structure: TBP>+≡

```

procedure :: insert_particle_fsr => flv_structure_insert_particle_fsr

```

<FKS regions: sub interfaces>+≡

```

module function flv_structure_insert_particle_fsr &
  (flv, i1, i2, flv_add) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i1, i2, flv_add
end function flv_structure_insert_particle_fsr

```

<FKS regions: procedures>+≡

```

module function flv_structure_insert_particle_fsr &
  (flv, i1, i2, flv_add) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i1, i2, flv_add
  if (flv%flst(i1) + flv_add == 0 .or. flv%flst(i2) + flv_add == 0) then
    flv_new = flv%insert_particle (i1, i2, -flv_add)
  else
    flv_new = flv%insert_particle (i1, i2, flv_add)
  end if
end function

```

```
end function flv_structure_insert_particle_fsr
```

Same as `insert_particle_fsr` but for ISR, the two particles are not exchangeable.

(FKS regions: flv structure: TBP)+≡

```
procedure :: insert_particle_isr => flv_structure_insert_particle_isr
```

(FKS regions: sub interfaces)+≡

```
module function flv_structure_insert_particle_isr &
  (flv, i_in, i_out, flv_add) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i_in, i_out, flv_add
end function flv_structure_insert_particle_isr
```

(FKS regions: procedures)+≡

```
module function flv_structure_insert_particle_isr &
  (flv, i_in, i_out, flv_add) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i_in, i_out, flv_add
  if (flv%flst(i_in) + flv_add == 0) then
    flv_new = flv%insert_particle (i_in, i_out, -flv_add)
  else
    flv_new = flv%insert_particle (i_in, i_out, flv_add)
  end if
end function flv_structure_insert_particle_isr
```

Removes the particles at position `i1` and `i2` and inserts a new particle at position `i1`.

(FKS regions: flv structure: TBP)+≡

```
procedure :: insert_particle => flv_structure_insert_particle
```

(FKS regions: sub interfaces)+≡

```
module function flv_structure_insert_particle &
  (flv, i1, i2, particle) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i1, i2, particle
end function flv_structure_insert_particle
```

(FKS regions: procedures)+≡

```
module function flv_structure_insert_particle &
  (flv, i1, i2, particle) result (flv_new)
  type(flv_structure_t) :: flv_new
  class(flv_structure_t), intent(in) :: flv
  integer, intent(in) :: i1, i2, particle
  type(flv_structure_t) :: flv_tmp
  integer :: n1, n2
  integer :: new_tag
  n1 = size (flv%flst); n2 = n1 - 1
  allocate (flv_new%flst (n2), flv_new%tag (n2))
  flv_new%nlegs = n2
  flv_new%n_in = flv%n_in
  new_tag = maxval(flv%tag) + 1
```

```

if (i1 < i2) then
  flv_tmp = flv%remove_particle (i1)
  flv_tmp = flv_tmp%remove_particle (i2 - 1)
else if (i2 < i1) then
  flv_tmp = flv%remove_particle(i2)
  flv_tmp = flv_tmp%remove_particle(i1 - 1)
else
  call msg_fatal ("flv_structure_insert_particle: Indices are identical!")
end if
if (i1 == 1) then
  flv_new%flst(1) = particle
  flv_new%flst(2 : n2) = flv_tmp%flst(1 : n2 - 1)
  flv_new%tag(1) = new_tag
  flv_new%tag(2 : n2) = flv_tmp%tag(1 : n2 - 1)
else if (i1 == n1 .or. i1 == n2) then
  flv_new%flst(1 : n2 - 1) = flv_tmp%flst(1 : n2 - 1)
  flv_new%flst(n2) = particle
  flv_new%tag(1 : n2 - 1) = flv_tmp%tag(1 : n2 - 1)
  flv_new%tag(n2) = new_tag
else
  flv_new%flst(1 : i1 - 1) = flv_tmp%flst(1 : i1 - 1)
  flv_new%flst(i1) = particle
  flv_new%flst(i1 + 1 : n2) = flv_tmp%flst(i1 : n2 - 1)
  flv_new%tag(1 : i1 - 1) = flv_tmp%tag(1 : i1 - 1)
  flv_new%tag(i1) = new_tag
  flv_new%tag(i1 + 1 : n2) = flv_tmp%tag(i1 : n2 - 1)
end if
call flv_new%compute_prt_symm_fs (flv_new%n_in)
end function flv_structure_insert_particle

```

Counts the number of occurrences of a particle in a flavor array

```

(FKS regions: flv structure: TBP)+≡
  procedure :: count_particle => flv_structure_count_particle

(FKS regions: sub interfaces)+≡
  module function flv_structure_count_particle (flv, part) result (n)
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: part
    integer :: n
  end function flv_structure_count_particle

(FKS regions: procedures)+≡
  module function flv_structure_count_particle (flv, part) result (n)
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: part
    integer :: n
    n = count (flv%flst == part)
  end function flv_structure_count_particle

```

Initializer for flavor structures

```

(FKS regions: flv structure: TBP)+≡
  procedure :: init => flv_structure_init

```

<FKS regions: sub interfaces>+≡

```

module subroutine flv_structure_init (flv, aval, n_in, tags)
  class(flv_structure_t), intent(inout) :: flv
  integer, intent(in), dimension(:) :: aval
  integer, intent(in) :: n_in
  integer, intent(in), dimension(:), optional :: tags
end subroutine flv_structure_init

```

<FKS regions: procedures>+≡

```

module subroutine flv_structure_init (flv, aval, n_in, tags)
  class(flv_structure_t), intent(inout) :: flv
  integer, intent(in), dimension(:) :: aval
  integer, intent(in) :: n_in
  integer, intent(in), dimension(:), optional :: tags
  integer :: i, n
  integer, dimension(:), allocatable :: aval_unique
  integer, dimension(:), allocatable :: mult
  n = size (aval)
  allocate (flv%flst (n), flv%tag (n))
  flv%flst = aval
  if (present (tags)) then
    flv%tag = tags
  else
    do i = 1, n
      flv%tag(i) = i
    end do
  end if
  flv%nlegs = n
  flv%n_in = n_in
  call flv%compute_prt_symm_fs (flv%n_in)
end subroutine flv_structure_init

```

<FKS regions: flv structure: TBP>+≡

```

procedure :: compute_prt_symm_fs => flv_structure_compute_prt_symm_fs

```

<FKS regions: sub interfaces>+≡

```

module subroutine flv_structure_compute_prt_symm_fs (flv, n_in)
  class(flv_structure_t), intent(inout) :: flv
  integer, intent(in) :: n_in
end subroutine flv_structure_compute_prt_symm_fs

```

<FKS regions: procedures>+≡

```

module subroutine flv_structure_compute_prt_symm_fs (flv, n_in)
  class(flv_structure_t), intent(inout) :: flv
  integer, intent(in) :: n_in
  integer, dimension(:), allocatable :: flst_unique
  integer, dimension(:), allocatable :: mult
  integer :: i
  flst_unique = remove_duplicates_from_int_array (flv%flst(n_in + 1 :))
  allocate (mult(size (flst_unique)))
  do i = 1, size (flst_unique)
    mult(i) = count (flv%flst(n_in + 1 :) == flst_unique(i))
  end do
  flv%prtsymm_fs = one / product (gamma (real (mult + 1, default)))
end subroutine flv_structure_compute_prt_symm_fs

```

```

<FKS regions: flv structure: TBP>+≡
  procedure :: write => flv_structure_write

<FKS regions: sub interfaces>+≡
  module subroutine flv_structure_write (flv, unit)
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in), optional :: unit
  end subroutine flv_structure_write

<FKS regions: procedures>+≡
  module subroutine flv_structure_write (flv, unit)
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, '(A)') char (flv%to_string ())
  end subroutine flv_structure_write

<FKS regions: flv structure: TBP>+≡
  procedure :: to_string => flv_structure_to_string

<FKS regions: sub interfaces>+≡
  module function flv_structure_to_string (flv) result (flv_string)
    type(string_t) :: flv_string
    class(flv_structure_t), intent(in) :: flv
  end function flv_structure_to_string

<FKS regions: procedures>+≡
  module function flv_structure_to_string (flv) result (flv_string)
    type(string_t) :: flv_string
    class(flv_structure_t), intent(in) :: flv
    integer :: i, n
    if (allocated (flv%flst)) then
      flv_string = var_str ("[")
      n = size (flv%flst)
      do i = 1, n - 1
        flv_string = flv_string // str (flv%flst(i)) // var_str(",")
      end do
      flv_string = flv_string // str (flv%flst(n)) // var_str("]")
    else
      flv_string = var_str ("[not allocated]")
    end if
  end function flv_structure_to_string

```

Creates the underlying Born flavor structure for a given real flavor structure if the particle at position `emitter` is removed

```

<FKS regions: flv structure: TBP>+≡
  procedure :: create_uborn => flv_structure_create_uborn

<FKS regions: sub interfaces>+≡
  module function flv_structure_create_uborn &
    (flv, emitter, nlo_correction_type) result(flv_uborn)
    type(flv_structure_t) :: flv_uborn
    class(flv_structure_t), intent(in) :: flv
    type(string_t), intent(in) :: nlo_correction_type
    integer, intent(in) :: emitter
  end function flv_structure_create_uborn

```


<FKS regions: procedures>+≡

```

module function flv_structure_create_uborn &
    (flv, emitter, nlo_correction_type) result(flv_uborn)
    type(flv_structure_t) :: flv_uborn
    class(flv_structure_t), intent(in) :: flv
    type(string_t), intent(in) :: nlo_correction_type
    integer, intent(in) :: emitter
    integer n_legs
    integer :: f1, f2
    integer :: gauge_boson

    n_legs = size(flv%flst)
    allocate (flv_uborn%flst (n_legs - 1), flv_uborn%tag (n_legs - 1))
    gauge_boson = determine_gauge_boson_to_be_inserted ()

    if (emitter > flv%n_in) then
        f1 = flv%flst(n_legs); f2 = flv%flst(n_legs - 1)
        if (is_massless_vector (f1)) then
            !!! Emitted particle is a gluon or photon => just remove it
            flv_uborn = flv%remove_particle(n_legs)
        else if (is_fermion (f1) .and. is_fermion (f2) .and. f1 + f2 == 0) then
            !!! Emission type is a gauge boson splitting into two fermions
            flv_uborn = flv%insert_particle(n_legs - 1, n_legs, gauge_boson)
        else
            call msg_error ("Create underlying Born: Unsupported splitting type.")
            call msg_error (char (str (flv%flst)))
            call msg_fatal ("FKS - FAIL")
        end if
    else if (emitter > 0) then
        f1 = flv%flst(n_legs); f2 = flv%flst(emitter)
        if (is_massless_vector (f1)) then
            flv_uborn = flv%remove_particle(n_legs)
        else if (is_fermion (f1) .and. is_massless_vector (f2)) then
            flv_uborn = flv%insert_particle (emitter, n_legs, -f1)
        else if (is_fermion (f1) .and. is_fermion (f2) .and. f1 == f2) then
            flv_uborn = flv%insert_particle(emitter, n_legs, gauge_boson)
        end if
    else
        flv_uborn = flv%remove_particle (n_legs)
    end if

contains
    integer function determine_gauge_boson_to_be_inserted ()
        select case (char (nlo_correction_type))
        case ("QCD")
            determine_gauge_boson_to_be_inserted = GLUON
        case ("EW")
            determine_gauge_boson_to_be_inserted = PHOTON
        case ("Full")
            call msg_fatal ("NLO correction type 'Full' not yet implemented!")
        case default
            call msg_fatal ("Invalid NLO correction type! Valid inputs " // &
                "are: QCD, EW and Full (default: QCD)")
        end select
    end function

```

```

        end function determine_gauge_boson_to_be_inserted

    end function flv_structure_create_uborn

    <FKS regions: flv structure: TBP>+≡
        procedure :: init_mass_color_and_charge => &
            flv_structure_init_mass_color_and_charge
    <FKS regions: sub interfaces>+≡
        module subroutine flv_structure_init_mass_color_and_charge (flv, model)
            class(flv_structure_t), intent(inout) :: flv
            type(model_t), intent(in) :: model
            end subroutine flv_structure_init_mass_color_and_charge
    <FKS regions: procedures>+≡
        module subroutine flv_structure_init_mass_color_and_charge (flv, model)
            class(flv_structure_t), intent(inout) :: flv
            type(model_t), intent(in) :: model
            integer :: i
            type(flavor_t) :: flavor
            allocate (flv%massive (flv%nlegs), flv%colored(flv%nlegs), &
                flv%charge(flv%nlegs))
            do i = 1, flv%nlegs
                call flavor%init (flv%flst(i), model)
                flv%massive(i) = flavor%get_mass () > 0
                flv%colored(i) = &
                    is_quark (flv%flst(i)) .or. is_gluon (flv%flst(i))
                flv%charge(i) = flavor%get_charge ()
            end do
            end subroutine flv_structure_init_mass_color_and_charge

    <FKS regions: flv structure: TBP>+≡
        procedure :: get_last_two => flv_structure_get_last_two
    <FKS regions: sub interfaces>+≡
        module function flv_structure_get_last_two (flv, n) result (flst_last)
            integer, dimension(2) :: flst_last
            class(flv_structure_t), intent(in) :: flv
            integer, intent(in) :: n
            end function flv_structure_get_last_two
    <FKS regions: procedures>+≡
        module function flv_structure_get_last_two (flv, n) result (flst_last)
            integer, dimension(2) :: flst_last
            class(flv_structure_t), intent(in) :: flv
            integer, intent(in) :: n
            flst_last = [flv%flst(n - 1), flv%flst(n)]
            end function flv_structure_get_last_two

    <FKS regions: flv structure: TBP>+≡
        procedure :: final => flv_structure_final
    <FKS regions: sub interfaces>+≡
        module subroutine flv_structure_final (flv)
            class(flv_structure_t), intent(inout) :: flv
            end subroutine flv_structure_final

```

<FKS regions: procedures>+≡

```
module subroutine flv_structure_final (flv)
  class(flv_structure_t), intent(inout) :: flv
  if (allocated (flv%flst)) deallocate (flv%flst)
  if (allocated (flv%tag)) deallocate (flv%tag)
  if (allocated (flv%massive)) deallocate (flv%massive)
  if (allocated (flv%colored)) deallocate (flv%colored)
  if (allocated (flv%charge)) deallocate (flv%charge)
end subroutine flv_structure_final
```

<FKS regions: types>+≡

```
type :: flv_perm_t
  integer, dimension(:,:), allocatable :: perms
contains
  <FKS regions: flavor permutation: TBP>
end type flv_perm_t
```

<FKS regions: flavor permutation: TBP>≡

```
procedure :: init => flv_perm_init
```

<FKS regions: sub interfaces>+≡

```
module subroutine flv_perm_init &
  (perm, flv_in, flv_ref, n_first, n_last, with_tag)
  class(flv_perm_t), intent(out) :: perm
  type(flv_structure_t), intent(in) :: flv_in, flv_ref
  integer, intent(in) :: n_first, n_last
  logical, intent(in) :: with_tag
end subroutine flv_perm_init
```

<FKS regions: procedures>+≡

```
module subroutine flv_perm_init &
  (perm, flv_in, flv_ref, n_first, n_last, with_tag)
  class(flv_perm_t), intent(out) :: perm
  type(flv_structure_t), intent(in) :: flv_in, flv_ref
  integer, intent(in) :: n_first, n_last
  logical, intent(in) :: with_tag
  integer :: flv1, flv2, tmp
  integer :: tag1, tag2
  integer :: i, j, j_min, i_perm
  integer, dimension(:,:), allocatable :: perm_list_tmp
  type(flv_structure_t) :: flv_copy
  logical :: condition
  logical, dimension(:), allocatable :: already_correct
  flv_copy = flv_in
  allocate (perm_list_tmp (factorial (n_last - n_first - 1), 2))
  allocate (already_correct (flv_in%nlegs))
  already_correct = flv_in%flst == flv_ref%flst
  if (with_tag) &
    already_correct = already_correct .and. (flv_in%tag == flv_ref%tag)
  j_min = n_first + 1
  i_perm = 0
  do i = n_first + 1, n_last
    flv1 = flv_ref%flst(i)
    tag1 = flv_ref%tag(i)
```

```

do j = j_min, n_last
  if (already_correct(i) .or. already_correct(j)) cycle
  flv2 = flv_copy%flst(j)
  tag2 = flv_copy%tag(j)
  condition = (flv1 == flv2) .and. i /= j
  if (with_tag) condition = condition .and. (tag1 == tag2)
  if (condition) then
    i_perm = i_perm + 1
    tmp = flv_copy%flst(i)
    flv_copy%flst(i) = flv2
    flv_copy%flst(j) = tmp
    tmp = flv_copy%tag(i)
    flv_copy%tag(i) = tag2
    flv_copy%tag(j) = tmp
    perm_list_tmp (i_perm, 1) = i
    perm_list_tmp (i_perm, 2) = j
    exit
  end if
end do
j_min = j_min + 1
end do
allocate (perm%perms (i_perm, 2))
perm%perms = perm_list_tmp (1 : i_perm, :)
deallocate (perm_list_tmp)
call flv_copy%final ()
end subroutine flv_perm_init

```

(FKS regions: flavor permutation: TBP)+≡
 procedure :: write => flv_perm_write

(FKS regions: sub interfaces)+≡
 module subroutine flv_perm_write (perm, unit)
 class(flv_perm_t), intent(in) :: perm
 integer, intent(in), optional :: unit
end subroutine flv_perm_write

(FKS regions: procedures)+≡
 module subroutine flv_perm_write (perm, unit)
 class(flv_perm_t), intent(in) :: perm
 integer, intent(in), optional :: unit
 integer :: i, n, u
 u = given_output_unit (unit); if (u < 0) return
 write (u, "(A)") "Flavor permutation list: "
 n = size (perm%perms, dim = 1)
 if (n > 0) then
 do i = 1, n
 write (u, "(A1,I1,1X,I1,A1)", advance = "no") "[", &
 perm%perms(i,1), perm%perms(i,2), "]"
 if (i < n) write (u, "(A4)", advance = "no") " //" "
 end do
 write (u, "(A)") ""
 else
 write (u, "(A)") "[Empty]"
 end if
end subroutine flv_perm_write

```

<FKS regions: flavor permutation: TBP>+≡
  procedure :: reset => flv_perm_final
  procedure :: final => flv_perm_final

<FKS regions: sub interfaces>+≡
  module subroutine flv_perm_final (perm)
    class(flv_perm_t), intent(inout) :: perm
  end subroutine flv_perm_final

<FKS regions: procedures>+≡
  module subroutine flv_perm_final (perm)
    class(flv_perm_t), intent(inout) :: perm
    if (allocated (perm%perms)) deallocate (perm%perms)
  end subroutine flv_perm_final

<FKS regions: flavor permutation: TBP>+≡
  generic :: apply => &
    apply_flv_structure, apply_index, apply_ftuple
  procedure :: apply_flv_structure => flv_perm_apply_flv_structure
  procedure :: apply_index => flv_perm_apply_index
  procedure :: apply_ftuple => flv_perm_apply_ftuple

<FKS regions: sub interfaces>+≡
  elemental module function flv_perm_apply_flv_structure &
    (perm, flv_in, invert) result (flv_out)
    type(flv_structure_t) :: flv_out
    class(flv_perm_t), intent(in) :: perm
    type(flv_structure_t), intent(in) :: flv_in
    logical, intent(in), optional :: invert
  end function flv_perm_apply_flv_structure

<FKS regions: procedures>+≡
  elemental module function flv_perm_apply_flv_structure &
    (perm, flv_in, invert) result (flv_out)
    type(flv_structure_t) :: flv_out
    class(flv_perm_t), intent(in) :: perm
    type(flv_structure_t), intent(in) :: flv_in
    logical, intent(in), optional :: invert
    integer :: i, i1, i2
    integer :: p1, p2, incr
    integer :: flv_tmp, tag_tmp
    logical :: inv
    inv = .false.; if (present(invert)) inv = invert
    flv_out = flv_in
    if (inv) then
      p1 = 1
      p2 = size (perm%perms, dim = 1)
      incr = 1
    else
      p1 = size (perm%perms, dim = 1)
      p2 = 1
      incr = -1
    end if
    do i = p1, p2, incr

```

```

        i1 = perm%perms(i,1)
        i2 = perm%perms(i,2)
        flv_tmp = flv_out%flst(i1)
        tag_tmp = flv_out%tag(i1)
        flv_out%flst(i1) = flv_out%flst(i2)
        flv_out%flst(i2) = flv_tmp
        flv_out%tag(i1) = flv_out%tag(i2)
        flv_out%tag(i2) = tag_tmp
    end do
end function flv_perm_apply_flv_structure

```

<FKS regions: sub interfaces>+≡

```

    elemental module function flv_perm_apply_index &
        (perm, i_in) result (i_out)
        integer :: i_out
        class(flv_perm_t), intent(in) :: perm
        integer, intent(in) :: i_in
    end function flv_perm_apply_index

```

<FKS regions: procedures>+≡

```

    elemental module function flv_perm_apply_index &
        (perm, i_in) result (i_out)
        integer :: i_out
        class(flv_perm_t), intent(in) :: perm
        integer, intent(in) :: i_in
        integer :: i, i1, i2
        i_out = i_in
        do i = size (perm%perms(:,1)), 1, -1
            i1 = perm%perms(i,1)
            i2 = perm%perms(i,2)
            if (i_out == i1) then
                i_out = i2
            else if (i_out == i2) then
                i_out = i1
            end if
        end do
    end function flv_perm_apply_index

```

<FKS regions: sub interfaces>+≡

```

    elemental module function flv_perm_apply_ftuple &
        (perm, f_in) result (f_out)
        type(ftuple_t) :: f_out
        class(flv_perm_t), intent(in) :: perm
        type(ftuple_t), intent(in) :: f_in
    end function flv_perm_apply_ftuple

```

<FKS regions: procedures>+≡

```

    elemental module function flv_perm_apply_ftuple &
        (perm, f_in) result (f_out)
        type(ftuple_t) :: f_out
        class(flv_perm_t), intent(in) :: perm
        type(ftuple_t), intent(in) :: f_in
        integer :: i, i1, i2
        f_out = f_in

```

```

do i = size (perm%perms, dim = 1), 1, -1
  i1 = perm%perms(i,1)
  i2 = perm%perms(i,2)
  if (f_out%ireg(1) == i1) then
    f_out%ireg(1) = i2
  else if (f_out%ireg(1) == i2) then
    f_out%ireg(1) = i1
  end if
  if (f_out%ireg(2) == i1) then
    f_out%ireg(2) = i2
  else if (f_out%ireg(2) == i2) then
    f_out%ireg(2) = i1
  end if
end do
if (f_out%ireg(1) > f_out%ireg(2)) f_out%ireg = f_out%ireg([2,1])
end function flv_perm_apply_ftuple

```

(FKS regions: flavor permutation: TBP)+≡

```

procedure :: eqv => flv_perm_eqv

```

(FKS regions: sub interfaces)+≡

```

module function flv_perm_eqv &
  (perm, flv1, flv2, with_tag) result (valid)
  logical :: valid
  class(flv_perm_t), intent(in) :: perm
  type(flv_structure_t), intent(in) :: flv1, flv2
  logical, intent(in) :: with_tag
end function flv_perm_eqv

```

(FKS regions: procedures)+≡

```

module function flv_perm_eqv &
  (perm, flv1, flv2, with_tag) result (valid)
  logical :: valid
  class(flv_perm_t), intent(in) :: perm
  type(flv_structure_t), intent(in) :: flv1, flv2
  logical, intent(in) :: with_tag
  type(flv_structure_t) :: flv_tmp
  flv_tmp = perm%apply (flv2, invert = .true.)
  valid = all (flv_tmp%flst == flv1%flst)
  if (with_tag) valid = valid .and. all (flv_tmp%tag == flv1%tag)
  call flv_tmp%final ()
end function flv_perm_eqv

```

A singular region is a partition of phase space which is associated with an individual emitter and, if relevant, resonance. It is associated with an α_r - and resonance-index, with a real flavor structure and its underlying Born flavor structure. To compute the FKS weights, it is relevant to know all the other particle indices which can result in a divergent phase space configuration, which are collected in the `ftuples`-array.

Some singular regions might behave physically identical. E.g. a real flavor structure associated with three-jet production is $[11, -11, 2, -2, 21, 21]$. Here, there are two possible `ftuples` which contribute to the same $u \rightarrow ug$ splitting, namely $(3, 5)$ and $(3, 6)$. The resulting singular regions will be identical. To

avoid this, one singular region is associated with the multiplicity factor `mult`. When computing the subtraction terms for each singular region, the result is then simply multiplied by this factor.

The `double_fsr`-flag indicates whether the singular region should also be supplied by a symmetry factor, explained below.

```

(FKS regions: public)+≡
    public :: singular_region_t

(FKS regions: types)+≡
    type :: singular_region_t
        integer :: alr
        integer :: i_res
        type(flv_structure_t) :: flst_real
        type(flv_structure_t) :: flst_uborn
        integer :: mult
        integer :: emitter
        integer :: nregions
        integer :: real_index
        type(ftuple_t), dimension(:), allocatable :: ftuples
        integer :: uborn_index
        logical :: double_fsr = .false.
        logical :: soft_divergence = .false.
        logical :: coll_divergence = .false.
        type(string_t) :: nlo_correction_type
        integer, dimension(:), allocatable :: i_reg_to_i_con
        logical :: pseudo_isr = .false.
        logical :: sc_required = .false.
        integer :: eqv_index = 0
    contains
    (FKS regions: singular region: TBP)
    end type singular_region_t

(FKS regions: singular region: TBP)≡
    procedure :: init => singular_region_init

(FKS regions: sub interfaces)+≡
    module subroutine singular_region_init (sregion, alr, mult, i_res, &
        flst_real, flst_uborn, flv_born, emitter, ftuples, equivalences, &
        nlo_correction_type)
        class(singular_region_t), intent(out) :: sregion
        integer, intent(in) :: alr, mult, i_res
        type(flv_structure_t), intent(in) :: flst_real
        type(flv_structure_t), intent(in) :: flst_uborn
        type(flv_structure_t), dimension(:), intent(in) :: flv_born
        integer, intent(in) :: emitter
        type(ftuple_t), intent(inout), dimension(:) :: ftuples
        logical, intent(inout), dimension(:, :) :: equivalences
        type(string_t), intent(in) :: nlo_correction_type
    end subroutine singular_region_init

(FKS regions: procedures)+≡
    module subroutine singular_region_init (sregion, alr, mult, i_res, &
        flst_real, flst_uborn, flv_born, emitter, ftuples, equivalences, &
        nlo_correction_type)
        class(singular_region_t), intent(out) :: sregion

```



```

integer, intent(in) :: alr, mult, i_res
type(flv_structure_t), intent(in) :: flst_real
type(flv_structure_t), intent(in) :: flst_uborn
type(flv_structure_t), dimension(:), intent(in) :: flv_born
integer, intent(in) :: emitter
type(ftuple_t), intent(inout), dimension(:) :: ftuples
logical, intent(inout), dimension(:, :) :: equivalences
type(string_t), intent(in) :: nlo_correction_type
integer :: i
call debug_input_values ()
sregion%alr = alr
sregion%mult = mult
sregion%i_res = i_res
sregion%flst_real = flst_real
sregion%flst_uborn = flst_uborn
sregion%emitter = emitter
sregion%nlo_correction_type = nlo_correction_type
sregion%nregions = size (ftuples)
allocate (sregion%ftuples (sregion%nregions))
sregion%ftuples = ftuples
do i = 1, size(flv_born)
  if (flv_born(i) .equiv. sregion%flst_uborn) then
    sregion%uborn_index = i
    exit
  end if
end do
sregion%sc_required = any (sregion%flst_uborn%flst == GLUON) .or. &
  any (sregion%flst_uborn%flst == PHOTON)
contains
subroutine debug_input_values()
  if (debug_on) call msg_debug2 (D_SUBTRACTION, "singular_region_init")
  if (debug2_active (D_SUBTRACTION)) then
    print *, 'alr = ', alr
    print *, 'mult = ', mult
    print *, 'i_res = ', i_res
    call flst_real%write ()
    call flst_uborn%write ()
    print *, 'emitter = ', emitter
    call print_equivalence_matrix (ftuples, equivalences)
  end if
end subroutine debug_input_values
end subroutine singular_region_init

```

<FKS regions: singular region: TBP>+≡

procedure :: write => singular_region_write

<FKS regions: sub interfaces>+≡

```

module subroutine singular_region_write (sregion, unit, maxnregions)
  class(singular_region_t), intent(in) :: sregion
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: maxnregions
end subroutine singular_region_write

```

<FKS regions: procedures>+≡

```

module subroutine singular_region_write (sregion, unit, maxnregions)

```

```

class(singular_region_t), intent(in) :: sregion
integer, intent(in), optional :: unit
integer, intent(in), optional :: maxnregions
character(len=7), parameter :: flst_format = "(I3,A1)"
character(len=7), parameter :: ireg_space_format = "(7X,A1)"
integer :: nreal, nborn, i, u, mr
integer :: nleft, nright, nreg, nreg_diff
u = given_output_unit (unit); if (u < 0) return
mr = sregion%nregions; if (present (maxnregions)) mr = maxnregions
nreal = size (sregion%flst_real%flst)
nborn = size (sregion%flst_uborn%flst)
call write_vline (u)
write (u, '(A1)', advance = 'no') '['
do i = 1, nreal - 1
    write (u, flst_format, advance = 'no') sregion%flst_real%flst(i), ', '
end do
write (u, flst_format, advance = 'no') sregion%flst_real%flst(nreal), ']'
call write_vline (u)
write (u, '(I6)', advance = 'no') sregion%real_index
call write_vline (u)
write (u, '(I3)', advance = 'no') sregion%emitter
call write_vline (u)
write (u, '(I3)', advance = 'no') sregion%mult
call write_vline (u)
write (u, '(I4)', advance = 'no') sregion%nregions
call write_vline (u)
if (sregion%i_res > 0) then
    write (u, '(I3)', advance = 'no') sregion%i_res
    call write_vline (u)
end if
nreg = sregion%nregions
if (nreg == mr) then
    nleft = 0
    nright = 0
else
    nreg_diff = mr - nreg
    nleft = nreg_diff / 2
    if (mod(nreg_diff, 2) == 0) then
        nright = nleft
    else
        nright = nleft + 1
    end if
end if
if (nleft > 0) then
    do i = 1, nleft
        write(u, ireg_space_format, advance='no') ' '
    end do
end if
write (u, '(A)', advance = 'no') char (ftuple_string (sregion%ftuples, .false.))
call write_vline (u)
write (u, '(A1)', advance = 'no') '['
do i = 1, nborn - 1
    write(u, flst_format, advance = 'no') sregion%flst_uborn%flst(i), ', '
end do

```

```

write (u, flst_format, advance = 'no') sregion%flst_uborn%flst(nborn), ']'
call write_vline (u)
write (u, '(I7)', advance = 'no') sregion%uborn_index
call write_vline (u)
if (sregion%nlo_correction_type == "EW") then
  write (u, '(A3)', advance = 'no') 'ew'
else if (sregion%nlo_correction_type == "QCD") then
  write (u, '(A4)', advance = 'no') 'qcd'
else
  write (u, '(A5)', advance = 'no') 'none'
end if
write (u, '(A)')
end subroutine singular_region_write

```

<FKS regions: singular region: TBP>+≡

```

procedure :: write_latex => singular_region_write_latex

```

<FKS regions: sub interfaces>+≡

```

module subroutine singular_region_write_latex (region, unit)
  class(singular_region_t), intent(in) :: region
  integer, intent(in), optional :: unit
end subroutine singular_region_write_latex

```

<FKS regions: procedures>+≡

```

module subroutine singular_region_write_latex (region, unit)
  class(singular_region_t), intent(in) :: region
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(I2,A3,A,A3,I2,A3,I1,A3,I1,A3,A,A3,I2,A3,A,A3)" &
    region%alr, " & ", char (region%flst_real%to_string ()), &
    " & ", region%real_index, " & ", region%emitter, " & ", &
    region%mult, " & ", char (ftuple_string (region%ftuples, .true.)), &
    " & ", region%uborn_index, " & ", char (region%flst_uborn%to_string ()), &
    " \\")
end subroutine singular_region_write_latex

```

In case of a $g \rightarrow gg$ splitting, the factor

$$\frac{2E_{\text{em}}}{E_{\text{em}} + E_{\text{rad}}}$$

is multiplied to the real matrix element. This way, the symmetry of the splitting is used and only one singular region has to be taken into account. However, the factor ensures that there is only a soft singularity if the radiated parton becomes soft.

<FKS regions: singular region: TBP>+≡

```

procedure :: set_splitting_info => singular_region_set_splitting_info

```

<FKS regions: sub interfaces>+≡

```

module subroutine singular_region_set_splitting_info (region, n_in)
  class(singular_region_t), intent(inout) :: region
  integer, intent(in) :: n_in
end subroutine singular_region_set_splitting_info

```

<FKS regions: procedures>+≡

```

module subroutine singular_region_set_splitting_info (region, n_in)
  class(singular_region_t), intent(inout) :: region
  integer, intent(in) :: n_in
  integer :: i1, i2
  integer :: reg
  region%double_fsr = .false.
  region%soft_divergence = .false.
  associate (ftuple => region%ftuples)
    do reg = 1, region%nregions
      call ftuple(reg)%get (i1, i2)
      if (i1 /= region%emitter .or. i2 /= region%flst_real%nlegs) then
        cycle
      else
        if (ftuple(reg)%splitting_type == V_TO_VV .or. &
           ftuple(reg)%splitting_type == F_TO_FV ) then
          region%soft_divergence = .true.
        end if

        if (i1 == 0) then
          region%coll_divergence = &
            .not. all (region%flst_real%massive(1:n_in))
        else
          region%coll_divergence = .not. region%flst_real%massive(i1)
        end if

        if (ftuple(reg)%splitting_type == V_TO_VV) then
          if (all (ftuple(reg)%ireg > n_in)) &
            region%double_fsr = &
              all (is_gluon (region%flst_real%flst(ftuple(reg)%ireg)))
          exit
        else if (ftuple(reg)%splitting_type == UNDEFINED_SPLITTING) then
          call msg_fatal ("All splittings should be defined!")
        end if
      end if
    end do
    if (.not. region%soft_divergence .and. .not. region%coll_divergence) &
      call msg_fatal ("Singular region defined without divergence!")
  end associate
end subroutine singular_region_set_splitting_info

```

<FKS regions: singular region: TBP>+≡

```

procedure :: double_fsr_factor => singular_region_double_fsr_factor

```

<FKS regions: sub interfaces>+≡

```

module function singular_region_double_fsr_factor (region, p) result (val)
  class(singular_region_t), intent(in) :: region
  type(vector4_t), intent(in), dimension(:) :: p
  real(default) :: val
end function singular_region_double_fsr_factor

```

<FKS regions: procedures>+≡

```

module function singular_region_double_fsr_factor (region, p) result (val)
  class(singular_region_t), intent(in) :: region
  type(vector4_t), intent(in), dimension(:) :: p

```

```

real(default) :: val
real(default) :: E_rad, E_em
if (region%double_fsr) then
  E_em = energy (p(region%emitter))
  E_rad = energy (p(region%flst_real%nlegs))
  val = two * E_em / (E_em + E_rad)
else
  val = one
end if
end function singular_region_double_fsr_factor

```

(FKS regions: singular region: TBP)+≡
 procedure :: has_soft_divergence => singular_region_has_soft_divergence

(FKS regions: sub interfaces)+≡
 module function singular_region_has_soft_divergence (region) result (div)
 logical :: div
 class(singular_region_t), intent(in) :: region
 end function singular_region_has_soft_divergence

(FKS regions: procedures)+≡
 module function singular_region_has_soft_divergence (region) result (div)
 logical :: div
 class(singular_region_t), intent(in) :: region
 div = region%soft_divergence
 end function singular_region_has_soft_divergence

(FKS regions: singular region: TBP)+≡
 procedure :: has_collinear_divergence => &
 singular_region_has_collinear_divergence

(FKS regions: sub interfaces)+≡
 module function singular_region_has_collinear_divergence &
 (region) result (div)
 logical :: div
 class(singular_region_t), intent(in) :: region
 end function singular_region_has_collinear_divergence

(FKS regions: procedures)+≡
 module function singular_region_has_collinear_divergence &
 (region) result (div)
 logical :: div
 class(singular_region_t), intent(in) :: region
 div = region%coll_divergence
 end function singular_region_has_collinear_divergence

(FKS regions: singular region: TBP)+≡
 procedure :: has_identical_ftuples => singular_region_has_identical_ftuples

(FKS regions: sub interfaces)+≡
 elemental module function singular_region_has_identical_ftuples &
 (sregion) result (value)
 logical :: value
 class(singular_region_t), intent(in) :: sregion
 end function singular_region_has_identical_ftuples

```

(FKS regions: procedures)+≡
  elemental module function singular_region_has_identical_ftuples &
    (sregion) result (value)
    logical :: value
    class(singular_region_t), intent(in) :: sregion
    integer :: alr
    value = .false.
    do alr = 1, sregion%nregions
      value = value .or. (count (sregion%ftuples(alr) == sregion%ftuples) > 1)
    end do
  end function singular_region_has_identical_ftuples

```

```

(FKS regions: interfaces)+≡
  interface assignment(=)
    module procedure singular_region_assign
  end interface

```

```

(FKS regions: sub interfaces)+≡
  module subroutine singular_region_assign (reg_out, reg_in)
    type(singular_region_t), intent(out) :: reg_out
    type(singular_region_t), intent(in) :: reg_in
  end subroutine singular_region_assign

```

```

(FKS regions: procedures)+≡
  module subroutine singular_region_assign (reg_out, reg_in)
    type(singular_region_t), intent(out) :: reg_out
    type(singular_region_t), intent(in) :: reg_in
    reg_out%alr = reg_in%alr
    reg_out%i_res = reg_in%i_res
    reg_out%flst_real = reg_in%flst_real
    reg_out%flst_uborn = reg_in%flst_uborn
    reg_out%mult = reg_in%mult
    reg_out%emitter = reg_in%emitter
    reg_out%nregions = reg_in%nregions
    reg_out%real_index = reg_in%real_index
    reg_out%uborn_index = reg_in%uborn_index
    reg_out%double_fsr = reg_in%double_fsr
    reg_out%soft_divergence = reg_in%soft_divergence
    reg_out%coll_divergence = reg_in%coll_divergence
    reg_out%nlo_correction_type = reg_in%nlo_correction_type
    if (allocated (reg_in%ftuples)) then
      allocate (reg_out%ftuples (size (reg_in%ftuples)))
      reg_out%ftuples = reg_in%ftuples
    else
      call msg_bug ("singular_region_assign: Trying to copy a " // &
        "singular region without allocated ftuples!")
    end if
  end subroutine singular_region_assign

```

Two singular regions match if they would produce the same amplitude. For this we have to check that their real and underlying Born flavor structures are equivalent, as determined by the `prc_core`. However, since there are more aspects of a singular region that make it unique, we have to check other attributes as

well.

<FKS regions: interfaces>+≡

```
interface operator(.match.)
  module procedure singular_region_match
end interface
```

<FKS regions: sub interfaces>+≡

```
module function singular_region_match (reg1, reg2) result (match)
  type(singular_region_t), intent(in) :: reg1, reg2
  logical :: match
end function singular_region_match
```

<FKS regions: procedures>+≡

```
module function singular_region_match (reg1, reg2) result (match)
  type(singular_region_t), intent(in) :: reg1, reg2
  logical :: match
  match = all ([reg1%flst_real%eqv_index, reg2%flst_real%eqv_index] > 0)
  match = match .and. (reg1%flst_real%eqv_index == reg2%flst_real%eqv_index)
  match = match .and. (reg1%flst_uborn%eqv_index == reg2%flst_uborn%eqv_index)
  match = match .and. (reg1%mult == reg2%mult)
  match = match .and. (reg1%emitter == reg2%emitter)
  match = match .and. (reg1%nregions == reg2%nregions)
  match = match .and. (reg1%double_fsr .eqv. reg2%double_fsr)
  match = match .and. (reg1%soft_divergence .eqv. reg2%soft_divergence)
  match = match .and. (reg1%coll_divergence .eqv. reg2%coll_divergence)
  match = match .and. (char (reg1%nlo_correction_type) == char (reg2%nlo_correction_type))
  if (match) match = match .and. (all (reg1%ftuples == reg2%ftuples))
end function singular_region_match
```

<FKS regions: types>+≡

```
type :: resonance_mapping_t
  type(resonance_history_t), dimension(:), allocatable :: res_histories
  integer, dimension(:), allocatable :: alr_to_i_res
  integer, dimension(:, :), allocatable :: i_res_to_alr
  type(vector4_t), dimension(:), allocatable :: p_res
contains
  <FKS regions: resonance mapping: TBP>
end type resonance_mapping_t
```

Testing: Init resonance mapping for $\mu\mu b\bar{b}$ final state.

<FKS regions: resonance mapping: TBP>≡

```
procedure :: init => resonance_mapping_init
```

<FKS regions: sub interfaces>+≡

```
module subroutine resonance_mapping_init (res_map, res_hist)
  class(resonance_mapping_t), intent(inout) :: res_map
  type(resonance_history_t), intent(in), dimension(:) :: res_hist
end subroutine resonance_mapping_init
```

<FKS regions: procedures>+≡

```
module subroutine resonance_mapping_init (res_map, res_hist)
  class(resonance_mapping_t), intent(inout) :: res_map
  type(resonance_history_t), intent(in), dimension(:) :: res_hist
  integer :: n_hist, i_hist1, i_hist2, n_contributors
```

```

n_contributors = 0
n_hist = size (res_hist)
allocate (res_map%res_histories (n_hist))
do i_hist1 = 1, n_hist
  if (i_hist1 + 1 <= n_hist) then
    do i_hist2 = i_hist1 + 1, n_hist
      if (.not. (res_hist(i_hist1) .contains. res_hist(i_hist2))) &
        n_contributors = n_contributors + &
          res_hist(i_hist2)%n_resonances
    end do
  else
    n_contributors = n_contributors + res_hist(i_hist1)%n_resonances
  end if
end do
allocate (res_map%p_res (n_contributors))
res_map%res_histories = res_hist
res_map%p_res = vector4_null
end subroutine resonance_mapping_init

```

(FKS regions: resonance mapping: TBP)+≡

```

procedure :: set_alr_to_i_res => resonance_mapping_set_alr_to_i_res

```

(FKS regions: sub interfaces)+≡

```

module subroutine resonance_mapping_set_alr_to_i_res &
  (res_map, regions, alr_new_to_old)
  class(resonance_mapping_t), intent(inout) :: res_map
  type(singular_region_t), intent(in), dimension(:) :: regions
  integer, intent(out), dimension(:), allocatable :: alr_new_to_old
end subroutine resonance_mapping_set_alr_to_i_res

```

(FKS regions: procedures)+≡

```

module subroutine resonance_mapping_set_alr_to_i_res &
  (res_map, regions, alr_new_to_old)
  class(resonance_mapping_t), intent(inout) :: res_map
  type(singular_region_t), intent(in), dimension(:) :: regions
  integer, intent(out), dimension(:), allocatable :: alr_new_to_old
  integer :: alr, i_res
  integer :: alr_new, n_alr_res
  integer :: k
  if (debug_on) call msg_debug &
    (D_SUBTRACTION, "resonance_mapping_set_alr_to_i_res")
  n_alr_res = 0
  do alr = 1, size (regions)
    do i_res = 1, size (res_map%res_histories)
      if (res_map%res_histories(i_res)%contains_leg &
        (regions(alr)%emitter)) &
        n_alr_res = n_alr_res + 1
    end do
  end do

  allocate (res_map%alr_to_i_res (n_alr_res))
  allocate (res_map%i_res_to_alr (size (res_map%res_histories), 10))
  res_map%i_res_to_alr = 0
  allocate (alr_new_to_old (n_alr_res))
  alr_new = 1

```



```

do alr = 1, size (regions)
  do i_res = 1, size (res_map%res_histories)
    if (res_map%res_histories(i_res)%contains_leg &
        (regions(alr)%emitter)) then
      res_map%alr_to_i_res (alr_new) = i_res
      alr_new_to_old (alr_new) = alr
      alr_new = alr_new + 1
    end if
  end do
end do

do i_res = 1, size (res_map%res_histories)
  k = 1
  do alr = 1, size (regions)
    if (res_map%res_histories(i_res)%contains_leg &
        (regions(alr)%emitter)) then
      res_map%i_res_to_alr (i_res, k) = alr
      k = k + 1
    end if
  end do
end do
if (debug_active (D_SUBTRACTION)) then
  print *, 'i_res_to_alr:'
  do i_res = 1, size(res_map%i_res_to_alr, dim=1)
    print *, res_map%i_res_to_alr (i_res, :)
  end do
  print *, 'alr_new_to_old:', alr_new_to_old
end if
end subroutine resonance_mapping_set_alr_to_i_res

```

(FKS regions: resonance mapping: TBP)+≡
 procedure :: get_resonance_history => resonance_mapping_get_resonance_history

(FKS regions: sub interfaces)+≡
 module function resonance_mapping_get_resonance_history &
 (res_map, alr) result (res_hist)
 type(resonance_history_t) :: res_hist
 class(resonance_mapping_t), intent(in) :: res_map
 integer, intent(in) :: alr
 end function resonance_mapping_get_resonance_history

(FKS regions: procedures)+≡
 module function resonance_mapping_get_resonance_history &
 (res_map, alr) result (res_hist)
 type(resonance_history_t) :: res_hist
 class(resonance_mapping_t), intent(in) :: res_map
 integer, intent(in) :: alr
 res_hist = res_map%res_histories(res_map%alr_to_i_res (alr))
 end function resonance_mapping_get_resonance_history

(FKS regions: resonance mapping: TBP)+≡
 procedure :: write => resonance_mapping_write

```

<FKS regions: sub interfaces>+≡
    module subroutine resonance_mapping_write (res_map)
        class(resonance_mapping_t), intent(in) :: res_map
    end subroutine resonance_mapping_write

<FKS regions: procedures>+≡
    module subroutine resonance_mapping_write (res_map)
        class(resonance_mapping_t), intent(in) :: res_map
        integer :: i_res
        do i_res = 1, size (res_map%res_histories)
            call res_map%res_histories(i_res)%write ()
        end do
    end subroutine resonance_mapping_write

<FKS regions: resonance mapping: TBP>+≡
    procedure :: get_resonance_value => resonance_mapping_get_resonance_value

<FKS regions: sub interfaces>+≡
    module function resonance_mapping_get_resonance_value &
        (res_map, i_res, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: i_res
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: i_gluon
    end function resonance_mapping_get_resonance_value

<FKS regions: procedures>+≡
    module function resonance_mapping_get_resonance_value &
        (res_map, i_res, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: i_res
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: i_gluon
        p_map = res_map%res_histories(i_res)%mapping (p, i_gluon)
    end function resonance_mapping_get_resonance_value

<FKS regions: resonance mapping: TBP>+≡
    procedure :: get_resonance_all => resonance_mapping_get_resonance_all

<FKS regions: sub interfaces>+≡
    module function resonance_mapping_get_resonance_all &
        (res_map, alr, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: alr
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: i_gluon
    end function resonance_mapping_get_resonance_all

<FKS regions: procedures>+≡
    module function resonance_mapping_get_resonance_all &
        (res_map, alr, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map

```

```

integer, intent(in) :: alr
type(vector4_t), intent(in), dimension(:) :: p
integer, intent(in), optional :: i_gluon
integer :: i_res
p_map = zero
do i_res = 1, size (res_map%res_histories)
  associate (res => res_map%res_histories(i_res))
    if (any (res_map%i_res_to_alr (i_res, :) == alr)) &
      p_map = p_map + res%mapping (p, i_gluon)
  end associate
end do
end function resonance_mapping_get_resonance_all

```

(FKS regions: resonance mapping: TBP)+≡

```

procedure :: get_weight => resonance_mapping_get_weight

```

(FKS regions: sub interfaces)+≡

```

module function resonance_mapping_get_weight (res_map, alr, p) result (pfr)
  real(default) :: pfr
  class(resonance_mapping_t), intent(in) :: res_map
  integer, intent(in) :: alr
  type(vector4_t), intent(in), dimension(:) :: p
end function resonance_mapping_get_weight

```

(FKS regions: procedures)+≡

```

module function resonance_mapping_get_weight (res_map, alr, p) result (pfr)
  real(default) :: pfr
  class(resonance_mapping_t), intent(in) :: res_map
  integer, intent(in) :: alr
  type(vector4_t), intent(in), dimension(:) :: p
  real(default) :: sumpfr
  integer :: i_res
  sumpfr = zero
  do i_res = 1, size (res_map%res_histories)
    sumpfr = sumpfr + res_map%get_resonance_value (i_res, p)
  end do
  pfr = res_map%get_resonance_value (res_map%alr_to_i_res (alr), p) / sumpfr
end function resonance_mapping_get_weight

```

(FKS regions: resonance mapping: TBP)+≡

```

procedure :: get_resonance_alr => resonance_mapping_get_resonance_alr

```

(FKS regions: sub interfaces)+≡

```

module function resonance_mapping_get_resonance_alr &
  (res_map, alr, p, i_gluon) result (p_map)
  real(default) :: p_map
  class(resonance_mapping_t), intent(in) :: res_map
  integer, intent(in) :: alr
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), optional :: i_gluon
end function resonance_mapping_get_resonance_alr

```

(FKS regions: procedures)+≡

```

module function resonance_mapping_get_resonance_alr &
  (res_map, alr, p, i_gluon) result (p_map)

```

```

real(default) :: p_map
class(resonance_mapping_t), intent(in) :: res_map
integer, intent(in) :: alr
type(vector4_t), intent(in), dimension(:) :: p
integer, intent(in), optional :: i_gluon
integer :: i_res
i_res = res_map%alr_to_i_res (alr)
p_map = res_map%res_histories(i_res)%mapping (p, i_gluon)
end function resonance_mapping_get_resonance_alr

```

(FKS regions: interfaces)+≡

```

interface assignment(=)
  module procedure resonance_mapping_assign
end interface

```

(FKS regions: sub interfaces)+≡

```

module subroutine resonance_mapping_assign (res_map_out, res_map_in)
  type(resonance_mapping_t), intent(out) :: res_map_out
  type(resonance_mapping_t), intent(in) :: res_map_in
end subroutine resonance_mapping_assign

```

(FKS regions: procedures)+≡

```

module subroutine resonance_mapping_assign (res_map_out, res_map_in)
  type(resonance_mapping_t), intent(out) :: res_map_out
  type(resonance_mapping_t), intent(in) :: res_map_in
  if (allocated (res_map_in%res_histories)) then
    allocate (res_map_out%res_histories (size (res_map_in%res_histories)))
    res_map_out%res_histories = res_map_in%res_histories
  end if
  if (allocated (res_map_in%alr_to_i_res)) then
    allocate (res_map_out%alr_to_i_res (size (res_map_in%alr_to_i_res)))
    res_map_out%alr_to_i_res = res_map_in%alr_to_i_res
  end if
  if (allocated (res_map_in%i_res_to_alr)) then
    allocate (res_map_out%i_res_to_alr (size (res_map_in%i_res_to_alr, 1), &
      size (res_map_in%i_res_to_alr, 2)))
    res_map_out%i_res_to_alr = res_map_in%i_res_to_alr
  end if
  if (allocated (res_map_in%p_res)) then
    allocate (res_map_out%p_res (size (res_map_in%p_res)))
    res_map_out%p_res = res_map_in%p_res
  end if
end subroutine resonance_mapping_assign

```

Every FKS mapping should store the $\sum_{\alpha} d_{ij}^{-1}$ and $\sum_{\alpha} d_{ij,\text{soft}}^{-1}$. Also we keep the option open to use a normlization factor, which ensures $\sum_{\alpha} S_{\alpha} = 1$.

(FKS regions: types)+≡

```

type, abstract :: fks_mapping_t
  real(default) :: sumdi_j
  real(default) :: sumdi_j_soft
  logical :: pseudo_isr = .false.
  real(default) :: normalization_factor = one
contains

```

```

    <FKS regions: fks mapping: TBP>
    end type fks_mapping_t

<FKS regions: public>+≡
    public :: fks_mapping_default_t

<FKS regions: types>+≡
    type, extends (fks_mapping_t) :: fks_mapping_default_t
        real(default) :: exp_1, exp_2
        integer :: n_in
    contains
    <FKS regions: fks mapping default: TBP>
    end type fks_mapping_default_t

<FKS regions: public>+≡
    public :: fks_mapping_resonances_t

<FKS regions: types>+≡
    type, extends (fks_mapping_t) :: fks_mapping_resonances_t
        real(default) :: exp_1, exp_2
        type(resonance_mapping_t) :: res_map
        integer :: i_con = 0
    contains
    <FKS regions: fks mapping resonances: TBP>
    end type fks_mapping_resonances_t

<FKS regions: public>+≡
    public :: operator(.equiv.)
    public :: operator(.equivtag.)

<FKS regions: interfaces>+≡
    interface operator(.equiv.)
        module procedure flv_structure_equivalent_no_tag
    end interface

    interface operator(.equivtag.)
        module procedure flv_structure_equivalent_with_tag
    end interface

    interface assignment(=)
        module procedure flv_structure_assign_flv
        module procedure flv_structure_assign_integer
    end interface

<FKS regions: public>+≡
    public :: region_data_t

<FKS regions: types>+≡
    type :: region_data_t
        type(singular_region_t), dimension(:), allocatable :: regions
        type(flv_structure_t), dimension(:), allocatable :: flv_born
        type(flv_structure_t), dimension(:), allocatable :: flv_real
        integer, dimension(:), allocatable :: eqv_flv_index_born
        integer, dimension(:), allocatable :: eqv_flv_index_real

```

```

integer, dimension(:), allocatable :: emitters
integer :: n_regions = 0
integer :: n_emitters = 0
integer :: n_flv_born = 0
integer :: n_flv_real = 0
integer :: n_in = 0
integer :: n_legs_born = 0
integer :: n_legs_real = 0
integer :: n_phs = 0
integer :: alpha_power = 0
integer :: alphas_power = 0
type(string_t) :: nlo_correction_type
class(fks_mapping_t), allocatable :: fks_mapping
integer, dimension(:), allocatable :: resonances
type(resonance_contributors_t), dimension(:), allocatable :: alr_contributors
integer, dimension(:), allocatable :: alr_to_i_contributor
integer, dimension(:), allocatable :: i_phs_to_i_con
contains
<FKS regions: reg data: TBP>
end type region_data_t

```

Gfortran 7/8/9/ bug, has to remain in the main module:

```

<FKS regions: reg data: TBP>≡
  procedure :: allocate_fks_mappings => region_data_allocate_fks_mappings

<FKS regions: main procedures>≡
  subroutine region_data_allocate_fks_mappings (reg_data, mapping_type)
    class(region_data_t), intent(inout) :: reg_data
    integer, intent(in) :: mapping_type
    select case (mapping_type)
    case (FKS_DEFAULT)
      allocate (fks_mapping_default_t :: reg_data%fks_mapping)
    case (FKS_RESONANCES)
      allocate (fks_mapping_resonances_t :: reg_data%fks_mapping)
    case default
      call msg_fatal ("Init region_data: FKS mapping not implemented!")
    end select
  end subroutine region_data_allocate_fks_mappings

<FKS regions: reg data: TBP>+≡
  procedure :: init => region_data_init

<FKS regions: sub interfaces>+≡
  module subroutine region_data_init (reg_data, n_in, model, flavor_born, &
    flavor_real, nlo_correction_type, alpha_pow, alphas_pow)
    class(region_data_t), intent(out) :: reg_data
    integer, intent(in) :: n_in, alpha_pow, alphas_pow
    type(model_t), intent(in) :: model
    integer, intent(in), dimension(:, :) :: flavor_born, flavor_real
    type(string_t), intent(in) :: nlo_correction_type
  end subroutine region_data_init

<FKS regions: procedures>+≡
  module subroutine region_data_init (reg_data, n_in, model, flavor_born, &

```

```

        flavor_real, nlo_correction_type, alpha_pow, alphas_pow)
class(region_data_t), intent(out) :: reg_data
integer, intent(in) :: n_in, alpha_pow, alphas_pow
type(model_t), intent(in) :: model
integer, intent(in), dimension(:, :) :: flavor_born, flavor_real
type(string_t), intent(in) :: nlo_correction_type
integer, dimension(:, :), allocatable :: flv_real_tmp
type(ftuple_list_t), dimension(:), allocatable :: ftuples
integer, dimension(:), allocatable :: emitter
type(flv_structure_t), dimension(:), allocatable :: flst_alr
integer :: i, n_real
integer :: n_flv_real_before_check
reg_data%n_in = n_in
reg_data%alpha_power = alpha_pow
reg_data%alphas_power = alphas_pow
reg_data%n_flv_born = size (flavor_born, dim = 2)
reg_data%n_legs_born = size (flavor_born, dim = 1)
reg_data%n_legs_real = reg_data%n_legs_born + 1
reg_data%nlo_correction_type = nlo_correction_type
n_flv_real_before_check = size (flavor_real, dim = 2)
allocate (reg_data%flv_born (reg_data%n_flv_born))
allocate (flv_real_tmp (reg_data%n_legs_real, n_flv_real_before_check))
do i = 1, reg_data%n_flv_born
    call reg_data%flv_born(i)%init (flavor_born (:, i), n_in)
end do
n_real = 0
do i = 1, n_flv_real_before_check
    if (nlo_correction_type == "EW") then
        if (.not. (query_coupling_powers &
            (flavor_real (:, i), reg_data%alpha_power + 1, &
            reg_data%alphas_power))) cycle
    end if
    n_real = n_real + 1
    flv_real_tmp (:, n_real) = flavor_real (:, i)
end do
allocate (reg_data%flv_real (n_real))
do i = 1, n_real
    call reg_data%flv_real(i)%init (flv_real_tmp (:, i), n_in)
end do

call reg_data%find_regions (model, ftuples, emitter, flst_alr)
call reg_data%init_singular_regions (ftuples, emitter, &
    flst_alr, nlo_correction_type)
reg_data%n_flv_real = maxval (reg_data%regions%real_index)
call reg_data%find_emitters ()
call reg_data%set_mass_color_and_charge (model)
call reg_data%set_splitting_info ()
end subroutine region_data_init

```

<FKS regions: reg data: TBP>+≡

```

    procedure :: init_resonance_information => &
        region_data_init_resonance_information

```

<FKS regions: sub interfaces>+≡

```

        module subroutine region_data_init_resonance_information (reg_data)
            class(region_data_t), intent(inout) :: reg_data
            end subroutine region_data_init_resonance_information
    <FKS regions: procedures>+≡
    module subroutine region_data_init_resonance_information (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        call reg_data%enlarge_singular_regions_with_resonances ()
        call reg_data%find_resonances ()
    end subroutine region_data_init_resonance_information

    <FKS regions: reg data: TBP>+≡
    procedure :: set_resonance_mappings => region_data_set_resonance_mappings

    <FKS regions: sub interfaces>+≡
    module subroutine region_data_set_resonance_mappings &
        (reg_data, resonance_histories)
        class(region_data_t), intent(inout) :: reg_data
        type(resonance_history_t), intent(in), dimension(:) :: resonance_histories
    end subroutine region_data_set_resonance_mappings

    <FKS regions: procedures>+≡
    module subroutine region_data_set_resonance_mappings &
        (reg_data, resonance_histories)
        class(region_data_t), intent(inout) :: reg_data
        type(resonance_history_t), intent(in), dimension(:) :: resonance_histories
        select type (map => reg_data%fks_mapping)
            type is (fks_mapping_resonances_t)
                call map%res_map%init (resonance_histories)
            end select
    end subroutine region_data_set_resonance_mappings

    <FKS regions: reg data: TBP>+≡
    procedure :: setup_fks_mappings => region_data_setup_fks_mappings

    <FKS regions: sub interfaces>+≡
    module subroutine region_data_setup_fks_mappings (reg_data, template, n_in)
        class(region_data_t), intent(inout) :: reg_data
        type(fks_template_t), intent(in) :: template
        integer, intent(in) :: n_in
    end subroutine region_data_setup_fks_mappings

    <FKS regions: procedures>+≡
    module subroutine region_data_setup_fks_mappings (reg_data, template, n_in)
        class(region_data_t), intent(inout) :: reg_data
        type(fks_template_t), intent(in) :: template
        integer, intent(in) :: n_in
        call reg_data%allocate_fks_mappings (template%mapping_type)
        select type (map => reg_data%fks_mapping)
            type is (fks_mapping_default_t)
                call map%set_parameter (n_in, template%fks_dij_exp1, &
                    template%fks_dij_exp2)
            end select
    end subroutine region_data_setup_fks_mappings

```


So far, we have only created singular regions for a non-resonant case. When resonance mappings are required, we have more singular regions, since they must now be identified by their emitter-resonance pair index, where the emitter must be compatible with the resonance.

```

(FKS regions: reg data: TBP)+≡
  procedure :: enlarge_singular_regions_with_resonances &
    => region_data_enlarge_singular_regions_with_resonances

(FKS regions: sub interfaces)+≡
  module subroutine region_data_enlarge_singular_regions_with_resonances &
    (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    end subroutine region_data_enlarge_singular_regions_with_resonances

(FKS regions: procedures)+≡
  module subroutine region_data_enlarge_singular_regions_with_resonances &
    (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr
    integer, dimension(:), allocatable :: alr_new_to_old
    integer :: n_alr_new
    type(singular_region_t), dimension(:), allocatable :: save_regions
    if (debug_on) call msg_debug &
      (D_SUBTRACTION, "region_data_enlarge_singular_regions_with_resonances")
    call debug_input_values ()
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_default_t)
      return
    type is (fks_mapping_resonances_t)
      allocate (save_regions (reg_data%n_regions))
      do alr = 1, reg_data%n_regions
        save_regions(alr) = reg_data%regions(alr)
      end do

      associate (res_map => fks_mapping%res_map)
        call res_map%set_alr_to_i_res (reg_data%regions, alr_new_to_old)
        deallocate (reg_data%regions)
        n_alr_new = size (alr_new_to_old)
        reg_data%n_regions = n_alr_new
        allocate (reg_data%regions (n_alr_new))
        do alr = 1, n_alr_new
          reg_data%regions(alr) = save_regions(alr_new_to_old (alr))
          reg_data%regions(alr)%i_res = res_map%alr_to_i_res (alr)
        end do
      end associate
    end select

contains

  subroutine debug_input_values ()
    if (debug2_active (D_SUBTRACTION)) then
      call reg_data%write ()
    end if
  end subroutine debug_input_values

```

```

end subroutine region_data_enlarge_singular_regions_with_resonances

<FKS regions: reg data: TBP>+≡
  procedure :: set_isr_pseudo_regions => region_data_set_isr_pseudo_regions

<FKS regions: sub interfaces>+≡
  module subroutine region_data_set_isr_pseudo_regions (reg_data)
    class(region_data_t), intent(inout) :: reg_data
  end subroutine region_data_set_isr_pseudo_regions

<FKS regions: procedures>+≡
  module subroutine region_data_set_isr_pseudo_regions (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr
    integer :: n_alr_new
    !!! Subroutine called for threshold factorization ->
    !!! Size of singular regions at this point is fixed
    type(singular_region_t), dimension(2) :: save_regions
    integer, dimension(4) :: alr_new_to_old
    do alr = 1, reg_data%n_regions
      save_regions(alr) = reg_data%regions(alr)
    end do
    n_alr_new = reg_data%n_regions * 2
    alr_new_to_old = [1, 1, 2, 2]
    deallocate (reg_data%regions)
    allocate (reg_data%regions (n_alr_new))
    reg_data%n_regions = n_alr_new
    do alr = 1, n_alr_new
      reg_data%regions(alr) = save_regions(alr_new_to_old (alr))
      call add_pseudo_emitters (reg_data%regions(alr))
      if (mod (alr, 2) == 0) reg_data%regions(alr)%pseudo_isr = .true.
    end do
  contains
    subroutine add_pseudo_emitters (sregion)
      type(singular_region_t), intent(inout) :: sregion
      type(ftuple_t), dimension(2) :: ftuples_save
      integer :: alr
      do alr = 1, 2
        ftuples_save(alr) = sregion%ftuples(alr)
      end do
      deallocate (sregion%ftuples)
      sregion%nregions = sregion%nregions * 2
      allocate (sregion%ftuples (sregion%nregions))
      do alr = 1, sregion%nregions
        sregion%ftuples(alr) = ftuples_save (alr_new_to_old(alr))
        if (mod (alr, 2) == 0) sregion%ftuples(alr)%pseudo_isr = .true.
      end do
    end subroutine add_pseudo_emitters
  end subroutine region_data_set_isr_pseudo_regions

```

This subroutine splits up the ftuple-list of the singular regions into interference-free lists, i.e. lists which only contain the same emitter. This is relevant for factorized NLO calculations. In the current implementation, it is hand-tailored

for the threshold computation, but should be generalized further in the future.

```

(FKS regions: reg data: TBP)+≡
  procedure :: split_up_interference_regions_for_threshold => &
    region_data_split_up_interference_regions_for_threshold

(FKS regions: sub interfaces)+≡
  module subroutine region_data_split_up_interference_regions_for_threshold &
    (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    end subroutine region_data_split_up_interference_regions_for_threshold

(FKS regions: procedures)+≡
  module subroutine region_data_split_up_interference_regions_for_threshold &
    (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr, i_ftuple
    integer :: current_emitter
    integer :: i1, i2
    integer :: n_new_reg
    type(ftuple_t), dimension(2) :: ftuples
    do alr = 1, reg_data%n_regions
      associate (region => reg_data%regions(alr))
        current_emitter = region%emitter
        n_new_reg = 0
        do i_ftuple = 1, region%nregions
          call region%ftuples(i_ftuple)%get (i1, i2)
          if (i1 == current_emitter) then
            n_new_reg = n_new_reg + 1
            ftuples(n_new_reg) = region%ftuples(i_ftuple)
          end if
        end do
        deallocate (region%ftuples)
        allocate (region%ftuples(n_new_reg))
        region%ftuples = ftuples (1 : n_new_reg)
        region%nregions = n_new_reg
      end associate
    end do
    reg_data%fks_mapping%normalization_factor = 0.5_default
  end subroutine region_data_split_up_interference_regions_for_threshold

(FKS regions: reg data: TBP)+≡
  procedure :: set_mass_color_and_charge => &
    region_data_set_mass_color_and_charge

(FKS regions: sub interfaces)+≡
  module subroutine region_data_set_mass_color_and_charge (reg_data, model)
    class(region_data_t), intent(inout) :: reg_data
    type(model_t), intent(in) :: model
    end subroutine region_data_set_mass_color_and_charge

(FKS regions: procedures)+≡
  module subroutine region_data_set_mass_color_and_charge (reg_data, model)
    class(region_data_t), intent(inout) :: reg_data
    type(model_t), intent(in) :: model
    integer :: i
    do i = 1, reg_data%n_regions

```

```

        associate (region => reg_data%regions(i))
            call region%flst_uborn%init_mass_color_and_charge (model)
            call region%flst_real%init_mass_color_and_charge (model)
        end associate
    end do
do i = 1, reg_data%n_flv_born
    call reg_data%flv_born(i)%init_mass_color_and_charge (model)
end do
do i = 1, size (reg_data%flv_real)
    call reg_data%flv_real(i)%init_mass_color_and_charge (model)
end do
end subroutine region_data_set_mass_color_and_charge

```

<FKS regions: reg data: TBP>+≡

```

    procedure :: uses_resonances => region_data_uses_resonances

```

<FKS regions: sub interfaces>+≡

```

    module function region_data_uses_resonances (reg_data) result (val)
        logical :: val
        class(region_data_t), intent(in) :: reg_data
    end function region_data_uses_resonances

```

<FKS regions: procedures>+≡

```

    module function region_data_uses_resonances (reg_data) result (val)
        logical :: val
        class(region_data_t), intent(in) :: reg_data
        select type (fks_mapping => reg_data%fks_mapping)
            type is (fks_mapping_resonances_t)
                val = .true.
            class default
                val = .false.
        end select
    end function region_data_uses_resonances

```

Creates a list containing the emitter of each singular region.

<FKS regions: reg data: TBP>+≡

```

    procedure :: get_emitter_list => region_data_get_emitter_list

```

<FKS regions: sub interfaces>+≡

```

    pure module function region_data_get_emitter_list &
        (reg_data) result (emitters)
        class(region_data_t), intent(in) :: reg_data
        integer, dimension(:), allocatable :: emitters
    end function region_data_get_emitter_list

```

<FKS regions: procedures>+≡

```

    pure module function region_data_get_emitter_list (reg_data) result (emitters)
        class(region_data_t), intent(in) :: reg_data
        integer, dimension(:), allocatable :: emitters
        integer :: i
        allocate (emitters (reg_data%n_regions))
        do i = 1, reg_data%n_regions
            emitters(i) = reg_data%regions(i)%emitter
        end do
    end function region_data_get_emitter_list

```

Returns the number of emitters not equal to 0 to avoid double counting between emitters 0, 1 and 2.

```
<FKS regions: reg data: TBP>+≡
  procedure :: get_n_emitters_sc => region_data_get_n_emitters_sc
```

```
<FKS regions: sub interfaces>+≡
  module function region_data_get_n_emitters_sc &
    (reg_data) result (n_emitters_sc)
    class(region_data_t), intent(in) :: reg_data
    integer :: n_emitters_sc
  end function region_data_get_n_emitters_sc
```

```
<FKS regions: procedures>+≡
  module function region_data_get_n_emitters_sc &
    (reg_data) result (n_emitters_sc)
    class(region_data_t), intent(in) :: reg_data
    integer :: n_emitters_sc
    n_emitters_sc = count (reg_data%emitters /= 0)
  end function region_data_get_n_emitters_sc
```

```
<FKS regions: reg data: TBP>+≡
  procedure :: get_associated_resonances => &
    region_data_get_associated_resonances
```

```
<FKS regions: sub interfaces>+≡
  module function region_data_get_associated_resonances &
    (reg_data, emitter) result (res)
    integer, dimension(:), allocatable :: res
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: emitter
  end function region_data_get_associated_resonances
```

```
<FKS regions: procedures>+≡
  module function region_data_get_associated_resonances &
    (reg_data, emitter) result (res)
    integer, dimension(:), allocatable :: res
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: emitter
    integer :: alr, i
    integer :: n_res
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
      n_res = 0

      do alr = 1, reg_data%n_regions
        if (reg_data%regions(alr)%emitter == emitter) &
          n_res = n_res + 1
      end do

      if (n_res > 0) then
        allocate (res (n_res))
      else
        return
      end if
      i = 1
```

```

        do alr = 1, reg_data%n_regions
            if (reg_data%regions(alr)%emitter == emitter) then
                res (i) = fks_mapping%res_map%alr_to_i_res (alr)
                i = i + 1
            end if
        end do
    end select
end function region_data_get_associated_resonances

(FKS regions: reg data: TBP)+≡
    procedure :: emitter_is_compatible_with_resonance => &
        region_data_emitter_is_compatible_with_resonance

(FKS regions: sub interfaces)+≡
    module function region_data_emitter_is_compatible_with_resonance &
        (reg_data, i_res, emitter) result (compatible)
        logical :: compatible
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_res, emitter
    end function region_data_emitter_is_compatible_with_resonance

(FKS regions: procedures)+≡
    module function region_data_emitter_is_compatible_with_resonance &
        (reg_data, i_res, emitter) result (compatible)
        logical :: compatible
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_res, emitter
        integer :: i_res_alr, alr
        compatible = .false.
        select type (fks_mapping => reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            do alr = 1, reg_data%n_regions
                i_res_alr = fks_mapping%res_map%alr_to_i_res (alr)
                if (i_res_alr == i_res .and. reg_data%get_emitter(alr) == emitter) then
                    compatible = .true.
                    exit
                end if
            end do
        end select
    end function region_data_emitter_is_compatible_with_resonance

(FKS regions: reg data: TBP)+≡
    procedure :: emitter_is_in_resonance => region_data_emitter_is_in_resonance

(FKS regions: sub interfaces)+≡
    module function region_data_emitter_is_in_resonance &
        (reg_data, i_res, emitter) result (exist)
        logical :: exist
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_res, emitter
    end function region_data_emitter_is_in_resonance

(FKS regions: procedures)+≡
    module function region_data_emitter_is_in_resonance &

```

```

        (reg_data, i_res, emitter) result (exist)
logical :: exist
class(region_data_t), intent(in) :: reg_data
integer, intent(in) :: i_res, emitter
integer :: i
exist = .false.
select type (fks_mapping => reg_data%fks_mapping)
type is (fks_mapping_resonances_t)
    associate (res_history => fks_mapping%res_map%res_histories(i_res))
        do i = 1, res_history%n_resonances
            exist = exist .or. &
                any (res_history%resonances(i)%contributors%c == emitter)
        end do
    end associate
end select
end function region_data_emitter_is_in_resonance

```

(FKS regions: reg data: TBP)+≡

```

procedure :: get_contributors => region_data_get_contributors

```

(FKS regions: sub interfaces)+≡

```

module subroutine region_data_get_contributors &
    (reg_data, i_res, emitter, c, success)
class(region_data_t), intent(in) :: reg_data
integer, intent(in) :: i_res, emitter
integer, intent(inout), dimension(:), allocatable :: c
logical, intent(out) :: success
end subroutine region_data_get_contributors

```

(FKS regions: procedures)+≡

```

module subroutine region_data_get_contributors &
    (reg_data, i_res, emitter, c, success)
class(region_data_t), intent(in) :: reg_data
integer, intent(in) :: i_res, emitter
integer, intent(inout), dimension(:), allocatable :: c
logical, intent(out) :: success
integer :: i
success = .false.
select type (fks_mapping => reg_data%fks_mapping)
type is (fks_mapping_resonances_t)
    associate (res_history => fks_mapping%res_map%res_histories (i_res))
        do i = 1, res_history%n_resonances
            if (any (res_history%resonances(i)%contributors%c == emitter)) then
                allocate (c (size (res_history%resonances(i)%contributors%c)))
                c = res_history%resonances(i)%contributors%c
                success = .true.
                exit
            end if
        end do
    end associate
end select
end subroutine region_data_get_contributors

```

(FKS regions: reg data: TBP)+≡

```

procedure :: get_emitter => region_data_get_emitter

```

```

(FKS regions: sub interfaces)+≡
    pure module function region_data_get_emitter &
        (reg_data, alr) result (emitter)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: alr
        integer :: emitter
    end function region_data_get_emitter

(FKS regions: procedures)+≡
    pure module function region_data_get_emitter (reg_data, alr) result (emitter)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: alr
        integer :: emitter
        emitter = reg_data%regions(alr)%emitter
    end function region_data_get_emitter

(FKS regions: reg data: TBP)+≡
    procedure :: map_real_to_born_index => region_data_map_real_to_born_index

(FKS regions: sub interfaces)+≡
    module function region_data_map_real_to_born_index &
        (reg_data, real_index) result (uborn_index)
        integer :: uborn_index
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: real_index
    end function region_data_map_real_to_born_index

(FKS regions: procedures)+≡
    module function region_data_map_real_to_born_index &
        (reg_data, real_index) result (uborn_index)
        integer :: uborn_index
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: real_index
        integer :: alr
        uborn_index = 0
        do alr = 1, size (reg_data%regions)
            if (reg_data%regions(alr)%real_index == real_index) then
                uborn_index = reg_data%regions(alr)%uborn_index
                exit
            end if
        end do
    end function region_data_map_real_to_born_index

(FKS regions: reg data: TBP)+≡
    generic :: get_flv_states_born => get_flv_states_born_single, &
        get_flv_states_born_array
    procedure :: get_flv_states_born_single => &
        region_data_get_flv_states_born_single
    procedure :: get_flv_states_born_array => &
        region_data_get_flv_states_born_array

(FKS regions: sub interfaces)+≡
    module function region_data_get_flv_states_born_array &
        (reg_data) result (flv_states)
        integer, dimension(:,:), allocatable :: flv_states

```



```

        class(region_data_t), intent(in) :: reg_data
    end function region_data_get_flv_states_born_array
    module function region_data_get_flv_states_born_single &
        (reg_data, i_flv) result (flv_states)
        integer, dimension(:), allocatable :: flv_states
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_flv
    end function region_data_get_flv_states_born_single
<FKS regions: procedures>+=
    module function region_data_get_flv_states_born_array &
        (reg_data) result (flv_states)
        integer, dimension(:,:), allocatable :: flv_states
        class(region_data_t), intent(in) :: reg_data
        integer :: i_flv
        allocate (flv_states (reg_data%n_legs_born, reg_data%n_flv_born))
        do i_flv = 1, reg_data%n_flv_born
            flv_states(:, i_flv) = reg_data%flv_born(i_flv)%flst
        end do
    end function region_data_get_flv_states_born_array

    module function region_data_get_flv_states_born_single &
        (reg_data, i_flv) result (flv_states)
        integer, dimension(:), allocatable :: flv_states
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_flv
        allocate (flv_states (reg_data%n_legs_born))
        flv_states = reg_data%flv_born(i_flv)%flst
    end function region_data_get_flv_states_born_single

<FKS regions: reg data: TBP>+=
    generic :: get_flv_states_real => &
        get_flv_states_real_single, get_flv_states_real_array
    procedure :: get_flv_states_real_single => &
        region_data_get_flv_states_real_single
    procedure :: get_flv_states_real_array => &
        region_data_get_flv_states_real_array

<FKS regions: sub interfaces>+=
    module function region_data_get_flv_states_real_single &
        (reg_data, i_flv) result (flv_states)
        integer, dimension(:), allocatable :: flv_states
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_flv
    end function region_data_get_flv_states_real_single
    module function region_data_get_flv_states_real_array &
        (reg_data) result (flv_states)
        integer, dimension(:,:), allocatable :: flv_states
        class(region_data_t), intent(in) :: reg_data
    end function region_data_get_flv_states_real_array

<FKS regions: procedures>+=
    module function region_data_get_flv_states_real_single &
        (reg_data, i_flv) result (flv_states)
        integer, dimension(:), allocatable :: flv_states

```

```

class(region_data_t), intent(in) :: reg_data
integer, intent(in) :: i_flv
integer :: i_reg
allocate (flv_states (reg_data%n_legs_real))
do i_reg = 1, reg_data%n_regions
  if (i_flv == reg_data%regions(i_reg)%real_index) then
    flv_states = reg_data%regions(i_reg)%flst_real%flst
    exit
  end if
end do
end function region_data_get_flv_states_real_single

module function region_data_get_flv_states_real_array &
  (reg_data) result (flv_states)
  integer, dimension(:,:), allocatable :: flv_states
  class(region_data_t), intent(in) :: reg_data
  integer :: i_flv
  allocate (flv_states (reg_data%n_legs_real, reg_data%n_flv_real))
  do i_flv = 1, reg_data%n_flv_real
    flv_states (:, i_flv) = reg_data%get_flv_states_real (i_flv)
  end do
end function region_data_get_flv_states_real_array

<FKS regions: reg data: TBP>+≡
  procedure :: get_all_flv_states => region_data_get_all_flv_states

<FKS regions: sub interfaces>+≡
  module subroutine region_data_get_all_flv_states &
    (reg_data, flv_born, flv_real)
    class(region_data_t), intent(in) :: reg_data
    integer, dimension(:,:), allocatable, intent(out) :: flv_born, flv_real
  end subroutine region_data_get_all_flv_states

<FKS regions: procedures>+≡
  module subroutine region_data_get_all_flv_states &
    (reg_data, flv_born, flv_real)
    class(region_data_t), intent(in) :: reg_data
    integer, dimension(:,:), allocatable, intent(out) :: flv_born, flv_real
    allocate (flv_born (reg_data%n_legs_born, reg_data%n_flv_born))
    flv_born = reg_data%get_flv_states_born ()
    allocate (flv_real (reg_data%n_legs_real, reg_data%n_flv_real))
    flv_real = reg_data%get_flv_states_real ()
  end subroutine region_data_get_all_flv_states

<FKS regions: reg data: TBP>+≡
  procedure :: get_n_in => region_data_get_n_in

<FKS regions: sub interfaces>+≡
  module function region_data_get_n_in (reg_data) result (n_in)
    integer :: n_in
    class(region_data_t), intent(in) :: reg_data
  end function region_data_get_n_in

<FKS regions: procedures>+≡
  module function region_data_get_n_in (reg_data) result (n_in)

```

```

integer :: n_in
class(region_data_t), intent(in) :: reg_data
n_in = reg_data%n_in
end function region_data_get_n_in

<FKS regions: reg data: TBP>+≡
  procedure :: get_n_legs_real => region_data_get_n_legs_real

<FKS regions: sub interfaces>+≡
  module function region_data_get_n_legs_real (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
  end function region_data_get_n_legs_real

<FKS regions: procedures>+≡
  module function region_data_get_n_legs_real (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
    n_legs = reg_data%n_legs_real
  end function region_data_get_n_legs_real

<FKS regions: reg data: TBP>+≡
  procedure :: get_n_legs_born => region_data_get_n_legs_born

<FKS regions: sub interfaces>+≡
  module function region_data_get_n_legs_born (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
  end function region_data_get_n_legs_born

<FKS regions: procedures>+≡
  module function region_data_get_n_legs_born (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
    n_legs = reg_data%n_legs_born
  end function region_data_get_n_legs_born

<FKS regions: reg data: TBP>+≡
  procedure :: get_n_flv_real => region_data_get_n_flv_real

<FKS regions: sub interfaces>+≡
  module function region_data_get_n_flv_real (reg_data) result (n_flv)
    integer :: n_flv
    class(region_data_t), intent(in) :: reg_data
  end function region_data_get_n_flv_real

<FKS regions: procedures>+≡
  module function region_data_get_n_flv_real (reg_data) result (n_flv)
    integer :: n_flv
    class(region_data_t), intent(in) :: reg_data
    n_flv = reg_data%n_flv_real
  end function region_data_get_n_flv_real

<FKS regions: reg data: TBP>+≡
  procedure :: get_n_flv_born => region_data_get_n_flv_born

```

```

(FKS regions: sub interfaces)+≡
  module function region_data_get_n_flv_born (reg_data) result (n_flv)
    integer :: n_flv
    class(region_data_t), intent(in) :: reg_data
  end function region_data_get_n_flv_born

```

```

(FKS regions: procedures)+≡
  module function region_data_get_n_flv_born (reg_data) result (n_flv)
    integer :: n_flv
    class(region_data_t), intent(in) :: reg_data
    n_flv = reg_data%n_flv_born
  end function region_data_get_n_flv_born

```

Returns $S_i = \frac{1}{\mathcal{D}_{d_i}}$ or $S_{ij} = \frac{1}{\mathcal{D}_{d_{ij}}}$ for one particular singular region. At this point, the flavor array should be rearranged in such a way that the emitted particle is at the last position of the flavor structure list.

```

(FKS regions: reg data: TBP)+≡
  generic :: get_svalue => get_svalue_last_pos, get_svalue_ij
  procedure :: get_svalue_last_pos => region_data_get_svalue_last_pos
  procedure :: get_svalue_ij => region_data_get_svalue_ij

```

```

(FKS regions: sub interfaces)+≡
  module function region_data_get_svalue_ij &
    (reg_data, p_real, alr, i, j, i_res) result (sval)
    class(region_data_t), intent(inout) :: reg_data
    type(vector4_t), intent(in), dimension(:) :: p_real
    integer, intent(in) :: alr, i, j
    integer, intent(in) :: i_res
    real(default) :: sval
  end function region_data_get_svalue_ij
  module function region_data_get_svalue_last_pos &
    (reg_data, p, alr, emitter, i_res) result (sval)
    class(region_data_t), intent(inout) :: reg_data
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: alr, emitter
    integer, intent(in) :: i_res
    real(default) :: sval
  end function region_data_get_svalue_last_pos

```

```

(FKS regions: procedures)+≡
  module function region_data_get_svalue_ij &
    (reg_data, p_real, alr, i, j, i_res) result (sval)
    class(region_data_t), intent(inout) :: reg_data
    type(vector4_t), intent(in), dimension(:) :: p_real
    integer, intent(in) :: alr, i, j
    integer, intent(in) :: i_res
    real(default) :: sval
    associate (map => reg_data%fks_mapping)
      call map%compute_sumdij (reg_data%regions(alr), p_real)
      select type (map)
        type is (fks_mapping_resonances_t)
          map%i_con = reg_data%alr_to_i_contributor (alr)
        end select
      map%pseudo_isr = reg_data%regions(alr)%pseudo_isr
      sval = map%svalue (p_real, i, j, i_res) * map%normalization_factor
    end associate
  end function region_data_get_svalue_ij

```

```

end associate
end function region_data_get_svalue_ij

module function region_data_get_svalue_last_pos &
  (reg_data, p, alr, emitter, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: alr, emitter
  integer, intent(in) :: i_res
  real(default) :: sval
  sval = reg_data%get_svalue (p, alr, emitter, reg_data%n_legs_real, i_res)
end function region_data_get_svalue_last_pos

```

The same as above, but for the soft limit.

(FKS regions: reg data: TBP)+≡

```

procedure :: get_svalue_soft => region_data_get_svalue_soft

```

(FKS regions: sub interfaces)+≡

```

module function region_data_get_svalue_soft &
  (reg_data, p_born, p_soft, alr, emitter, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p_born
  type(vector4_t), intent(in) :: p_soft
  integer, intent(in) :: alr, emitter, i_res
  real(default) :: sval
end function region_data_get_svalue_soft

```

(FKS regions: procedures)+≡

```

module function region_data_get_svalue_soft &
  (reg_data, p_born, p_soft, alr, emitter, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p_born
  type(vector4_t), intent(in) :: p_soft
  integer, intent(in) :: alr, emitter, i_res
  real(default) :: sval
  associate (map => reg_data%fks_mapping)
    call map%compute_sumdij_soft (reg_data%regions(alr), p_born, p_soft)
    select type (map)
      type is (fks_mapping_resonances_t)
        map%i_con = reg_data%alr_to_i_contributor (alr)
      end select
    map%pseudo_isr = reg_data%regions(alr)%pseudo_isr
    sval = map%svalue_soft (p_born, p_soft, emitter, i_res) * &
      map%normalization_factor
  end associate
end function region_data_get_svalue_soft

```

This subroutine starts with a specification of N - and $N + 1$ -particle configurations, `flst_born` and `flst_real`, saved in `reg_data`. From these, it creates a list of fundamental tuples, a list of emitters and a list containing the $N + 1$ -particle configuration, rearranged in such a way that the emitter-radiation pair is last (`flst_alr`). For the $e^+ e^- \rightarrow u \bar{u} g$ - example, the generated objects are shown in table 27.2. Note that at this point, `flst_alr` is arranged in such a way that the emitter can only be equal to $n_{legs} - 1$ for final-state radiation or 0, 1,

or 2 for initial-state radiation. Further, it occurs that regions can be equivalent. For example in table 27.2 the regions corresponding to $\text{alr} = 1$ and $\text{alr} = 3$ as well as $\text{alr} = 2$ and $\text{alr} = 4$ describe the same physics and are therefore equivalent.

```

(FKS regions: reg data: TBP)+≡
  procedure :: find_regions => region_data_find_regions

(FKS regions: sub interfaces)+≡
  module subroutine region_data_find_regions &
    (reg_data, model, ftuples, emitters, flst_alr)
    class(region_data_t), intent(in) :: reg_data
    type(model_t), intent(in) :: model
    type(ftuple_list_t), intent(out), dimension(:), allocatable :: ftuples
    integer, intent(out), dimension(:), allocatable :: emitters
    type(flv_structure_t), intent(out), dimension(:), allocatable :: flst_alr
  end subroutine region_data_find_regions

(FKS regions: procedures)+≡
  module subroutine region_data_find_regions &
    (reg_data, model, ftuples, emitters, flst_alr)
    class(region_data_t), intent(in) :: reg_data
    type(model_t), intent(in) :: model
    type(ftuple_list_t), intent(out), dimension(:), allocatable :: ftuples
    integer, intent(out), dimension(:), allocatable :: emitters
    type(flv_structure_t), intent(out), dimension(:), allocatable :: flst_alr
    type(ftuple_list_t), dimension(:,:), allocatable :: ftuples_tmp
    integer, dimension(:,:), allocatable :: ftuple_index
    integer :: n_born, n_real
    integer :: n_legreal
    integer :: i_born, i_real, i_ftuple
    integer :: last_registered_i_born, last_registered_i_real

    n_born = size (reg_data%flv_born)
    n_real = size (reg_data%flv_real)
    n_legreal = size (reg_data%flv_real(1)%flst)
    allocate (emitters (0))
    allocate (flst_alr (0))
    allocate (ftuples (0))
    i_ftuple = 0
    last_registered_i_born = 0; last_registered_i_real = 0

    do i_real = 1, n_real
      do i_born = 1, n_born
        call setup_flsts_emitters_and_ftuples_fsr &
          (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
        call setup_flsts_emitters_and_ftuples_isr &
          (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
      end do
    end do

contains
  function incr_i_ftuple_if_required (i_born, i_real, i_ftuple_in) result (i_ftuple)
    integer :: i_ftuple
    integer, intent(in) :: i_born, i_real, i_ftuple_in
    if (last_registered_i_born /= i_born .or. last_registered_i_real /= i_real) then

```

```

        last_registered_i_born = i_born
        last_registered_i_real = i_real
        i_ftuple = i_ftuple_in + 1
    else
        i_ftuple = i_ftuple_in
    end if
end function incr_i_ftuple_if_required

subroutine setup_flsts_emitters_and_ftuples_fsr &
    (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
    integer, intent(in) :: i_real, i_born
    integer, intent(inout) :: i_ftuple
    type(flv_structure_t), intent(inout), dimension(:), allocatable :: flst_alr
    integer, intent(inout), dimension(:), allocatable :: emitters
    type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
    type(ftuple_list_t) :: ftuples_tmp
    type(flv_structure_t) :: flst_alr_tmp
    type(ftuple_t) :: current_ftuple
    integer :: leg1, leg2
    logical :: valid
    associate (flv_born => reg_data%flv_born(i_born), &
        flv_real => reg_data%flv_real(i_real))
    do leg1 = reg_data%n_in + 1, n_legreal
    do leg2 = leg1 + 1, n_legreal
        valid = flv_real%valid_pair(leg1, leg2, flv_born, model)
        if (valid) then
            if (is_vector(flv_real%flst(leg1)) .and. &
                is_fermion(flv_real%flst(leg2))) then
                flst_alr_tmp = create_alr (flv_real, &
                    reg_data%n_in, leg2, leg1)
            else
                flst_alr_tmp = create_alr (flv_real, &
                    reg_data%n_in, leg1, leg2)
            end if
            flst_alr = [flst_alr, flst_alr_tmp]
            emitters = [emitters, n_legreal - 1]
            call current_ftuple%set (leg1, leg2)
            call current_ftuple%determine_splitting_type_fsr &
                (flv_real, leg1, leg2)
            call current_ftuple%determine_sub_correction_type &
                (flv_born, flv_real, leg1, leg2)
            i_ftuple = incr_i_ftuple_if_required (i_born, i_real, i_ftuple)
            if (i_ftuple > size (ftuples)) then
                call ftuples_tmp%append (current_ftuple)
                ftuples = [ftuples, ftuples_tmp]
            else
                call ftuples(i_ftuple)%append (current_ftuple)
            end if
        end if
    end do
    end do
    end associate
end subroutine setup_flsts_emitters_and_ftuples_fsr

```

```

subroutine setup_flsts_emitters_and_ftuples_isr &
  (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
  integer, intent(in) :: i_real, i_born
  integer, intent(inout) :: i_ftuple
  type(flv_structure_t), intent(inout), dimension(:), allocatable :: flst_alr
  integer, intent(inout), dimension(:), allocatable :: emitters
  type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
  type(ftuple_list_t) :: ftuples_tmp
  type(flv_structure_t) :: flst_alr_tmp
  type(ftuple_t) :: current_ftuple
  integer :: leg, emitter
  logical :: valid1, valid2
  associate (flv_born => reg_data%flv_born(i_born), &
    flv_real => reg_data%flv_real(i_real))
    do leg = reg_data%n_in + 1, n_legreal
      valid1 = flv_real%valid_pair(1, leg, flv_born, model)
      if (reg_data%n_in > 1) then
        valid2 = flv_real%valid_pair(2, leg, flv_born, model)
      else
        valid2 = .false.
      end if
      if (valid1 .and. valid2) then
        emitter = 0
      else if (valid1 .and. .not. valid2) then
        emitter = 1
      else if (.not. valid1 .and. valid2) then
        emitter = 2
      else
        emitter = -1
      end if
      if (valid1 .or. valid2) then
        flst_alr_tmp = create_alr (flv_real, reg_data%n_in, emitter, leg)
        flst_alr = [flst_alr, flst_alr_tmp]
        emitters = [emitters, emitter]
        call current_ftuple%set(emitter, leg)
        call current_ftuple%determine_splitting_type_isr &
          (flv_real, emitter, leg)
        call current_ftuple%determine_sub_correction_type &
          (flv_born, flv_real, emitter, leg)
        i_ftuple = incr_i_ftuple_if_required (i_born, i_real, i_ftuple)
        if (i_ftuple > size (ftuples)) then
          call ftuples_tmp%append (current_ftuple)
          ftuples = [ftuples, ftuples_tmp]
        else
          call ftuples(i_ftuple)%append (current_ftuple)
        end if
      end if
    end do
  end associate
end subroutine setup_flsts_emitters_and_ftuples_isr

end subroutine region_data_find_regions

```

We transfer the mapping of flavor structures that lead to the same ampli-

tude (with structure functions already accounted for!) to the Born and real flv_structure of each singular_region. We then use this information, besides other data of each singular_region, to determine which produce the same amplitude for the non-subtracted real and real subtraction terms and set up the equivalence index mapping for each region.

(FKS regions: reg data: TBP)+≡

```
procedure :: find_eqv_regions => region_data_find_eqv_regions
```

(FKS regions: sub interfaces)+≡

```
module subroutine region_data_find_eqv_regions (reg_data, optimize)
  class(region_data_t), intent(inout) :: reg_data
  logical, intent(in) :: optimize
end subroutine region_data_find_eqv_regions
```

(FKS regions: procedures)+≡

```
module subroutine region_data_find_eqv_regions (reg_data, optimize)
  class(region_data_t), intent(inout) :: reg_data
  logical, intent(in) :: optimize
  integer :: n_reg, alr1, alr2
  n_reg = reg_data%n_regions
  if (optimize) then
    do alr1 = 1, n_reg
      reg_data%regions(alr1)%flst_uborn%eqv_index = &
        reg_data%eqv_flv_index_born(reg_data%regions(alr1)%uborn_index)
      reg_data%regions(alr1)%flst_real%eqv_index = &
        reg_data%eqv_flv_index_real(reg_data%regions(alr1)%real_index)
    end do
    do alr1 = 1, n_reg
      do alr2 = 1, alr1
        if (reg_data%regions(alr2).match.reg_data%regions(alr1)) then
          reg_data%regions(alr1)%eqv_index = alr2
          exit
        end if
      end do
    end do
  else
    do alr1 = 1, n_reg
      reg_data%regions(alr1)%eqv_index = alr1
    end do
  end if
end subroutine region_data_find_eqv_regions
```

Creates singular regions according to table 27.1. It scans all regions in table 27.2 and records the real flavor structures. If they are equivalent, the flavor structure is not recorded, but the multiplicity of the present one is increased.

(FKS regions: reg data: TBP)+≡

```
procedure :: init_singular_regions => region_data_init_singular_regions
```

(FKS regions: sub interfaces)+≡

```
module subroutine region_data_init_singular_regions &
  (reg_data, ftuples, emitter, flv_alr, nlo_correction_type)
  class(region_data_t), intent(inout) :: reg_data
  type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
  type(string_t), intent(in) :: nlo_correction_type
```

```

        integer, intent(in), dimension(:) :: emitter
        type(flv_structure_t), intent(in), dimension(:) :: flv_alr
    end subroutine region_data_init_singular_regions

(FKS regions: procedures)+≡
module subroutine region_data_init_singular_regions &
    (reg_data, ftuples, emitter, flv_alr, nlo_correction_type)
    class(region_data_t), intent(inout) :: reg_data
    type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
    type(string_t), intent(in) :: nlo_correction_type
    type(string_t), dimension(:), allocatable :: nlo_correction_type_dyn
    integer, intent(in), dimension(:) :: emitter
    integer :: n_independent_flv
    type(flv_structure_t), intent(in), dimension(:) :: flv_alr
    type(flv_structure_t), dimension(:), allocatable :: flv_uborn, &
        flv_alr_registered
    integer, dimension(:), allocatable :: mult
    integer, dimension(:), allocatable :: flst_emitter
    integer :: n_regions, maxregions
    integer, dimension(:), allocatable :: index
    integer :: i, i_flv, n_legs
    logical :: equiv, valid_fs_splitting, pure_corr_type, &
        corr_type_valid, non_singular_reg
    integer :: i_first, i_reg, i_reg_prev
    integer, dimension(:), allocatable :: region_to_ftuple, alr_limits
    integer, dimension(:), allocatable :: equiv_index

    maxregions = size (emitter)
    n_legs = flv_alr(1)%nlegs

    allocate (flv_uborn (maxregions))
    allocate (flv_alr_registered (maxregions))
    allocate (mult (maxregions))
    mult = 0
    allocate (flst_emitter (maxregions))
    allocate (index (0))
    allocate (region_to_ftuple (maxregions))
    allocate (equiv_index (maxregions))
    allocate (nlo_correction_type_dyn (maxregions))

    call setup_region_mappings (n_independent_flv, alr_limits, region_to_ftuple)
    nlo_correction_type_dyn = nlo_correction_type
    i_first = 1
    i_reg = 1
    SCAN_FLAVORS: do i_flv = 1, n_independent_flv
        SCAN_FTUPLES: do i = i_first, i_first + alr_limits (i_flv) - 1
            equiv = .false.
            corr_type_valid = .true.
            non_singular_reg = .false.
            if (i == i_first) then
                flv_alr_registered(i_reg) = flv_alr(i)
                if (nlo_correction_type == "EW" .and. &
                    reg_data%alphas_power > 0) then
                    nlo_correction_type_dyn (i_reg) = &
                        set_dynamic_correction_type (i)
                end if
            end if
            i_reg = i_reg + 1
        end do
    end do

```

```

end if
flv_uborn(i_reg) = flv_alr(i)%create_uborn (emitter(i), &
      nlo_correction_type_dyn (i_reg))
flst_emitter(i_reg) = emitter(i)
equiv_index(i_reg) = region_to_ftuple(i)
if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
  corr_type_valid = (nlo_correction_type_dyn (i_reg) == "EW" .and. &
    query_coupling_powers (flv_uborn(i_reg)%flst, &
      reg_data%alpha_power, reg_data%alphas_power)) &
    .or. (nlo_correction_type_dyn (i_reg) == "QCD" .and. &
      query_coupling_powers (flv_uborn(i_reg)%flst, &
        reg_data%alpha_power + 1, reg_data%alphas_power - 1))
  non_singular_reg = .not. corr_type_valid .and. &
    qcd_ew_interferences (flv_alr_registered(i_reg)%flst) &
    .and. query_coupling_powers (flv_alr_registered(i_reg)%flst, &
      reg_data%alpha_power+2, reg_data%alphas_power-1) &
    .and. .not. qcd_ew_interferences (flv_uborn(i_reg)%flst) &
    .and. nlo_correction_type_dyn (i_reg) == "QCD"
  if (non_singular_reg) nlo_correction_type_dyn (i_reg) = "none"
end if
if (corr_type_valid .or. non_singular_reg) then
  mult(i_reg) = mult(i_reg) + 1
  index = [index, region_to_real_index(ftuples, i)]
  i_reg = i_reg + 1
end if
else
  !!! Check for equivalent flavor structures
  do i_reg_prev = 1, i_reg - 1
    if (emitter(i) == flst_emitter(i_reg_prev) .and. emitter(i) > reg_data%n_in) then
      valid_fs_splitting = check_fs_splitting &
        (flv_alr(i)%get_last_two(n_legs), &
          flv_alr_registered(i_reg_prev)%get_last_two(n_legs), &
          flv_alr(i)%tag(n_legs - 1), &
          flv_alr_registered(i_reg_prev)%tag(n_legs - 1))
      if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
        nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
      end if
      pure_corr_type = nlo_correction_type_dyn (i_reg) &
        == nlo_correction_type_dyn (i_reg_prev)
      if ((flv_alr(i) .equiv. flv_alr_registered(i_reg_prev)) &
        .and. valid_fs_splitting .and. pure_corr_type) then
        mult(i_reg_prev) = mult(i_reg_prev) + 1
        equiv = .true.
        call ftuples(region_to_real_index(ftuples, i))%set_equiv &
          (equiv_index(i_reg_prev), region_to_ftuple(i))
        exit
      end if
    else if (emitter(i) == flst_emitter(i_reg_prev) .and. emitter(i) <= reg_data%n_in)
      if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
        nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
      end if
      pure_corr_type = nlo_correction_type_dyn (i_reg) &
        == nlo_correction_type_dyn (i_reg_prev)
      if ((flv_alr(i) .equiv. flv_alr_registered(i_reg_prev)) &

```

```

        .and. pure_corr_type) then
        mult(i_reg_prev) = mult(i_reg_prev) + 1
        equiv = .true.
        call ftuples(region_to_real_index(ftuples, i))%set_equiv &
            (equiv_index(i_reg_prev), region_to_ftuple(i))
        exit
    end if
end if
end do
if (.not. equiv) then
    flv_alr_registered(i_reg) = flv_alr(i)
    if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
        nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
    end if
    flv_uborn(i_reg) = flv_alr(i)%create_uborn (emitter(i), &
        nlo_correction_type_dyn (i_reg))
    flst_emitter(i_reg) = emitter(i)
    equiv_index (i_reg) = region_to_ftuple(i)
    if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
        corr_type_valid = (nlo_correction_type_dyn (i_reg) == "EW" .and. &
            query_coupling_powers (flv_uborn(i_reg)%flst, &
            reg_data%alpha_power, reg_data%alphas_power)) &
            .or. (nlo_correction_type_dyn (i_reg) == "QCD" .and. &
            query_coupling_powers (flv_uborn(i_reg)%flst, &
            reg_data%alpha_power + 1, reg_data%alphas_power - 1))
        non_singular_reg = .not. corr_type_valid .and. &
            qcd_ew_interferences (flv_alr_registered(i_reg)%flst) &
            .and. query_coupling_powers (flv_alr_registered(i_reg)%flst, &
            reg_data%alpha_power+2, reg_data%alphas_power-1) &
            .and. .not. qcd_ew_interferences (flv_uborn(i_reg)%flst) &
            .and. nlo_correction_type_dyn (i_reg) == "QCD"
        if (non_singular_reg) nlo_correction_type_dyn (i_reg) = "none"
    end if
    if (corr_type_valid .or. non_singular_reg) then
        mult(i_reg) = mult(i_reg) + 1
        index = [index, region_to_real_index(ftuples, i)]
        i_reg = i_reg + 1
    end if
end if
end if
end do SCAN_FTUPLES
i_first = i_first + alr_limits(i_flv)
end do SCAN_FLAVORS
n_regions = i_reg - 1

allocate (reg_data%regions (n_regions))
reg_data%n_regions = n_regions
call account_for_regions_from_other_uborns (ftuples)
call init_regions_with_permuted_flavors ()
call assign_real_indices ()

deallocate (flv_uborn)
deallocate (flv_alr_registered)
deallocate (mult)

```

```

deallocate (flst_emitter)
deallocate (index)
deallocate (region_to_ftuple)
deallocate (equiv_index)

contains

subroutine account_for_regions_from_other_uborns (ftuples)
  type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
  integer :: alr1, alr2, i
  type(ftuple_t), dimension(:), allocatable :: ftuples_alr1, ftuples_alr2
  logical, dimension(:,:), allocatable :: equivalences
  do alr1 = 1, n_regions
    do alr2 = 1, n_regions
      if (index(alr1) == index(alr2)) cycle
      if (flv_alr_registered(alr1) .equiv. flv_alr_registered(alr2)) then
        call ftuples(index(alr1))%to_array (ftuples_alr1, equivalences, .false.)
        call ftuples(index(alr2))%to_array (ftuples_alr2, equivalences, .false.)
        do i = 1, size (ftuples_alr2)
          if (.not. any (ftuple_equal_ireg (ftuples_alr1, ftuples_alr2(i)))) then
            call ftuples(index(alr1))%append (ftuples_alr2(i))
          end if
        end do
      end if
    end do
  end do
end subroutine account_for_regions_from_other_uborns

subroutine setup_region_mappings (n_independent_flv, &
  alr_limits, region_to_ftuple)
  integer, intent(inout) :: n_independent_flv
  integer, intent(inout), dimension(:), allocatable :: alr_limits
  integer, intent(inout), dimension(:), allocatable :: region_to_ftuple
  integer :: i, j, i_flv
  if (any (ftuples%get_n_tuples() == 0)) &
    call msg_fatal ("Inconsistent collection of FKS pairs!")
  n_independent_flv = size (ftuples)
  alr_limits = ftuples%get_n_tuples()
  if (.not. (sum (alr_limits) == maxregions)) &
    call msg_fatal ("Too many regions!")
  j = 1
  do i_flv = 1, n_independent_flv
    do i = 1, alr_limits(i_flv)
      region_to_ftuple(j) = i
      j = j + 1
    end do
  end do
end subroutine setup_region_mappings

subroutine check_permutation (perm, flv_perm, flv_orig, i_reg)
  type(flv_perm_t), intent(in) :: perm
  type(flv_structure_t), intent(in) :: flv_perm, flv_orig
  integer, intent(in) :: i_reg
  type(flv_structure_t) :: flv_tmp

```

```

flv_tmp = perm%apply (flv_orig, invert = .true.)
if (.not. all (flv_tmp%flst == flv_perm%flst)) then
  print *, 'Fail at: ', i_reg
  print *, 'Original flavor structure: ', flv_orig%flst
  call perm%write ()
  print *, 'Permuted flavor: ', flv_perm%flst
  print *, 'Should be: ', flv_tmp%flst
  call msg_fatal ("Permutation does not reproduce original flavor!")
end if
end subroutine check_permutation

subroutine init_regions_with_permuted_flavors ()
  type(flv_perm_t) :: perm_list
  type(ftuple_t), dimension(:), allocatable :: ftuple_array
  logical, dimension(:,:), allocatable :: equivalences
  integer :: i, j
  do j = 1, n_regions
    do i = 1, reg_data%n_flv_born
      if (reg_data%flv_born(i) .equiv. flv_uborn(j)) then
        call perm_list%reset ()
        call perm_list%init (reg_data%flv_born(i), flv_uborn(j), &
          reg_data%n_in, reg_data%n_legs_born, .true.)
        flv_uborn(j) = perm_list%apply (flv_uborn(j))
        flv_alr_registered(j) = perm_list%apply (flv_alr_registered(j))
        flst_emitter(j) = perm_list%apply (flst_emitter(j))
      end if
    end do
    call ftuples(index(j))%to_array (ftuple_array, equivalences, .false.)
    do i = 1, size (reg_data%flv_real)
      if (reg_data%flv_real(i) .equiv. flv_alr_registered(j)) then
        call perm_list%reset ()
        call perm_list%init (flv_alr_registered(j), reg_data%flv_real(i), &
          reg_data%n_in, reg_data%n_legs_real, .false.)
        if (debug_active (D_SUBTRACTION)) call check_permutation &
          (perm_list, reg_data%flv_real(i), flv_alr_registered(j), j)
        ftuple_array = perm_list%apply (ftuple_array)
        call ftuple_sort_array (ftuple_array, equivalences)
      end if
    end do
    call reg_data%regions(j)%init (j, mult(j), 0, flv_alr_registered(j), &
      flv_uborn(j), reg_data%flv_born, flst_emitter(j), ftuple_array, &
      equivalences, nlo_correction_type_dyn (j))
    if (allocated (ftuple_array)) deallocate (ftuple_array)
    if (allocated (equivalences)) deallocate (equivalences)
  end do
end subroutine init_regions_with_permuted_flavors

subroutine assign_real_indices ()
  type(flv_structure_t) :: current_flv_real
  type(flv_structure_t), dimension(:), allocatable :: these_flv
  integer :: i_real, current_uborn_index
  integer :: i, j, this_i_real
  allocate (these_flv (size (flv_alr_registered)))
  i_real = 1

```

```

associate (regions => reg_data%regions)
do i = 1, reg_data%n_regions
do j = 1, size (these_flv)
if (.not. allocated (these_flv(j)%flst)) then
this_i_real = i_real
call these_flv(i_real)%init (flv_alr_registered(i)%flst, reg_data%n_in)
i_real = i_real + 1
exit
else if (all (these_flv(j)%flst == flv_alr_registered(i)%flst)) then
this_i_real = j
exit
end if
end do
regions(i)%real_index = this_i_real
end do
end associate
deallocate (these_flv)
end subroutine assign_real_indices

function check_fs_splitting (flv1, flv2, tag1, tag2) result (valid)
logical :: valid
integer, intent(in), dimension(2) :: flv1, flv2
integer, intent(in) :: tag1, tag2
if (flv1(1) + flv1(2) == 0) then
valid = abs(flvl(1)) == abs(flvl(2)) .and. abs(flvl(2)) == abs(flvl(2))
else
valid = flvl(1) == flvl(1) .and. flvl(2) == flvl(2) .and. tag1 == tag2
end if
end function check_fs_splitting

function set_dynamic_correction_type (i_flv_alr) result (nlo_corr_type_dyn)
type(string_t) :: nlo_corr_type_dyn
type(ftuple_t) :: ftuple_tmp
integer, intent(in) :: i_flv_alr
ftuple_tmp = ftuples (region_to_real_index(ftuples, i_flv_alr))%get_ftuple &
(region_to_ftuple(i_flv_alr))
if (ftuple_tmp%qcd_split) then
nlo_corr_type_dyn = var_str ("QCD")
else
nlo_corr_type_dyn = var_str ("EW")
end if
end function set_dynamic_correction_type
end subroutine region_data_init_singular_regions

```

Create an array containing all emitters and resonances of `region_data`.

<FKS regions: reg data: TBP>+≡

```
procedure :: find_emitters => region_data_find_emitters
```

<FKS regions: sub interfaces>+≡

```
module subroutine region_data_find_emitters (reg_data)
class(region_data_t), intent(inout) :: reg_data
end subroutine region_data_find_emitters
```

<FKS regions: procedures>+≡

```
module subroutine region_data_find_emitters (reg_data)
```

```

class(region_data_t), intent(inout) :: reg_data
integer :: alr, j, n_em, em
integer, dimension(:), allocatable :: em_count
allocate (em_count(reg_data%n_regions))
em_count = -1
n_em = 0

!!!Count the number of different emitters
do alr = 1, reg_data%n_regions
  em = reg_data%regions(alr)%emitter
  if (.not. any (em_count == em)) then
    n_em = n_em + 1
    em_count(alr) = em
  end if
end do

if (n_em < 1) call msg_fatal ("region_data_find_emitters: No emitters found!")
reg_data%n_emitters = n_em
allocate (reg_data%emitters (reg_data%n_emitters))
reg_data%emitters = -1

j = 1
do alr = 1, size (reg_data%regions)
  em = reg_data%regions(alr)%emitter
  if (.not. any (reg_data%emitters == em)) then
    reg_data%emitters(j) = em
    j = j + 1
  end if
end do
end subroutine region_data_find_emitters

```

(FKS regions: reg data: TBP)+≡

```

procedure :: find_resonances => region_data_find_resonances

```

(FKS regions: sub interfaces)+≡

```

module subroutine region_data_find_resonances (reg_data)
  class(region_data_t), intent(inout) :: reg_data
  end subroutine region_data_find_resonances

```

(FKS regions: procedures)+≡

```

module subroutine region_data_find_resonances (reg_data)
  class(region_data_t), intent(inout) :: reg_data
  integer :: alr, j, k, n_res, n_contr
  integer :: res
  integer, dimension(10) :: res_count
  type(resonance_contributors_t), dimension(10) :: contributors_count
  type(resonance_contributors_t) :: contributors
  integer :: i_res, emitter
  logical :: share_emitter
  res_count = -1
  n_res = 0; n_contr = 0

```

```

!!! Count the number of different resonances
do alr = 1, reg_data%n_regions
  select type (fks_mapping => reg_data%fks_mapping)

```



```

type is (fks_mapping_resonances_t)
  res = fks_mapping%res_map%alr_to_i_res (alr)
  if (.not. any (res_count == res)) then
    n_res = n_res + 1
    res_count(alr) = res
  end if
end select
end do

if (n_res > 0) allocate (reg_data%resonances (n_res))

j = 1
select type (fks_mapping => reg_data%fks_mapping)
type is (fks_mapping_resonances_t)
  do alr = 1, size (reg_data%regions)
    res = fks_mapping%res_map%alr_to_i_res (alr)
    if (.not. any (reg_data%resonances == res)) then
      reg_data%resonances(j) = res
      j = j + 1
    end if
  end do

  allocate (reg_data%alr_to_i_contributor (size (reg_data%regions)))
  do alr = 1, size (reg_data%regions)
    i_res = fks_mapping%res_map%alr_to_i_res (alr)
    emitter = reg_data%regions(alr)%emitter
    call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
    if (.not. share_emitter) cycle
    if (.not. any (contributors_count == contributors)) then
      n_contr = n_contr + 1
      contributors_count(alr) = contributors
    end if
    if (allocated (contributors%c)) deallocate (contributors%c)
  end do
  allocate (reg_data%alr_contributors (n_contr))
  j = 1
  do alr = 1, size (reg_data%regions)
    i_res = fks_mapping%res_map%alr_to_i_res (alr)
    emitter = reg_data%regions(alr)%emitter
    call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
    if (.not. share_emitter) cycle
    if (.not. any (reg_data%alr_contributors == contributors)) then
      reg_data%alr_contributors(j) = contributors
      reg_data%alr_to_i_contributor (alr) = j
      j = j + 1
    else
      do k = 1, size (reg_data%alr_contributors)
        if (reg_data%alr_contributors(k) == contributors) exit
      end do
      reg_data%alr_to_i_contributor (alr) = k
    end if
    if (allocated (contributors%c)) deallocate (contributors%c)
  end do
end select

```

```

        call reg_data%extend_ftuples (n_res)
        call reg_data%set_contributors ()

    end subroutine region_data_find_resonances

<FKS regions: reg data: TBP>+≡
    procedure :: set_i_phs_to_i_con => region_data_set_i_phs_to_i_con

<FKS regions: sub interfaces>+≡
    module subroutine region_data_set_i_phs_to_i_con (reg_data)
        class(region_data_t), intent(inout) :: reg_data
    end subroutine region_data_set_i_phs_to_i_con

<FKS regions: procedures>+≡
    module subroutine region_data_set_i_phs_to_i_con (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        integer :: alr
        integer :: i_res, emitter, i_con, i_phs, i_em
        type(phs_identifier_t), dimension(:), allocatable :: phs_id_tmp
        logical :: share_emitter, phs_exist
        type(resonance_contributors_t) :: contributors
        allocate (phs_id_tmp (reg_data%n_phs))
        if (allocated (reg_data%resonances)) then
            allocate (reg_data%i_phs_to_i_con (reg_data%n_phs))
            do i_em = 1, size (reg_data%emitters)
                emitter = reg_data%emitters(i_em)
                do i_res = 1, size (reg_data%resonances)
                    if (reg_data%emitter_is_compatible_with_resonance (i_res, emitter)) then
                        alr = find_alr (emitter, i_res)
                        if (alr == 0) call msg_fatal ("Could not find requested alpha region!")
                        i_con = reg_data%alr_to_i_contributor (alr)
                        call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
                        if (.not. share_emitter) cycle
                        call check_for_phs_identifier &
                            (phs_id_tmp, reg_data%n_in, emitter, contributors%c, phs_exist, i_phs)
                        if (phs_id_tmp(i_phs)%emitter < 0) then
                            phs_id_tmp(i_phs)%emitter = emitter
                            allocate (phs_id_tmp(i_phs)%contributors (size (contributors%c)))
                            phs_id_tmp(i_phs)%contributors = contributors%c
                        end if
                        reg_data%i_phs_to_i_con (i_phs) = i_con
                    end if
                end do
                if (allocated (contributors%c)) deallocate (contributors%c)
            end do
        end do
    end if
contains
    function find_alr (emitter, i_res) result (alr)
        integer :: alr
        integer, intent(in) :: emitter, i_res
        integer :: i
        do i = 1, reg_data%n_regions
            if (reg_data%regions(i)%emitter == emitter .and. &
                reg_data%regions(i)%i_res == i_res) then
                alr = i
            end if
        end do
    end function

```

```

        return
    end if
end do
alr = 0
end function find_alr
end subroutine region_data_set_i_phs_to_i_con

```

(FKS regions: reg data: TBP)+≡

```

procedure :: set_alr_to_i_phs => region_data_set_alr_to_i_phs

```

(FKS regions: sub interfaces)+≡

```

module subroutine region_data_set_alr_to_i_phs &
    (reg_data, phs_identifiers, alr_to_i_phs)
class(region_data_t), intent(inout) :: reg_data
type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
integer, intent(out), dimension(:) :: alr_to_i_phs
end subroutine region_data_set_alr_to_i_phs

```

(FKS regions: procedures)+≡

```

module subroutine region_data_set_alr_to_i_phs &
    (reg_data, phs_identifiers, alr_to_i_phs)
class(region_data_t), intent(inout) :: reg_data
type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
integer, intent(out), dimension(:) :: alr_to_i_phs
integer :: alr, i_phs
integer :: emitter, i_res
type(resonance_contributors_t) :: contributors
logical :: share_emitter, phs_exist
do alr = 1, reg_data%n_regions
    associate (region => reg_data%regions(alr))
        emitter = region%emitter
        i_res = region%i_res
        if (i_res /= 0) then
            call reg_data%get_contributors (i_res, emitter, &
                contributors%c, share_emitter)
            if (.not. share_emitter) cycle
        end if
        if (allocated (contributors%c)) then
            call check_for_phs_identifier (phs_identifiers, reg_data%n_in, &
                emitter, contributors%c, phs_exist = phs_exist, i_phs = i_phs)
        else
            call check_for_phs_identifier (phs_identifiers, reg_data%n_in, &
                emitter, phs_exist = phs_exist, i_phs = i_phs)
        end if
        if (.not. phs_exist) &
            call msg_fatal ("phs identifiers are not set up correctly!")
        alr_to_i_phs(alr) = i_phs
    end associate
    if (allocated (contributors%c)) deallocate (contributors%c)
end do
end subroutine region_data_set_alr_to_i_phs

```

(FKS regions: reg data: TBP)+≡

```

procedure :: set_contributors => region_data_set_contributors

```

```

<FKS regions: sub interfaces>+≡
    module subroutine region_data_set_contributors (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        end subroutine region_data_set_contributors
<FKS regions: procedures>+≡
    module subroutine region_data_set_contributors (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        integer :: alr, i_res, i_reg, i_con
        integer :: i1, i2, i_em
        integer, dimension(:), allocatable :: contributors
        logical :: share_emitter
        do alr = 1, size (reg_data%regions)
            associate (sregion => reg_data%regions(alr))
                allocate (sregion%i_reg_to_i_con (sregion%nregions))
                do i_reg = 1, sregion%nregions
                    call sregion%ftuples(i_reg)%get (i1, i2)
                    i_em = get_emitter_index (i1, i2, reg_data%n_legs_real)
                    i_res = sregion%ftuples(i_reg)%i_res
                    call reg_data%get_contributors &
                        (i_res, i_em, contributors, share_emitter)
                    !!! Lookup contributor index
                    do i_con = 1, size (reg_data%alr_contributors)
                        if (all (reg_data%alr_contributors(i_con)%c == contributors)) &
                            then
                            sregion%i_reg_to_i_con (i_reg) = i_con
                            exit
                        end if
                    end do
                    deallocate (contributors)
                end do
            end associate
        end do
contains
        function get_emitter_index (i1, i2, n) result (i_em)
            integer :: i_em
            integer, intent(in) :: i1, i2, n
            if (i1 == n) then
                i_em = i2
            else
                i_em = i1
            end if
        end function get_emitter_index
    end subroutine region_data_set_contributors

```

This extension of the ftuples is still too naive as it assumes that the same resonances are possible for all ftuples

```

<FKS regions: reg data: TBP>+≡
    procedure :: extend_ftuples => region_data_extend_ftuples
<FKS regions: sub interfaces>+≡
    module subroutine region_data_extend_ftuples (reg_data, n_res)
        class(region_data_t), intent(inout) :: reg_data
        integer, intent(in) :: n_res
        end subroutine region_data_extend_ftuples

```

(FKS regions: procedures)+≡

```

module subroutine region_data_extend_ftuples (reg_data, n_res)
  class(region_data_t), intent(inout) :: reg_data
  integer, intent(in) :: n_res
  integer :: alr, n_reg_save
  integer :: i_reg, i_res, i_em, k
  type(ftuple_t), dimension(:), allocatable :: ftuple_save
  integer :: n_new
  do alr = 1, size (reg_data%regions)
    associate (sregion => reg_data%regions(alr))
      n_reg_save = sregion%nregions
      allocate (ftuple_save (n_reg_save))
      ftuple_save = sregion%ftuples
      n_new = count_n_new_ftuples (sregion, n_res)
      deallocate (sregion%ftuples)
      sregion%nregions = n_new
      allocate (sregion%ftuples (n_new))
      k = 1
      do i_res = 1, n_res
        do i_reg = 1, n_reg_save
          associate (ftuple_new => sregion%ftuples(k))
            i_em = ftuple_save(i_reg)%ireg(1)
            if (reg_data%emitter_is_in_resonance (i_res, i_em)) then
              call ftuple_new%set (i_em, ftuple_save(i_reg)%ireg(2))
              ftuple_new%i_res = i_res
              ftuple_new%splitting_type = ftuple_save(i_reg)%splitting_type
              k = k + 1
            end if
          end associate
        end do
      end do
    end associate
    deallocate (ftuple_save)
  end do
contains
  function count_n_new_ftuples (sregion, n_res) result (n_new)
    integer :: n_new
    type(singular_region_t), intent(in) :: sregion
    integer, intent(in) :: n_res
    integer :: i_reg, i_res, i_em
    n_new = 0
    do i_reg = 1, sregion%nregions
      do i_res = 1, n_res
        i_em = sregion%ftuples(i_reg)%ireg(1)
        if (reg_data%emitter_is_in_resonance (i_res, i_em)) &
          n_new = n_new + 1
      end do
    end do
  end function count_n_new_ftuples
end subroutine region_data_extend_ftuples

```

(FKS regions: reg data: TBP)+≡

```

procedure :: get_flavor_indices => region_data_get_flavor_indices

```

```

(FKS regions: sub interfaces)+≡
    module function region_data_get_flavor_indices &
        (reg_data, born) result (i_flv)
        integer, dimension(:), allocatable :: i_flv
        class(region_data_t), intent(in) :: reg_data
        logical, intent(in) :: born
    end function region_data_get_flavor_indices

(FKS regions: procedures)+≡
    module function region_data_get_flavor_indices (reg_data, born) result (i_flv)
        integer, dimension(:), allocatable :: i_flv
        class(region_data_t), intent(in) :: reg_data
        logical, intent(in) :: born
        allocate (i_flv (reg_data%n_regions))
        if (born) then
            i_flv = reg_data%regions%uborn_index
        else
            i_flv = reg_data%regions%real_index
        end if
    end function region_data_get_flavor_indices

(FKS regions: reg data: TBP)+≡
    procedure :: get_matrix_element_index => region_data_get_matrix_element_index

(FKS regions: sub interfaces)+≡
    module function region_data_get_matrix_element_index &
        (reg_data, i_reg) result (i_me)
        integer :: i_me
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_reg
    end function region_data_get_matrix_element_index

(FKS regions: procedures)+≡
    module function region_data_get_matrix_element_index &
        (reg_data, i_reg) result (i_me)
        integer :: i_me
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_reg
        i_me = reg_data%regions(i_reg)%real_index
    end function region_data_get_matrix_element_index

(FKS regions: reg data: TBP)+≡
    procedure :: compute_number_of_phase_spaces &
        => region_data_compute_number_of_phase_spaces

(FKS regions: sub interfaces)+≡
    module subroutine region_data_compute_number_of_phase_spaces (reg_data)
        class(region_data_t), intent(inout) :: reg_data
    end subroutine region_data_compute_number_of_phase_spaces

(FKS regions: procedures)+≡
    module subroutine region_data_compute_number_of_phase_spaces (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        integer :: i_em, i_res, i_phs
        integer :: emitter
        type(resonance_contributors_t) :: contributors

```

```

integer, parameter :: n_max_phs = 10
type(phs_identifer_t), dimension(n_max_phs) :: phs_id_tmp
logical :: share_emitter, phs_exist
if (allocated (reg_data%resonances)) then
  reg_data%n_phs = 0
  do i_em = 1, size (reg_data%emitters)
    emitter = reg_data%emitters(i_em)
    do i_res = 1, size (reg_data%resonances)
      if (reg_data%emitter_is_compatible_with_resonance (i_res, emitter)) then
        call reg_data%get_contributors &
          (i_res, emitter, contributors%c, share_emitter)
        if (.not. share_emitter) cycle
        call check_for_phs_identifer (phs_id_tmp, reg_data%n_in, &
          emitter, contributors%c, phs_exist, i_phs)
        if (.not. phs_exist) then
          reg_data%n_phs = reg_data%n_phs + 1
          if (reg_data%n_phs > n_max_phs) call msg_fatal &
            ("Buffer of phase space identifiere: Too much phase spaces!")
          call phs_id_tmp(i_phs)%init (emitter, contributors%c)
        end if
      end if
    end do
    if (allocated (contributors%c)) deallocate (contributors%c)
  end do
end do
else
  reg_data%n_phs = size (remove_duplicates_from_int_array &
    (reg_data%emitters))
end if
end subroutine region_data_compute_number_of_phase_spaces

```

(FKS regions: reg data: TBP)+≡

```

procedure :: get_n_phs => region_data_get_n_phs

```

(FKS regions: sub interfaces)+≡

```

module function region_data_get_n_phs (reg_data) result (n_phs)
  integer :: n_phs
  class(region_data_t), intent(in) :: reg_data
end function region_data_get_n_phs

```

(FKS regions: procedures)+≡

```

module function region_data_get_n_phs (reg_data) result (n_phs)
  integer :: n_phs
  class(region_data_t), intent(in) :: reg_data
  n_phs = reg_data%n_phs
end function region_data_get_n_phs

```

(FKS regions: reg data: TBP)+≡

```

procedure :: set_splitting_info => region_data_set_splitting_info

```

(FKS regions: sub interfaces)+≡

```

module subroutine region_data_set_splitting_info (reg_data)
  class(region_data_t), intent(inout) :: reg_data
end subroutine region_data_set_splitting_info

```

```

(FKS regions: procedures)+≡
module subroutine region_data_set_splitting_info (reg_data)
  class(region_data_t), intent(inout) :: reg_data
  integer :: alr
  do alr = 1, reg_data%n_regions
    call reg_data%regions(alr)%set_splitting_info (reg_data%n_in)
  end do
end subroutine region_data_set_splitting_info

(FKS regions: reg data: TBP)+≡
procedure :: init_phs_identifiers => region_data_init_phs_identifiers

(FKS regions: sub interfaces)+≡
module subroutine region_data_init_phs_identifiers (reg_data, phs_id)
  class(region_data_t), intent(in) :: reg_data
  type(phs_identifier_t), intent(out), dimension(:), allocatable :: phs_id
end subroutine region_data_init_phs_identifiers

(FKS regions: procedures)+≡
module subroutine region_data_init_phs_identifiers (reg_data, phs_id)
  class(region_data_t), intent(in) :: reg_data
  type(phs_identifier_t), intent(out), dimension(:), allocatable :: phs_id
  integer :: i_em, i_res, i_phs
  integer :: emitter
  type(resonance_contributors_t) :: contributors
  logical :: share_emitter, phs_exist
  allocate (phs_id (reg_data%n_phs))
  do i_em = 1, size (reg_data%emitters)
    emitter = reg_data%emitters(i_em)
    if (allocated (reg_data%resonances)) then
      do i_res = 1, size (reg_data%resonances)
        call reg_data%get_contributors (i_res, emitter, &
          contributors%c, share_emitter)
        if (.not. share_emitter) cycle
        call check_for_phs_identifier &
          (phs_id, reg_data%n_in, emitter, contributors%c, &
            phs_exist, i_phs)
        if (.not. phs_exist) &
          call phs_id(i_phs)%init (emitter, contributors%c)
        if (allocated (contributors%c)) deallocate (contributors%c)
      end do
    else
      call check_for_phs_identifier (phs_id, reg_data%n_in, emitter, &
        phs_exist = phs_exist, i_phs = i_phs)
      if (.not. phs_exist) call phs_id(i_phs)%init (emitter)
    end if
  end do
end subroutine region_data_init_phs_identifiers

```

Gathers all ftuples from all ALRs. There are at most $n \cdot (n - 1)$ ftuples with i and j in the final state and up to $3n$ ftuples with i in the initial state.

```

(FKS regions: reg data: TBP)+≡
procedure :: get_all_ftuples => region_data_get_all_ftuples

```


<FKS regions: sub interfaces>+≡

```

module subroutine region_data_get_all_ftuples (reg_data, ftuples)
  class(region_data_t), intent(in) :: reg_data
  type(ftuple_t), intent(inout), dimension(:), allocatable :: ftuples
end subroutine region_data_get_all_ftuples

```

<FKS regions: procedures>+≡

```

module subroutine region_data_get_all_ftuples (reg_data, ftuples)
  class(region_data_t), intent(in) :: reg_data
  type(ftuple_t), intent(inout), dimension(:), allocatable :: ftuples
  type(ftuple_t), dimension(:), allocatable :: ftuple_tmp
  integer :: i, j, alr, n_fs
  j = 0
  n_fs = reg_data%n_legs_real - reg_data%n_in
  allocate (ftuple_tmp (n_fs * (n_fs - 1) + 3 * n_fs))
  do i = 1, reg_data%n_regions
    associate (region => reg_data%regions(i))
      do alr = 1, region%nregions
        if (.not. any &
          (ftuple_equal_ireg (region%ftuples(alr), ftuple_tmp))) then
          j = j + 1
          ftuple_tmp(j) = region%ftuples(alr)
        end if
      end do
    end associate
  end do
  allocate (ftuples (j))
  ftuples = ftuple_tmp(1:j)
  deallocate (ftuple_tmp)
end subroutine region_data_get_all_ftuples

```

<FKS regions: reg data: TBP>+≡

```

procedure :: write_to_file => region_data_write_to_file

```

<FKS regions: sub interfaces>+≡

```

module subroutine region_data_write_to_file &
  (reg_data, proc_id, latex, os_data)
  class(region_data_t), intent(inout) :: reg_data
  type(string_t), intent(in) :: proc_id
  logical, intent(in) :: latex
  type(os_data_t), intent(in) :: os_data
end subroutine region_data_write_to_file

```

<FKS regions: procedures>+≡

```

module subroutine region_data_write_to_file &
  (reg_data, proc_id, latex, os_data)
  class(region_data_t), intent(inout) :: reg_data
  type(string_t), intent(in) :: proc_id
  logical, intent(in) :: latex
  type(os_data_t), intent(in) :: os_data
  type(string_t) :: filename
  integer :: u
  integer :: status

  if (latex) then

```

```

        filename = proc_id // "_fks_regions.tex"
    else
        filename = proc_id // "_fks_regions.out"
    end if
    u = free_unit ()
    open (u, file=char(filename), action = "write", status="replace")
    if (latex) then
        call reg_data%write_latex (u)
        close (u)
        call os_data%build_latex_file &
            (proc_id // "_fks_regions", stat_out = status)
        if (status /= 0) &
            call msg_error (char ("Failed to compile " // filename))
    else
        call reg_data%write (u)
        close (u)
    end if
end subroutine region_data_write_to_file

```

(FKS regions: reg data: TBP)+≡

```

    procedure :: write_latex => region_data_write_latex

```

(FKS regions: sub interfaces)+≡

```

    module subroutine region_data_write_latex (reg_data, unit)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in), optional :: unit
    end subroutine region_data_write_latex

```

(FKS regions: procedures)+≡

```

    module subroutine region_data_write_latex (reg_data, unit)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in), optional :: unit
        integer :: i, u
        u = given_output_unit (); if (present (unit)) u = unit
        write (u, "(A)") "\documentclass{article}"
        write (u, "(A)") "\begin{document}"
        write (u, "(A)") "%FKS region data, automatically created by WHIZARD"
        write (u, "(A)") "\begin{table}"
        write (u, "(A)") "\begin{center}"
        write (u, "(A)") "\begin{tabular} {|c|c|c|c|c|c|c|c|}"
        write (u, "(A)") "\hline"
        write (u, "(A)") "$\alpha_r$ & $f_r$ & $i_r$ & $\varepsilon$ & " // &
            "$\varSigma$ & $\mathcal{P}_{\rm FKS}$ & $i_b$ & $f_b$ \\"
        write (u, "(A)") "\hline"
        do i = 1, reg_data%n_regions
            call reg_data%regions(i)%write_latex (u)
        end do
        write (u, "(A)") "\hline"
        write (u, "(A)") "\end{tabular}"
        write (u, "(A)") "\caption{List of singular regions}"
        write (u, "(A)") "\begin{description}"
        write (u, "(A)") "\item[$\alpha_r$] Index of the singular region"
        write (u, "(A)") "\item[$f_r$] Real flavor structure"
        write (u, "(A)") "\item[$i_r$] Index of the associated real flavor structure"
        write (u, "(A)") "\item[$\varepsilon$] Emitter"
    end subroutine

```

```

write (u, "(A)") "\item[$\varsigma$] Multiplicity"
      !!! The symbol used by 0908.4272 for multiplicities
write (u, "(A)") "\item[$\mathcal{P}_{\rm{FKS}}$] The set of singular FKS-pairs"
write (u, "(A)") "\item[$i_b$] Underlying Born index"
write (u, "(A)") "\item[$f_b$] Underlying Born flavor structure"
write (u, "(A)") "\end{description}"
write (u, "(A)") "\end{center}"
write (u, "(A)") "\end{table}"
write (u, "(A)") "\end{document}"
end subroutine region_data_write_latex

```

Creates a table with information about all singular regions and writes it to a file.

```

(FKS regions: reg data: TBP)+≡
  procedure :: write => region_data_write

(FKS regions: sub interfaces)+≡
  module subroutine region_data_write (reg_data, unit)
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in), optional :: unit
  end subroutine region_data_write

(FKS regions: procedures)+≡
  module subroutine region_data_write (reg_data, unit)
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in), optional :: unit
    integer :: j
    integer :: maxnregions, i_reg_max
    type(string_t) :: flst_title, ftuple_title
    integer :: n_res, u
    u = given_output_unit (unit); if (u < 0) return
    maxnregions = 1; i_reg_max = 1
    do j = 1, reg_data%n_regions
      if (size (reg_data%regions(j)%ftuples) > maxnregions) then
        maxnregions = reg_data%regions(j)%nregions
        i_reg_max = j
      end if
    end do
    flst_title = '(A' // flst_title_format(reg_data%n_legs_real) // ')'
    ftuple_title = '(A' // ftuple_title_format() // ')'
    write (u, '(A,1X,I4)') 'Total number of regions: ', size(reg_data%regions)
    write (u, '(A4)', advance = 'no') ' alr'
    call write_vline (u)
    write (u, char (flst_title), advance = 'no') 'flst_real'
    call write_vline (u)
    write (u, '(A6)', advance = 'no') 'i_real'
    call write_vline (u)
    write (u, '(A3)', advance = 'no') 'em'
    call write_vline (u)
    write (u, '(A3)', advance = 'no') 'mult'
    call write_vline (u)
    write (u, '(A4)', advance = 'no') 'nreg'
    call write_vline (u)
    if (allocated (reg_data%fks_mapping)) then
      select type (fks_mapping => reg_data%fks_mapping)

```

```

        type is (fks_mapping_resonances_t)
        write (u, '(A3)', advance = 'no') 'res'
        call write_vline (u)
    end select
end if
write (u, char (ftuple_title), advance = 'no') 'ftuples'
call write_vline (u)
flst_title = '(A' // flst_title_format(reg_data%n_legs_born) // ')'
write (u, char (flst_title), advance = 'no') 'flst_born'
call write_vline (u)
write (u, '(A7)', advance = 'no') 'i_born'
call write_vline (u)
write (u, '(A4)') 'corr'
do j = 1, reg_data%n_regions
    write (u, '(I4)', advance = 'no') j
    call reg_data%regions(j)%write (u, maxnregions)
end do
call write_separator (u)
if (allocated (reg_data%fks_mapping)) then
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
        write (u, '(A)')
        write (u, '(A)') &
            "The FKS regions are combined with resonance information: "
        n_res = size (fks_mapping%res_map%res_histories)
        write (u, '(A,1X,I1)') "Number of QCD resonance histories: ", n_res
        do j = 1, n_res
            write (u, '(A,1X,I1)') "i_res = ", j
            call fks_mapping%res_map%res_histories(j)%write (u)
            call write_separator (u)
        end do
    end select
end if

contains

function flst_title_format (n) result (frmt)
    integer, intent(in) :: n
    type(string_t) :: frmt
    character(len=2) :: frmt_char
    write (frmt_char, '(I2)') 4 * n + 1
    frmt = var_str (frmt_char)
end function flst_title_format

function ftuple_title_format () result (frmt)
    type(string_t) :: frmt
    integer :: n_ftuple_char
    !!! An ftuple (x,x) consists of five characters. In the string, they
    !!! are separated by maxnregions - 1 commas. In total these are
    !!! 5 * maxnregions + maxnregions - 1 = 6 * maxnregions - 1 characters.
    !!! The {} brackets at add two additional characters.
    n_ftuple_char = 6 * maxnregions + 1
    !!! If there are resonances, each ftuple with a resonance adds a ";x"
    !!! to the ftuple

```

```

        n_ftuple_char = n_ftuple_char + &
        2 * count (reg_data%regions(i_reg_max)%ftuples%i_res > 0)
        !!! Pseudo-ISR regions are denoted with a * at the end
        n_ftuple_char = n_ftuple_char + &
        count (reg_data%regions(i_reg_max)%ftuples%pseudo_isr)
        frmt = str (n_ftuple_char)
    end function ftuple_title_format

end subroutine region_data_write

<FKS regions: procedures>+≡
subroutine write_vline (u)
    integer, intent(in) :: u
    character(len=10), parameter :: sep_format = "(1X,A2,1X)"
    write (u, sep_format, advance = 'no') '||'
end subroutine write_vline

<FKS regions: public>+≡
public :: assignment(=)

<FKS regions: interfaces>+≡
interface assignment(=)
    module procedure region_data_assign
end interface

<FKS regions: sub interfaces>+≡
module subroutine region_data_assign (reg_data_out, reg_data_in)
    type(region_data_t), intent(out) :: reg_data_out
    type(region_data_t), intent(in) :: reg_data_in
end subroutine region_data_assign

<FKS regions: procedures>+≡
module subroutine region_data_assign (reg_data_out, reg_data_in)
    type(region_data_t), intent(out) :: reg_data_out
    type(region_data_t), intent(in) :: reg_data_in
    integer :: i
    if (allocated (reg_data_in%regions)) then
        allocate (reg_data_out%regions (size (reg_data_in%regions)))
        do i = 1, size (reg_data_in%regions)
            reg_data_out%regions(i) = reg_data_in%regions(i)
        end do
    else
        call msg_warning &
            ("Copying region data without allocated singular regions!")
    end if
    if (allocated (reg_data_in%flv_born)) then
        allocate (reg_data_out%flv_born (size (reg_data_in%flv_born)))
        do i = 1, size (reg_data_in%flv_born)
            reg_data_out%flv_born(i) = reg_data_in%flv_born(i)
        end do
    else
        call msg_warning &
            ("Copying region data without allocated born flavor structure!")
    end if
end if

```

```

if (allocated (reg_data_in%flv_real)) then
  allocate (reg_data_out%flv_real (size (reg_data_in%flv_real)))
  do i = 1, size (reg_data_in%flv_real)
    reg_data_out%flv_real(i) = reg_data_in%flv_real(i)
  end do
else
  call msg_warning ("Copying region data without allocated real flavor structure!")
end if
if (allocated (reg_data_in%emitters)) then
  allocate (reg_data_out%emitters (size (reg_data_in%emitters)))
  do i = 1, size (reg_data_in%emitters)
    reg_data_out%emitters(i) = reg_data_in%emitters(i)
  end do
else
  call msg_warning ("Copying region data without allocated emitters!")
end if
reg_data_out%n_regions = reg_data_in%n_regions
reg_data_out%n_emitters = reg_data_in%n_emitters
reg_data_out%n_flv_born = reg_data_in%n_flv_born
reg_data_out%n_flv_real = reg_data_in%n_flv_real
reg_data_out%n_in = reg_data_in%n_in
reg_data_out%n_legs_born = reg_data_in%n_legs_born
reg_data_out%n_legs_real = reg_data_in%n_legs_real
if (allocated (reg_data_in%fks_mapping)) then
  select type (fks_mapping_in => reg_data_in%fks_mapping)
  type is (fks_mapping_default_t)
    allocate (fks_mapping_default_t :: reg_data_out%fks_mapping)
    select type (fks_mapping_out => reg_data_out%fks_mapping)
    type is (fks_mapping_default_t)
      fks_mapping_out = fks_mapping_in
    end select
  type is (fks_mapping_resonances_t)
    allocate (fks_mapping_resonances_t :: reg_data_out%fks_mapping)
    select type (fks_mapping_out => reg_data_out%fks_mapping)
    type is (fks_mapping_resonances_t)
      fks_mapping_out = fks_mapping_in
    end select
  end select
else
  call msg_warning ("Copying region data without allocated FKS regions!")
end if
if (allocated (reg_data_in%resonances)) then
  allocate (reg_data_out%resonances (size (reg_data_in%resonances)))
  reg_data_out%resonances = reg_data_in%resonances
end if
reg_data_out%n_phs = reg_data_in%n_phs
if (allocated (reg_data_in%alr_contributors)) then
  allocate (reg_data_out%alr_contributors (size (reg_data_in%alr_contributors)))
  reg_data_out%alr_contributors = reg_data_in%alr_contributors
end if
if (allocated (reg_data_in%alr_to_i_contributor)) then
  allocate (reg_data_out%alr_to_i_contributor &
    (size (reg_data_in%alr_to_i_contributor)))
  reg_data_out%alr_to_i_contributor = reg_data_in%alr_to_i_contributor

```

```

end if
end subroutine region_data_assign

```

Returns the index of the real flavor structure an ftuple belongs to.

(FKS regions: procedures)+≡

```

function region_to_real_index (list, i) result(index)
  type(ftuple_list_t), intent(in), dimension(:), allocatable :: list
  integer, intent(in) :: i
  integer, dimension(:), allocatable :: nreg
  integer :: index, j
  allocate (nreg (0))
  index = 0
  do j = 1, size (list)
    nreg = [nreg, sum (list(:j)%get_n_tuples ())]
    if (j == 1) then
      if (i <= nreg(j)) then
        index = j
        exit
      end if
    else
      if (i > nreg(j - 1) .and. i <= nreg(j)) then
        index = j
        exit
      end if
    end if
  end do
end function region_to_real_index

```

Final state emission: Rearrange the flavor array in such a way that the emitted particle is last and the emitter is second last. *i1* is the index of the emitter, *i2* is the index of the emitted particle.

Initial state emission: Just put the emitted particle to the last position.

(FKS regions: procedures)+≡

```

function create_alr (flv1, n_in, i_em, i_rad) result(flv2)
  type(flv_structure_t), intent(in) :: flv1
  integer, intent(in) :: n_in
  integer, intent(in) :: i_em, i_rad
  type(flv_structure_t) :: flv2
  integer :: n
  n = size (flv1%flst)
  allocate (flv2%flst (n), flv2%tag (n))
  flv2%nlegs = n
  flv2%n_in = n_in
  if (i_em > n_in) then
    flv2%flst(1 : n_in) = flv1%flst(1 : n_in)
    flv2%flst(n - 1) = flv1%flst(i_em)
    flv2%flst(n) = flv1%flst(i_rad)
    flv2%tag(1 : n_in) = flv1%tag(1 : n_in)
    flv2%tag(n - 1) = flv1%tag(i_em)
    flv2%tag(n) = flv1%tag(i_rad)
    call fill_remaining_flavors (n_in, .true.)
  else
    flv2%flst(1 : n_in) = flv1%flst(1 : n_in)

```

```

        flv2%flst(n) = flv1%flst(i_rad)
        flv2%tag(1 : n_in) = flv1%tag(1 : n_in)
        flv2%tag(n) = flv1%tag(i_rad)
        call fill_remaining_flavors (n_in, .false.)
    end if
    call flv2%compute_prt_symm_fs (flv2%n_in)
contains

```

Order remaining particles according to their original position

```

(FKS regions: procedures)+≡
    subroutine fill_remaining_flavors (n_in, final_final)
        integer, intent(in) :: n_in
        logical, intent(in) :: final_final
        integer :: i, j
        logical :: check
        j = n_in + 1
        do i = n_in + 1, n
            if (final_final) then
                check = (i /= i_em .and. i /= i_rad)
            else
                check = (i /= i_rad)
            end if
            if (check) then
                flv2%flst(j) = flv1%flst(i)
                flv2%tag(j) = flv1%tag(i)
                j = j + 1
            end if
        end do
    end subroutine fill_remaining_flavors
end function create_alr

```

```

(FKS regions: reg data: TBP)+≡
    procedure :: has_pseudo_isr => region_data_has_pseudo_isr

```

```

(FKS regions: sub interfaces)+≡
    module function region_data_has_pseudo_isr (reg_data) result (flag)
        logical :: flag
        class(region_data_t), intent(in) :: reg_data
    end function region_data_has_pseudo_isr

```

```

(FKS regions: procedures)+≡
    module function region_data_has_pseudo_isr (reg_data) result (flag)
        logical :: flag
        class(region_data_t), intent(in) :: reg_data
        flag = any (reg_data%regions%pseudo_isr)
    end function region_data_has_pseudo_isr

```

Performs consistency checks on `region_data`. Up to now only checks that no `ftuple` appears more than once.

```

(FKS regions: reg data: TBP)+≡
    procedure :: check_consistency => region_data_check_consistency

```

```

(FKS regions: sub interfaces)+≡
    module subroutine region_data_check_consistency (reg_data, fail_fatal, unit)
        class(region_data_t), intent(in) :: reg_data

```



```

        logical, intent(in) :: fail_fatal
        integer, intent(in), optional :: unit
    end subroutine region_data_check_consistency

(FKS regions: procedures)+≡
module subroutine region_data_check_consistency (reg_data, fail_fatal, unit)
    class(region_data_t), intent(in) :: reg_data
    logical, intent(in) :: fail_fatal
    integer, intent(in), optional :: unit
    integer :: u
    integer :: i_reg, alr
    integer :: i1, f1, f2
    logical :: undefined_ftuples, same_ftuple_indices, valid_splitting
    logical, dimension(4) :: no_fail
    u = given_output_unit(unit); if (u < 0) return
    no_fail = .true.
    call msg_message ("Check that no negative ftuple indices occur", unit = u)
    do i_reg = 1, reg_data%n_regions
        if (any (reg_data%regions(i_reg)%ftuples%has_negative_elements ())) then
            !!! This error is so severe that we stop immediately
            call msg_fatal ("Negative ftuple indices!")
        end if
    end do
    call msg_message ("Success!", unit = u)
    call msg_message ("Check that there is no ftuple with identical elements", unit = u)
    do i_reg = 1, reg_data%n_regions
        if (any (reg_data%regions(i_reg)%ftuples%has_identical_elements ())) then
            !!! This error is so severe that we stop immediately
            call msg_fatal ("Identical ftuple indices!")
        end if
    end do
    call msg_message ("Success!", unit = u)
    call msg_message ("Check that there are no duplicate ftuples in a region", unit = u)
    do i_reg = 1, reg_data%n_regions
        if (reg_data%regions(i_reg)%has_identical_ftuples ()) then
            if (no_fail(1)) then
                call msg_error ("FAIL: ", unit = u)
                no_fail(1) = .false.
            end if
            write (u, '(A,1x,I3)') 'i_reg:', i_reg
        end if
    end do
    if (no_fail(1)) call msg_message ("Success!", unit = u)
    call msg_message ("Check that ftuples add up to a valid splitting", unit = u)
    do i_reg = 1, reg_data%n_regions
        do alr = 1, reg_data%regions(i_reg)%nregions
            associate (region => reg_data%regions(i_reg))
                i1 = region%ftuples(alr)%ireg(1)
                if (i1 == 0) i1 = 1 !!! Gluon emission from both initial-state particles
                f1 = region%flst_real%flst(i1)
                f2 = region%flst_real%flst(region%ftuples(alr)%ireg(2))
                ! Flip PDG sign of IS fermions to allow a q -> g q splitting
                ! in which the ftuple has the flavors (q,q).
                if (i1 <= reg_data%n_in .and. is_fermion(f1)) then
                    f1 = -f1
                end if
            end associate
        end do
    end do

```

```

        end if
        valid_splitting = f1 + f2 == 0 &
            .or. (is_gluon(f1) .and. is_gluon(f2)) &
            .or. (is_massive_vector(f1) .and. is_photon(f2)) &
            .or. is_fermion_vector_splitting (f1, f2)
        if (.not. valid_splitting) then
            if (no_fail(2)) then
                call msg_error ("FAIL: ", unit = u)
                no_fail(2) = .false.
            end if
            write (u, '(A,1x,I3)') 'i_reg:', i_reg
            exit
        end if
    end associate
end do
end do
if (no_fail(2)) call msg_message ("Success!", unit = u)
call msg_message ("Check that at least one ftuple contains the emitter", unit = u)
do i_reg = 1, reg_data%n_regions
    associate (region => reg_data%regions(i_reg))
        if (.not. any (region%emitter == region%ftuples%ireg(1))) then
            if (no_fail(3)) then
                call msg_error ("FAIL: ", unit = u)
                no_fail(3) = .false.
            end if
            write (u, '(A,1x,I3)') 'i_reg:', i_reg
        end if
    end associate
end do
if (no_fail(3)) call msg_message ("Success!", unit = u)
call msg_message ("Check that each region has at least one ftuple &
    &with index n + 1", unit = u)
do i_reg = 1, reg_data%n_regions
    if (.not. any (reg_data%regions(i_reg)%ftuples%ireg(2) == reg_data%n_legs_real)) then
        if (no_fail(4)) then
            call msg_error ("FAIL: ", unit = u)
            no_fail(4) = .false.
        end if
        write (u, '(A,1x,I3)') 'i_reg:', i_reg
    end if
end do
if (no_fail(4)) call msg_message ("Success!", unit = u)
if (.not. all (no_fail)) &
    call abort_with_message ("Stop due to inconsistent region data!")

contains
subroutine abort_with_message (msg)
    character(len=*), intent(in) :: msg
    if (fail_fatal) then
        call msg_fatal (msg)
    else
        call msg_error (msg, unit = u)
    end if
end subroutine abort_with_message

```

```

function is_fermion_vector_splitting (pdg_1, pdg_2) result (value)
  logical :: value
  integer, intent(in) :: pdg_1, pdg_2
  value = (is_fermion (pdg_1) .and. is_massless_vector (pdg_2)) .or. &
    (is_fermion (pdg_2) .and. is_massless_vector (pdg_1))
end function
end subroutine region_data_check_consistency

```

<FKS regions: reg data: TBP>+≡

```

procedure :: requires_spin_correlations => &
  region_data_requires_spin_correlations

```

<FKS regions: sub interfaces>+≡

```

module function region_data_requires_spin_correlations &
  (reg_data) result (flag)
  class(region_data_t), intent(in) :: reg_data
  logical :: flag
end function region_data_requires_spin_correlations

```

<FKS regions: procedures>+≡

```

module function region_data_requires_spin_correlations &
  (reg_data) result (flag)
  class(region_data_t), intent(in) :: reg_data
  logical :: flag
  integer :: alr
  flag = .false.
  do alr = 1, reg_data%n_regions
    flag = reg_data%regions(alr)%sc_required
    if (flag) return
  end do
end function region_data_requires_spin_correlations

```

We have to apply the symmetry factor for identical particles of the real flavor structure to the born squared matrix element. The corresponding factor from the born flavor structure has to be cancelled.

<FKS regions: reg data: TBP>+≡

```

procedure :: born_to_real_symm_factor_fs => &
  region_data_born_to_real_symm_factor_fs

```

<FKS regions: sub interfaces>+≡

```

module function region_data_born_to_real_symm_factor_fs &
  (reg_data, alr) result (factor)
  class(region_data_t), intent(in) :: reg_data
  integer, intent(in) :: alr
  real(default) :: factor
end function region_data_born_to_real_symm_factor_fs

```

<FKS regions: procedures>+≡

```

module function region_data_born_to_real_symm_factor_fs &
  (reg_data, alr) result (factor)
  class(region_data_t), intent(in) :: reg_data
  integer, intent(in) :: alr
  real(default) :: factor
  associate (flv_real => reg_data%regions(alr)%flst_real, &

```

```

        flv_uborn => reg_data%regions(alr)%flst_uborn
        factor = flv_real%prt_symm_fs / flv_uborn%prt_symm_fs
    end associate
end function region_data_born_to_real_symm_factor_fs

<FKS regions: reg data: TBP>+≡
    procedure :: final => region_data_final

<FKS regions: sub interfaces>+≡
    module subroutine region_data_final (reg_data)
        class(region_data_t), intent(inout) :: reg_data
    end subroutine region_data_final

<FKS regions: procedures>+≡
    module subroutine region_data_final (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        if (allocated (reg_data%regions)) deallocate (reg_data%regions)
        if (allocated (reg_data%flv_born)) deallocate (reg_data%flv_born)
        if (allocated (reg_data%flv_real)) deallocate (reg_data%flv_real)
        if (allocated (reg_data%emitters)) deallocate (reg_data%emitters)
        if (allocated (reg_data%fks_mapping)) deallocate (reg_data%fks_mapping)
        if (allocated (reg_data%resonances)) deallocate (reg_data%resonances)
        if (allocated (reg_data%alr_contributors)) &
            deallocate (reg_data%alr_contributors)
        if (allocated (reg_data%alr_to_i_contributor)) &
            deallocate (reg_data%alr_to_i_contributor)
    end subroutine region_data_final

<FKS regions: fks mapping: TBP>≡
    procedure (fks_mapping_dij), deferred :: dij

<FKS regions: interfaces>+≡
    abstract interface
        function fks_mapping_dij (map, p, i, j, i_con) result (d)
            import
            real(default) :: d
            class(fks_mapping_t), intent(in) :: map
            type(vector4_t), intent(in), dimension(:) :: p
            integer, intent(in) :: i, j
            integer, intent(in), optional :: i_con
        end function fks_mapping_dij
    end interface

<FKS regions: fks mapping: TBP>+≡
    procedure (fks_mapping_compute_sumdij), deferred :: compute_sumdij

<FKS regions: interfaces>+≡
    abstract interface
        subroutine fks_mapping_compute_sumdij (map, sregion, p_real)
            import
            class(fks_mapping_t), intent(inout) :: map
            type(singular_region_t), intent(in) :: sregion
            type(vector4_t), intent(in), dimension(:) :: p_real
        end subroutine fks_mapping_compute_sumdij
    end interface

```

```

<FKS regions: fks mapping: TBP>+≡
  procedure (fks_mapping_svalue), deferred :: svalue

<FKS regions: interfaces>+≡
  abstract interface
    function fks_mapping_svalue (map, p, i, j, i_res) result (value)
      import
      real(default) :: value
      class(fks_mapping_t), intent(in) :: map
      type(vector4_t), intent(in), dimension(:) :: p
      integer, intent(in) :: i, j
      integer, intent(in), optional :: i_res
    end function fks_mapping_svalue
  end interface

  procedure (fks_mapping_dij_soft), deferred :: dij_soft

<FKS regions: interfaces>+≡
  abstract interface
    function fks_mapping_dij_soft (map, p_born, p_soft, em, i_con) result (d)
      import
      real(default) :: d
      class(fks_mapping_t), intent(in) :: map
      type(vector4_t), intent(in), dimension(:) :: p_born
      type(vector4_t), intent(in) :: p_soft
      integer, intent(in) :: em
      integer, intent(in), optional :: i_con
    end function fks_mapping_dij_soft
  end interface

  procedure (fks_mapping_compute_sumdij_soft), deferred :: compute_sumdij_soft

<FKS regions: interfaces>+≡
  abstract interface
    subroutine fks_mapping_compute_sumdij_soft (map, sregion, p_born, p_soft)
      import
      class(fks_mapping_t), intent(inout) :: map
      type(singular_region_t), intent(in) :: sregion
      type(vector4_t), intent(in), dimension(:) :: p_born
      type(vector4_t), intent(in) :: p_soft
    end subroutine fks_mapping_compute_sumdij_soft
  end interface

  procedure (fks_mapping_svalue_soft), deferred :: svalue_soft

<FKS regions: interfaces>+≡
  abstract interface
    function fks_mapping_svalue_soft (map, p_born, p_soft, em, i_res) result (value)
      import
      real(default) :: value
      class(fks_mapping_t), intent(in) :: map
      type(vector4_t), intent(in), dimension(:) :: p_born
      type(vector4_t), intent(in) :: p_soft

```

```

integer, intent(in) :: em
integer, intent(in), optional :: i_res
end function fks_mapping_svalue_soft
end interface

```

```

(FKS regions: fks mapping default: TBP)≡
  procedure :: set_parameter => fks_mapping_default_set_parameter

```

```

(FKS regions: sub interfaces)+≡
  module subroutine fks_mapping_default_set_parameter &
    (map, n_in, dij_exp1, dij_exp2)
    class(fks_mapping_default_t), intent(inout) :: map
    integer, intent(in) :: n_in
    real(default), intent(in) :: dij_exp1, dij_exp2
  end subroutine fks_mapping_default_set_parameter

```

```

(FKS regions: procedures)+≡
  module subroutine fks_mapping_default_set_parameter &
    (map, n_in, dij_exp1, dij_exp2)
    class(fks_mapping_default_t), intent(inout) :: map
    integer, intent(in) :: n_in
    real(default), intent(in) :: dij_exp1, dij_exp2
    map%n_in = n_in
    map%exp_1 = dij_exp1
    map%exp_2 = dij_exp2
  end subroutine fks_mapping_default_set_parameter

```

Computes the d_{ij} -quantities defined als follows:

$$\begin{aligned}
d_{0i} &= [E_i^2 (1 - y_i)]^{p_2} \\
, d_{1i} &= [2E_i^2 (1 - y_i)]^{p_2} \\
, d_{2i} &= [2E_i^2 (1 + y_i)]^{p_2} \\
, &
\end{aligned}$$

for initial state regions and

$$d_{ij} = \left[2(k_i \cdot k_j) \frac{E_i E_j}{(E_i + E_j)^2} \right]^{p_1}$$

for final state regions, c.f. [1002.2581, Eq. 4.23f]. The exponents p_1 and p_2 can be used for tuning the efficiency of the mapping and are set to 1 per default.

```

(FKS regions: fks mapping default: TBP)+≡
  procedure :: dij => fks_mapping_default_dij

(FKS regions: sub interfaces)+≡
  module function fks_mapping_default_dij (map, p, i, j, i_con) result (d)
    real(default) :: d
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_con
  end function fks_mapping_default_dij

```

<FKS regions: procedures>+≡

```

module function fks_mapping_default_dij (map, p, i, j, i_con) result (d)
  real(default) :: d
  class(fks_mapping_default_t), intent(in) :: map
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: i, j
  integer, intent(in), optional :: i_con
  d = zero
  if (map%pseudo_isr) then
    d = dij_threshold_gluon_from_top (i, j, p, map%exp_1)
  else if (i > map%n_in .and. j > map%n_in) then
    d = dij_fsr (p(i), p(j), map%exp_1)
  else
    d = dij_isr (map%n_in, i, j, p, map%exp_2)
  end if
contains

  function dij_fsr (p1, p2, expo) result (d_ij)
    real(default) :: d_ij
    type(vector4_t), intent(in) :: p1, p2
    real(default), intent(in) :: expo
    real(default) :: E1, E2
    E1 = p1%p(0); E2 = p2%p(0)
    d_ij = (two * p1 * p2 * E1 * E2 / (E1 + E2)**2)**expo
  end function dij_fsr

  function dij_threshold_gluon_from_top (i, j, p, expo) result (d_ij)
    real(default) :: d_ij
    integer, intent(in) :: i, j
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: expo
    type(vector4_t) :: p_top
    if (i == THR_POS_B) then
      p_top = p(THR_POS_WP) + p(THR_POS_B)
    else
      p_top = p(THR_POS_WM) + p(THR_POS_BBAR)
    end if
    d_ij = dij_fsr (p_top, p(j), expo)
  end function dij_threshold_gluon_from_top

  function dij_isr (n_in, i, j, p, expo) result (d_ij)
    real(default) :: d_ij
    integer, intent(in) :: n_in, i, j
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: expo
    real(default) :: E, y
    select case (n_in)
    case (1)
      call get_emitter_variables (1, i, j, p, E, y)
      d_ij = (E**2 * (one - y**2))**expo
    case (2)
      if ((i == 0 .and. j > 2) .or. (j == 0 .and. i > 2)) then
        call get_emitter_variables (0, i, j, p, E, y)
        d_ij = (E**2 * (one - y**2))**expo
      end if
    end select
  end function dij_isr

```

```

        else if ((i == 1 .and. j > 2) .or. (j == 1 .and. i > 2)) then
            call get_emitter_variables (1, i, j, p, E, y)
            d_ij = (two * E**2 * (one - y))**expo
        else if ((i == 2 .and. j > 2) .or. (j == 2 .and. i > 2)) then
            call get_emitter_variables (2, i, j, p, E, y)
            d_ij = (two * E**2 * (one + y))**expo
        end if
    end select
end function dij_isr

subroutine get_emitter_variables (i_check, i, j, p, E, y)
    integer, intent(in) :: i_check, i, j
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(out) :: E, y
    if (j == i_check) then
        E = energy (p(i))
        y = polar_angle_ct (p(i))
    else
        E = energy (p(j))
        y = polar_angle_ct(p(j))
    end if
end subroutine get_emitter_variables

end function fks_mapping_default_dij

```

Computes the quantity

$$\mathcal{D} = \sum_k \frac{1}{d_{0k}} + \sum_{kl} \frac{1}{d_{kl}}.$$

where the sum goes over all ftuples of a single singular region.

(FKS regions: fks_mapping_default: TBP)+≡

```

    procedure :: compute_sumdij => fks_mapping_default_compute_sumdij

```

(FKS regions: sub interfaces)+≡

```

    module subroutine fks_mapping_default_compute_sumdij (map, sregion, p_real)
        class(fks_mapping_default_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_real
    end subroutine fks_mapping_default_compute_sumdij

```

(FKS regions: procedures)+≡

```

    module subroutine fks_mapping_default_compute_sumdij (map, sregion, p_real)
        class(fks_mapping_default_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_real
        real(default) :: d
        integer :: i_ftuple, i, j

        associate (ftuples => sregion%ftuples)
            d = zero
            do i_ftuple = 1, sregion%nregions
                call ftuples(i_ftuple)%get (i, j)
                map%pseudo_isr = ftuples(i_ftuple)%pseudo_isr
                d = d + one / map%dij (p_real, i, j)
            end do
        end associate
    end subroutine fks_mapping_default_compute_sumdij

```



```

        end do
    end associate
    map%sumdij = d
end subroutine fks_mapping_default_compute_sumdij

```

Computes

$$S_i = \frac{1}{\mathcal{D}d_{0i}}$$

or

$$S_{ij} = \frac{1}{\mathcal{D}d_{ij}},$$

respectively.

```

<FKS regions: fks mapping default: TBP>+=
  procedure :: svalue => fks_mapping_default_svalue

<FKS regions: sub interfaces>+=
  module function fks_mapping_default_svalue &
    (map, p, i, j, i_res) result (value)
    real(default) :: value
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_res
  end function fks_mapping_default_svalue

<FKS regions: procedures>+=
  module function fks_mapping_default_svalue &
    (map, p, i, j, i_res) result (value)
    real(default) :: value
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_res
    value = one / (map%dij (p, i, j) * map%sumdij)
  end function fks_mapping_default_svalue

```

In the soft limit, our treatment of the divergencies requires a modification of the mapping functions. Recall that there, the ratios of the d -functions must approach either 1 or 0. This means

$$\frac{d_{lm}}{d_{0m}} = \frac{(2k_l \cdot k_m) [E_l E_m / (E_l + E_m)^2]}{E_m^2 (1 - y^2)} \Big|_{k_m = E_m \hat{k}} \frac{E_l E_m^2}{(E_l + E_m)^2} \frac{2k_l \cdot \hat{k}}{E_m^2 (1 - y^2)} \xrightarrow{E_m \rightarrow 0} \frac{2k_l \cdot \hat{k}}{E_l} (1 - y^2),$$

where we have written the gluon momentum in terms of the soft momentum \hat{k} . In the same limit

$$\frac{d_{lm}}{d_{nm}} = \frac{k_l \cdot \hat{k}}{k_n \cdot \hat{k}} \frac{E_n}{E_l}.$$

From these equations we can deduce the soft limit of d :

$$\begin{aligned} d_0^{\text{soft}} &= 1 - y^2, \\ d_1^{\text{soft}} &= 2(1 - y), \\ d_2^{\text{soft}} &= 2(1 + y), \\ d_i^{\text{soft}} &= \frac{2k_i \cdot \hat{k}}{E_i}. \end{aligned}$$

```

(FKS regions: fks mapping default: TBP)+≡
  procedure :: dij_soft => fks_mapping_default_dij_soft

(FKS regions: sub interfaces)+≡
  module function fks_mapping_default_dij_soft &
    (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
  end function fks_mapping_default_dij_soft

(FKS regions: procedures)+≡
  module function fks_mapping_default_dij_soft &
    (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
    if (map%pseudo_isr) then
      d = dij_soft_threshold_gluon_from_top (em, p_born, p_soft, map%exp_1)
    else if (em <= map%n_in) then
      d = dij_soft_isr (map%n_in, p_soft, map%exp_2)
    else
      d = dij_soft_fsr (p_born(em), p_soft, map%exp_1)
    end if
  contains

  function dij_soft_threshold_gluon_from_top &
    (em, p_born, p_soft, expo) result (dij_soft)
    real(default) :: dij_soft
    integer, intent(in) :: em
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    real(default), intent(in) :: expo
    type(vector4_t) :: p_top
    if (em == THR_POS_B) then
      p_top = p_born(THR_POS_WP) + p_born(THR_POS_B)
    else
      p_top = p_born(THR_POS_WM) + p_born(THR_POS_BBAR)
    end if
    dij_soft = dij_soft_fsr (p_top, p_soft, expo)

```

```

end function dij_soft_threshold_gluon_from_top

function dij_soft_fsr (p_em, p_soft, expo) result (dij_soft)
  real(default) :: dij_soft
  type(vector4_t), intent(in) :: p_em, p_soft
  real(default), intent(in) :: expo
  dij_soft = (two * p_em * p_soft / p_em%p(0))**expo
end function dij_soft_fsr

function dij_soft_isr (n_in, p_soft, expo) result (dij_soft)
  real(default) :: dij_soft
  integer, intent(in) :: n_in
  type(vector4_t), intent(in) :: p_soft
  real(default), intent(in) :: expo
  real(default) :: y
  y = polar_angle_ct (p_soft)
  select case (n_in)
  case (1)
    dij_soft = one - y**2
  case (2)
    select case (em)
    case (0)
      dij_soft = one - y**2
    case (1)
      dij_soft = two * (one - y)
    case (2)
      dij_soft = two * (one + y)
    case default
      dij_soft = zero
      call msg_fatal ("fks_mappings_default_dij_soft: n_in > 2")
    end select
  case default
    dij_soft = zero
    call msg_fatal ("fks_mappings_default_dij_soft: n_in > 2")
  end select
  dij_soft = dij_soft**expo
end function dij_soft_isr
end function fks_mapping_default_dij_soft

```

Computes the sum of all soft dijs required to normalize the soft S functions `s_alpha_soft` similar to `fks_mapping_default_compute_sumdij`. In the soft limit however, we need to skip all ftuples (i, j) in which j does not correspond to the emitted particle because those d_{ij} s are finite and thus their contribution to the soft S function vanishes in the limit of soft radiation. Technically, they would not vanish if computed here because the fixed `p_soft` at this point would not fit their actual emitter.

```

<FKS regions: fks mapping default: TBP>+≡
  procedure :: compute_sumdij_soft => fks_mapping_default_compute_sumdij_soft
<FKS regions: sub interfaces>+≡
  module subroutine fks_mapping_default_compute_sumdij_soft &
    (map, sregion, p_born, p_soft)
    class(fks_mapping_default_t), intent(inout) :: map
    type(singular_region_t), intent(in) :: sregion

```

```

        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
    end subroutine fks_mapping_default_compute_sumdij_soft

<FKS regions: procedures>+≡
    module subroutine fks_mapping_default_compute_sumdij_soft &
        (map, sregion, p_born, p_soft)
        class(fks_mapping_default_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
        real(default) :: d
        integer :: i_ftuple, i, j
        integer :: nlegs
        d = zero
        nlegs = size (sregion%flst_real%flst)
        associate (ftuples => sregion%ftuples)
            do i_ftuple = 1, sregion%nregions
                call ftuples(i_ftuple)%get (i ,j)
                if (j == nlegs) then
                    map%pseudo_isr = ftuples(i_ftuple)%pseudo_isr
                    d = d + one / map%dij_soft (p_born, p_soft, i)
                end if
            end do
        end associate
        map%sumdij_soft = d
    end subroutine fks_mapping_default_compute_sumdij_soft

<FKS regions: fks mapping default: TBP>+≡
    procedure :: svalue_soft => fks_mapping_default_svalue_soft

<FKS regions: sub interfaces>+≡
    module function fks_mapping_default_svalue_soft &
        (map, p_born, p_soft, em, i_res) result (value)
        real(default) :: value
        class(fks_mapping_default_t), intent(in) :: map
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
        integer, intent(in) :: em
        integer, intent(in), optional :: i_res
    end function fks_mapping_default_svalue_soft

<FKS regions: procedures>+≡
    module function fks_mapping_default_svalue_soft &
        (map, p_born, p_soft, em, i_res) result (value)
        real(default) :: value
        class(fks_mapping_default_t), intent(in) :: map
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
        integer, intent(in) :: em
        integer, intent(in), optional :: i_res
        value = one / (map%sumdij_soft * map%dij_soft (p_born, p_soft, em))
    end function fks_mapping_default_svalue_soft

```

```

<FKS regions: interfaces>+≡
  interface assignment(=)
    module procedure fks_mapping_default_assign
  end interface

<FKS regions: sub interfaces>+≡
  module subroutine fks_mapping_default_assign (fks_map_out, fks_map_in)
    type(fks_mapping_default_t), intent(out) :: fks_map_out
    type(fks_mapping_default_t), intent(in) :: fks_map_in
  end subroutine fks_mapping_default_assign

<FKS regions: procedures>+≡
  module subroutine fks_mapping_default_assign (fks_map_out, fks_map_in)
    type(fks_mapping_default_t), intent(out) :: fks_map_out
    type(fks_mapping_default_t), intent(in) :: fks_map_in
    fks_map_out%exp_1 = fks_map_in%exp_1
    fks_map_out%exp_2 = fks_map_in%exp_2
    fks_map_out%n_in = fks_map_in%n_in
  end subroutine fks_mapping_default_assign

```

The $d_{ij,k}$ -functions for the resonance mapping are basically the same as in the default case, but the kinematical values here must be evaluated in the resonance frame of reference. The energy of parton i in a given resonance frame with momentum p_{res} is

$$E_i = \frac{p_i^0 \cdot p_{res}}{m_{res}}.$$

However, since the expressions only depend on ratios of four-momenta, we leave out the denominator because it will cancel out anyway.

```

<FKS regions: fks mapping resonances: TBP>≡
  procedure :: dij => fks_mapping_resonances_dij

<FKS regions: sub interfaces>+≡
  module function fks_mapping_resonances_dij (map, p, i, j, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_con
  end function fks_mapping_resonances_dij

<FKS regions: procedures>+≡
  module function fks_mapping_resonances_dij (map, p, i, j, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_con
    real(default) :: E1, E2
    integer :: ii_con
    if (present (i_con)) then
      ii_con = i_con
    else
      call msg_fatal ("Resonance mappings require resonance index as input!")
    end if
  end function

```

```

d = 0
if (i /= j) then
  if (i > 2 .and. j > 2) then
    associate (p_res => map%res_map%p_res (ii_con))
      E1 = p(i) * p_res
      E2 = p(j) * p_res
      d = two * p(i) * p(j) * E1 * E2 / (E1 + E2)**2
    end associate
  else
    call msg_fatal ("Resonance mappings are not implemented for ISR")
  end if
end if
end function fks_mapping_resonances_dij

```

Computes

$$S_{\alpha} = \frac{P^{f_r(\alpha)} d^{-1}(\alpha)}{\sum_{f'_r \in T(F_r(\alpha))} P^{f'_r} \sum_{\alpha' \in S_r(f'_r)} d^{-1}(\alpha')}.$$

(FKS regions: fks mapping resonances: TBP)+≡

```

procedure :: compute_sumdij => fks_mapping_resonances_compute_sumdij

```

(FKS regions: sub interfaces)+≡

```

module subroutine fks_mapping_resonances_compute_sumdij &
  (map, sregion, p_real)
  class(fks_mapping_resonances_t), intent(inout) :: map
  type(singular_region_t), intent(in) :: sregion
  type(vector4_t), intent(in), dimension(:) :: p_real
end subroutine fks_mapping_resonances_compute_sumdij

```

(FKS regions: procedures)+≡

```

module subroutine fks_mapping_resonances_compute_sumdij (map, sregion, p_real)
  class(fks_mapping_resonances_t), intent(inout) :: map
  type(singular_region_t), intent(in) :: sregion
  type(vector4_t), intent(in), dimension(:) :: p_real
  real(default) :: d, pfr
  integer :: i_res, i_reg, i, j, i_con
  integer :: nlegreal

  nlegreal = size (p_real)
  d = zero
  do i_reg = 1, sregion%nregions
    associate (ftuple => sregion%ftuples(i_reg))
      call ftuple%get (i, j)
      i_res = ftuple%i_res
    end associate
    pfr = map%res_map%get_resonance_value (i_res, p_real, nlegreal)
    i_con = sregion%i_reg_to_i_con (i_reg)
    d = d + pfr / map%dij (p_real, i, j, i_con)
  end do
  map%sumdij = d
end subroutine fks_mapping_resonances_compute_sumdij

```

(FKS regions: fks mapping resonances: TBP)+≡

```

procedure :: svalue => fks_mapping_resonances_svalue

```

```

(FKS regions: sub interfaces)+≡
  module function fks_mapping_resonances_svalue &
    (map, p, i, j, i_res) result (value)
    real(default) :: value
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_res
  end function fks_mapping_resonances_svalue

(FKS regions: procedures)+≡
  module function fks_mapping_resonances_svalue &
    (map, p, i, j, i_res) result (value)
    real(default) :: value
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_res
    real(default) :: pfr
    integer :: i_gluon
    i_gluon = size (p)
    pfr = map%res_map%get_resonance_value (i_res, p, i_gluon)
    value = pfr / (map%dij (p, i, j, map%i_con) * map%sumdij)
  end function fks_mapping_resonances_svalue

(FKS regions: fks mapping resonances: TBP)+≡
  procedure :: get_resonance_weight => &
    fks_mapping_resonances_get_resonance_weight

(FKS regions: sub interfaces)+≡
  module function fks_mapping_resonances_get_resonance_weight &
    (map, alr, p) result (pfr)
    real(default) :: pfr
    class(fks_mapping_resonances_t), intent(in) :: map
    integer, intent(in) :: alr
    type(vector4_t), intent(in), dimension(:) :: p
  end function fks_mapping_resonances_get_resonance_weight

(FKS regions: procedures)+≡
  module function fks_mapping_resonances_get_resonance_weight &
    (map, alr, p) result (pfr)
    real(default) :: pfr
    class(fks_mapping_resonances_t), intent(in) :: map
    integer, intent(in) :: alr
    type(vector4_t), intent(in), dimension(:) :: p
    pfr = map%res_map%get_weight (alr, p)
  end function fks_mapping_resonances_get_resonance_weight

```

As above, the soft limit of $d_{ij,k}$ must be computed in the resonance frame of reference.

```

(FKS regions: fks mapping resonances: TBP)+≡
  procedure :: dij_soft => fks_mapping_resonances_dij_soft

(FKS regions: sub interfaces)+≡
  module function fks_mapping_resonances_dij_soft &

```

```

        (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
end function fks_mapping_resonances_dij_soft

<FKS regions: procedures>+≡
module function fks_mapping_resonances_dij_soft &
    (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
    real(default) :: E1, E2
    integer :: ii_con
    type(vector4_t) :: pb
    if (present (i_con)) then
        ii_con = i_con
    else
        call msg_fatal ("fks_mapping_resonances requires resonance index")
    end if
    associate (p_res => map%res_map%p_res(ii_con))
        pb = p_born(em)
        E1 = pb * p_res
        E2 = p_soft * p_res
        d = two * pb * p_soft * E1 * E2 / E1**2
    end associate
end function fks_mapping_resonances_dij_soft

<FKS regions: fks mapping resonances: TBP>+≡
procedure :: compute_sumdij_soft => fks_mapping_resonances_compute_sumdij_soft

<FKS regions: sub interfaces>+≡
module subroutine fks_mapping_resonances_compute_sumdij_soft &
    (map, sregion, p_born, p_soft)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(singular_region_t), intent(in) :: sregion
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
end subroutine fks_mapping_resonances_compute_sumdij_soft

<FKS regions: procedures>+≡
module subroutine fks_mapping_resonances_compute_sumdij_soft &
    (map, sregion, p_born, p_soft)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(singular_region_t), intent(in) :: sregion
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    real(default) :: d
    real(default) :: pfr

```



```

integer :: i_res, i, j, i_reg, i_con
integer :: nlegs

d = zero
nlegs = size (sregion%flst_real%flst)
do i_reg = 1, sregion%nregions
  associate (ftuple => sregion%ftuples(i_reg))
    call ftuple%get(i, j)
    i_res = ftuple%i_res
  end associate
  pfr = map%res_map%get_resonance_value (i_res, p_born)
  i_con = sregion%i_reg_to_i_con (i_reg)
  if (j == nlegs) d = d + pfr / map%dij_soft (p_born, p_soft, i, i_con)
end do
map%sumdij_soft = d
end subroutine fks_mapping_resonances_compute_sumdij_soft

```

(FKS regions: fks mapping resonances: TBP)+≡
 procedure :: svalue_soft => fks_mapping_resonances_svalue_soft

(FKS regions: sub interfaces)+≡
 module function fks_mapping_resonances_svalue_soft &
 (map, p_born, p_soft, em, i_res) result (value)
 real(default) :: value
 class(fks_mapping_resonances_t), intent(in) :: map
 type(vector4_t), intent(in), dimension(:) :: p_born
 type(vector4_t), intent(in) :: p_soft
 integer, intent(in) :: em
 integer, intent(in), optional :: i_res
 end function fks_mapping_resonances_svalue_soft

(FKS regions: procedures)+≡
 module function fks_mapping_resonances_svalue_soft &
 (map, p_born, p_soft, em, i_res) result (value)
 real(default) :: value
 class(fks_mapping_resonances_t), intent(in) :: map
 type(vector4_t), intent(in), dimension(:) :: p_born
 type(vector4_t), intent(in) :: p_soft
 integer, intent(in) :: em
 integer, intent(in), optional :: i_res
 real(default) :: pfr
 pfr = map%res_map%get_resonance_value (i_res, p_born)
 value = pfr / (map%sumdij_soft * map%dij_soft &
 (p_born, p_soft, em, map%i_con))
 end function fks_mapping_resonances_svalue_soft

(FKS regions: fks mapping resonances: TBP)+≡
 procedure :: set_resonance_momentum => &
 fks_mapping_resonances_set_resonance_momentum

(FKS regions: sub interfaces)+≡
 module subroutine fks_mapping_resonances_set_resonance_momentum (map, p)
 class(fks_mapping_resonances_t), intent(inout) :: map
 type(vector4_t), intent(in) :: p
 end subroutine fks_mapping_resonances_set_resonance_momentum

```

<FKS regions: procedures>+≡
  module subroutine fks_mapping_resonances_set_resonance_momentum (map, p)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(vector4_t), intent(in) :: p
    map%res_map%p_res = p
  end subroutine fks_mapping_resonances_set_resonance_momentum

<FKS regions: fks mapping resonances: TBP>+≡
  procedure :: set_resonance_momenta => &
    fks_mapping_resonances_set_resonance_momenta

<FKS regions: sub interfaces>+≡
  module subroutine fks_mapping_resonances_set_resonance_momenta (map, p)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(vector4_t), intent(in), dimension(:) :: p
  end subroutine fks_mapping_resonances_set_resonance_momenta

<FKS regions: procedures>+≡
  module subroutine fks_mapping_resonances_set_resonance_momenta (map, p)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    map%res_map%p_res = p
  end subroutine fks_mapping_resonances_set_resonance_momenta

<FKS regions: interfaces>+≡
  interface assignment(=)
    module procedure fks_mapping_resonances_assign
  end interface

<FKS regions: sub interfaces>+≡
  module subroutine fks_mapping_resonances_assign (fks_map_out, fks_map_in)
    type(fks_mapping_resonances_t), intent(out) :: fks_map_out
    type(fks_mapping_resonances_t), intent(in) :: fks_map_in
  end subroutine fks_mapping_resonances_assign

<FKS regions: procedures>+≡
  module subroutine fks_mapping_resonances_assign (fks_map_out, fks_map_in)
    type(fks_mapping_resonances_t), intent(out) :: fks_map_out
    type(fks_mapping_resonances_t), intent(in) :: fks_map_in
    fks_map_out%exp_1 = fks_map_in%exp_1
    fks_map_out%exp_2 = fks_map_in%exp_2
    fks_map_out%res_map = fks_map_in%res_map
  end subroutine fks_mapping_resonances_assign

<FKS regions: public>+≡
  public :: create_resonance_histories_for_threshold

<FKS regions: sub interfaces>+≡
  module function create_resonance_histories_for_threshold &
    () result (res_history)
    type(resonance_history_t) :: res_history
  end function create_resonance_histories_for_threshold

```

<FKS regions: procedures>+≡

```

module function create_resonance_histories_for_threshold &
  () result (res_history)
  type(resonance_history_t) :: res_history
  res_history%n_resonances = 2
  allocate (res_history%resonances (2))
  allocate (res_history%resonances(1)%contributors%c(2))
  allocate (res_history%resonances(2)%contributors%c(2))
  res_history%resonances(1)%contributors%c = [THR_POS_WP, THR_POS_B]
  res_history%resonances(2)%contributors%c = [THR_POS_WM, THR_POS_BBAR]
end function create_resonance_histories_for_threshold

```

<FKS regions: public>+≡

```

public :: setup_region_data_for_test

```

<FKS regions: sub interfaces>+≡

```

module subroutine setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, &
  nlo_corr_type, alpha_pow, alphas_pow)
  integer, intent(in) :: n_in, alpha_pow, alphas_pow
  integer, intent(in), dimension(:, :) :: flv_born, flv_real
  type(string_t), intent(in) :: nlo_corr_type
  type(region_data_t), intent(out) :: reg_data
end subroutine setup_region_data_for_test

```

<FKS regions: procedures>+≡

```

module subroutine setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, &
  nlo_corr_type, alpha_pow, alphas_pow)
  integer, intent(in) :: n_in, alpha_pow, alphas_pow
  integer, intent(in), dimension(:, :) :: flv_born, flv_real
  type(string_t), intent(in) :: nlo_corr_type
  type(region_data_t), intent(out) :: reg_data
  type(model_t), pointer :: test_model => null ()
  call create_test_model (var_str ("SM"), test_model)
  call test_model%set_real (var_str ("me"), 0._default)
  call test_model%set_real (var_str ("mmu"), 0._default)
  call test_model%set_real (var_str ("mtau"), 0._default)
  call test_model%set_real (var_str ("ms"), 0._default)
  call test_model%set_real (var_str ("mc"), 0._default)
  call test_model%set_real (var_str ("mb"), 0._default)
  call reg_data%init (n_in, test_model, flv_born, flv_real, nlo_corr_type, alpha_pow, &
    alphas_pow)
end subroutine setup_region_data_for_test

```

27.3.1 Unit tests

```

<fks_regions_ut.f90>≡
  <File header>

  module fks_regions_ut
    use unit_tests
    use fks_regions_uti

    <Standard module head>

    <FKS regions: public test>

    contains

    <FKS regions: test driver>

  end module fks_regions_ut
<fks_regions_uti.f90>≡
  <File header>

  module fks_regions_uti

    <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use models

    use fks_regions

    <Standard module head>

    <FKS regions: test declarations>

    contains

    <FKS regions: tests>

  end module fks_regions_uti
<FKS regions: public test>≡
  public :: fks_regions_test
<FKS regions: test driver>≡
  subroutine fks_regions_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    call test(fks_regions_1, "fks_regions_1", &
      "Test flavor structure utilities", u, results)
    call test(fks_regions_2, "fks_regions_2", &
      "Test singular regions for final-state radiation for n = 2", &
      u, results)
    call test(fks_regions_3, "fks_regions_3", &
      "Test singular regions for final-state radiation for n = 3", &
      u, results)
    call test(fks_regions_4, "fks_regions_4", &
      "Test singular regions for final-state radiation for n = 4", &

```

```

        u, results)
call test(fks_regions_5, "fks_regions_5", &
        "Test singular regions for final-state radiation for n = 5", &
        u, results)
call test(fks_regions_6, "fks_regions_6", &
        "Test singular regions for initial-state radiation", &
        u, results)
call test(fks_regions_7, "fks_regions_7", &
        "Check Latex output", u, results)
call test(fks_regions_8, "fks_regions_8", &
        "Test singular regions for initial-state photon contributions", &
        u, results)
end subroutine fks_regions_test

```

<FKS regions: test declarations>≡
public :: fks_regions_1

<FKS regions: tests>≡
subroutine fks_regions_1 (u)
integer, intent(in) :: u
type(flv_structure_t) :: flv_born, flv_real
type(model_t), pointer :: test_model => null ()
write (u, "(A)") "* Test output: fks_regions_1"
write (u, "(A)") "* Purpose: Test utilities of flavor structure manipulation"
write (u, "(A)")

call create_test_model (var_str ("SM"), test_model)

flv_born = [11, -11, 2, -2]
flv_real = [11, -11, 2, -2, 21]
flv_born%n_in = 2; flv_real%n_in = 2
write (u, "(A)") "* Valid splittings of ee -> uu"
write (u, "(A)") "Born Flavors: "
call flv_born%write (u)
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "3, 4 (2, -2) : ", flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-2, 2) : ", flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 21) : ", flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (21, 2) : ", flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-2, 21): ", flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (21, -2): ", flv_real%valid_pair (5, 4, flv_born, test_model)
call write_separator (u)

call flv_born%final ()
call flv_real%final ()

flv_born = [2, -2, 11, -11]
flv_real = [2, -2, 11, -11, 21]
flv_born%n_in = 2; flv_real%n_in = 2
write (u, "(A)") "* Valid splittings of uu -> ee"
write (u, "(A)") "Born Flavors: "
call flv_born%write (u)
write (u, "(A)") "Real Flavors: "

```

call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (2, -2) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-2, 2) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (21, -2): " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-2, 21): " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (21, 2) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (2, 21) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
call flv_real%final ()
flv_real = [21, -2, 11, -11, -2]
flv_real%n_in = 2
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (21, -2): " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-2, 21): " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (-2, -2): " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-2, -2): " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (-2, 21): " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (21, -2): " , flv_real%valid_pair (1, 5, flv_born, test_model)
call flv_real%final ()
flv_real = [2, 21, 11, -11, 2]
flv_real%n_in = 2
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (2, 21) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (21, 2) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (2, 21) : " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (21, 2) : " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (2, 2) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (2, 2) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
call write_separator (u)

call flv_born%final ()
call flv_real%final ()

flv_born = [11, -11, 2, -2, 21]
flv_real = [11, -11, 2, -2, 21]
flv_born%n_in = 2; flv_real%n_in = 2
write (u, "(A)") "* Valid splittings of ee -> uug"
write (u, "(A)") "Born Flavors: "
call flv_born%write (u)
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "3, 4 (2, -2) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-2, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 21) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (21, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-2, 21): " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (21, -2): " , flv_real%valid_pair (5, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 6 (2, 21) : " , flv_real%valid_pair (3, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 3 (21, 2) : " , flv_real%valid_pair (6, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 6 (-2, 21): " , flv_real%valid_pair (4, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 4 (21, -2): " , flv_real%valid_pair (6, 4, flv_born, test_model)
write (u, "(A,L1)") "5, 6 (21, 21): " , flv_real%valid_pair (5, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 5 (21, 21): " , flv_real%valid_pair (6, 5, flv_born, test_model)

```

```

call flv_real%final ()
flv_real = [11, -11, 2, -2, 1, -1]
flv_real%n_in = 2
write (u, "(A)") "Real Flavours (exemplary g -> dd splitting): "
call flv_real%write (u)
write (u, "(A,L1)") "3, 4 (2, -2) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-2, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 1) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (1, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-2, 1) : " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (1, -2) : " , flv_real%valid_pair (5, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 6 (2, -1) : " , flv_real%valid_pair (3, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 3 (-1, 2) : " , flv_real%valid_pair (6, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 6 (-2, -1): " , flv_real%valid_pair (4, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 4 (-1, -2): " , flv_real%valid_pair (6, 4, flv_born, test_model)
write (u, "(A,L1)") "5, 6 (1, -1) : " , flv_real%valid_pair (5, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 5 (-1, 1) : " , flv_real%valid_pair (6, 5, flv_born, test_model)
call write_separator (u)

call flv_born%final ()
call flv_real%final ()

flv_born = [6, -5, 2, -1 ]
flv_real = [6, -5, 2, -1, 21]
flv_born%n_in = 1; flv_real%n_in = 1
write (u, "(A)") "* Valid splittings of t -> b u d~"
write (u, "(A)") "Born Flavours: "
call flv_born%write (u)
write (u, "(A)") "Real Flavours: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (6, -5) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "1, 3 (6, 2) : " , flv_real%valid_pair (1, 3, flv_born, test_model)
write (u, "(A,L1)") "1, 4 (6, -1) : " , flv_real%valid_pair (1, 4, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-5, 6) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "3, 1 (2, 6) : " , flv_real%valid_pair (3, 1, flv_born, test_model)
write (u, "(A,L1)") "4, 1 (-1, 6) : " , flv_real%valid_pair (4, 1, flv_born, test_model)
write (u, "(A,L1)") "2, 3 (-5, 2) : " , flv_real%valid_pair (2, 3, flv_born, test_model)
write (u, "(A,L1)") "2, 4 (-5, -1): " , flv_real%valid_pair (2, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 2 (2, -5) : " , flv_real%valid_pair (3, 2, flv_born, test_model)
write (u, "(A,L1)") "4, 2 (-1, -5): " , flv_real%valid_pair (4, 2, flv_born, test_model)
write (u, "(A,L1)") "3, 4 (2, -1) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-1, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (6, 21) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (21, 6) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-5, 21): " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (21, 5) : " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 21) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (21, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-1, 21): " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (21, -1): " , flv_real%valid_pair (5, 4, flv_born, test_model)

call flv_born%final ()
call flv_real%final ()

```



```

end subroutine fks_regions_1

<FKS regions: test declarations>+=
public :: fks_regions_2

<FKS regions: tests>+=
subroutine fks_regions_2 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_2"
  write (u, "(A)") "* Create singular regions for processes with up to four singular regions"
  write (u, "(A)") "* ee -> qq with QCD corrections"
  write (u, "(A)")

  n_flv_born = 1; n_flv_real = 1
  n_legs_born = 4; n_legs_real = 5
  n_in = 2

  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flv_born (:, 1) = [11, -11, 2, -2]
  flv_real (:, 1) = [11, -11, 2, -2, 21]
  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> qq with EW corrections"
  write (u, "(A)")

  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flv_born (:, 1) = [11, -11, 2, -2]
  flv_real (:, 1) = [11, -11, 2, -2, 22]

  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 2, 0)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> tt"
  write (u, "(A)")
  write (u, "(A)") "* This process has four singular regions because they are not equivalent."

```

```

n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2

allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))
flv_born (:, 1) = [11, -11, 6, -6, 6, -6]
flv_real (:, 1) = [11, -11, 6, -6, 6, -6, 21]
call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
end subroutine fks_regions_2

```

<FKS regions: test declarations>+≡

```
public :: fks_regions_3
```

<FKS regions: tests>+≡

```

subroutine fks_regions_3 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in, i, j
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_3"
  write (u, "(A)") "* Create singular regions for processes with three final-state particles"

  write (u, "(A)") "* ee -> qqg"
  write (u, "(A)")
  n_flv_born = 1; n_flv_real = 2
  n_legs_born = 5; n_legs_real = 6
  n_in = 2
  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))

  flv_born (:, 1) = [11, -11, 2, -2, 21]
  flv_real (:, 1) = [11, -11, 2, -2, 21, 21]
  flv_real (:, 2) = [11, -11, 2, -2, 1, -1]

  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 1)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> qqA"
  write (u, "(A)")
  n_flv_born = 1; n_flv_real = 2
  n_legs_born = 5; n_legs_real = 6

```

```

n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, 2, -2, 22]
flv_real (:, 1) = [11, -11, 2, -2, 22, 22]
flv_real (:, 2) = [11, -11, 2, -2, 11, -11]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 3, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> jet jet jet"
write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
write (u, "(A)")
n_flv_born = 5; n_flv_real = 22
n_legs_born = 5; n_legs_real = 6
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -4, 4, 21]
flv_born (:, 2) = [11, -11, -2, 2, 21]
flv_born (:, 3) = [11, -11, -5, 5, 21]
flv_born (:, 4) = [11, -11, -3, 3, 21]
flv_born (:, 5) = [11, -11, -1, 1, 21]
flv_real (:, 1) = [11, -11, -4, -4, 4, 4]
flv_real (:, 2) = [11, -11, -4, -2, 2, 4]
flv_real (:, 3) = [11, -11, -4, 4, 21, 21]
flv_real (:, 4) = [11, -11, -4, -5, 4, 5]
flv_real (:, 5) = [11, -11, -4, -3, 4, 3]
flv_real (:, 6) = [11, -11, -4, -1, 2, 3]
flv_real (:, 7) = [11, -11, -4, -1, 4, 1]
flv_real (:, 8) = [11, -11, -2, -2, 2, 2]
flv_real (:, 9) = [11, -11, -2, 2, 21, 21]
flv_real (:, 10) = [11, -11, -2, -5, 2, 5]
flv_real (:, 11) = [11, -11, -2, -3, 2, 3]
flv_real (:, 12) = [11, -11, -2, -3, 4, 1]
flv_real (:, 13) = [11, -11, -2, -1, 2, 1]
flv_real (:, 14) = [11, -11, -5, -5, 5, 5]
flv_real (:, 15) = [11, -11, -5, -3, 3, 5]
flv_real (:, 16) = [11, -11, -5, -1, 1, 5]
flv_real (:, 17) = [11, -11, -5, 5, 21, 21]
flv_real (:, 18) = [11, -11, -3, -3, 3, 3]
flv_real (:, 19) = [11, -11, -3, -1, 1, 3]
flv_real (:, 20) = [11, -11, -3, 3, 21, 21]
flv_real (:, 21) = [11, -11, -1, -1, 1, 1]
flv_real (:, 22) = [11, -11, -1, 1, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 1)

```

```

call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> L L A"
write (u, "(A)") "* with L = e2:E2:e3:E3"
write (u, "(A)")
n_flv_born = 2; n_flv_real = 6
n_legs_born = 5; n_legs_real = 6
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -15, 15, 22]
flv_born (:, 2) = [11, -11, -13, 13, 22]

flv_real (:, 1) = [11, -11, -15, -15, 15, 15]
flv_real (:, 2) = [11, -11, -15, -13, 13, 13]
flv_real (:, 3) = [11, -11, -13, -15, 13, 15]
flv_real (:, 4) = [11, -11, -15, 15, 22, 22]
flv_real (:, 5) = [11, -11, -13, -13, 13, 13]
flv_real (:, 6) = [11, -11, -13, 13, 22, 22]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 3, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

end subroutine fks_regions_3

<FKS regions: test declarations>+≡
public :: fks_regions_4

<FKS regions: tests>+≡
subroutine fks_regions_4 (u)
integer, intent(in) :: u
integer :: n_flv_born, n_flv_real
integer :: n_legs_born, n_legs_real
integer :: n_in
integer, dimension(:,:), allocatable :: flv_born, flv_real
type(region_data_t) :: reg_data
write (u, "(A)") "* Test output: fks_regions_4"
write (u, "(A)") "* Create singular regions for processes with four final-state particles"
write (u, "(A)") "* ee -> 4 jet"
write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
write (u, "(A)")
n_flv_born = 22; n_flv_real = 22
n_legs_born = 6; n_legs_real = 7
n_in = 2

```

```

allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -4, -4, 4, 4]
flv_born (:, 2) = [11, -11, -4, -2, 2, 4]
flv_born (:, 3) = [11, -11, -4, 4, 21, 21]
flv_born (:, 4) = [11, -11, -4, -5, 4, 5]
flv_born (:, 5) = [11, -11, -4, -3, 4, 3]
flv_born (:, 6) = [11, -11, -4, -1, 2, 3]
flv_born (:, 7) = [11, -11, -4, -1, 4, 1]
flv_born (:, 8) = [11, -11, -2, -2, 2, 2]
flv_born (:, 9) = [11, -11, -2, 2, 21, 21]
flv_born (:, 10) = [11, -11, -2, -5, 2, 5]
flv_born (:, 11) = [11, -11, -2, -3, 2, 3]
flv_born (:, 12) = [11, -11, -2, -3, 4, 1]
flv_born (:, 13) = [11, -11, -2, -1, 2, 1]
flv_born (:, 14) = [11, -11, -5, -5, 5, 5]
flv_born (:, 15) = [11, -11, -5, -3, 3, 5]
flv_born (:, 16) = [11, -11, -5, -1, 1, 5]
flv_born (:, 17) = [11, -11, -5, 5, 21, 21]
flv_born (:, 18) = [11, -11, -3, -3, 3, 3]
flv_born (:, 19) = [11, -11, -3, -1, 1, 3]
flv_born (:, 20) = [11, -11, -3, -3, 21, 21]
flv_born (:, 21) = [11, -11, -1, -1, 1, 1]
flv_born (:, 22) = [11, -11, -1, 1, 21, 21]
flv_real (:, 1) = [11, -11, -4, -4, 4, 4, 21]
flv_real (:, 2) = [11, -11, -4, -2, 2, 4, 21]
flv_real (:, 3) = [11, -11, -4, 4, 21, 21, 21]
flv_real (:, 4) = [11, -11, -4, -5, 4, 5, 21]
flv_real (:, 5) = [11, -11, -4, -3, 4, 3, 21]
flv_real (:, 6) = [11, -11, -4, -1, 2, 3, 21]
flv_real (:, 7) = [11, -11, -4, -1, 4, 1, 21]
flv_real (:, 8) = [11, -11, -2, -2, 2, 2, 21]
flv_real (:, 9) = [11, -11, -2, 2, 21, 21, 21]
flv_real (:, 10) = [11, -11, -2, -5, 2, 5, 21]
flv_real (:, 11) = [11, -11, -2, -3, 2, 3, 21]
flv_real (:, 12) = [11, -11, -2, -3, 4, 1, 21]
flv_real (:, 13) = [11, -11, -2, -1, 2, 1, 21]
flv_real (:, 14) = [11, -11, -5, -5, 5, 5, 21]
flv_real (:, 15) = [11, -11, -5, -3, 3, 5, 21]
flv_real (:, 16) = [11, -11, -5, -1, 1, 5, 21]
flv_real (:, 17) = [11, -11, -5, 5, 21, 21, 21]
flv_real (:, 18) = [11, -11, -3, -3, 3, 3, 21]
flv_real (:, 19) = [11, -11, -3, -1, 1, 3, 21]
flv_real (:, 20) = [11, -11, -3, 3, 21, 21, 21]
flv_real (:, 21) = [11, -11, -1, -1, 1, 1, 21]
flv_real (:, 22) = [11, -11, -1, 1, 21, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

```

```

call write_separator (u)

write (u, "(A)") "* ee -> bbmumu with QCD corrections"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -5, 5, -13, 13]
flv_real (:, 1) = [11, -11, -5, 5, -13, 13, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> bbmumu with EW corrections"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -5, 5, -13, 13]
flv_real (:, 1) = [11, -11, -5, 5, -13, 13, 22]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

end subroutine fks_regions_4

<FKS regions: test declarations>+≡
public :: fks_regions_5

<FKS regions: tests>+≡
subroutine fks_regions_5 (u)
integer, intent(in) :: u
integer :: n_flv_born, n_flv_real
integer :: n_legs_born, n_legs_real
integer :: n_in
integer, dimension(:,:), allocatable :: flv_born, flv_real
type(region_data_t) :: reg_data
write (u, "(A)") "* Test output: fks_regions_5"
write (u, "(A)") "* Create singular regions for processes with five final-state particles"

```

```

write (u, "(A)") "* ee -> 5 jet"
write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
write (u, "(A)")
n_flv_born = 22; n_flv_real = 67
n_legs_born = 7; n_legs_real = 8
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:,1) = [11,-11,-4,-4,4,4,21]
flv_born (:,2) = [11,-11,-4,-2,2,4,21]
flv_born (:,3) = [11,-11,-4,4,21,21,21]
flv_born (:,4) = [11,-11,-4,-5,4,5,21]
flv_born (:,5) = [11,-11,-4,-3,4,3,21]
flv_born (:,6) = [11,-11,-4,-1,2,3,21]
flv_born (:,7) = [11,-11,-4,-1,4,1,21]
flv_born (:,8) = [11,-11,-2,-2,2,2,21]
flv_born (:,9) = [11,-11,-2,2,21,21,21]
flv_born (:,10) = [11,-11,-2,-5,2,5,21]
flv_born (:,11) = [11,-11,-2,-3,2,3,21]
flv_born (:,12) = [11,-11,-2,-3,4,1,21]
flv_born (:,13) = [11,-11,-2,-1,2,1,21]
flv_born (:,14) = [11,-11,-5,-5,5,5,21]
flv_born (:,15) = [11,-11,-5,-3,3,5,21]
flv_born (:,16) = [11,-11,-5,-1,1,5,21]
flv_born (:,17) = [11,-11,-5,5,21,21,21]
flv_born (:,18) = [11,-11,-3,-3,3,3,21]
flv_born (:,19) = [11,-11,-3,-1,1,3,21]
flv_born (:,20) = [11,-11,-3,3,21,21,21]
flv_born (:,21) = [11,-11,-1,-1,1,1,21]
flv_born (:,22) = [11,-11,-1,1,21,21,21]

flv_real (:,1) = [11,-11,-4,-4,-4,4,4]
flv_real (:,2) = [11,-11,-4,-4,-2,2,4]
flv_real (:,3) = [11,-11,-4,-4,4,4,21]
flv_real (:,4) = [11,-11,-4,-4,-5,4,4]
flv_real (:,5) = [11,-11,-4,-4,-3,4,4]
flv_real (:,6) = [11,-11,-4,-4,-1,2,4]
flv_real (:,7) = [11,-11,-4,-4,-1,4,4]
flv_real (:,8) = [11,-11,-4,-2,-2,2,4]
flv_real (:,9) = [11,-11,-4,-2,2,4,21]
flv_real (:,10) = [11,-11,-4,-2,-5,2,4]
flv_real (:,11) = [11,-11,-4,-2,-3,2,4]
flv_real (:,12) = [11,-11,-4,-2,-3,4,4]
flv_real (:,13) = [11,-11,-4,-2,-1,2,4]
flv_real (:,14) = [11,-11,-4,-2,-1,4,4]
flv_real (:,15) = [11,-11,-4,4,21,21,21]
flv_real (:,16) = [11,-11,-4,-5,4,5,21]
flv_real (:,17) = [11,-11,-4,-5,-5,4,5]
flv_real (:,18) = [11,-11,-4,-5,-3,4,5]
flv_real (:,19) = [11,-11,-4,-5,-1,2,5]
flv_real (:,20) = [11,-11,-4,-5,-1,4,5]
flv_real (:,21) = [11,-11,-4,-3,4,3,21]

```

```

flv_real (:,22) = [11,-11,-4,-3,-3,4,3,3]
flv_real (:,23) = [11,-11,-4,-3,-1,2,3,3]
flv_real (:,24) = [11,-11,-4,-3,-1,4,1,3]
flv_real (:,25) = [11,-11,-4,-1,2,3,21,21]
flv_real (:,26) = [11,-11,-4,-1,4,1,21,21]
flv_real (:,27) = [11,-11,-4,-1,-1,2,1,3]
flv_real (:,28) = [11,-11,-4,-1,-1,4,1,1]
flv_real (:,29) = [11,-11,-2,-2,-2,2,2,2]
flv_real (:,30) = [11,-11,-2,-2,2,2,21,21]
flv_real (:,31) = [11,-11,-2,-2,-5,2,2,5]
flv_real (:,32) = [11,-11,-2,-2,-3,2,2,3]
flv_real (:,33) = [11,-11,-2,-2,-3,2,4,1]
flv_real (:,34) = [11,-11,-2,-2,-1,2,2,1]
flv_real (:,35) = [11,-11,-2,2,21,21,21,21]
flv_real (:,36) = [11,-11,-2,-5,2,5,21,21]
flv_real (:,37) = [11,-11,-2,-5,-5,2,5,5]
flv_real (:,38) = [11,-11,-2,-5,-3,2,3,5]
flv_real (:,39) = [11,-11,-2,-5,-3,4,1,5]
flv_real (:,40) = [11,-11,-2,-5,-1,2,1,5]
flv_real (:,41) = [11,-11,-2,-3,2,3,21,21]
flv_real (:,42) = [11,-11,-2,-3,4,1,21,21]
flv_real (:,43) = [11,-11,-2,-3,-3,2,3,3]
flv_real (:,44) = [11,-11,-2,-3,-3,4,1,3]
flv_real (:,45) = [11,-11,-2,-3,-1,2,1,3]
flv_real (:,46) = [11,-11,-2,-3,-1,4,1,1]
flv_real (:,47) = [11,-11,-2,-1,2,1,21,21]
flv_real (:,48) = [11,-11,-2,-1,-1,2,1,1]
flv_real (:,49) = [11,-11,-5,-5,-5,5,5,5]
flv_real (:,50) = [11,-11,-5,-5,-3,3,5,5]
flv_real (:,51) = [11,-11,-5,-5,-1,1,5,5]
flv_real (:,52) = [11,-11,-5,-5,5,5,21,21]
flv_real (:,53) = [11,-11,-5,-3,-3,3,3,5]
flv_real (:,54) = [11,-11,-5,-3,-1,1,3,5]
flv_real (:,55) = [11,-11,-5,-3,3,5,21,21]
flv_real (:,56) = [11,-11,-5,-1,-1,1,1,5]
flv_real (:,57) = [11,-11,-5,-1,1,5,21,21]
flv_real (:,58) = [11,-11,-5,5,21,21,21,21]
flv_real (:,59) = [11,-11,-3,-3,-3,3,3,3]
flv_real (:,60) = [11,-11,-3,-3,-1,1,3,3]
flv_real (:,61) = [11,-11,-3,-3,3,3,21,21]
flv_real (:,62) = [11,-11,-3,-1,-1,1,1,3]
flv_real (:,63) = [11,-11,-3,-1,1,3,21,21]
flv_real (:,64) = [11,-11,-3,3,21,21,21,21]
flv_real (:,65) = [11,-11,-1,-1,-1,1,1,1]
flv_real (:,66) = [11,-11,-1,-1,1,1,21,21]
flv_real (:,67) = [11,-11,-1,1,21,21,21,21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 3)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

```



```

end subroutine fks_regions_5

<FKS regions: test declarations>+≡
public :: fks_regions_6

<FKS regions: tests>+≡
subroutine fks_regions_6 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  integer :: i, j
  integer, dimension(10) :: flavors
  write (u, "(A)") "* Test output: fks_regions_6"
  write (u, "(A)") "* Create table of singular regions for Drell Yan"
  write (u, "(A)")

  n_flv_born = 10; n_flv_real = 30
  n_legs_born = 4; n_legs_real = 5
  n_in = 2
  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flavors = [-5, -4, -3, -2, -1, 1, 2, 3, 4, 5]
  do i = 1, n_flv_born
    flv_born (3:4, i) = [11, -11]
  end do
  do j = 1, n_flv_born
    flv_born (1, j) = flavors (j)
    flv_born (2, j) = -flavors (j)
  end do

  do i = 1, n_flv_real
    flv_real (3:4, i) = [11, -11]
  end do
  i = 1
  do j = 1, n_flv_real
    if (mod (j, 3) == 1) then
      flv_real (1, j) = flavors (i)
      flv_real (2, j) = -flavors (i)
      flv_real (5, j) = 21
    else if (mod (j, 3) == 2) then
      flv_real (1, j) = flavors (i)
      flv_real (2, j) = 21
      flv_real (5, j) = flavors (i)
    else
      flv_real (1, j) = 21
      flv_real (2, j) = -flavors (i)
      flv_real (5, j) = -flavors (i)
      i = i + 1
    end if
  end do
end do

```

```

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

call write_separator (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

write (u, "(A)") "* Create table of singular regions for hadronic top decay"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 4; n_legs_real = 5
n_in = 1
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [6, -5, 2, -1]
flv_real (:, 1) = [6, -5, 2, -1, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 0, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

call write_separator (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

write (u, "(A)") "* Create table of singular regions for dijet s sbar -> jet jet"
write (u, "(A)") "* With jet = u:d:gl"
write (u, "(A)")

n_flv_born = 3; n_flv_real = 3
n_legs_born = 4; n_legs_real = 5
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))
do i = 1, n_flv_born
    flv_born (1:2, i) = [3, -3]
end do
flv_born (3, :) = [1, 2, 21]
flv_born (4, :) = [-1, -2, 21]

do i = 1, n_flv_real
    flv_real (1:2, i) = [3, -3]
end do
flv_real (3, :) = [1, 2, 21]
flv_real (4, :) = [-1, -2, 21]
flv_real (5, :) = [21, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 0, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

```

```

        call reg_data%final ()

    end subroutine fks_regions_6

<FKS regions: test declarations>+≡
    public :: fks_regions_7

<FKS regions: tests>+≡
    subroutine fks_regions_7 (u)
        integer, intent(in) :: u
        integer :: n_flv_born, n_flv_real
        integer :: n_legs_born, n_legs_real
        integer :: n_in
        integer, dimension(:,:), allocatable :: flv_born, flv_real
        type(region_data_t) :: reg_data
        write (u, "(A)") "* Test output: fks_regions_7"
        write (u, "(A)") "* Create table of singular regions for ee -> qq"
        write (u, "(A)")

        n_flv_born = 1; n_flv_real = 1
        n_legs_born = 4; n_legs_real = 5
        n_in = 2

        allocate (flv_born (n_legs_born, n_flv_born))
        allocate (flv_real (n_legs_real, n_flv_real))
        flv_born (:, 1) = [11, -11, 2, -2]
        flv_real (:, 1) = [11, -11, 2, -2, 21]
        call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
        call reg_data%write_latex (u)
        call reg_data%final ()

    end subroutine fks_regions_7

<FKS regions: test declarations>+≡
    public :: fks_regions_8

<FKS regions: tests>+≡
    subroutine fks_regions_8 (u)
        integer, intent(in) :: u
        integer :: n_flv_born, n_flv_real
        integer :: n_legs_born, n_legs_real
        integer :: n_in
        integer, dimension(:,:), allocatable :: flv_born, flv_real
        type(region_data_t) :: reg_data
        integer :: i, j
        integer, dimension(10) :: flavors
        write (u, "(A)") "* Test output: fks_regions_8"
        write (u, "(A)") "* Create table of singular regions for ee -> ee"
        write (u, "(A)")

        n_flv_born = 1; n_flv_real = 3
        n_legs_born = 4; n_legs_real = 5
        n_in = 2
        allocate (flv_born (n_legs_born, n_flv_born))

```

```

allocate (flv_real (n_legs_real, n_flv_real))
flv_born (:, 1) = [11, -11, -11, 11]

flv_real (:, 1) = [11, -11, -11, 11, 22]
flv_real (:, 2) = [11, 22, -11, 11, 11]
flv_real (:, 3) = [22, -11, 11, -11, -11]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 2, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)
call reg_data%final ()

end subroutine fks_regions_8

```

27.4 NLO infrastructure and data

This module contains the settings and data infrastructure.

```

<nlo_data.f90>≡
  <File header>

  module nlo_data

    <Use kinds>
    <Use strings>
    use constants, only: zero
    use lorentz
    use variables, only: var_list_t
    use physics_defs, only: NO_FACTORIZATION, FACTORIZATION_THRESHOLD

    <Standard module head>

    <NLO data: public>

    <NLO data: parameters>

    <NLO data: types>

    interface
    <NLO data: sub interfaces>
    end interface

  end module nlo_data

<nlo_data_sub.f90>≡
  <File header>

  submodule (nlo_data) nlo_data_s

    use diagnostics
    use string_utils, only: split_string, read_ival, string_contains_word
    use io_units

```

```

    use format_defs, only: FMT_15
    use physics_defs, only: THR_POS_WP, THR_POS_WM
    use physics_defs, only: THR_POS_B, THR_POS_BBAR

    implicit none

contains

    <NLO data: procedures>

end submodule nlo_data_s

<NLO data: parameters>≡
    integer, parameter, public :: FKS_DEFAULT = 1
    integer, parameter, public :: FKS_RESONANCES = 2

    integer, dimension(2), parameter, public :: ASSOCIATED_LEG_PAIR = [1, 3]

<NLO data: public>≡
    public :: fks_template_t

<NLO data: types>≡
    type :: fks_template_t
        logical :: subtraction_disabled = .false.
        integer :: mapping_type = FKS_DEFAULT
        logical :: count_kinematics = .false.
        real(default) :: fks_dij_exp1
        real(default) :: fks_dij_exp2
        real(default) :: xi_min
        real(default) :: y_max
        real(default) :: xi_cut, delta_o, delta_i
        type(string_t), dimension(:), allocatable :: excluded_resonances
        integer :: n_f
    contains
        <NLO data: fks template: TBP>
    end type fks_template_t

<NLO data: fks template: TBP>≡
    procedure :: write => fks_template_write

<NLO data: sub interfaces>≡
    module subroutine fks_template_write (template, unit)
        class(fks_template_t), intent(in) :: template
        integer, intent(in), optional :: unit
    end subroutine fks_template_write

<NLO data: procedures>≡
    module subroutine fks_template_write (template, unit)
        class(fks_template_t), intent(in) :: template
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u,'(1x,A)') 'FKS Template: '
        write (u,'(1x,A)', advance = 'no') 'Mapping Type: '

```

```

select case (template%mapping_type)
case (FKS_DEFAULT)
  write (u,'(A)') 'Default'
case (FKS_RESONANCES)
  write (u,'(A)') 'Resonances'
case default
  write (u,'(A)') 'Unkown'
end select
write (u,'(1x,A,ES4.3,ES4.3)') 'd_ij exponentials: ', &
  template%fks_dij_exp1, template%fks_dij_exp2
write (u, '(1x,A,ES4.3,ES4.3)') 'xi_cut: ', &
  template%xi_cut
write (u, '(1x,A,ES4.3,ES4.3)') 'delta_o: ', &
  template%delta_o
write (u, '(1x,A,ES4.3,ES4.3)') 'delta_i: ', &
  template%delta_i
end subroutine fks_template_write

```

Set FKS parameters. ξ_{cut} , δ_o and δ_i steer the ratio of the integrated and real subtraction.

```

<NLO data: fks template: TBP>+=
  procedure :: set_parameters => fks_template_set_parameters

<NLO data: sub interfaces>+=
  module subroutine fks_template_set_parameters (template, &
    exp1, exp2, xi_min, y_max, xi_cut, delta_o, delta_i)
    class(fks_template_t), intent(inout) :: template
    real(default), intent(in) :: exp1, exp2
    real(default), intent(in) :: xi_min, y_max, &
      xi_cut, delta_o, delta_i
  end subroutine fks_template_set_parameters

<NLO data: procedures>+=
  module subroutine fks_template_set_parameters (template, &
    exp1, exp2, xi_min, y_max, xi_cut, delta_o, delta_i)
    class(fks_template_t), intent(inout) :: template
    real(default), intent(in) :: exp1, exp2
    real(default), intent(in) :: xi_min, y_max, &
      xi_cut, delta_o, delta_i
    template%fks_dij_exp1 = exp1
    template%fks_dij_exp2 = exp2
    template%xi_min = xi_min
    template%y_max = y_max
    template%xi_cut = xi_cut
    template%delta_o = delta_o
    template%delta_i = delta_i
  end subroutine fks_template_set_parameters

<NLO data: fks template: TBP>+=
  procedure :: set_mapping_type => fks_template_set_mapping_type

<NLO data: sub interfaces>+=
  module subroutine fks_template_set_mapping_type (template, val)
    class(fks_template_t), intent(inout) :: template
    integer, intent(in) :: val

```

```

        end subroutine fks_template_set_mapping_type
<NLO data: procedures>+≡
    module subroutine fks_template_set_mapping_type (template, val)
        class(fks_template_t), intent(inout) :: template
        integer, intent(in) :: val
        template%mapping_type = val
    end subroutine fks_template_set_mapping_type

<NLO data: fks template: TBP>+≡
    procedure :: set_counter => fks_template_set_counter

<NLO data: sub interfaces>+≡
    module subroutine fks_template_set_counter (template)
        class(fks_template_t), intent(inout) :: template
    end subroutine fks_template_set_counter

<NLO data: procedures>+≡
    module subroutine fks_template_set_counter (template)
        class(fks_template_t), intent(inout) :: template
        template%count_kinematics = .true.
    end subroutine fks_template_set_counter

<NLO data: public>+≡
    public :: get_threshold_momenta

<NLO data: sub interfaces>+≡
    module function get_threshold_momenta (p) result (p_thr)
        type(vector4_t), dimension(4) :: p_thr
        type(vector4_t), intent(in), dimension(:) :: p
    end function get_threshold_momenta

<NLO data: procedures>+≡
    module function get_threshold_momenta (p) result (p_thr)
        type(vector4_t), dimension(4) :: p_thr
        type(vector4_t), intent(in), dimension(:) :: p
        p_thr(1) = p(THR_POS_WP) + p(THR_POS_B)
        p_thr(2) = p(THR_POS_B)
        p_thr(3) = p(THR_POS_WM) + p(THR_POS_BBAR)
        p_thr(4) = p(THR_POS_BBAR)
    end function get_threshold_momenta

```

27.4.1 NLO settings and steering

```

<NLO data: public>+≡
    public :: nlo_settings_t

<NLO data: types>+≡
    type :: nlo_settings_t
        logical :: use_internal_color_correlations = .true.
        logical :: use_internal_spin_correlations = .false.
        logical :: use_resonance_mappings = .false.
        logical :: combined_integration = .false.
        logical :: fixed_order_nlo = .false.
        logical :: test_soft_limit = .false.

```

```

logical :: test_coll_limit = .false.
logical :: test_anti_coll_limit = .false.
integer, dimension(:), allocatable :: selected_alr
integer :: factorization_mode = NO_FACTORIZATION
!!! Probably not the right place for this. Revisit after refactoring
real(default) :: powheg_damping_scale = zero
type(fks_template_t) :: fks_template
type(string_t) :: virtual_selection
logical :: virtual_resonance_aware_collinear = .true.
logical :: use_born_scale = .false.
logical :: cut_all_real_sqmes = .false.
type(string_t) :: nlo_correction_type
logical :: reuse_amplitudes_fks = .false.
contains
<NLO data: nlo settings: TBP>
end type nlo_settings_t

```

```

<NLO data: nlo settings: TBP>≡
  procedure :: init => nlo_settings_init

<NLO data: sub interfaces>+≡
  module subroutine nlo_settings_init (nlo_settings, var_list, fks_template)
    class(nlo_settings_t), intent(inout) :: nlo_settings
    type(var_list_t), intent(in) :: var_list
    type(fks_template_t), intent(in), optional :: fks_template
  end subroutine nlo_settings_init

<NLO data: procedures>+≡
  module subroutine nlo_settings_init (nlo_settings, var_list, fks_template)
    class(nlo_settings_t), intent(inout) :: nlo_settings
    type(var_list_t), intent(in) :: var_list
    type(fks_template_t), intent(in), optional :: fks_template
    type(string_t) :: color_method
    if (present (fks_template)) nlo_settings%fks_template = fks_template
    color_method = var_list%get_sval (var_str ('$correlation_me_method'))
    if (color_method == "") &
      color_method = var_list%get_sval (var_str ('$method'))
    nlo_settings%use_internal_color_correlations = color_method == 'omega' &
      .or. color_method == 'threshold'
    nlo_settings%combined_integration = var_list%get_lval &
      (var_str ("?combined_nlo_integration"))
    nlo_settings%fixed_order_nlo = var_list%get_lval &
      (var_str ("?fixed_order_nlo_events"))
    nlo_settings%test_soft_limit = &
      var_list%get_lval (var_str ('?test_soft_limit'))
    nlo_settings%test_coll_limit = &
      var_list%get_lval (var_str ('?test_coll_limit'))
    nlo_settings%test_anti_coll_limit = &
      var_list%get_lval (var_str ('?test_anti_coll_limit'))
    call setup_alr_selection ()
    nlo_settings%virtual_selection = &
      var_list%get_sval (var_str ('$virtual_selection'))
    nlo_settings%virtual_resonance_aware_collinear = &
      var_list%get_lval (var_str ('?virtual_collinear_resonance_aware'))
    nlo_settings%powheg_damping_scale = &

```



```

        var_list%get_rval (var_str ('powheg_damping_scale'))
nlo_settings%use_born_scale = &
        var_list%get_lval (var_str ("?nlo_use_born_scale"))
nlo_settings%cut_all_real_sqmes = &
        var_list%get_lval (var_str ("?nlo_cut_all_real_sqmes"))
nlo_settings%nlo_correction_type = &
        var_list%get_sval (var_str ('$nlo_correction_type'))
nlo_settings%reuse_amplitudes_fks = &
        var_list%get_lval (var_str ('?nlo_reuse_amplitudes_fks'))
contains
subroutine setup_alr_selection ()
    type(string_t) :: alr_selection
    type(string_t), dimension(:), allocatable :: alr_split
    integer :: i, i1, i2
    alr_selection = var_list%get_sval (var_str ('$select_alpha_regions'))
    if (string_contains_word (alr_selection, var_str (","))) then
        call split_string (alr_selection, var_str (","), alr_split)
        allocate (nlo_settings%selected_alr (size (alr_split)))
        do i = 1, size (alr_split)
            nlo_settings%selected_alr(i) = read_ival(alr_split(i))
        end do
    else if (string_contains_word (alr_selection, var_str (":"))) then
        call split_string (alr_selection, var_str (":"), alr_split)
        if (size (alr_split) == 2) then
            i1 = read_ival (alr_split(1))
            i2 = read_ival (alr_split(2))
            allocate (nlo_settings%selected_alr (i2 - i1 + 1))
            do i = 1, i2 - i1 + 1
                nlo_settings%selected_alr(i) = read_ival (alr_split(i))
            end do
        else
            call msg_fatal ("select_alpha_regions: ':' specifies a range!")
        end if
    else if (len(alr_selection) == 1) then
        allocate (nlo_settings%selected_alr (1))
        nlo_settings%selected_alr(1) = read_ival (alr_selection)
    end if
    if (allocated (alr_split)) deallocate (alr_split)
end subroutine setup_alr_selection
end subroutine nlo_settings_init

```

<NLO data: nlo settings: TBP>+≡

```
procedure :: write => nlo_settings_write
```

<NLO data: sub interfaces>+≡

```

module subroutine nlo_settings_write (nlo_settings, unit)
    class(nlo_settings_t), intent(in) :: nlo_settings
    integer, intent(in), optional :: unit
end subroutine nlo_settings_write

```

<NLO data: procedures>+≡

```

module subroutine nlo_settings_write (nlo_settings, unit)
    class(nlo_settings_t), intent(in) :: nlo_settings
    integer, intent(in), optional :: unit
    integer :: i, u

```

```

u = given_output_unit (unit); if (u < 0) return
write (u, '(A)') 'nlo_settings:'
write (u, '(3X,A,L1)') 'internal_color_correlations = ', &
    nlo_settings%use_internal_color_correlations
write (u, '(3X,A,L1)') 'internal_spin_correlations = ', &
    nlo_settings%use_internal_spin_correlations
write (u, '(3X,A,L1)') 'use_resonance_mappings = ', &
    nlo_settings%use_resonance_mappings
write (u, '(3X,A,L1)') 'combined_integration = ', &
    nlo_settings%combined_integration
write (u, '(3X,A,L1)') 'test_soft_limit = ', &
    nlo_settings%test_soft_limit
write (u, '(3X,A,L1)') 'test_coll_limit = ', &
    nlo_settings%test_coll_limit
write (u, '(3X,A,L1)') 'test_anti_coll_limit = ', &
    nlo_settings%test_anti_coll_limit
if (allocated (nlo_settings%selected_alr)) then
    write (u, '(3x,A)', advance = "no") 'selected alpha regions = ['
    do i = 1, size (nlo_settings%selected_alr)
        write (u, '(A,I0)', advance = "no") ", ", &
            nlo_settings%selected_alr(i)
    end do
    write (u, '(A)') "]"
end if
write (u, '(3X,A,' // FMT_15 // ')') 'powheg_damping_scale = ', &
    nlo_settings%powheg_damping_scale
write (u, '(3X,A,A)') 'virtual_selection = ', &
    char (nlo_settings%virtual_selection)
write (u, '(3X,A,A)') 'Real factorization mode = ', &
    char (factorization_mode (nlo_settings%factorization_mode))
contains
function factorization_mode (fm)
    type(string_t) :: factorization_mode
    integer, intent(in) :: fm
    select case (fm)
    case (NO_FACTORIZATION)
        factorization_mode = var_str ("None")
    case (FACTORIZATION_THRESHOLD)
        factorization_mode = var_str ("Threshold")
    case default
        factorization_mode = var_str ("Undefined!")
    end select
end function factorization_mode
end subroutine nlo_settings_write

```

27.5 Virtual contribution to the cross section

This module implements the UV-finite virtual contribution of an NLO calculation together with the integrated (FKS) subtraction terms.

```
<virtual.f90>≡
  <File header>

  module virtual

    <Use kinds>
    <Use strings>
    use pdg_arrays
    use models
    use model_data, only: model_data_t, field_data_t
    use lorentz
    use nlo_data, only: nlo_settings_t
    use fks_regions

    <Standard module head>

    <Virtual: public>

    <Virtual: types>

    interface
    <Virtual: sub interfaces>
    end interface

  end module virtual

<virtual_sub.f90>≡
  <File header>

  submodule (virtual) virtual_s

    <Use debug>
    use constants
    use numeric_utils
    use diagnostics
    use physics_defs
    use sm_physics
    use flavors
    use nlo_data, only: ASSOCIATED_LEG_PAIR, get_threshold_momenta

    implicit none

  contains

    <Virtual: procedures>

  end submodule virtual_s

  <Virtual: public>≡
    public :: virtual_t
```

```

<Virtual: types>≡
  type :: virtual_t
    type(nlo_settings_t) :: settings
    real(default), dimension(:,:,:), allocatable :: gamma_0, gamma_p, c_flv
    real(default) :: fac_scale
    real(default), allocatable :: ren_scale
    real(default), allocatable :: es_scale2
    integer, dimension(:), allocatable :: n_is_neutrinos
    integer :: n_in, n_legs, n_flv
    logical :: bad_point = .false.
    type(string_t) :: selection
    real(default), dimension(:), allocatable :: sqme_born
    real(default), dimension(:), allocatable :: sqme_virt_fin
    real(default), dimension(:,:,:), allocatable :: sqme_color_c
    real(default), dimension(:,:,:), allocatable :: sqme_charge_c
    logical :: has_pdf = .false.
  contains
    <Virtual: virtual: TBP>
  end type virtual_t

<Virtual: virtual: TBP>≡
  procedure :: init => virtual_init

<Virtual: sub interfaces>≡
  module subroutine virtual_init &
    (virt, flv_born, n_in, settings, model, has_pdf)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in), dimension(:,:) :: flv_born
    integer, intent(in) :: n_in
    type(nlo_settings_t), intent(in) :: settings
    class(model_data_t), intent(in) :: model
    logical, intent(in) :: has_pdf
  end subroutine virtual_init

<Virtual: procedures>≡
  module subroutine virtual_init &
    (virt, flv_born, n_in, settings, model, has_pdf)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in), dimension(:,:) :: flv_born
    integer, intent(in) :: n_in
    type(nlo_settings_t), intent(in) :: settings
    class(model_data_t), intent(in) :: model
    logical, intent(in) :: has_pdf
    integer :: i_flv, n_corr
    n_corr = 2
    virt%n_legs = size (flv_born, 1); virt%n_flv = size (flv_born, 2)
    virt%n_in = n_in
    allocate (virt%sqme_born (virt%n_flv))
    allocate (virt%sqme_virt_fin (virt%n_flv))
    allocate (virt%sqme_color_c (virt%n_legs, virt%n_legs, virt%n_flv))
    allocate (virt%sqme_charge_c (virt%n_legs, virt%n_legs, virt%n_flv))
    allocate (virt%gamma_0 (virt%n_legs, virt%n_flv, n_corr), &
      virt%gamma_p (virt%n_legs, virt%n_flv, n_corr), &
      virt%c_flv (virt%n_legs, virt%n_flv, n_corr))
    call virt%init_constants (flv_born, settings%fks_template%n_f, model)

```

```

allocate (virt%n_is_neutrinos (virt%n_flv))
virt%n_is_neutrinos = 0
do i_flv = 1, virt%n_flv
  if (is_neutrino (flv_born(1, i_flv))) &
    virt%n_is_neutrinos(i_flv) = virt%n_is_neutrinos(i_flv) + 1
  if (is_neutrino (flv_born(2, i_flv))) &
    virt%n_is_neutrinos(i_flv) = virt%n_is_neutrinos(i_flv) + 1
end do
select case (char (settings%virtual_selection))
case ("Full", "OLP", "Subtraction")
  virt%selection = settings%virtual_selection
case default
  call msg_fatal ('Virtual selection: Possible values are "Full", "OLP" or "Subtraction')
end select
virt%settings = settings
virt%has_pdfs = has_pdfs
contains

function is_neutrino (flv) result (neutrino)
  integer, intent(in) :: flv
  logical :: neutrino
  neutrino = (abs(flv) == 12 .or. abs(flv) == 14 .or. abs(flv) == 16)
end function is_neutrino

end subroutine virtual_init

```

The virtual subtraction terms contain Casimir operators and derived constants, listed below:

$$C(q) = C(\bar{q}) = C_F, \quad (27.2)$$

$$C(g) = C_A, \quad (27.3)$$

$$\gamma(q) = \gamma(\bar{q}) = \frac{3}{2}C_F, \quad (27.4)$$

$$\gamma(g) = \frac{11}{6}C_A - \frac{2}{3}T_F N_f, \quad (27.5)$$

$$\gamma'(q) = \gamma'(\bar{q}) = \left(\frac{13}{2} - \frac{2\pi^2}{3} \right) C_F, \quad (27.6)$$

$$\gamma'(g) = \left(\frac{67}{9} - \frac{2\pi^2}{3} \right) C_A - \frac{23}{9}T_F N_f. \quad (27.7)$$

For uncolored particles, `virtual_init_constants` sets C , γ and γ' to zero.

```

<Virtual: virtual: TBP>+≡
  procedure :: init_constants => virtual_init_constants
<Virtual: sub interfaces>+≡
  module subroutine virtual_init_constants (virt, flv_born, nf_input, model)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in), dimension(:, :) :: flv_born
    integer, intent(in) :: nf_input
    type(string_t), dimension(2) :: corr_type
    class(model_data_t), intent(in) :: model
  end subroutine virtual_init_constants

```

{Virtual: procedures}+≡

```

module subroutine virtual_init_constants (virt, flv_born, nf_input, model)
  class(virtual_t), intent(inout) :: virt
  integer, intent(in), dimension(:,:) :: flv_born
  integer, intent(in) :: nf_input
  type(string_t), dimension(2) :: corr_type
  class(model_data_t), intent(in) :: model
  type(field_data_t), pointer :: field
  integer :: i_part, i_flv, pdg, i_corr
  real(default) :: nf, CA_factor, TR_sum
  real(default), dimension(:,:), allocatable :: CF_factor, TR_factor
  type(flavor_t) :: flv
  allocate (CF_factor (size (flv_born, 1), size (flv_born, 2)), &
    TR_factor (size (flv_born, 1), size (flv_born, 2)))
  corr_type (1) = "QCD"; corr_type (2) = "EW"
  do i_corr = 1, 2
    TR_sum = 0
    if (i_corr == 1) then
      CA_factor = CA; CF_factor = CF; TR_factor = TR
      nf = real(nf_input, default)
      TR_sum = nf * TR
    else
      CA_factor = zero
      do i_flv = 1, size (flv_born, 2)
        do i_part = 1, size (flv_born, 1)
          call flv%init (flv_born(i_part, i_flv), model)
          CF_factor(i_part, i_flv) = (flv%get_charge ())**2
          TR_factor(i_part, i_flv) = (flv%get_charge ())**2
          if (is_quark (flv_born (i_part, i_flv))) &
            TR_factor(i_part, i_flv) = NC * TR_factor(i_part, i_flv)
        end do
      end do
      do pdg = 1, nf_input
        field => model%get_field_ptr (pdg)
        TR_sum = TR_sum + NC*field%get_charge()**2
      end do
      do pdg = 11, 15, 2
        field => model%get_field_ptr (pdg)
        if (field%get_mass() > 0) exit
        TR_sum = TR_sum + field%get_charge()**2
      end do
    end if
    do i_flv = 1, size (flv_born, 2)
      do i_part = 1, size (flv_born, 1)
        if (is_massless_vectorboson (flv_born(i_part, i_flv), corr_type (i_corr))) then
          virt%gamma_0(i_part, i_flv, i_corr) = 11._default / 6._default * CA_factor &
            - two / three * TR_sum
          virt%gamma_p(i_part, i_flv, i_corr) = (67._default / 9._default &
            - two * pi**2 / three) * CA_factor &
            - 23._default / 9._default * TR_sum
          virt%c_flv(i_part, i_flv, i_corr) = CA_factor
        else if (is_corresponding_fermion (flv_born(i_part, i_flv), corr_type (i_corr))) then
          virt%gamma_0(i_part, i_flv, i_corr) = 1.5_default * CF_factor(i_part, i_flv)
          virt%gamma_p(i_part, i_flv, i_corr) = (6.5_default - two * pi**2 / three) * CF_fac

```

```

        virt%c_flv(i_part, i_flv, i_corr) = CF_factor(i_part, i_flv)
    else if (is_massive_vectorbosc (flv_born(i_part, i_flv), corr_type (i_corr))) then
        virt%gamma_0(i_part, i_flv, i_corr) = zero
        virt%gamma_p(i_part, i_flv, i_corr) = zero
        virt%c_flv(i_part, i_flv, i_corr) = CF_factor(i_part, i_flv)
    else
        virt%gamma_0(i_part, i_flv, i_corr) = zero
        virt%gamma_p(i_part, i_flv, i_corr) = zero
        virt%c_flv(i_part, i_flv, i_corr) = zero
    end if
end do
end do
end do
contains
function is_massless_vectorbosc (pdg_nr, nlo_corr_type)
    logical :: is_massless_vectorbosc
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_massless_vectorbosc = .false.
    if (nlo_corr_type == "QCD") then
        is_massless_vectorbosc = is_gluon (pdg_nr)
    else if (nlo_corr_type == "EW") then
        is_massless_vectorbosc = is_photon (pdg_nr)
    end if
end function is_massless_vectorbosc
function is_corresponding_fermion (pdg_nr, nlo_corr_type)
    logical :: is_corresponding_fermion
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_corresponding_fermion = .false.
    if (nlo_corr_type == "QCD") then
        is_corresponding_fermion = is_quark (pdg_nr)
    else if (nlo_corr_type == "EW") then
        is_corresponding_fermion = is_fermion (pdg_nr)
    end if
end function is_corresponding_fermion
function is_massive_vectorbosc (pdg_nr, nlo_corr_type)
    logical :: is_massive_vectorbosc
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_massive_vectorbosc = .false.
    if (nlo_corr_type == "EW") then
        is_massive_vectorbosc = is_massive_vector (pdg_nr)
    end if
end function is_massive_vectorbosc
end subroutine virtual_init_constants

```

Set the renormalization scale. If the input is zero, use the center-of-mass energy.

```

<Virtual: virtual: TBP>+=
    procedure :: set_ren_scale => virtual_set_ren_scale

<Virtual: sub interfaces>+=
    module subroutine virtual_set_ren_scale (virt, ren_scale)
        class(virtual_t), intent(inout) :: virt

```

```

        real(default), allocatable, intent(in) :: ren_scale
    end subroutine virtual_set_ren_scale

<Virtual: procedures>+≡
    module subroutine virtual_set_ren_scale (virt, ren_scale)
        class(virtual_t), intent(inout) :: virt
        real(default), allocatable, intent(in) :: ren_scale
        if (allocated (ren_scale)) then
            if (allocated (virt%ren_scale)) then
                virt%ren_scale = ren_scale
            else
                allocate (virt%ren_scale, source=ren_scale)
            end if
        end if
    end subroutine virtual_set_ren_scale

<Virtual: virtual: TBP>+≡
    procedure :: set_fac_scale => virtual_set_fac_scale

<Virtual: sub interfaces>+≡
    module subroutine virtual_set_fac_scale (virt, p, fac_scale)
        class(virtual_t), intent(inout) :: virt
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in), optional :: fac_scale
    end subroutine virtual_set_fac_scale

<Virtual: procedures>+≡
    module subroutine virtual_set_fac_scale (virt, p, fac_scale)
        class(virtual_t), intent(inout) :: virt
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in), optional :: fac_scale
        if (present (fac_scale)) then
            virt%fac_scale = fac_scale
        else
            virt%fac_scale = (p(1) + p(2))*1
        end if
    end subroutine virtual_set_fac_scale

<Virtual: virtual: TBP>+≡
    procedure :: set_ellis_sexton_scale => virtual_set_ellis_sexton_scale

<Virtual: sub interfaces>+≡
    module subroutine virtual_set_ellis_sexton_scale (virt, Q)
        class(virtual_t), intent(inout) :: virt
        real(default), allocatable, intent(in) :: Q
    end subroutine virtual_set_ellis_sexton_scale

<Virtual: procedures>+≡
    module subroutine virtual_set_ellis_sexton_scale (virt, Q)
        class(virtual_t), intent(inout) :: virt
        real(default), allocatable, intent(in) :: Q
        if (allocated (Q)) then
            if (allocated (virt%es_scale2)) then
                virt%es_scale2 = Q * Q
            else
                allocate (virt%es_scale2, source=Q*Q)
            end if
        end if
    end subroutine virtual_set_ellis_sexton_scale

```



```

        end if
    end if
end subroutine virtual_set_ellis_sexton_scale

```

The virtual-subtracted matrix element is given by the equation

$$\mathcal{V} = \frac{\alpha_s}{2\pi} \left(\mathcal{QB} + \sum \mathcal{I}_{ij} \mathcal{B}_{ij} + \mathcal{V}_{fin} \right), \quad (27.8)$$

The expressions for \mathcal{Q} can be found in equations 27.9 and 27.11. The expressions for \mathcal{I}_{ij} can be found in equations (27.13), (27.14), (27.29), depending on whether the particles involved in the radiation process are massive or massless.

If two or more flavor structures would produce the same amplitude we only compute one and use the `eqv_index` to copy the result to the others (if `reuse_amplitudes_fks` is true).

The Ellis-Sexton scale is set when explicitly allocated; if not it first is set to the renormalization scale; if that it is not set it will be set to the factorization scale which is the scale used for the virtual corrections.

```

<Virtual: virtual: TBP>+≡
    procedure :: evaluate => virtual_evaluate

<Virtual: sub interfaces>+≡
    module subroutine virtual_evaluate (virt, reg_data, alpha_coupling, &
        p_born, separate_uborns, sqme_virt)
        class(virtual_t), intent(inout) :: virt
        type(region_data_t), intent(in) :: reg_data
        real(default), dimension(2), intent(in) :: alpha_coupling
        type(vector4_t), intent(in), dimension(:) :: p_born
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), intent(inout) :: sqme_virt
    end subroutine virtual_evaluate

<Virtual: procedures>+≡
    module subroutine virtual_evaluate (virt, reg_data, alpha_coupling, &
        p_born, separate_uborns, sqme_virt)
        class(virtual_t), intent(inout) :: virt
        type(region_data_t), intent(in) :: reg_data
        real(default), dimension(2), intent(in) :: alpha_coupling
        type(vector4_t), intent(in), dimension(:) :: p_born
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), intent(inout) :: sqme_virt
        integer, dimension(:), allocatable :: eqv_flv_index
        real(default), dimension(:), allocatable :: sqme_virt_arr
        real(default) :: s, s_o_Q2, es_scale2
        real(default), dimension(reg_data%n_flv_born) :: QB, BI
        integer :: i_flv, ii_flv, alr, i_corr
        logical, dimension(:), allocatable :: flv_evaluated
        integer, dimension(:), allocatable :: corr_index
        logical :: alr_qcd, alr_ew
        allocate (flv_evaluated(reg_data%n_flv_born))
        allocate (sqme_virt_arr(reg_data%n_flv_born))
        sqme_virt_arr = zero
        flv_evaluated = .false.
        if (virt%bad_point) return
        if (allocated (virt%es_scale2)) then

```

```

        es_scale2 = virt%es_scale2
    else
        if (allocated (virt%ren_scale)) then
            es_scale2 = virt%ren_scale**2
        else
            es_scale2 = virt%fac_scale**2
        end if
    end if
    if (debug2_active (D_VIRTUAL)) then
        print *, 'Compute virtual component using alpha = ', alpha_coupling
        print *, 'Virtual selection: ', char (virt%selection)
        print *, 'virt%es_scale2 = ', es_scale2 !!! Debugging
    end if
    s = sum (p_born(1 : virt%n_in))**2
    if (virt%settings%factorization_mode == FACTORIZATION_THRESHOLD) &
        call set_s_for_threshold ()
    s_o_Q2 = s / es_scale2 * virt%settings%fks_template%xi_cut**2
    eqv_flv_index = reg_data%eqv_flv_index_born
    do i_flv = 1, reg_data%n_flv_born
        alr_qcd = .false.; alr_ew = .false.
        do alr = 1, reg_data%n_regions
            if (i_flv == reg_data%regions(alr)%uborn_index) then
                if (reg_data%regions(alr)%nlo_correction_type == "QCD") then
                    alr_qcd = .true.
                else if (reg_data%regions(alr)%nlo_correction_type == "EW") then
                    alr_ew = .true.
                end if
            end if
        end do
        if (alr_qcd .and. alr_ew) then
            allocate (corr_index (2))
            corr_index (1) = 1; corr_index (2) = 2
        else
            allocate (corr_index (1))
            corr_index (1) = 0
            if (alr_qcd) then
                corr_index (1) = 1
            else if (alr_ew) then
                corr_index (1) = 2
            end if
        end if
        if (.not. flv_evaluated(eqv_flv_index(i_flv)) .and. corr_index(1) > 0) then
            if (virt%selection == var_str ("Full") .or. virt%selection == var_str ("OLP")) then
                !!! A factor of alpha_coupling/twopi is assumed to be included in vfin
                sqme_virt_arr(i_flv) = sqme_virt_arr(i_flv) + virt%sqme_virt_fin(i_flv)
            end if
            do i_corr = 1, size (corr_index)
                QB = zero; BI = zero
                if (virt%selection == var_str ("Full") .or. &
                    virt%selection == var_str ("Subtraction")) then
                    call virt%evaluate_initial_state (i_flv, corr_index (i_corr), reg_data, QB)
                    call virt%compute_collinear_contribution &
                        (i_flv, corr_index (i_corr), p_born, sqrt(s), reg_data, QB)
                    select case (virt%settings%factorization_mode)

```

```

case (FACTORIZATION_THRESHOLD)
  call virt%compute_eikonals_threshold (i_flv, p_born, s_o_Q2, QB, BI)
case default
  call virt%compute_massive_self_eikonals &
    (i_flv, corr_index (i_corr), p_born, s_o_Q2, reg_data, QB)
  call virt%compute_eikonals &
    (i_flv, corr_index (i_corr), p_born, s_o_Q2, reg_data, BI)
end select
if (debug2_active (D_VIRTUAL)) then
  if (corr_index (i_corr) == 1) then
    print *, 'Correction type: QCD'
  else
    print *, 'Correction type: EW'
  end if
  print *, 'Evaluate i_flv: ', i_flv
  print *, 'sqme_born: ', virt%sqme_born (i_flv)
  print *, 'Q * sqme_born: ', alpha_coupling / twopi * QB(i_flv)
  print *, 'BI: ', alpha_coupling / twopi * BI(i_flv)
  print *, 'vfin: ', virt%sqme_virt_fin (i_flv)
end if
sqme_virt_arr(i_flv) = sqme_virt_arr(i_flv) &
  + alpha_coupling (corr_index (i_corr)) / twopi * (QB(i_flv) + BI(i_flv))
end if
end do
if (.not. (debug_active (D_VIRTUAL) .or. &
  debug2_active (D_VIRTUAL))) flv_evaluated(eqv_flv_index(i_flv)) = .true.
else
  sqme_virt_arr(i_flv) = sqme_virt_arr(eqv_flv_index(i_flv))
end if
if (separate_uborns) then
  sqme_virt(i_flv) = sqme_virt(i_flv) + sqme_virt_arr(i_flv)
else
  sqme_virt(1) = sqme_virt(1) + sqme_virt_arr(i_flv)
end if
deallocate (corr_index)
end do
if (debug2_active (D_VIRTUAL)) then
  call msg_debug2 (D_VIRTUAL, "virtual-subtracted matrix element(s): ")
  print *, sqme_virt
end if
do i_flv = 1, reg_data%n_flv_born
  if (virt%n_is_neutrinos(i_flv) > 0) &
    sqme_virt = sqme_virt * virt%n_is_neutrinos(i_flv) * two
end do
contains
subroutine set_s_for_threshold ()
  use ttv_formfactors, only: mls_to_mpole
  real(default) :: mtop2
  mtop2 = mls_to_mpole (sqrt(s))**2
  if (s < four * mtop2) s = four * mtop2
end subroutine set_s_for_threshold
end subroutine virtual_evaluate

```

```

<Virtual: virtual: TBP>+=
  procedure :: compute_eikonals => virtual_compute_eikonals

<Virtual: sub interfaces>+=
  module subroutine virtual_compute_eikonals (virtual, i_flv, i_corr, &
    p_born, s_o_Q2, reg_data, BI)
    class(virtual_t), intent(inout) :: virtual
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: s_o_Q2
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: BI
  end subroutine virtual_compute_eikonals

<Virtual: procedures>+=
  module subroutine virtual_compute_eikonals (virtual, i_flv, i_corr, &
    p_born, s_o_Q2, reg_data, BI)
    class(virtual_t), intent(inout) :: virtual
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: s_o_Q2
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: BI
    integer :: i, j
    real(default) :: I_ij, BI_tmp
    BI_tmp = zero
    ! TODO vincent_r: Split the procedure into one computing QCD eikonals
    ! and one computing QED eikonals.
    ! TODO vincent_r: In the best case, remove the dependency on
    ! reg_data completely.
    associate (flst_born => reg_data%flv_born(i_flv))
      do i = 1, virtual%n_legs
        do j = 1, virtual%n_legs
          if (i /= j) then
            if (i_corr == 1) then
              if (flst_born%colored(i) .and. flst_born%colored(j)) then
                I_ij = compute_eikonal_factor &
                  (p_born, flst_born%massive, i, j, s_o_Q2)
                BI_tmp = BI_tmp + &
                  virtual%sqme_color_c (i, j, i_flv) * I_ij
                if (debug2_active (D_VIRTUAL)) &
                  print *, 'b_ij: ', i, j, &
                    virtual%sqme_color_c (i, j, i_flv), 'I_ij: ', I_ij
              end if
            else if (i_corr == 2) then
              if (flst_born%charge (i) /= 0 .and. flst_born%charge(j) /= 0) then
                I_ij = compute_eikonal_factor (p_born, flst_born%massive, &
                  i, j, s_o_Q2)
                BI_tmp = BI_tmp + virtual%sqme_charge_c (i, j, i_flv) * I_ij
                if (debug2_active (D_VIRTUAL)) &
                  print *, 'b_ij: ', &
                    virtual%sqme_charge_c (i, j, i_flv), 'I_ij: ', I_ij
              end if
            end if
          end if
        end do
      end do
    end associate
    if (debug2_active (D_VIRTUAL)) then

```

```

        if (i_corr == 1) then
            print *, 'b_ij: ', i, j, &
                virtual%sqme_color_c (i, j, i_flv), 'I_ij: ', I_ij
        else if (i_corr == 2) then
            print *, 'b_ij: ', i, j, &
                virtual%sqme_charge_c (i, j, i_flv), 'I_ij: ', I_ij
        end if
    end if
end do
end do
if (virtual%settings%use_internal_color_correlations .or. i_corr == 2) &
    BI_tmp = BI_tmp * virtual%sqme_born (i_flv)
end associate
BI(i_flv) = BI(i_flv) + BI_tmp
end subroutine virtual_compute_eikonals

```

<Virtual: virtual: TBP>+≡

```

    procedure :: compute_eikonals_threshold => virtual_compute_eikonals_threshold

```

<Virtual: sub interfaces>+≡

```

    module subroutine virtual_compute_eikonals_threshold (virtual, i_flv, &
        p_born, s_o_Q2, QB, BI)
        class(virtual_t), intent(in) :: virtual
        integer, intent(in) :: i_flv
        type(vector4_t), intent(in), dimension(:) :: p_born
        real(default), intent(in) :: s_o_Q2
        real(default), intent(inout), dimension(:) :: QB
        real(default), intent(inout), dimension(:) :: BI
    end subroutine virtual_compute_eikonals_threshold

```

<Virtual: procedures>+≡

```

    module subroutine virtual_compute_eikonals_threshold (virtual, i_flv, &
        p_born, s_o_Q2, QB, BI)
        class(virtual_t), intent(in) :: virtual
        integer, intent(in) :: i_flv
        type(vector4_t), intent(in), dimension(:) :: p_born
        real(default), intent(in) :: s_o_Q2
        real(default), intent(inout), dimension(:) :: QB
        real(default), intent(inout), dimension(:) :: BI
        type(vector4_t), dimension(4) :: p_thr
        integer :: leg
        BI = zero; p_thr = get_threshold_momenta (p_born)
        call compute_massive_self_eikonals (virtual%sqme_born(i_flv), QB(i_flv))
        do leg = 1, 2
            BI(i_flv) = BI(i_flv) + evaluate_leg_pair (ASSOCIATED_LEG_PAIR(leg), i_flv)
        end do
contains
    subroutine compute_massive_self_eikonals (sqme_born, QB)
        real(default), intent(in) :: sqme_born
        real(default), intent(inout) :: QB
        integer :: i
        if (debug_on) call msg_debug2 (D_VIRTUAL, "compute_massive_self_eikonals")
        if (debug_on) call msg_debug2 (D_VIRTUAL, "s_o_Q2", s_o_Q2)
        if (debug_on) call msg_debug2 (D_VIRTUAL, "log (s_o_Q2)", log (s_o_Q2))
        do i = 1, 4

```

```

        QB = QB - (cf * (log (s_o_Q2) - 0.5_default * I_m_eps (p_thr(i)))) &
            * sqme_born
    end do
end subroutine compute_massive_self_eikonals

function evaluate_leg_pair (i_start, i_flv) result (b_ij_times_I)
    real(default) :: b_ij_times_I
    integer, intent(in) :: i_start, i_flv
    real(default) :: I_ij
    integer :: i, j
    b_ij_times_I = zero
    do i = i_start, i_start + 1
        do j = i_start, i_start + 1
            if (i /= j) then
                I_ij = compute_eikonal_factor &
                    (p_thr, [.true., .true., .true., .true.], i, j, s_o_Q2)
                b_ij_times_I = b_ij_times_I + &
                    virtual%sqme_color_c (i, j, i_flv) * I_ij
                if (debug2_active (D_VIRTUAL)) &
                    print *, 'b_ij: ', virtual%sqme_color_c (i, j, i_flv), 'I_ij: ', I_ij
            end if
        end do
    end do
    if (virtual%settings%use_internal_color_correlations) &
        b_ij_times_I = b_ij_times_I * virtual%sqme_born (i_flv)
    if (debug2_active (D_VIRTUAL)) then
        print *, 'internal color: ', virtual%settings%use_internal_color_correlations
        print *, 'b_ij_times_I = ', b_ij_times_I
        print *, 'QB = ', QB
    end if
end function evaluate_leg_pair
end subroutine virtual_compute_eikonals_threshold

```

```

<Virtual: virtual: TBP>+≡
    procedure :: set_bad_point => virtual_set_bad_point
<Virtual: sub interfaces>+≡
    module subroutine virtual_set_bad_point (virt, value)
        class(virtual_t), intent(inout) :: virt
        logical, intent(in) :: value
    end subroutine virtual_set_bad_point
<Virtual: procedures>+≡
    module subroutine virtual_set_bad_point (virt, value)
        class(virtual_t), intent(inout) :: virt
        logical, intent(in) :: value
        virt%bad_point = value
    end subroutine virtual_set_bad_point

```

The collinear limit of $\tilde{\mathcal{R}}$ can be integrated over the radiation degrees of freedom, giving the collinear contribution to the virtual component. Its general structure is $\mathcal{Q} \cdot \mathcal{B}$. The initial-state contribution to \mathcal{Q} is simply given by

$$\mathcal{Q} = -\log \frac{\mu_F^2}{Q^2} (\gamma(\mathcal{I}_1) + 2C(\mathcal{I}_1) \log(\xi_{\text{cut}}) + \gamma(\mathcal{I}_2) + 2C(\mathcal{I}_2) \log(\xi_{\text{cut}})), \quad (27.9)$$

where Q^2 is the Ellis-Sexton scale and γ is as in eqns. 27.4 and 27.5. `virtual_evaluate_initial_state` computes this quantity. The loop over the initial-state particles is only executed if we are dealing with a scattering process, because for decays there are no virtual initial-initial interactions.

```

<Virtual: virtual: TBP>+≡
  procedure :: evaluate_initial_state => virtual_evaluate_initial_state

<Virtual: sub interfaces>+≡
  module subroutine virtual_evaluate_initial_state &
    (virt, i_flv, i_corr, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    type(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_flv, i_corr
    real(default), intent(inout), dimension(:) :: QB
  end subroutine virtual_evaluate_initial_state

<Virtual: procedures>+≡
  module subroutine virtual_evaluate_initial_state &
    (virt, i_flv, i_corr, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    type(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_flv, i_corr
    real(default), intent(inout), dimension(:) :: QB
    real(default) :: sqme_born_virt, es_scale2
    integer :: i
    if (allocated (virt%es_scale2)) then
      es_scale2 = virt%es_scale2
    else
      if (allocated (virt%ren_scale)) then
        es_scale2 = virt%ren_scale**2
      else
        es_scale2 = virt%fac_scale**2
      end if
    end if
    sqme_born_virt = zero
    if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
      .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
      do i = 1, size (reg_data%flv_born(i_flv)%flst)
        if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
          sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
          exit
        end if
      end do
    else
      sqme_born_virt = virt%sqme_born (i_flv)
    end if
    if (virt%n_in == 2) then
      do i = 1, virt%n_in
        QB(i_flv) = QB(i_flv) - (virt%gamma_0 (i, i_flv, i_corr) &
          + two * virt%c_flv(i, i_flv, i_corr) &
          * log (virt%settings%fks_template%xi_cut)) &
          * log(virt%fac_scale**2 / es_scale2) * sqme_born_virt
      end do
    end if
  end subroutine virtual_evaluate_initial_state

```

Same as above, but for final-state particles. The collinear limit for final-state particles follows from the integral

$$I_{+, \alpha_r} = \int d\Phi_{n+1} \frac{\xi_+^{-1-2\epsilon}}{\xi^{-1-2\epsilon}} \mathcal{R}_{\alpha_r}.$$

We can distinguish three situations:

1. α_r contains a massive emitter. In this case, no collinear subtraction term is required and the integral above is irrelevant.
2. α_r contains a massless emitter, but resonances are not taken into account in the subtraction. Here, $\xi_{max} = \frac{2E_{em}}{\sqrt{s}}$ is the upper bound on ξ .
3. α_r contains a massless emitter and resonance-aware subtraction is used. Here, $\xi_{max} = \frac{2E_{em}}{\sqrt{k_{res}^2}}$.

Before version 2.4, only situations 1 and 2 were covered. The difference between situation 2 and 3 comes from the expansion of the plus-distribution in the integral above,

$$\xi_+^{-1-2\epsilon} = \xi^{-1-2\epsilon} + \frac{1}{2\epsilon} \delta(\xi) = \xi_{max}^{-1-2\epsilon} \left[(1-z)^{-1-2\epsilon} + \frac{\xi_{max}^{2\epsilon}}{2\epsilon} \delta(1-z) \right].$$

The expression from the standard FKS literature is given by \mathcal{Q} is given by

$$\begin{aligned} \mathcal{Q} = \sum_{k=n_{in}}^{n_L^{(B)}} & \left[\gamma'(\mathcal{I}_k) - \log \frac{s\delta_o}{2Q^2} \left(\gamma(\mathcal{I}_k) - 2C(\mathcal{I}_k) \log \frac{2E_k}{\xi_{cut}\sqrt{s}} \right) \right. \\ & \left. + 2C(\mathcal{I}_k) \left(\log^2 \frac{2E_k}{\sqrt{s}} - \log^2 \xi_{cut} \right) - 2\gamma(\mathcal{I}_k) \log \frac{2E_k}{\sqrt{s}} \right]. \end{aligned} \quad (27.10)$$

$n_L^{(B)}$ is the number of legs at Born level. Here, ξ_{max} is implicitly present in the ratios in the logarithms. Using the resonance-aware ξ_{max} yields

$$\begin{aligned} \mathcal{Q} = \sum_{k=n_{in}}^{n_L^{(B)}} & \left[\gamma'(\mathcal{I}_k) + 2 \left(\log \frac{\sqrt{s}}{2E_{em}} + \log \xi_{max} \right) \left(\log \frac{\sqrt{s}}{2E_{em}} + \log \xi_{max} + \log \frac{Q^2}{s} \right) C(\mathcal{I}_k) \right. \\ & \left. + 2 \log \xi_{max} \left(\log \xi_{max} - \log \frac{Q^2}{k_{res}^2} \right) C(\mathcal{I}_k) + \left(\log \frac{Q^2}{k_{res}^2} - 2 \log \xi_{max} \right) \gamma(\mathcal{I}_k) \right]. \end{aligned} \quad (27.11)$$

Equation 27.11 leads to 27.10 with the substitutions $\xi_{max} \rightarrow \frac{2E_{em}}{\sqrt{s}}$ and $k_{res}^2 \rightarrow s$. `virtual_compute_collinear_contribution` only implements the second one.

<Virtual: virtual: TBP>+≡

```
procedure :: compute_collinear_contribution &
=> virtual_compute_collinear_contribution
```



```

<Virtual: sub interfaces>+=
  module subroutine virtual_compute_collinear_contribution &
    (virt, i_flv, i_corr, p_born, sqrts, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), dimension(:), intent(in) :: p_born
    real(default), intent(in) :: sqrts
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: QB
  end subroutine virtual_compute_collinear_contribution

<Virtual: procedures>+=
  module subroutine virtual_compute_collinear_contribution &
    (virt, i_flv, i_corr, p_born, sqrts, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), dimension(:), intent(in) :: p_born
    real(default), intent(in) :: sqrts
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: QB
    real(default) :: s1, s2, s3, s4, s5
    real(default) :: sqme_born_virt
    integer :: alr, em, i
    real(default) :: E_em, xi_max, log_xi_max, E_tot2, es_scale2
    logical, dimension(virt%n_flv, virt%n_legs) :: evaluated
    integer :: i_contr
    type(vector4_t) :: k_res
    type(lorentz_transformation_t) :: L_to_resonance
    evaluated = .false.
    if (allocated (virt%es_scale2)) then
      es_scale2 = virt%es_scale2
    else
      if (allocated (virt%ren_scale)) then
        es_scale2 = virt%ren_scale**2
      else
        es_scale2 = virt%fac_scale**2
      end if
    end if
    sqme_born_virt = zero
    if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
      .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
      do i = 1, size (reg_data%flv_born(i_flv)%flst)
        if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
          sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
          exit
        end if
      end do
    else
      sqme_born_virt = virt%sqme_born (i_flv)
    end if
    do alr = 1, reg_data%n_regions
      if (i_flv /= reg_data%regions(alr)%uborn_index) cycle
      em = reg_data%regions(alr)%emitter
      if (em <= virt%n_in) cycle
      if (evaluated(i_flv, em)) cycle

```

```

!!! Collinear terms only for massless particles
if (reg_data%regions(alr)%flst_uborn%massive(em)) cycle
E_em = p_born(em)%p(0)
if (allocated (reg_data%alr_contributors)) then
  i_contr = reg_data%alr_to_i_contributor (alr)
  k_res = get_resonance_momentum (p_born, reg_data%alr_contributors(i_contr)%c)
  E_tot2 = k_res%p(0)**2
  L_to_resonance = inverse (boost (k_res, k_res**1))
  xi_max = two * space_part_norm (L_to_resonance * p_born(em)) / k_res%p(0)
else
  E_tot2 = sqrts**2
  xi_max = two * E_em / sqrts
end if
log_xi_max = log (xi_max)
associate (xi_cut => virt%settings%fks_template%xi_cut, delta_o => virt%settings%fks_template%delta_o)
if (virt%settings%virtual_resonance_aware_collinear) then
  if (debug_active (D_VIRTUAL)) &
    call msg_debug (D_VIRTUAL, "Using resonance-aware collinear subtraction")
  s1 = virt%gamma_p(em, i_flv, i_corr)
  s2 = two * (log (sqrts / (two * E_em)) + log_xi_max) * &
    (log (sqrts / (two * E_em)) + log_xi_max + log (es_scale2 / sqrts**2)) &
    * virt%c_flv(em, i_flv, i_corr)
  s3 = two * log_xi_max * &
    (log_xi_max - log (es_scale2 / E_tot2)) * virt%c_flv(em, i_flv, i_corr)
  s4 = (log (es_scale2 / E_tot2) - two * log_xi_max) &
    * virt%gamma_0(em, i_flv, i_corr)
  QB(i_flv) = QB(i_flv) + (s1 + s2 + s3 + s4) * sqme_born_virt
else
  if (debug_active (D_VIRTUAL)) &
    call msg_debug (D_VIRTUAL, "Using old-fashioned collinear subtraction")
  s1 = virt%gamma_p(em, i_flv, i_corr)
  s2 = log (delta_o * sqrts**2 / (two * es_scale2)) &
    * virt%gamma_0(em, i_flv, i_corr)
  s3 = log (delta_o * sqrts**2 / (two * es_scale2)) * two &
    * virt%c_flv(em, i_flv, i_corr) * log (two * E_em / (xi_cut * sqrts))
  ! s4 = two * virt%c_flv(em, i_flv, i_corr) * (log (two * E_em / sqrts)**2 - log (xi_cut * sqrts))
  s4 = two * virt%c_flv(em, i_flv, i_corr) * & ! a**2 - b**2 = (a - b) * (a + b), for bet
    (log (two * E_em / sqrts) + log (xi_cut)) * (log (two * E_em / sqrts) - log (xi_cut))
  s5 = two * virt%gamma_0(em, i_flv, i_corr) * log (two * E_em / sqrts)
  QB(i_flv) = QB(i_flv) + (s1 - s2 + s3 + s4 - s5) * sqme_born_virt
end if
end associate
evaluated(i_flv, em) = .true.
end do
end subroutine virtual_compute_collinear_contribution

```

For the massless-massive case and $i = j$ we get the massive self-eikonal of (A.10) in arXiv:0908.4272, given as

$$\mathcal{I}_{ii} = \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{\beta} \log \frac{1 + \beta}{1 - \beta}. \quad (27.12)$$

$\langle \text{Virtual: virtual: TBP} \rangle + \equiv$

```

procedure :: compute_massive_self_eikonals => &

```

```

        virtual_compute_massive_self_eikonals
    <Virtual: sub interfaces>+≡
    module subroutine virtual_compute_massive_self_eikonals (virt, &
        i_flv, i_corr, p_born, s_over_Q2, reg_data, QB)
        class(virtual_t), intent(inout) :: virt
        integer, intent(in) :: i_flv, i_corr
        type(vector4_t), intent(in), dimension(:) :: p_born
        real(default), intent(in) :: s_over_Q2
        type(region_data_t), intent(in) :: reg_data
        real(default), intent(inout), dimension(:) :: QB
    end subroutine virtual_compute_massive_self_eikonals
    <Virtual: procedures>+≡
    module subroutine virtual_compute_massive_self_eikonals (virt, &
        i_flv, i_corr, p_born, s_over_Q2, reg_data, QB)
        class(virtual_t), intent(inout) :: virt
        integer, intent(in) :: i_flv, i_corr
        type(vector4_t), intent(in), dimension(:) :: p_born
        real(default), intent(in) :: s_over_Q2
        type(region_data_t), intent(in) :: reg_data
        real(default), intent(inout), dimension(:) :: QB
        real(default) :: sqme_born_virt
        integer :: i
        logical :: massive
        sqme_born_virt = zero
        if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
            .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
            do i = 1, size (reg_data%flv_born(i_flv)%flst)
                if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
                    sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
                    exit
                end if
            end do
        else
            sqme_born_virt = virt%sqme_born (i_flv)
        end if
        do i = 1, virt%n_legs
            massive = reg_data%flv_born(i_flv)%massive(i)
            if (massive) then
                if (virt%c_flv (i, i_flv, i_corr) /= 0) then
                    QB(i_flv) = QB(i_flv) - (virt%c_flv (i, i_flv, i_corr) &
                        * (log (s_over_Q2) - 0.5_default * I_m_eps (p_born(i)))) &
                        * sqme_born_virt
                end if
            end if
        end do
    end subroutine virtual_compute_massive_self_eikonals

```

The following code implements the \mathcal{I}_{ij} -function. The complete formulas can be found in arXiv:0908.4272 (A.1-A.17) and are also discussed in arXiv:1002.2581 in Appendix A. The implementation may differ in the detail from the formulas presented in the above paper. The parameter ξ_{cut} is unphysically and cancels with appropriate factors in the real subtraction. We keep the additional parameter for debug usage. The implemented formulas are then defined as follows:

massless-massless case $p^2 = 0, k^2 = 0$,

$$\begin{aligned} \mathcal{I}_{ij} = & \frac{1}{2} \log^2 \frac{\xi_{\text{cut}}^2 s}{Q^2} + \log \frac{\xi_{\text{cut}}^2 s}{Q^2} \log \frac{k_i k_j}{2E_i E_j} - \text{Li}_2 \left(\frac{k_i k_j}{2E_i E_j} \right) \\ & + \frac{1}{2} \log^2 \frac{k_i k_j}{2E_i E_j} - \log \left(1 - \frac{k_i k_j}{2E_i E_j} \right) \log \frac{k_i k_j}{2E_i E_j}. \end{aligned} \quad (27.13)$$

massive-massive case $p^2 \neq 0, k^2 \neq 0$,

$$\mathcal{I}_{ij} = \frac{1}{2} I_0(k_i, k_j) \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{2} I_\epsilon(k_i, k_j) \quad (27.14)$$

with

$$I_0(k_i, k_j) = \frac{1}{\beta} \log \frac{1 + \beta}{1 - \beta}, \quad \beta = \sqrt{1 - \frac{k_i^2 k_j^2}{(k_i \cdot k_j)^2}} \quad (27.15)$$

and a rather involved expression for I_ϵ :

$$I_\epsilon(k_i, k_j) = (K(z_j) - K(z_i)) \frac{1 - \vec{\beta}_i \cdot \vec{\beta}_j}{\sqrt{a(1-b)}}, \quad (27.16)$$

$$\vec{\beta}_i = \frac{\vec{k}_i}{k_i^0}, \quad (27.17)$$

$$a = \beta_i^2 + \beta_j^2 - 2\vec{\beta}_i \cdot \vec{\beta}_j, \quad (27.18)$$

$$x_i = \frac{\beta_i^2 - \vec{\beta}_i \cdot \vec{\beta}_j}{a}, \quad (27.19)$$

$$x_j = \frac{\beta_j^2 - \vec{\beta}_i \cdot \vec{\beta}_j}{a} = 1 - x_i, \quad (27.20)$$

$$b = \frac{\beta_i^2 \beta_j^2 - (\vec{\beta}_i \cdot \vec{\beta}_j)^2}{a}, \quad (27.21)$$

$$c = \sqrt{\frac{b}{4a}}, \quad (27.22)$$

$$z_+ = \frac{1 + \sqrt{1-b}}{\sqrt{b}}, \quad (27.23)$$

$$z_- = \frac{1 - \sqrt{1-b}}{\sqrt{b}}, \quad (27.24)$$

$$z_i = \frac{\sqrt{x_i^2 + 4c^2} - x_i}{2c}, \quad (27.25)$$

$$z_j = \frac{\sqrt{x_j^2 + 4c^2} + x_j}{2c}, \quad (27.26)$$

$$K(z) = -\frac{1}{2} \log^2 \frac{(z - z_-)(z_+ - z)}{(z_+ + z)(z_- + z)} - 2\text{Li}_2 \left(\frac{2z_-(z_+ - z)}{(z_+ - z_-)(z_- + z)} \right) \quad (27.27)$$

$$- 2\text{Li}_2 \left(-\frac{2z_+(z_- + z)}{(z_+ - z_-)(z_+ - z)} \right) \quad (27.28)$$

massless-massive case $p^2 = 0, k^2 \neq 0$,

$$\mathcal{I}_{ij} = \frac{1}{2} \left[\frac{1}{2} \log^2 \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{\pi^2}{6} \right] + \frac{1}{2} I_0(k_i, k_j) \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{2} I_\epsilon(k_i, k_j) \quad (27.29)$$

with

$$I_0(p, k) = \log \frac{(\hat{p} \cdot \hat{k})^2}{\hat{k}^2}, \quad (27.30)$$

$$I_\epsilon(p, k) = -2 \left[\frac{1}{4} \log^2 \frac{1-\beta}{1+\beta} + \log \frac{\hat{p} \cdot \hat{k}}{1+\beta} \log \frac{\hat{p} \cdot \hat{k}}{1-\beta} + \text{Li}_2 \left(1 - \frac{\hat{p} \cdot \hat{k}}{1+\beta} \right) + \text{Li}_2 \left(1 - \frac{\hat{p} \cdot \hat{k}}{1-\beta} \right) \right], \quad (27.31)$$

using

$$\hat{p} = \frac{p}{p^0}, \quad \hat{k} = \frac{k}{k^0}, \quad \beta = \frac{|\vec{k}|}{k^0}, \quad (27.32)$$

$$\text{Li}_2(1-x) + \text{Li}_2(1-x^{-1}) = -\frac{1}{2} \log^2 x. \quad (27.33)$$

<Virtual: procedures>+≡

```
function compute_eikonal_factor (p_born, massive, i, j, s_o_Q2) result (I_ij)
  real(default) :: I_ij
  type(vector4_t), intent(in), dimension(:) :: p_born
  logical, dimension(:), intent(in) :: massive
  integer, intent(in) :: i, j
  real(default), intent(in) :: s_o_Q2
  if (massive(i) .and. massive(j)) then
    I_ij = compute_Imm (p_born(i), p_born(j), s_o_Q2)
  else if (.not. massive(i) .and. massive(j)) then
    I_ij = compute_I0m (p_born(i), p_born(j), s_o_Q2)
  else if (massive(i) .and. .not. massive(j)) then
    I_ij = compute_I0m (p_born(j), p_born(i), s_o_Q2)
  else
    I_ij = compute_I00 (p_born(i), p_born(j), s_o_Q2)
  end if
end function compute_eikonal_factor
```

```
function compute_I00 (pi, pj, s_o_Q2) result (I)
  type(vector4_t), intent(in) :: pi, pj
  real(default), intent(in) :: s_o_Q2
  real(default) :: I
  real(default) :: Ei, Ej
  real(default) :: pij, Eij
  real(default) :: s1, s2, s3, s4, s5
  real(default) :: arglog
  real(default), parameter :: tiny_value = epsilon(1.0)
  s1 = 0; s2 = 0; s3 = 0; s4 = 0; s5 = 0
  Ei = pi%p(0); Ej = pj%p(0)
  pij = pi * pj; Eij = Ei * Ej
  s1 = 0.5_default * log(s_o_Q2)**2
  s2 = log(s_o_Q2) * log(pij / (two * Eij))
  s3 = Li2 (pij / (two * Eij))
```

```

s4 = 0.5_default * log (pij / (two * Eij))**2
arglog = one - pij / (two * Eij)
if (arglog > tiny_value) then
    s5 = log(arglog) * log(pij / (two * Eij))
else
    s5 = zero
end if
I = s1 + s2 - s3 + s4 - s5
end function compute_I00

function compute_I0m (ki, kj, s_o_Q2) result (I)
    type(vector4_t), intent(in) :: ki, kj
    real(default), intent(in) :: s_o_Q2
    real(default) :: I
    real(default) :: logsomu
    real(default) :: s1, s2, s3
    s1 = 0; s2 = 0; s3 = 0
    logsomu = log(s_o_Q2)
    s1 = 0.5 * (0.5 * logsomu**2 - pi**2 / 6)
    s2 = 0.5 * I_0m_0 (ki, kj) * logsomu
    s3 = 0.5 * I_0m_eps (ki, kj)
    I = s1 + s2 - s3
end function compute_I0m

function compute_Imm (pi, pj, s_o_Q2) result (I)
    type(vector4_t), intent(in) :: pi, pj
    real(default), intent(in) :: s_o_Q2
    real(default) :: I
    real(default) :: s1, s2
    s1 = 0.5 * log(s_o_Q2) * I_mm_0(pi, pj)
    s2 = 0.5 * I_mm_eps(pi, pj)
    I = s1 - s2
end function compute_Imm

function I_m_eps (p) result (I)
    type(vector4_t), intent(in) :: p
    real(default) :: I
    real(default) :: beta
    beta = space_part_norm (p)/p%p(0)
    if (beta < tiny_07) then
        I = four * (one + beta**2/3 + beta**4/5 + beta**6/7)
    else
        I = two * log((one + beta) / (one - beta)) / beta
    end if
end function I_m_eps

function I_0m_eps (p, k) result (I)
    type(vector4_t), intent(in) :: p, k
    real(default) :: I
    type(vector4_t) :: pp, kp
    real(default) :: beta

    pp = p / p%p(0); kp = k / k%p(0)

```

```

    beta = sqrt (one - kp*kp)
    I = -2*(log((one - beta) / (one + beta))**2/4 + log((pp*kp) / (one + beta))*log((pp*kp) / (one
        + Li2(one - (pp*kp) / (one + beta)) + Li2(one - (pp*kp) / (one - beta)))
end function I_0m_eps

function I_0m_0 (p, k) result (I)
    type(vector4_t), intent(in) :: p, k
    real(default) :: I
    type(vector4_t) :: pp, kp

    pp = p / p%p(0); kp = k / k%p(0)
    I = log((pp*kp)**2 / kp**2)
end function I_0m_0

function I_mm_eps (p1, p2) result (I)
    type(vector4_t), intent(in) :: p1, p2
    real(default) :: I
    type(vector4_t) :: q1, q2
    type(vector3_t) :: beta1, beta2
    real(default) :: a, b
    real(default) :: zp, zm, z1, z2, x1, x2
    real(default) :: zmb, z1b
    real(default) :: K1, K2, b1, b2
    real(default) :: nu, a_kl, m12, m22
    beta1 = space_part (p1) / energy(p1)
    beta2 = space_part (p2) / energy(p2)
    if (min (one - beta1**1, one - beta2**1) < tiny_07) then
        if (beta1**1 < beta2**1) then
            call switch_beta (beta1, beta2)
            q1 = p2
            q2 = p1
        else
            q1 = p1
            q2 = p2
        end if
        b1 = beta1**1
        b2 = beta2**1
        m12 = q1**2
        m22 = q2**2
        a_kl = ((q1*q2) + sqrt((q1*q2)**2 - q1**2*q2**2))/m12
        nu = (a_kl**2 * m12 - m22) / two / (a_kl * p1%p(0) - q2%p(0))
        K1 = 0.5_default * log ((one - b1) / (one + b1))**2 &
            + two * Li2 (one - (one - b1)*(a_kl*q1%p(0)/nu)) &
            + two * Li2 (one - (one + b1)*(a_kl*q1%p(0)/nu))
        K2 = 0.5_default * log((one - b2) / (one + b2))**2 &
            + two * Li2 (one - (one - b2)*(q2%p(0)/nu)) &
            + two * Li2 (one - (one + b2)*(q2%p(0)/nu))
        I = (K2 - K1) / sqrt(one - m12*m22/(q1*q2)**2)
    else
        a = beta1**2 + beta2**2 - 2 * beta1 * beta2
        b = beta1**2 * beta2**2 - (beta1 * beta2)**2
        if (beta1**1 > beta2**1) call switch_beta (beta1, beta2)
        b2 = beta2**1
        if (beta1 == vector3_null) then

```

```

        I = (-0.5 * log ((one - b2) / (one + b2))**2 - two * Li2 (-two * b2 / (one - b2))) &
            * one / sqrt (a - b)
        return
    end if
    x1 = beta1**2 - beta1 * beta2
    x2 = beta2**2 - beta1 * beta2
    zp = sqrt (a) + sqrt (a - b)
    zm = sqrt (a) - sqrt (a - b)
    zmb = one / zp
    z1 = sqrt (x1**2 + b) - x1
    z2 = sqrt (x2**2 + b) + x2
    z1b = one / (sqrt (x1**2 + b) + x1)
    K1 = - 0.5_default * log (((z1b - zmb) * (zp - z1)) / ((zp + z1) * (z1b + zmb)))**2 &
        - two * Li2 ((two * zmb * (zp - z1)) / ((zp - zm) * (zmb + z1b))) &
        - two * Li2 ((-two * zp * (zm + z1)) / ((zp - zm) * (zp - z1)))
    K2 = - 0.5_default * log (((z2 - zm) * (zp - z2)) / ((zp + z2) * (z2 + zm)))**2 &
        - two * Li2 ((two * zm * (zp - z2)) / ((zp - zm) * (zm + z2))) &
        - two * Li2 ((-two * zp * (zm + z2)) / ((zp - zm) * (zp - z2)))
    I = (K2 - K1) * (one - beta1 * beta2) / sqrt (a - b)
end if
contains
subroutine switch_beta (beta1, beta2)
    type(vector3_t), intent(inout) :: beta1, beta2
    type(vector3_t) :: beta_tmp
    beta_tmp = beta1
    beta1 = beta2
    beta2 = beta_tmp
end subroutine switch_beta
end function I_mm_eps

function I_mm_0 (k1, k2) result (I)
    type(vector4_t), intent(in) :: k1, k2
    real(default) :: I
    real(default) :: beta, kquotient
    kquotient = k1**2 * k2**2 / (k1 * k2)**2
    if (kquotient > tiny_13) then
        beta = sqrt (one - kquotient)
        I = log ((one + beta) / (one - beta)) / beta
    else
        beta = one - kquotient / two
        I = log (two * (one + beta) / kquotient) / beta
    end if
end function I_mm_0

```

```

<Virtual: virtual: TBP>+≡
    procedure :: final => virtual_final

<Virtual: sub interfaces>+≡
    module subroutine virtual_final (virtual)
        class(virtual_t), intent(inout) :: virtual
    end subroutine virtual_final

<Virtual: procedures>+≡
    module subroutine virtual_final (virtual)
        class(virtual_t), intent(inout) :: virtual
    end subroutine virtual_final

```



```
    if (allocated (virtual%gamma_0)) deallocate (virtual%gamma_0)
    if (allocated (virtual%gamma_p)) deallocate (virtual%gamma_p)
    if (allocated (virtual%c_flv)) deallocate (virtual%c_flv)
    if (allocated (virtual%n_is_neutrinos)) deallocate (virtual%n_is_neutrinos)
end subroutine virtual_final
```

27.6 Real Subtraction

```
<real_subtraction.f90>≡
  <File header>

  module real_subtraction

    <Use kinds with double>
    <Use strings>
    use physics_defs
    use lorentz
    use flavors
    use phs_fks, only: real_kinematics_t, isr_kinematics_t
    use phs_fks, only: I_PLUS, I_MINUS
    use phs_fks, only: SQRTS_VAR, SQRTS_FIXED
    use phs_fks, only: phs_point_set_t

    use fks_regions
    use nlo_data

    <Standard module head>

    <Real subtraction: public>

    <Real subtraction: parameters>

    <Real subtraction: types>

    <Real subtraction: interfaces>

    interface
    <Real subtraction: sub interfaces>
    end interface

  end module real_subtraction

<real_subtraction_sub.f90>≡
  <File header>

  submodule (real_subtraction) real_subtraction_s

    <Use debug>
    use io_units
    use format_defs, only: FMT_15
    use string_utils
    use constants
    use numeric_utils
    use diagnostics
    use pdg_arrays
    use sm_physics
    use models
    use ttv_formfactors, only: mls_to_mpole

    implicit none
```

```
contains

⟨Real subtraction: procedures⟩

end submodule real_subtraction_s
```

Soft subtraction terms

```
⟨Real subtraction: parameters⟩≡
  integer, parameter, public :: INTEGRATION = 0
  integer, parameter, public :: FIXED_ORDER_EVENTS = 1
```

Translates the NLO purpose into a string. However, this purpose is never set and this routine is nowhere used.

```
⟨Real subtraction: procedures⟩≡
  function nlo_purpose (purpose) result (of_purpose)
    type(string_t) :: of_purpose
    integer, intent(in) :: purpose
    select case (purpose)
    case (INTEGRATION)
      of_purpose = var_str ("Integration")
    case (FIXED_ORDER_EVENTS)
      of_purpose = var_str ("Fixed order NLO events")
    case default
      of_purpose = var_str ("Undefined!")
    end select
  end function nlo_purpose
```

In the soft limit, the real matrix element behaves as

$$\mathcal{R}_{\text{soft}} = 4\pi\alpha_s \left[\sum_{i \neq j} \mathcal{B}_{ij} \frac{k_i \cdot k_j}{(k_i \cdot k)(k_j \cdot k)} - \mathcal{B} \sum_i \frac{k_i^2}{(k_i \cdot k)^2} C_i \right],$$

where k denotes the momentum of the emitted parton. The quantity \mathcal{B}_{ij} is called the color-correlated Born matrix element defined as

$$\mathcal{B}_{ij} = \frac{1}{2s} \sum_{\substack{\text{colors} \\ \text{spins}}} \mathcal{M}_{\{c_k\}} \left(\mathcal{M}_{\{c_k\}}^\dagger \right)_{\substack{c_i \rightarrow c'_i \\ c_j \rightarrow c'_j}} T_{c_i, c'_i}^a T_{c_j, c'_j}^a.$$

```
⟨Real subtraction: types⟩≡
  type :: soft_subtraction_t
    type(region_data_t), pointer :: reg_data => null ()
    real(default), dimension(:,:), allocatable :: momentum_matrix
    logical :: use_resonance_mappings = .false.
    type(vector4_t) :: p_soft = vector4_null
    logical :: use_internal_color_correlations = .true.
    logical :: use_internal_spin_correlations = .false.
    logical :: xi2_expanded = .true.
    integer :: factorization_mode = NO_FACTORIZATION
contains
```

```

    <Real subtraction: soft sub: TBP>
    end type soft_subtraction_t

    <Real subtraction: soft sub: TBP>≡
    procedure :: init => soft_subtraction_init

    <Real subtraction: sub interfaces>≡
    module subroutine soft_subtraction_init (sub_soft, reg_data)
        class(soft_subtraction_t), intent(inout) :: sub_soft
        type(region_data_t), intent(in), target :: reg_data
    end subroutine soft_subtraction_init

    <Real subtraction: procedures>+≡
    module subroutine soft_subtraction_init (sub_soft, reg_data)
        class(soft_subtraction_t), intent(inout) :: sub_soft
        type(region_data_t), intent(in), target :: reg_data
        sub_soft%reg_data => reg_data
        allocate (sub_soft%momentum_matrix (reg_data%n_legs_born, &
            reg_data%n_legs_born))
    end subroutine soft_subtraction_init

    <Real subtraction: soft sub: TBP>+≡
    procedure :: requires_boost => soft_subtraction_requires_boost

    <Real subtraction: sub interfaces>+≡
    module function soft_subtraction_requires_boost &
        (sub_soft, sqrts) result (requires_boost)
        logical :: requires_boost
        class(soft_subtraction_t), intent(in) :: sub_soft
        real(default), intent(in) :: sqrts
    end function soft_subtraction_requires_boost

    <Real subtraction: procedures>+≡
    module function soft_subtraction_requires_boost &
        (sub_soft, sqrts) result (requires_boost)
        logical :: requires_boost
        class(soft_subtraction_t), intent(in) :: sub_soft
        real(default), intent(in) :: sqrts
        real(default) :: mtop
        logical :: above_threshold
        if (sub_soft%factorization_mode == FACTORIZATION_THRESHOLD) then
            mtop = mls_to_mpole (sqrts)
            above_threshold = sqrts**2 - four * mtop**2 > zero
        else
            above_threshold = .false.
        end if
        requires_boost = sub_soft%use_resonance_mappings .or. above_threshold
    end function soft_subtraction_requires_boost

```

The treatment of the momentum k follows the discussion about the soft limit of the partition functions (see [1002.2581], p. 29 and C. Weiss' PhD Thesis, p. 24). The parton momentum is pulled out, $k = E\hat{k}$. In fact, we will substitute \hat{k} for k throughout the code, because the energy will factor out of the equation when the soft \mathcal{S} -function is multiplied. The momentum `p_soft` represents the soft

limit of the radiated particle divided by its energy. It is a unit vector, because $k^2 = (k^0)^2 - (\hat{k})^2 = 0$.

The soft momentum is constructed by first creating a unit vector parallel to the emitter's Born momentum. This unit vector is then rotated about the corresponding angles y and ϕ to match the direction of the real radiation in the soft limit.

(Real subtraction: soft sub: TBP)+≡

```
procedure :: create_softvec_fsr => soft_subtraction_create_softvec_fsr
```

(Real subtraction: sub interfaces)+≡

```
module subroutine soft_subtraction_create_softvec_fsr &
  (sub_soft, p_born, y, phi, emitter, xi_ref_momentum)
  class(soft_subtraction_t), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: y, phi
  integer, intent(in) :: emitter
  type(vector4_t), intent(in) :: xi_ref_momentum
end subroutine soft_subtraction_create_softvec_fsr
```

(Real subtraction: procedures)+≡

```
module subroutine soft_subtraction_create_softvec_fsr &
  (sub_soft, p_born, y, phi, emitter, xi_ref_momentum)
  class(soft_subtraction_t), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: y, phi
  integer, intent(in) :: emitter
  type(vector4_t), intent(in) :: xi_ref_momentum
  type(vector3_t) :: dir
  type(vector4_t) :: p_em
  type(lorentz_transformation_t) :: rot
  type(lorentz_transformation_t) :: boost_to_rest_frame
  logical :: requires_boost
  associate (p_soft => sub_soft%p_soft)
    p_soft%p(0) = one
    requires_boost = sub_soft%requires_boost (two * p_born(1)%p(0))
    if (requires_boost) then
      boost_to_rest_frame = inverse (boost (xi_ref_momentum, xi_ref_momentum**1))
      p_em = boost_to_rest_frame * p_born(emitter)
    else
      p_em = p_born(emitter)
    end if
    p_soft%p(1:3) = p_em%p(1:3) / space_part_norm (p_em)
    dir = create_orthogonal (space_part (p_em))
    rot = rotation (y, sqrt(one - y**2), dir)
    p_soft = rot * p_soft
    if (.not. vanishes (phi)) then
      dir = space_part (p_em) / space_part_norm (p_em)
      rot = rotation (cos(phi), sin(phi), dir)
      p_soft = rot * p_soft
    end if
    if (requires_boost) p_soft = inverse (boost_to_rest_frame) * p_soft
  end associate
end subroutine soft_subtraction_create_softvec_fsr
```

For initial-state emissions, the soft vector is just a unit vector with the same direction as the radiated particle. As y for ISR is defined independently of the emitter, also p_{soft} is the same for all initial state emitters.

```

<Real subtraction: soft sub: TBP>+≡
  procedure :: create_softvec_isr => soft_subtraction_create_softvec_isr

<Real subtraction: sub interfaces>+≡
  module subroutine soft_subtraction_create_softvec_isr (sub_soft, y, phi)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    real(default), intent(in) :: y, phi
  end subroutine soft_subtraction_create_softvec_isr

<Real subtraction: procedures>+≡
  module subroutine soft_subtraction_create_softvec_isr (sub_soft, y, phi)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    real(default), intent(in) :: y, phi
    real(default) :: sin_theta
    sin_theta = sqrt(one - y**2)
    associate (p => sub_soft%p_soft%p)
      p(0) = one
      p(1) = sin_theta * sin(phi)
      p(2) = sin_theta * cos(phi)
      p(3) = y
    end associate
  end subroutine soft_subtraction_create_softvec_isr

```

The soft vector for the real mismatch is basically the same as for usual FSR, except for the scaling with the total gluon energy. Moreover, the resulting vector is rotated into the frame where the 3-axis points along the direction of the emitter. This is necessary because in the collinear limit, the approximation

$$k_i = \frac{k_i^0}{k_j^0} \bar{k}_j = \frac{\xi \sqrt{s}}{2k_j^0} \bar{k}_j$$

is used. The collinear limit is not included in the soft mismatch yet, but we keep the rotation for future usage here already (the performance loss is negligible).

```

<Real subtraction: soft sub: TBP>+≡
  procedure :: create_softvec_mismatch => &
    soft_subtraction_create_softvec_mismatch

<Real subtraction: sub interfaces>+≡
  module subroutine soft_subtraction_create_softvec_mismatch &
    (sub_soft, E, y, phi, p_em)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    real(default), intent(in) :: E, phi, y
    type(vector4_t), intent(in) :: p_em
  end subroutine soft_subtraction_create_softvec_mismatch

<Real subtraction: procedures>+≡
  module subroutine soft_subtraction_create_softvec_mismatch &
    (sub_soft, E, y, phi, p_em)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    real(default), intent(in) :: E, phi, y
    type(vector4_t), intent(in) :: p_em
    real(default) :: sin_theta

```

```

type(lorentz_transformation_t) :: rot_em_off_3_axis
sin_theta = sqrt (one - y**2)
associate (p => sub_soft%p_soft%p)
  p(0) = E
  p(1) = E * sin_theta * sin(phi)
  p(2) = E * sin_theta * cos(phi)
  p(3) = E * y
end associate
rot_em_off_3_axis = rotation_to_2nd (3, space_part (p_em))
sub_soft%p_soft = rot_em_off_3_axis * sub_soft%p_soft
end subroutine soft_subtraction_create_softvec_mismatch

```

Computation of the soft limit of R_α . Note that what we are actually integrating (in the case of final-state radiation) is the quantity $f(0, y)/\xi$, where

$$f(\xi, y) = \frac{J(\xi, y, \phi)}{\xi} \xi^2 R_\alpha.$$

J/ξ is computed by the phase space generator. The additional factor of ξ^{-1} is supplied in the `evaluate_region_fsr`-routine. Thus, we are left with a factor of ξ^2 . A look on the expression for the soft limit of R_α below reveals that we are factoring out the gluon energy E_i in the denominator. Therefore, we have a factor $\xi^2/E_i^2 = 4/q^2$.

Note that the same routine is used also for the computation of the soft mismatch. There, the gluon energy is not factored out from the soft vector, so that we are left with the ξ^2 -factor, which will eventually be cancelled out again. So, we just multiply with 1. Both cases are distinguished by the flag `xi2_expanded`.

Note that for the soft subtraction term, also the S functions are computed in the soft limit. The input momenta are thus the real momenta in the soft limit, i.e. the Born momenta given by `p_born`.

(Real subtraction: soft sub: TBP)+≡

```

procedure :: compute => soft_subtraction_compute

```

(Real subtraction: sub interfaces)+≡

```

module function soft_subtraction_compute (sub_soft, p_born, &
  born_ij, y, q2, alpha_coupling, alr, emitter, i_res) result (sqme)
  real(default) :: sqme
  class(soft_subtraction_t), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in), dimension(:,:) :: born_ij
  real(default), intent(in) :: y
  real(default), intent(in) :: q2, alpha_coupling
  integer, intent(in) :: alr, emitter, i_res
end function soft_subtraction_compute

```

(Real subtraction: procedures)+≡

```

module function soft_subtraction_compute (sub_soft, p_born, &
  born_ij, y, q2, alpha_coupling, alr, emitter, i_res) result (sqme)
  real(default) :: sqme
  class(soft_subtraction_t), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in), dimension(:,:) :: born_ij

```

```

real(default), intent(in) :: y
real(default), intent(in) :: q2, alpha_coupling
integer, intent(in) :: alr, emitter, i_res
real(default) :: s_alpha_soft
real(default) :: kb
real(default) :: xi2_factor

if (.not. vector_set_is_cms (p_born, sub_soft%reg_data%n_in)) then
  call vector4_write_set (p_born, show_mass = .true., &
    check_conservation = .true.)
  call msg_fatal ("Soft subtraction: phase space point must be in CMS")
end if
if (debug2_active (D_SUBTRACTION)) then
  select case (char (sub_soft%reg_data%regions(alr)%nlo_correction_type))
  case ("QCD")
    print *, 'Compute soft subtraction using alpha_s = ', alpha_coupling
  case ("EW")
    print *, 'Compute soft subtraction using alpha_qed = ', alpha_coupling
  end select
end if

s_alpha_soft = sub_soft%reg_data%get_svalue_soft (p_born, &
  sub_soft%p_soft, alr, emitter, i_res)
if (s_alpha_soft > one + tiny_07) call msg_fatal ("s_alpha_soft > 1!")
if (debug2_active (D_SUBTRACTION)) &
  call msg_print_color ('s_alpha_soft', s_alpha_soft, COL_YELLOW)
select case (sub_soft%factorization_mode)
case (NO_FACTORIZATION)
  kb = sub_soft%evaluate_factorization_default (p_born, born_ij)
case (FACTORIZATION_THRESHOLD)
  kb = sub_soft%evaluate_factorization_threshold (thr_leg(emitter), p_born, born_ij)
end select
if (debug_on) call msg_debug2 (D_SUBTRACTION, 'KB', kb)
sqme = four * pi * alpha_coupling * s_alpha_soft * kb
if (sub_soft%xi2_expanded) then
  xi2_factor = four / q2
else
  xi2_factor = one
end if
if (emitter <= sub_soft%reg_data%n_in) then
  sqme = xi2_factor * (one - y**2) * sqme
else
  sqme = xi2_factor * (one - y) * sqme
end if
if (sub_soft%reg_data%regions(alr)%double_fsr) sqme = sqme * two
end function soft_subtraction_compute

```

We loop over all external legs and do not take care to leave out non-colored ones because `born_ij` is constructed in such a way that it is only non-zero for colored entries.

(Real subtraction: soft sub: TBP)+≡

```

procedure :: evaluate_factorization_default => &
  soft_subtraction_evaluate_factorization_default

```



```

<Real subtraction: sub interfaces>+≡
  module function soft_subtraction_evaluate_factorization_default &
    (sub_soft, p, born_ij) result (kb)
    real(default) :: kb
    class(soft_subtraction_t), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in), dimension(:, :) :: born_ij
  end function soft_subtraction_evaluate_factorization_default

<Real subtraction: procedures>+≡
  module function soft_subtraction_evaluate_factorization_default &
    (sub_soft, p, born_ij) result (kb)
    real(default) :: kb
    class(soft_subtraction_t), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in), dimension(:, :) :: born_ij
    integer :: i, j
    kb = zero
    call sub_soft%compute_momentum_matrix (p)
    do i = 1, size (p)
      do j = 1, size (p)
        kb = kb + sub_soft%momentum_matrix (i, j) * born_ij (i, j)
      end do
    end do
  end function soft_subtraction_evaluate_factorization_default

```

We have to multiply this with $\xi^2(1-y)$. Further, when applying the soft \mathcal{S} -function, the energy of the radiated particle is factored out. Thus we have $\xi^2/E_{em}^2(1-y) = 4/q_0^2(1-y)$. Computes the quantity $\mathcal{K}_{ij} = \frac{k_i \cdot k_j}{(k_i \cdot k)(k_j \cdot k)}$.

```

<Real subtraction: soft sub: TBP>+≡
  procedure :: compute_momentum_matrix => &
    soft_subtraction_compute_momentum_matrix

<Real subtraction: sub interfaces>+≡
  module subroutine soft_subtraction_compute_momentum_matrix &
    (sub_soft, p_born)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p_born
  end subroutine soft_subtraction_compute_momentum_matrix

<Real subtraction: procedures>+≡
  module subroutine soft_subtraction_compute_momentum_matrix &
    (sub_soft, p_born)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default) :: num, deno1, deno2
    integer :: i, j
    do i = 1, sub_soft%reg_data%n_legs_born
      do j = 1, sub_soft%reg_data%n_legs_born
        if (i <= j) then
          num = p_born(i) * p_born(j)
          deno1 = p_born(i) * sub_soft%p_soft
          deno2 = p_born(j) * sub_soft%p_soft
          sub_soft%momentum_matrix(i, j) = num / (deno1 * deno2)
        else

```

```

        !!! momentum matrix is symmetric.
        sub_soft%momentum_matrix(i, j) = sub_soft%momentum_matrix(j, i)
    end if
end do
end do
end subroutine soft_subtraction_compute_momentum_matrix

```

<Real subtraction: soft sub: TBP>+≡

```

procedure :: evaluate_factorization_threshold => &
    soft_subtraction_evaluate_factorization_threshold

```

<Real subtraction: sub interfaces>+≡

```

module function soft_subtraction_evaluate_factorization_threshold &
    (sub_soft, leg, p_born, born_ij) result (kb)
    real(default) :: kb
    class(soft_subtraction_t), intent(inout) :: sub_soft
    integer, intent(in) :: leg
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in), dimension(:, :) :: born_ij
end function soft_subtraction_evaluate_factorization_threshold

```

<Real subtraction: procedures>+≡

```

module function soft_subtraction_evaluate_factorization_threshold &
    (sub_soft, leg, p_born, born_ij) result (kb)
    real(default) :: kb
    class(soft_subtraction_t), intent(inout) :: sub_soft
    integer, intent(in) :: leg
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in), dimension(:, :) :: born_ij
    type(vector4_t), dimension(4) :: p
    p = get_threshold_momenta (p_born)
    kb = evaluate_leg_pair (ASSOCIATED_LEG_PAIR (leg))
    if (debug2_active (D_SUBTRACTION)) call show_debug ()

```

contains

```

function evaluate_leg_pair (i_start) result (kbb)
    real(default) :: kbb
    integer, intent(in) :: i_start
    integer :: i1, i2
    real(default) :: numerator, deno1, deno2
    kbb = zero
    do i1 = i_start, i_start + 1
        do i2 = i_start, i_start + 1
            numerator = p(i1) * p(i2)
            deno1 = p(i1) * sub_soft%p_soft
            deno2 = p(i2) * sub_soft%p_soft
            kbb = kbb + numerator * born_ij (i1, i2) / deno1 / deno2
        end do
    end do
    if (debug2_active (D_SUBTRACTION)) then
        do i1 = i_start, i_start + 1
            do i2 = i_start, i_start + 1
                call msg_print_color('i1', i1, COL_PEACH)
                call msg_print_color('i2', i2, COL_PEACH)
            end do
        end do
    end if
end function evaluate_leg_pair

```

```

        call msg_print_color('born_ij (i1,i2)', born_ij (i1,i2), &
            COL_PINK)
        print *, 'Top momentum: ', p(1)%p
    end do
end do
end if
end function evaluate_leg_pair

subroutine show_debug ()
    integer :: i
    call msg_print_color &
        ('soft_subtraction_evaluate_factorization_threshold', COL_GREEN)
    do i = 1, 4
        print *, 'sqrt(p(i)**2) = ', sqrt(p(i)**2)
    end do
end subroutine show_debug

end function soft_subtraction_evaluate_factorization_threshold

<Real subtraction: soft sub: TBP>+≡
    procedure :: i_xi_ref => soft_subtraction_i_xi_ref

<Real subtraction: sub interfaces>+≡
    module function soft_subtraction_i_xi_ref &
        (sub_soft, alr, i_phs) result (i_xi_ref)
        integer :: i_xi_ref
        class(soft_subtraction_t), intent(in) :: sub_soft
        integer, intent(in) :: alr, i_phs
    end function soft_subtraction_i_xi_ref

<Real subtraction: procedures>+≡
    module function soft_subtraction_i_xi_ref &
        (sub_soft, alr, i_phs) result (i_xi_ref)
        integer :: i_xi_ref
        class(soft_subtraction_t), intent(in) :: sub_soft
        integer, intent(in) :: alr, i_phs
        if (sub_soft%use_resonance_mappings) then
            i_xi_ref = sub_soft%reg_data%alr_to_i_contributor (alr)
        else if (sub_soft%factorization_mode == FACTORIZATION_THRESHOLD) then
            i_xi_ref = i_phs
        else
            i_xi_ref = 1
        end if
    end function soft_subtraction_i_xi_ref

<Real subtraction: soft sub: TBP>+≡
    procedure :: final => soft_subtraction_final

<Real subtraction: sub interfaces>+≡
    module subroutine soft_subtraction_final (sub_soft)
        class(soft_subtraction_t), intent(inout) :: sub_soft
    end subroutine soft_subtraction_final

<Real subtraction: procedures>+≡
    module subroutine soft_subtraction_final (sub_soft)

```

```

class(soft_subtraction_t), intent(inout) :: sub_soft
if (associated (sub_soft%reg_data)) nullify (sub_soft%reg_data)
if (allocated (sub_soft%momentum_matrix)) &
    deallocate (sub_soft%momentum_matrix)
end subroutine soft_subtraction_final

```

27.6.1 Soft mismatch

```

⟨Real subtraction: public⟩≡
public :: soft_mismatch_t

```

```

⟨Real subtraction: types⟩+≡
type :: soft_mismatch_t
    type(region_data_t), pointer :: reg_data => null ()
    real(default), dimension(:), allocatable :: sqme_born
    real(default), dimension(:,:,:), allocatable :: sqme_born_color_c
    real(default), dimension(:,:,:), allocatable :: sqme_born_charge_c
    type(real_kinematics_t), pointer :: real_kinematics => null ()
    type(soft_subtraction_t) :: sub_soft
contains
⟨Real subtraction: soft mismatch: TBP⟩
end type soft_mismatch_t

```

```

⟨Real subtraction: soft mismatch: TBP⟩≡
procedure :: init => soft_mismatch_init

```

```

⟨Real subtraction: sub interfaces⟩+≡
module subroutine soft_mismatch_init (soft_mismatch, reg_data, &
    real_kinematics, factorization_mode)
    class(soft_mismatch_t), intent(inout) :: soft_mismatch
    type(region_data_t), intent(in), target :: reg_data
    type(real_kinematics_t), intent(in), target :: real_kinematics
    integer, intent(in) :: factorization_mode
end subroutine soft_mismatch_init

```

```

⟨Real subtraction: procedures⟩+≡
module subroutine soft_mismatch_init (soft_mismatch, reg_data, &
    real_kinematics, factorization_mode)
    class(soft_mismatch_t), intent(inout) :: soft_mismatch
    type(region_data_t), intent(in), target :: reg_data
    type(real_kinematics_t), intent(in), target :: real_kinematics
    integer, intent(in) :: factorization_mode
    soft_mismatch%reg_data => reg_data
    allocate (soft_mismatch%sqme_born (reg_data%n_flv_born))
    allocate (soft_mismatch%sqme_born_color_c (reg_data%n_legs_born, &
        reg_data%n_legs_born, reg_data%n_flv_born))
    allocate (soft_mismatch%sqme_born_charge_c (reg_data%n_legs_born, &
        reg_data%n_legs_born, reg_data%n_flv_born))
    call soft_mismatch%sub_soft%init (reg_data)
    soft_mismatch%sub_soft%xi2_expanded = .false.
    soft_mismatch%real_kinematics => real_kinematics
    soft_mismatch%sub_soft%factorization_mode = factorization_mode
end subroutine soft_mismatch_init

```

Main routine to compute the soft mismatch. Loops over all singular regions. There, it first creates the soft vector, then the necessary soft real matrix element. These inputs are then used to get the numerical value of the soft mismatch.

```

<Real subtraction: soft mismatch: TBP>+≡
  procedure :: evaluate => soft_mismatch_evaluate

<Real subtraction: sub interfaces>+≡
  module function soft_mismatch_evaluate &
    (soft_mismatch, alpha_s) result (sqme_mismatch)
    real(default) :: sqme_mismatch
    class(soft_mismatch_t), intent(inout) :: soft_mismatch
    real(default), intent(in) :: alpha_s
  end function soft_mismatch_evaluate

<Real subtraction: procedures>+≡
  module function soft_mismatch_evaluate &
    (soft_mismatch, alpha_s) result (sqme_mismatch)
    real(default) :: sqme_mismatch
    class(soft_mismatch_t), intent(inout) :: soft_mismatch
    real(default), intent(in) :: alpha_s
    integer :: alr, i_born, emitter, i_res, i_phs, i_con
    real(default) :: xi, y, q2, s
    real(default) :: E_gluon
    type(vector4_t) :: p_em
    real(default) :: sqme_alr, sqme_soft
    type(vector4_t), dimension(:), allocatable :: p_born
    sqme_mismatch = zero
    associate (real_kinematics => soft_mismatch%real_kinematics)
      xi = real_kinematics%xi_mismatch
      y = real_kinematics%y_mismatch
      s = real_kinematics%cms_energy2
      E_gluon = sqrt (s) * xi / two

      if (debug_active (D_MISMATCH)) then
        print *, 'Evaluating soft mismatch: '
        print *, 'Phase space: '
        call vector4_write_set (real_kinematics%p_born_cms%get_momenta(1), &
          show_mass = .true.)
        print *, 'xi: ', xi, 'y: ', y, 's: ', s, 'E_gluon: ', E_gluon
      end if

      allocate (p_born (soft_mismatch%reg_data%n_legs_born))

      do alr = 1, soft_mismatch%reg_data%n_regions

        i_phs = real_kinematics%alr_to_i_phs (alr)
        if (soft_mismatch%reg_data%has_pseudo_isr ()) then
          i_con = 1
          p_born = &
            soft_mismatch%real_kinematics%p_born_onshell%get_momenta(1)
        else
          i_con = soft_mismatch%reg_data%alr_to_i_contributor (alr)
          p_born = soft_mismatch%real_kinematics%p_born_cms%get_momenta(1)
        end if
        q2 = real_kinematics%xi_ref_momenta(i_con)**2

```

```

emitter = soft_mismatch%reg_data%regions(alr)%emitter
p_em = p_born (emitter)
i_res = soft_mismatch%reg_data%regions(alr)%i_res
i_born = soft_mismatch%reg_data%regions(alr)%uborn_index

call print_debug_alr ()

call soft_mismatch%sub_soft%create_softvec_mismatch &
(E_gluon, y, real_kinematics%phi, p_em)
if (debug_active (D_MISMATCH)) &
print *, 'Created soft vector: ', &
soft_mismatch%sub_soft%p_soft%p

select type (fks_mapping => soft_mismatch%reg_data%fks_mapping)
type is (fks_mapping_resonances_t)
call fks_mapping%set_resonance_momentum &
(real_kinematics%xi_ref_momenta(i_con))
end select

sqme_soft = soft_mismatch%sub_soft%compute &
(p_born, soft_mismatch%sqme_born_color_c(:, :, i_born), y, &
q2, alpha_s, alr, emitter, i_res)

sqme_alr = soft_mismatch%compute (alr, xi, y, p_em, &
real_kinematics%xi_ref_momenta(i_con), &
soft_mismatch%sub_soft%p_soft, &
soft_mismatch%sqme_born(i_born), sqme_soft, &
alpha_s, s)

if (debug_on) call msg_debug (D_MISMATCH, 'sqme_alr: ', sqme_alr)
sqme_mismatch = sqme_mismatch + sqme_alr

end do
end associate
contains
subroutine print_debug_alr ()
if (debug_active (D_MISMATCH)) then
print *, 'alr: ', alr
print *, 'i_phs: ', i_phs, 'i_con: ', i_con, 'i_res: ', i_res
print *, 'emitter: ', emitter, 'i_born: ', i_born
print *, 'emitter momentum: ', p_em%p
print *, 'resonance momentum: ', &
soft_mismatch%real_kinematics%xi_ref_momenta(i_con)%p
print *, 'q2: ', q2
end if
end subroutine print_debug_alr
end function soft_mismatch_evaluate

```

Computes the soft mismatch in a given α_r ,

$$I_{s+, \alpha_r} = \int d\Phi_B \int_0^\infty d\xi \int_{-1}^1 dy \int_0^{2\pi} d\phi \frac{s\xi}{(4\pi)^3} \\ \times \left\{ \tilde{R}_{\alpha_r} \left(e^{-\frac{2k_{em} \cdot k_{res}}{k_{res}^2}} - e^{-\xi} \right) - \frac{32\pi\alpha_s C_{em}}{s\xi^2} B_{fb(\alpha_r)} (1-y)^{-1} \left[e^{-\frac{2k_{em} \cdot k_{res}}{k_{res}^2} \frac{k_{em}^0}{k_{em}^0}} - e^{-\xi} \right] \right\}.$$

(Real subtraction: soft mismatch: TBP)+≡

procedure :: compute => soft_mismatch_compute

(Real subtraction: sub interfaces)+≡

```
module function soft_mismatch_compute &
  (soft_mismatch, alr, xi, y, p_em, p_res, p_soft, &
   sqme_born, sqme_soft, alpha_s, s) result (sqme_mismatch)
  real(default) :: sqme_mismatch
  class(soft_mismatch_t), intent(in) :: soft_mismatch
  integer, intent(in) :: alr
  real(default), intent(in) :: xi, y
  type(vector4_t), intent(in) :: p_em, p_res, p_soft
  real(default), intent(in) :: sqme_born, sqme_soft
  real(default), intent(in) :: alpha_s, s
end function soft_mismatch_compute
```

(Real subtraction: procedures)+≡

```
module function soft_mismatch_compute &
  (soft_mismatch, alr, xi, y, p_em, p_res, p_soft, &
   sqme_born, sqme_soft, alpha_s, s) result (sqme_mismatch)
  real(default) :: sqme_mismatch
  class(soft_mismatch_t), intent(in) :: soft_mismatch
  integer, intent(in) :: alr
  real(default), intent(in) :: xi, y
  type(vector4_t), intent(in) :: p_em, p_res, p_soft
  real(default), intent(in) :: sqme_born, sqme_soft
  real(default), intent(in) :: alpha_s, s
  real(default) :: q2, expo, sm1, sm2, jacobian

  q2 = p_res**2
  expo = - two * p_soft * p_res / q2
  !!! Divide by 1 - y to factor out the corresponding
  !!! factor in the soft matrix element
  sm1 = sqme_soft / (one - y) * ( exp(expo) - exp(- xi) )
  if (debug_on) call msg_debug2 &
    (D_MISMATCH, 'sqme_soft in mismatch ', sqme_soft)

  sm2 = zero
  if (soft_mismatch%reg_data%regions(alr)%has_collinear_divergence ()) then
    expo = - two * p_em * p_res / q2 * &
      p_soft%p(0) / p_em%p(0)
    sm2 = 32 * pi * alpha_s * cf / (s * xi**2) * sqme_born * &
      ( exp(expo) - exp(- xi) ) / (one - y)
  end if

  jacobian = soft_mismatch%real_kinematics%jac_mismatch * &
    s * xi / (8 * twopi3)
```

```

        sqme_mismatch = (sm1 - sm2) * jacobian

    end function soft_mismatch_compute

    <Real subtraction: soft mismatch: TBP>+≡
    procedure :: final => soft_mismatch_final

    <Real subtraction: sub interfaces>+≡
    module subroutine soft_mismatch_final (soft_mismatch)
        class(soft_mismatch_t), intent(inout) :: soft_mismatch
    end subroutine soft_mismatch_final

    <Real subtraction: procedures>+≡
    module subroutine soft_mismatch_final (soft_mismatch)
        class(soft_mismatch_t), intent(inout) :: soft_mismatch
        call soft_mismatch%sub_soft%final ()
        if (associated (soft_mismatch%reg_data)) nullify (soft_mismatch%reg_data)
        if (allocated (soft_mismatch%sqme_born)) &
            deallocate (soft_mismatch%sqme_born)
        if (allocated (soft_mismatch%sqme_born_color_c)) &
            deallocate (soft_mismatch%sqme_born_color_c)
        if (allocated (soft_mismatch%sqme_born_charge_c)) &
            deallocate (soft_mismatch%sqme_born_charge_c)
        if (associated (soft_mismatch%real_kinematics)) &
            nullify (soft_mismatch%real_kinematics)
    end subroutine soft_mismatch_final

```

27.6.2 Collinear and soft-collinear subtraction terms

This data type deals with the calculation of the collinear and soft-collinear contribution to the cross section.

```

    <Real subtraction: public>+≡
    public :: coll_subtraction_t

    <Real subtraction: types>+≡
    type :: coll_subtraction_t
        integer :: n_in, n_alr
        logical :: use_resonance_mappings = .false.
        real(default) :: CA = 0, CF = 0, TR = 0
    contains
        <Real subtraction: coll sub: TBP>
        end type coll_subtraction_t

    <Real subtraction: coll sub: TBP>≡
    procedure :: init => coll_subtraction_init

    <Real subtraction: sub interfaces>+≡
    module subroutine coll_subtraction_init (coll_sub, n_alr, n_in)
        class(coll_subtraction_t), intent(inout) :: coll_sub
        integer, intent(in) :: n_alr, n_in
    end subroutine coll_subtraction_init

```



```

⟨Real subtraction: procedures⟩ +=
  module subroutine coll_subtraction_init (coll_sub, n_alr, n_in)
    class(coll_subtraction_t), intent(inout) :: coll_sub
    integer, intent(in) :: n_alr, n_in
    coll_sub%n_in = n_in
    coll_sub%n_alr = n_alr
  end subroutine coll_subtraction_init

```

Set the corresponding algebra parameters of the underlying gauge group of the correction.

```

⟨Real subtraction: coll sub: TBP⟩ +=
  procedure :: set_parameters => coll_subtraction_set_parameters

⟨Real subtraction: sub interfaces⟩ +=
  module subroutine coll_subtraction_set_parameters (coll_sub, CA, CF, TR)
    class(coll_subtraction_t), intent(inout) :: coll_sub
    real(default), intent(in) :: CA, CF, TR
  end subroutine coll_subtraction_set_parameters

⟨Real subtraction: procedures⟩ +=
  module subroutine coll_subtraction_set_parameters (coll_sub, CA, CF, TR)
    class(coll_subtraction_t), intent(inout) :: coll_sub
    real(default), intent(in) :: CA, CF, TR
    coll_sub%CA = CA
    coll_sub%CF = CF
    coll_sub%TR = TR
  end subroutine coll_subtraction_set_parameters

```

This subroutine computes the collinear limit of $g^\alpha(\xi, y)$ introduced in eq. 27.34. Care is given to also enable the usage for the soft-collinear limit. This, we write all formulas in terms of soft-finite quantities.

We have to compute

$$\frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1-y)\xi^2 \mathcal{R}^\alpha(\Phi_{n+1})] |_{y=1}.$$

The Jacobian J is proportional to ξ , due to the d^3k_{n+1}/k_{n+1}^0 factor in the integration measure. It cancels the factor of ξ in the denominator. The remaining part of the Jacobian is multiplied in `evaluate_region_fsr` and is not relevant here. Inserting the splitting functions exemplarily for $q \rightarrow qg$ yields

$$g^\alpha = \frac{8\pi\alpha_s}{k_{\text{em}}^2} C_F (1-y) \xi^2 \frac{1+(1-z)^2}{z} \mathcal{B},$$

where we have chosen $z = E_{\text{rad}}/\bar{E}_{\text{em}}$ and \bar{E}_{em} denotes the emitter energy in the Born frame. The collinear final state imposes $\bar{k}_n = k_n + k_{n+1}$ for the connection between Φ_n - and Φ_{n+1} -phasepace and we get $1-z = E_{\text{em}}/\bar{E}_{\text{em}}$. The denominator can be rewritten by the constraint $\bar{k}_n^2 = (k_n + k_{n+1})^2 = 0$ to

$$k_{\text{em}}^2 = 2E_{\text{rad}}E_{\text{em}}(1-y)$$

which cancels the $(1-y)$ factor in the numerator, thus showing that the whole expression is indeed collinear-finite. We can further transform

$$E_{\text{rad}}E_{\text{em}} = z(1-z)\bar{E}_{\text{em}}^2$$

so that in total we have

$$g^\alpha = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} C_F \left(\frac{\xi}{z} \right)^2 (1 + (1-z)^2) \mathcal{B}$$

Follow up calculations give us

$$g^{\alpha, g \rightarrow gg} = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} C_A \frac{\xi}{z} \left\{ 2 \left(\frac{z}{1-z} \xi + \frac{1-z}{\frac{z}{\xi}} \right) \mathcal{B} + 4\xi z(1-z) \hat{k}_\perp^\mu \hat{k}_\perp^\nu \mathcal{B}_{\mu\nu} \right\},$$

$$g^{\alpha, g \rightarrow qq} = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} T_R \frac{\xi}{z} \left\{ \xi \mathcal{B} - 4\xi z(1-z) \hat{k}_\perp^\mu \hat{k}_\perp^\nu \mathcal{B}_{\mu\nu} \right\}.$$

The ratio z/ξ is finite in the soft limit

$$\frac{z}{\xi} = \frac{q^0}{2E_{\text{em}}}$$

so that ξ does not appear explicitly in the computation.

The argumentation above is valid for $q \rightarrow qg$ -splittings, but the general factorization is valid for general splittings, also for those involving spin correlations and QED splittings. Note that care has to be given to the definition of z . Further, we have factored out a factor of z to include in the ratio z/ξ , which has to be taken into account in the implementation of the splitting functions.

(Real subtraction: coll sub: TBP)+≡

```
procedure :: compute_fsr => coll_subtraction_compute_fsr
```

(Real subtraction: sub interfaces)+≡

```
module function coll_subtraction_compute_fsr (coll_sub, emitter, &
    flst, p_res, p_born, sqme_born, mom_times_sqme_spin_c, &
    xi, alpha_coupling, double_fsr) result (sqme)
    real(default) :: sqme
    class(coll_subtraction_t), intent(in) :: coll_sub
    integer, intent(in) :: emitter
    integer, dimension(:), intent(in) :: flst
    type(vector4_t), intent(in) :: p_res
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: sqme_born, mom_times_sqme_spin_c
    real(default), intent(in) :: xi, alpha_coupling
    logical, intent(in) :: double_fsr
end function coll_subtraction_compute_fsr
```

(Real subtraction: procedures)+≡

```
module function coll_subtraction_compute_fsr (coll_sub, emitter, &
    flst, p_res, p_born, sqme_born, mom_times_sqme_spin_c, &
    xi, alpha_coupling, double_fsr) result (sqme)
    real(default) :: sqme
    class(coll_subtraction_t), intent(in) :: coll_sub
    integer, intent(in) :: emitter
    integer, dimension(:), intent(in) :: flst
    type(vector4_t), intent(in) :: p_res
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: sqme_born, mom_times_sqme_spin_c
    real(default), intent(in) :: xi, alpha_coupling
    logical, intent(in) :: double_fsr
```

```

real(default) :: q0, z, p0, z_o_xi, onemz
integer :: nlegs, flv_em, flv_rad
nlegs = size (flst)
flv_rad = flst(nlegs); flv_em = flst(emitter)
q0 = p_res**1
p0 = p_res * p_born(emitter) / q0
!!! Here, z corresponds to 1-z in the formulas of arXiv:1002.2581;
!!! the integrand is symmetric under this variable change
z_o_xi = q0 / (two * p0)
z = xi * z_o_xi; onemz = one - z
if (is_gluon (flv_em) .and. is_gluon (flv_rad)) then
    sqme = coll_sub%CA * ( two * ( z / onemz * xi + onemz / z_o_xi ) * sqme_born &
        + four * xi * z * onemz * mom_times_sqme_spin_c )
else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
    sqme = coll_sub%TR * xi * (sqme_born - four * z * onemz * mom_times_sqme_spin_c)
else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = sqme_born * coll_sub%CF * (one + onemz**2) / z_o_xi
else
    sqme = zero
end if
sqme = sqme / (p0**2 * onemz * z_o_xi)
sqme = sqme * four * pi * alpha_coupling
if (double_fsr) sqme = sqme * onemz * two
end function coll_subtraction_compute_fsr

```

Like in the context of `coll_subtraction_compute_fsr` we compute the quantity

$$\lim_{y \rightarrow \pm 1} \left\{ \frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1-y^2)\xi^2 \mathcal{R}^\alpha(\Phi_{n+1})] \right\},$$

where the $(1-y^2)$ accounts for both $y = \pm 1$. Again, the Jacobian is proportional to ξ , so we drop the J/ξ factor. Note that it is important to take into account this missing factor of ξ in the computation of the Jacobian during phase-space generation both for fixed-beam and structure ISR. We consider only a $q \rightarrow qq$ splitting arguing that other splittings are identical in terms of the factors which cancel. It is given by

$$g^\alpha = \frac{8\pi\alpha_s}{-k_{\text{em}}^2} C_F (1-y^2) \xi^2 \frac{1+z^2}{1-z} \mathcal{B},$$

where g^α is defined akin to the one for FSR in eq. 27.34. Note the negative sign of k_{em}^2 to compensate the negative virtuality of the initial-state emitter. For ISR, z is defined with respect to the emitter energy entering the hard interaction, i.e.

$$z = \frac{E_{\text{beam}} - E_{\text{rad}}}{E_{\text{beam}}} = 1 - \frac{E_{\text{rad}}}{E_{\text{beam}}}.$$

Because $E_{\text{rad}} = E_{\text{beam}} \cdot \xi$, it is $z = 1 - \xi$, thus one factor of ξ is cancelled by $(1-z)$ in the denominator of g^α . The factor k_{em}^2 in the denominator is rewritten as

$$k_{\text{em}}^2 = (p_{\text{beam}} - p_{\text{rad}})^2 = -2p_{\text{beam}} \cdot p_{\text{rad}} = -2E_{\text{beam}} E_{\text{rad}} (1 \pm y) = -2E_{\text{beam}}^2 (1-z)(1 \pm y),$$

where we used

$$E_{\text{beam}} E_{\text{rad}} = E_{\text{beam}}^2 (1-z).$$

This leads to the cancellation of the corresponding $(1 \pm y)$ factor in $(1 - y^2)$, with the other factor becoming a simple factor of 2, and the remaining factor of ξ in the numerator. We thus end up with

$$g^\alpha = \frac{8\pi\alpha_s}{E_{\text{beam}}^2} C_F (1 + z^2) \mathcal{B},$$

which is soft-finite.

Note that here in `compute_isr`, `sqme_born` is supposed to be the squared Born matrix element convoluted with the real PDF.

(Real subtraction: coll sub: TBP)+≡

```
procedure :: compute_isr => coll_subtraction_compute_isr
```

(Real subtraction: sub interfaces)+≡

```
module function coll_subtraction_compute_isr &
  (coll_sub, emitter, flst, p_born, sqme_born, mom_times_sqme_spin_c, &
   xi, alpha_coupling, isr_mode) result (sqme)
  real(default) :: sqme
  class(coll_subtraction_t), intent(in) :: coll_sub
  integer, intent(in) :: emitter
  integer, dimension(:), intent(in) :: flst
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: sqme_born
  real(default), intent(in) :: mom_times_sqme_spin_c
  real(default), intent(in) :: xi, alpha_coupling
  integer, intent(in) :: isr_mode
end function coll_subtraction_compute_isr
```

(Real subtraction: procedures)+≡

```
module function coll_subtraction_compute_isr &
  (coll_sub, emitter, flst, p_born, sqme_born, mom_times_sqme_spin_c, &
   xi, alpha_coupling, isr_mode) result (sqme)
  real(default) :: sqme
  class(coll_subtraction_t), intent(in) :: coll_sub
  integer, intent(in) :: emitter
  integer, dimension(:), intent(in) :: flst
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: sqme_born
  real(default), intent(in) :: mom_times_sqme_spin_c
  real(default), intent(in) :: xi, alpha_coupling
  integer, intent(in) :: isr_mode
  real(default) :: z, onemz, p02
  integer :: nlegs, flv_em, flv_rad
  !!! p_born must be in lab frame.
  nlegs = size (flst)
  flv_rad = flst(nlegs); flv_em = flst(emitter)
  !!! No need to pay attention to n_in = 1, because this case always has a
  !!! massive initial-state particle and thus no collinear divergence.
  p02 = p_born(1)%p(0) * p_born(2)%p(0) / two
  z = one - xi; onemz = xi
  if (is_massless_vector (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = coll_sub%CA * (two * (z + z * onemz**2) * sqme_born + four * onemz**2 &
      / z * mom_times_sqme_spin_c)
  else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = coll_sub%CF * (one + z**2) * sqme_born
```

```

else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
  sqme = coll_sub%CF * (z * onemz * sqme_born + four * onemz**2 / z * mom_times_sqme_spin_c)
else if (is_massless_vector (flv_em) .and. is_fermion (flv_rad)) then
  sqme = coll_sub%TR * (z**2 + onemz**2) * onemz * sqme_born
else
  sqme = zero
end if
if (isr_mode == SQRTS_VAR) then
  sqme = sqme / p02 * z
else
  !!! We have no idea why this seems to work as there should be no factor
  !!! of z for the fixed-beam settings. This should definitely be understood in the
  !!! future!
  sqme = sqme / p02 / z
end if
sqme = sqme * four * pi * alpha_coupling
end function coll_subtraction_compute_isr

```

```

<Real subtraction: coll sub: TBP>+≡
  procedure :: final => coll_subtraction_final

<Real subtraction: sub interfaces>+≡
  module subroutine coll_subtraction_final (sub_coll)
    class(coll_subtraction_t), intent(inout) :: sub_coll
  end subroutine coll_subtraction_final

<Real subtraction: procedures>+≡
  module subroutine coll_subtraction_final (sub_coll)
    class(coll_subtraction_t), intent(inout) :: sub_coll
    sub_coll%use_resonance_mappings = .false.
  end subroutine coll_subtraction_final

```

27.6.3 Real Subtraction

We store a pointer to the `nlo_settings_t` object which holds tuning parameters, e.g. cutoffs for the subtraction terms.

```

<Real subtraction: public>+≡
  public :: real_subtraction_t

<Real subtraction: types>+≡
  type :: real_subtraction_t
    type(nlo_settings_t), pointer :: settings => null ()
    type(region_data_t), pointer :: reg_data => null ()
    type(real_kinematics_t), pointer :: real_kinematics => null ()
    type(isr_kinematics_t), pointer :: isr_kinematics => null ()
    real(default), dimension(:,:), allocatable :: sqme_real_non_sub
    real(default), dimension(:), allocatable :: sqme_born
    real(default), dimension(:,:), allocatable :: sf_factors
    real(default), dimension(:), allocatable :: sqme_real_arr
    real(default), dimension(:,:,:), allocatable :: sqme_born_color_c
    real(default), dimension(:,:,:), allocatable :: sqme_born_charge_c
    real(default), dimension(:,:,:), allocatable :: sqme_born_spin_c
    type(soft_subtraction_t) :: sub_soft

```

```

type(coll_subtraction_t) :: sub_coll
logical, dimension(:), allocatable :: sc_required
logical :: subtraction_deactivated = .false.
integer :: purpose = INTEGRATION
logical :: radiation_event = .true.
logical :: subtraction_event = .false.
integer, dimension(:), allocatable :: selected_alr
contains
<Real subtraction: real subtraction: TBP>
end type real_subtraction_t

```

Initializer

```

<Real subtraction: real subtraction: TBP>≡
  procedure :: init => real_subtraction_init

<Real subtraction: sub interfaces>+≡
  module subroutine real_subtraction_init (rsub, reg_data, settings)
    class(real_subtraction_t), intent(inout), target :: rsub
    type(region_data_t), intent(in), target :: reg_data
    type(nlo_settings_t), intent(in), target :: settings
  end subroutine real_subtraction_init

<Real subtraction: procedures>+≡
  module subroutine real_subtraction_init (rsub, reg_data, settings)
    class(real_subtraction_t), intent(inout), target :: rsub
    type(region_data_t), intent(in), target :: reg_data
    type(nlo_settings_t), intent(in), target :: settings
    integer :: alr
    if (debug_on) call msg_debug (D_SUBTRACTION, "real_subtraction_init")
    if (debug_on) call msg_debug (D_SUBTRACTION, "n_in", reg_data%n_in)
    if (debug_on) call msg_debug &
      (D_SUBTRACTION, "nlegs_born", reg_data%n_legs_born)
    if (debug_on) call msg_debug &
      (D_SUBTRACTION, "nlegs_real", reg_data%n_legs_real)
    if (debug_on) call msg_debug &
      (D_SUBTRACTION, "reg_data%n_regions", reg_data%n_regions)
    if (debug2_active (D_SUBTRACTION)) call reg_data%write ()
    rsub%reg_data => reg_data
    allocate (rsub%sqme_born (reg_data%n_flv_born))
    rsub%sqme_born = zero
    allocate (rsub%sf_factors (reg_data%n_regions, 0:reg_data%n_in))
    rsub%sf_factors = zero
    allocate (rsub%sqme_real_arr (reg_data%n_regions))
    rsub%sqme_real_arr = zero
    allocate (rsub%sqme_born_color_c &
      (reg_data%n_legs_born, reg_data%n_legs_born, reg_data%n_flv_born))
    rsub%sqme_born_color_c = zero
    allocate (rsub%sqme_born_charge_c &
      (reg_data%n_legs_born, reg_data%n_legs_born, reg_data%n_flv_born))
    rsub%sqme_born_charge_c = zero
    allocate (rsub%sqme_real_non_sub (reg_data%n_flv_real, reg_data%n_phs))
    rsub%sqme_real_non_sub = zero
    allocate (rsub%sc_required (reg_data%n_regions))
    do alr = 1, reg_data%n_regions
      rsub%sc_required(alr) = reg_data%regions(alr)%sc_required
    end do
  end subroutine real_subtraction_init

```

```

end do
if (rsub%requires_spin_correlations ()) then
  allocate (rsub%sqme_born_spin_c &
    (1:3, 1:3, reg_data%n_legs_born, reg_data%n_flv_born))
  rsub%sqme_born_spin_c = zero
end if
call rsub%sub_soft%init (reg_data)
call rsub%sub_coll%init (reg_data%n_regions, reg_data%n_in)
rsub%settings => settings
rsub%sub_soft%use_resonance_mappings = settings%use_resonance_mappings
rsub%sub_coll%use_resonance_mappings = settings%use_resonance_mappings
rsub%sub_soft%factorization_mode = settings%factorization_mode
end subroutine real_subtraction_init

```

<Real subtraction: real subtraction: TBP>+≡
 procedure :: set_real_kinematics => real_subtraction_set_real_kinematics

<Real subtraction: sub interfaces>+≡
 module subroutine real_subtraction_set_real_kinematics &
 (rsub, real_kinematics)
 class(real_subtraction_t), intent(inout) :: rsub
 type(real_kinematics_t), intent(in), target :: real_kinematics
 end subroutine real_subtraction_set_real_kinematics

<Real subtraction: procedures>+≡
 module subroutine real_subtraction_set_real_kinematics (rsub, real_kinematics)
 class(real_subtraction_t), intent(inout) :: rsub
 type(real_kinematics_t), intent(in), target :: real_kinematics
 rsub%real_kinematics => real_kinematics
 end subroutine real_subtraction_set_real_kinematics

<Real subtraction: real subtraction: TBP>+≡
 procedure :: set_isr_kinematics => real_subtraction_set_isr_kinematics

<Real subtraction: sub interfaces>+≡
 module subroutine real_subtraction_set_isr_kinematics (rsub, fractions)
 class(real_subtraction_t), intent(inout) :: rsub
 type(isr_kinematics_t), intent(in), target :: fractions
 end subroutine real_subtraction_set_isr_kinematics

<Real subtraction: procedures>+≡
 module subroutine real_subtraction_set_isr_kinematics (rsub, fractions)
 class(real_subtraction_t), intent(inout) :: rsub
 type(isr_kinematics_t), intent(in), target :: fractions
 rsub%isr_kinematics => fractions
 end subroutine real_subtraction_set_isr_kinematics

<Real subtraction: real subtraction: TBP>+≡
 procedure :: get_i_res => real_subtraction_get_i_res

<Real subtraction: sub interfaces>+≡
 module function real_subtraction_get_i_res (rsub, alr) result (i_res)
 integer :: i_res
 class(real_subtraction_t), intent(inout) :: rsub
 integer, intent(in) :: alr
 end function real_subtraction_get_i_res

```

⟨Real subtraction: procedures⟩+≡
module function real_subtraction_get_i_res (rsub, alr) result (i_res)
  integer :: i_res
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr
  select type (fks_mapping => rsub%reg_data%fks_mapping)
  type is (fks_mapping_resonances_t)
    i_res = fks_mapping%res_map%alr_to_i_res (alr)
  class default
    i_res = 0
  end select
end function real_subtraction_get_i_res

```

27.6.4 The real contribution to the cross section

In each singular region α , the real contribution to σ is given by the second summand of eqn. ??,

$$\sigma_{\text{real}}^{\alpha} = \int d\Phi_n \int_0^{2\pi} d\phi \int_{-1}^1 dy \int_0^{\xi_{\text{max}}} d\xi \left(\frac{1}{\xi} \right)_+ \left(\frac{1}{1-y} \right)_+ \underbrace{\frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1-y)\xi^2 \mathcal{R}^{\alpha}(\Phi_{n+1})]}_{g^{\alpha}(\xi, y)} \quad (27.34)$$

Writing out the plus-distribution and introducing $\tilde{\xi} = \xi/\xi_{\text{max}}$ to set the upper integration limit to 1, this turns out to be equal to

$$\begin{aligned} \sigma_{\text{real}}^{\alpha} = \int d\Phi_n \int_0^{2\pi} d\phi \int_{-1}^1 \frac{dy}{1-y} \left\{ \int_0^1 d\tilde{\xi} \left[\frac{g^{\alpha}(\tilde{\xi}\xi_{\text{max}}, y)}{\tilde{\xi}} - \underbrace{\frac{g^{\alpha}(0, y)}{\tilde{\xi}}}_{\text{soft}} - \underbrace{\frac{g^{\alpha}(\tilde{\xi}\xi_{\text{max}}, 1)}{\tilde{\xi}}}_{\text{coll.}} + \underbrace{\frac{g^{\alpha}(0, 1)}{\tilde{\xi}}}_{\text{coll.+soft}} \right] \right. \\ \left. + [\log \xi_{\text{max}}(y) g^{\alpha}(0, y) - \log \xi_{\text{max}}(1) g^{\alpha}(0, 1)] \right\}. \end{aligned} \quad (27.35)$$

This formula is implemented in `compute_sqme_real_fin`

If two or more singular regions would produce the same amplitude we only compute one and use the `eqv_index` to copy the result to the others (if `reuse_amplitudes_fks` is true).

```

⟨Real subtraction: real subtraction: TBP⟩+≡
  procedure :: compute => real_subtraction_compute

⟨Real subtraction: sub interfaces⟩+≡
module subroutine real_subtraction_compute (rsub, emitter, &
  i_phs, alpha_s, alpha_qed, separate_alrs, sqme)
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: emitter, i_phs
  logical, intent(in) :: separate_alrs
  real(default), intent(inout), dimension(:) :: sqme
  real(default), intent(in) :: alpha_s, alpha_qed
end subroutine real_subtraction_compute

```


<Real subtraction: procedures>+≡

```

module subroutine real_subtraction_compute (rsub, emitter, &
    i_phs, alpha_s, alpha_qed, separate_alrs, sqme)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: emitter, i_phs
    logical, intent(in) :: separate_alrs
    real(default), intent(inout), dimension(:) :: sqme
    real(default), dimension(:), allocatable :: sqme_alr_arr
    real(default), intent(in) :: alpha_s, alpha_qed
    real(default) :: sqme_alr, alpha_coupling
    integer :: alr, i_con, i_res, this_emitter
    logical :: same_emitter
    logical, dimension(:), allocatable :: alr_evaluated
    allocate (alr_evaluated(rsub%reg_data%n_regions))
    allocate (sqme_alr_arr(rsub%reg_data%n_regions))
    sqme_alr_arr = zero
    alr_evaluated = .false.
    do alr = 1, rsub%reg_data%n_regions
        if (.not. alr_evaluated(rsub%reg_data%regions(alr)%eqv_index)) then
            if (allocated (rsub%selected_alr)) then
                if (.not. any (rsub%selected_alr == alr)) cycle
            end if
            sqme_alr = zero
            if (emitter > rsub%isr_kinematics%n_in) then
                same_emitter = emitter == rsub%reg_data%regions(alr)%emitter
            else
                same_emitter = rsub%reg_data%regions(alr)%emitter <= rsub%isr_kinematics%n_in
            end if
            select case (char(rsub%reg_data%regions(alr)%nlo_correction_type))
            case ("QCD")
                alpha_coupling = alpha_s
            case ("EW")
                alpha_coupling = alpha_qed
            end select
            if (same_emitter .and. i_phs == rsub%real_kinematics%alr_to_i_phs (alr)) then
                i_res = rsub%get_i_res (alr)
                this_emitter = rsub%reg_data%regions(alr)%emitter
                sqme_alr = rsub%evaluate_emitter_region (alr, this_emitter, i_phs, &
                    i_res, alpha_coupling)
                i_con = rsub%get_i_contributor (alr)
                sqme_alr = sqme_alr * rsub%get_phs_factor (i_con)
            end if
            sqme_alr_arr(alr) = sqme_alr_arr(alr) + sqme_alr
            if (.not. (debug_active (D_SUBTRACTION) .or. debug2_active (D_SUBTRACTION))) then
                if (.not. allocated (rsub%selected_alr)) &
                    alr_evaluated(rsub%reg_data%regions(alr)%eqv_index) = .true.
            end if
        else if
            sqme_alr_arr(alr) = sqme_alr_arr(rsub%reg_data%regions(alr)%eqv_index)
        end if
        if (rsub%radiation_event .and. sqme_alr_arr(alr) /= zero) then
            rsub%sqme_real_arr(alr) = sqme_alr_arr(alr)
        end if
        if (separate_alrs) then

```

```

        sqme(alr) = sqme(alr) + sqme_alr_arr(alr)
    else
        sqme(1) = sqme(1) + sqme_alr_arr(alr)
    end if
end do
if (debug_on) then
    if (debug2_active (D_SUBTRACTION)) call check_s_alpha_consistency ()
end if
contains
subroutine check_s_alpha_consistency ()
    real(default) :: sum_s_alpha, sum_s_alpha_soft
    integer :: i_ftuple
    if (debug_on) call msg_debug2 (D_SUBTRACTION, "Check consistency of s_alpha: ")
    do alr = 1, rsub%reg_data%n_regions
        sum_s_alpha = rsub%sum_up_s_alpha(alr, i_phs)
        call msg_debug2 (D_SUBTRACTION, 'sum_s_alpha', sum_s_alpha)
        if (.not. nearly_equal(sum_s_alpha, one)) then
            call msg_bug ("The sum of all S functions should be equal to one!")
        end if
        sum_s_alpha_soft = rsub%sum_up_s_alpha_soft(alr, i_phs)
        call msg_debug2 (D_SUBTRACTION, 'sum_s_alpha_soft', sum_s_alpha_soft)
        if (.not. nearly_equal(sum_s_alpha_soft, one)) then
            call msg_bug ("The sum of all soft S functions should be equal to one!")
        end if
    end do
end subroutine check_s_alpha_consistency
end subroutine real_subtraction_compute

```

The emitter is fixed. We now have to decide whether we evaluate in ISR or FSR region, and also if resonances are used.

```

<Real subtraction: real subtraction: TBP>+≡
    procedure :: evaluate_emitter_region => &
        real_subtraction_evaluate_emitter_region
<Real subtraction: sub interfaces>+≡
    module function real_subtraction_evaluate_emitter_region (rsub, alr, &
        emitter, i_phs, i_res, alpha_coupling) result (sqme)
        real(default) :: sqme
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, emitter, i_phs, i_res
        real(default), intent(in) :: alpha_coupling
    end function real_subtraction_evaluate_emitter_region
<Real subtraction: procedures>+≡
    module function real_subtraction_evaluate_emitter_region (rsub, alr, &
        emitter, i_phs, i_res, alpha_coupling) result (sqme)
        real(default) :: sqme
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, emitter, i_phs, i_res
        real(default), intent(in) :: alpha_coupling
        if (emitter <= rsub%isr_kinematics%n_in) then
            sqme = rsub%evaluate_region_isr &
                (alr, emitter, i_phs, i_res, alpha_coupling)
        else
            select type (fks_mapping => rsub%reg_data%fks_mapping)

```

```

        type is (fks_mapping_resonances_t)
        call fks_mapping%set_resonance_momenta &
            (rsub%real_kinematics%xi_ref_momenta)
    end select
    sqme = rsub%evaluate_region_fsr (alr, emitter, i_phs, i_res, alpha_coupling)
end if
end function real_subtraction_evaluate_emitter_region

```

Sums up $\sum_{i_1, i_2} S_{i_1 i_2}$ for the given alr.

```

<Real subtraction: real subtraction: TBP>+≡
    procedure :: sum_up_s_alpha => real_subtraction_sum_up_s_alpha

<Real subtraction: sub interfaces>+≡
    module function real_subtraction_sum_up_s_alpha &
        (rsub, alr, i_phs) result (sum_s_alpha)
        real(default) :: sum_s_alpha
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, i_phs
    end function real_subtraction_sum_up_s_alpha

<Real subtraction: procedures>+≡
    module function real_subtraction_sum_up_s_alpha &
        (rsub, alr, i_phs) result (sum_s_alpha)
        real(default) :: sum_s_alpha
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, i_phs
        type(vector4_t), dimension(:), allocatable :: p_real
        integer :: i_res, i_ftuple, i1, i2
        allocate (p_real (rsub%reg_data%n_legs_real))
        if (rsub%reg_data%has_pseudo_isr ()) then
            p_real = rsub%real_kinematics%p_real_onshell(i_phs)%get_momenta (i_phs)
        else
            p_real = rsub%real_kinematics%p_real_cms%get_momenta (i_phs)
        end if
        i_res = rsub%get_i_res (alr)
        sum_s_alpha = zero
        do i_ftuple = 1, rsub%reg_data%regions(alr)%nregions
            call rsub%reg_data%regions(alr)%ftuples(i_ftuple)%get (i1, i2)
            sum_s_alpha = sum_s_alpha + rsub%reg_data%get_svalue (p_real, alr, i1, i2, i_res)
        end do
    end function real_subtraction_sum_up_s_alpha

```

Sums up $\sum_{i_1, i_2} S_{i_1 i_2}$ for the given alr. The soft S functions take the real momenta in the soft limit, i.e. the Born momenta. For each summand of `sum_s_alpha_soft` we take `p_soft` constructed from the emitter of the given alpha region also for ftuples in which the first integer i1 does not coincide with the emitter. This is necessary because only if we keep `p_soft` fixed, all soft S functions are computed with the same denominator and thus add up to 1.

```

<Real subtraction: real subtraction: TBP>+≡
    procedure :: sum_up_s_alpha_soft => real_subtraction_sum_up_s_alpha_soft

<Real subtraction: sub interfaces>+≡
    module function real_subtraction_sum_up_s_alpha_soft &
        (rsub, alr, i_phs) result (sum_s_alpha_soft)

```

```

        real(default) :: sum_s_alpha_soft
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, i_phs
    end function real_subtraction_sum_up_s_alpha_soft

<Real subtraction: procedures>+≡
module function real_subtraction_sum_up_s_alpha_soft &
    (rsub, alr, i_phs) result (sum_s_alpha_soft)
    real(default) :: sum_s_alpha_soft
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, i_phs
    type(vector4_t), dimension(:), allocatable :: p_born
    integer :: i_res, i_ftuple, i1, i2, emitter, nlegs
    allocate (p_born (rsub%reg_data%n_legs_born))
    if (rsub%reg_data%has_pseudo_isr ()) then
        p_born = rsub%real_kinematics%p_born_onshell%get_momenta (1)
    else
        p_born = rsub%real_kinematics%p_born_cms%get_momenta (1)
    end if
    i_res = rsub%get_i_res (alr)
    emitter = rsub%reg_data%regions(alr)%emitter
    associate (r => rsub%real_kinematics)
        if (emitter > rsub%sub_soft%reg_data%n_in) then
            call rsub%sub_soft%create_softvec_fsr (p_born, r%y_soft(i_phs), r%phi, &
                emitter, r%xi_ref_momenta(rsub%sub_soft%i_xi_ref (alr, i_phs)))
        else
            call rsub%sub_soft%create_softvec_isr (r%y_soft(i_phs), r%phi)
        end if
    end associate
    nlegs = rsub%reg_data%n_legs_real
    sum_s_alpha_soft = zero
    do i_ftuple = 1, rsub%reg_data%regions(alr)%nregions
        call rsub%reg_data%regions(alr)%ftuples(i_ftuple)%get (i1, i2)
        if (i2 == nlegs) then
            sum_s_alpha_soft = sum_s_alpha_soft + rsub%reg_data%get_svalue_soft &
                (p_born, rsub%sub_soft%p_soft, alr, i1, i_res)
        end if
    end do
end function real_subtraction_sum_up_s_alpha_soft

```

This subroutine computes the finite part of the real matrix element in an individual singular region. First, the radiation variables are fetched and \mathcal{R} is multiplied by the appropriate S_α -factors, region multiplicities and double-FSR factors. Then, it computes the soft, collinear, soft-collinear and remnant matrix elements and supplies the corresponding factor $1/\xi/(1-y)$ as well as the corresponding Jacobians.

```

<Real subtraction: real subtraction: TBP>+≡
procedure :: evaluate_region_fsr => real_subtraction_evaluate_region_fsr

<Real subtraction: sub interfaces>+≡
module function real_subtraction_evaluate_region_fsr (rsub, alr, &
    emitter, i_phs, i_res, alpha_coupling) result (sqme_tot)
    real(default) :: sqme_tot
    class(real_subtraction_t), intent(inout) :: rsub

```

```

integer, intent(in) :: alr, emitter, i_phs, i_res
real(default), intent(in) :: alpha_coupling
end function real_subtraction_evaluate_region_fsr

```

(Real subtraction: procedures)+≡

```

module function real_subtraction_evaluate_region_fsr (rsub, alr, &
  emitter, i_phs, i_res, alpha_coupling) result (sqme_tot)
  real(default) :: sqme_tot
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, emitter, i_phs, i_res
  real(default), intent(in) :: alpha_coupling
  real(default) :: sqme_rad, sqme_soft, sqme_coll, sqme_cs, sqme_remn
  sqme_rad = zero; sqme_soft = zero; sqme_coll = zero
  sqme_cs = zero; sqme_remn = zero
  associate (region => rsub%reg_data%regions(alr), &
    template => rsub%settings%fks_template)
    if (rsub%radiation_event) then
      sqme_rad = rsub%sqme_real_non_sub &
        (rsub%reg_data%get_matrix_element_index (alr), i_phs)
      call evaluate_fks_factors (sqme_rad, rsub%reg_data, &
        rsub%real_kinematics, alr, i_phs, emitter, i_res)
      call apply_kinematic_factors_radiation (sqme_rad, &
        rsub%real_kinematics, i_phs)
    end if
    if (rsub%subtraction_event .and. .not. (rsub%subtraction_deactivated &
      .or. region%nlo_correction_type == "none")) then
      if (debug2_active (D_SUBTRACTION)) then
        print *, "[real_subtraction_evaluate_region_fsr]"
        print *, "xi: ", rsub%real_kinematics%xi_max(i_phs) * &
          rsub%real_kinematics%xi_tilde
        print *, "y: ", rsub%real_kinematics%y(i_phs)
      end if
      call rsub%evaluate_subtraction_terms_fsr (alr, emitter, i_phs, &
        i_res, alpha_coupling, sqme_soft, sqme_coll, sqme_cs)
      call apply_kinematic_factors_subtraction_fsr (sqme_soft, &
        sqme_coll, sqme_cs, rsub%real_kinematics, i_phs)
      associate (symm_factor_fs => &
        rsub%reg_data%born_to_real_symm_factor_fs (alr))
        sqme_soft = sqme_soft * symm_factor_fs
        sqme_coll = sqme_coll * symm_factor_fs
        sqme_cs = sqme_cs * symm_factor_fs
      end associate
      sqme_remn = compute_sqme_remnant_fsr (sqme_soft, sqme_cs, &
        rsub%real_kinematics%xi_max(i_phs), template%xi_cut, &
        rsub%real_kinematics%xi_tilde)
      sqme_tot = - sqme_soft - sqme_coll + sqme_cs + sqme_remn
    else
      sqme_tot = sqme_rad
    end if
    sqme_tot = sqme_tot * rsub%real_kinematics%jac_rand(i_phs)
    sqme_tot = sqme_tot * rsub%reg_data%regions(alr)%mult
  end associate
  if (debug2_active (D_SUBTRACTION) .and. .not. &
    debug2_active (D_SUBTRACTION)) then
    call real_subtraction_register_debug_sqme (rsub, alr, emitter, &

```

```

        i_phs, sqme_rad, sqme_soft, sqme_coll=sqme_coll, sqme_cs=sqme_cs)
else if (debug2_active (D_SUBTRACTION)) then
    call write_computation_status_fsr ()
end if
contains
<Real subtraction: real subtraction evaluate region fsr: procedures>
subroutine write_computation_status_fsr (passed, total, region_type, full)
    integer, intent(in), optional :: passed, total
    character(*), intent(in), optional :: region_type
    integer :: i_born
    integer :: u
    real(default) :: xi
    logical :: yorn
    logical, intent(in), optional :: full
    yorn = .true.
    if (present (full)) yorn = full
    if (debug_on) call msg_debug &
        (D_SUBTRACTION, "real_subtraction_evaluate_region_fsr")
    u = given_output_unit (); if (u < 0) return
    i_born = rsub%reg_data%regions(alr)%uborn_index
    xi = rsub%real_kinematics%xi_max (i_phs) * rsub%real_kinematics%xi_tilde
    write (u,'(A,I2)') 'rsub%purpose: ', rsub%purpose
    write (u,'(A,I4)') 'alr: ', alr
    write (u,'(A,I3)') 'emitter: ', emitter
    write (u,'(A,I3)') 'i_phs: ', i_phs
    write (u,'(A,F6.4)') 'xi_max: ', rsub%real_kinematics%xi_max (i_phs)
    write (u,'(A,F6.4)') 'xi_cut: ', rsub%real_kinematics%xi_max(i_phs) * &
        rsub%settings%fks_template%xi_cut
    write (u,'(A,F6.4,2X,A,F6.4)') 'xi: ', xi, 'y: ', &
        rsub%real_kinematics%y (i_phs)
    if (yorn) then
        write (u,'(A,ES16.9)') 'sqme_born: ', rsub%sqme_born(i_born)
        write (u,'(A,ES16.9)') 'sqme_real: ', sqme_rad
        write (u,'(A,ES16.9)') 'sqme_soft: ', sqme_soft
        write (u,'(A,ES16.9)') 'sqme_coll: ', sqme_coll
        write (u,'(A,ES16.9)') 'sqme_coll-soft: ', sqme_cs
        write (u,'(A,ES16.9)') 'sqme_remn: ', sqme_remn
        write (u,'(A,ES16.9)') 'sqme_tot: ', sqme_tot
        if (present (passed) .and. present (total) .and. &
            present (region_type)) &
            write (u,'(A)') char (str (passed) // " of " // str (total) // &
                " " // region_type // " points passed in total")
    end if
    write (u,'(A,ES16.9)') 'jacobian - real: ', &
        rsub%real_kinematics%jac(i_phs)%jac(1)
    write (u,'(A,ES16.9)') 'jacobian - soft: ', &
        rsub%real_kinematics%jac(i_phs)%jac(2)
    write (u,'(A,ES16.9)') 'jacobian - coll: ', &
        rsub%real_kinematics%jac(i_phs)%jac(3)
end subroutine write_computation_status_fsr
end function real_subtraction_evaluate_region_fsr

```

Compares the real matrix element to the subtraction terms in the soft, the collinear or the soft-collinear limits. Used for debug purposes if ?test_anti_coll_limit,

?test_coll_limit and/or ?test_soft_limit are set in the Sindarin. sqme_soft and sqme_cs need to be provided if called for FSR and sqme_coll_plus, sqme_coll_minus, sqme_cs_plus as well as sqme_cs_minus need to be provided if called for ISR.

(Real subtraction: procedures)+≡

```
subroutine real_subtraction_register_debug_sqme (rsub, alr, emitter, i_phs, sqme_rad, sqme_soft,
    sqme_coll, sqme_cs, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
class(real_subtraction_t), intent(in) :: rsub
integer, intent(in) :: alr, emitter, i_phs
real(default), intent(in) :: sqme_rad, sqme_soft
real(default), intent(in), optional :: sqme_coll, sqme_cs, sqme_coll_plus, sqme_coll_minus, sq
real(default), dimension(:), allocatable, save :: sqme_rad_store
logical :: is_soft, is_collinear_plus, is_collinear_minus, is_fsr
real(default), parameter :: soft_threshold = 0.001_default
real(default), parameter :: coll_threshold = 0.99_default
real(default), parameter :: rel_smallness = 0.01_default
real(default) :: sqme_dummy, this_sqme_rad, y, xi_tilde
logical, dimension(:), allocatable, save :: count_alr

if (.not. allocated (sqme_rad_store)) then
    allocate (sqme_rad_store (rsub%reg_data%n_regions))
    sqme_rad_store = zero
end if
if (rsub%radiation_event) then
    sqme_rad_store(alr) = sqme_rad
else
    if (.not. allocated (count_alr)) then
        allocate (count_alr (rsub%reg_data%n_regions))
        count_alr = .false.
    end if

    if (is_massless_vector (rsub%reg_data%regions(alr)%flst_real%flst(rsub%reg_data%n_legs_real
        xi_tilde = rsub%real_kinematics%xi_tilde
        is_soft = xi_tilde < soft_threshold
    else
        is_soft = .false.
    end if
    y = rsub%real_kinematics%y(i_phs)
    is_collinear_plus = y > coll_threshold .and. &
        rsub%reg_data%regions(alr)%has_collinear_divergence()
    is_collinear_minus = -y > coll_threshold .and. &
        rsub%reg_data%regions(alr)%has_collinear_divergence()

    is_fsr = emitter > rsub%isr_kinematics%n_in

    if (is_fsr) then
        if (.not. present(sqme_coll) .or. .not. present(sqme_cs)) &
            call msg_error ("real_subtraction_register_debug_sqme: Wrong arguments for FSR")
        else
            if (.not. present(sqme_coll_plus) .or. .not. present(sqme_coll_minus) &
                .or. .not. present(sqme_cs_plus) .or. .not. present(sqme_cs_minus)) &
                call msg_error ("real_subtraction_register_debug_sqme: Wrong arguments for ISR")
            end if

            this_sqme_rad = sqme_rad_store(alr)
```

```

if (is_soft .and. .not. is_collinear_plus .and. .not. is_collinear_minus) then
  if ( .not. nearly_equal (this_sqme_rad, sqme_soft, &
    abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
    call msg_print_color (char ("Soft MEs do not match in region " // str (alr)), COL_RED)
  else
    call msg_print_color (char ("sqme_soft OK in region " // str (alr)), COL_GREEN)
  end if
  print *, 'this_sqme_rad, sqme_soft = ', this_sqme_rad, sqme_soft
end if

if (is_collinear_plus .and. .not. is_soft) then
  if (is_fsr) then
    if ( .not. nearly_equal (this_sqme_rad, sqme_coll, &
      abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
      call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
    else
      call msg_print_color (char ("sqme_coll OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_coll = ', this_sqme_rad, sqme_coll
  else
    if ( .not. nearly_equal (this_sqme_rad, sqme_coll_plus, &
      abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
      call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
    else
      call msg_print_color (char ("sqme_coll_plus OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_coll_plus = ', this_sqme_rad, sqme_coll_plus
  end if
end if

if (is_collinear_minus .and. .not. is_soft) then
  if (.not. is_fsr) then
    if ( .not. nearly_equal (this_sqme_rad, sqme_coll_minus, &
      abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
      call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
    else
      call msg_print_color (char ("sqme_coll_minus OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_coll_minus = ', this_sqme_rad, sqme_coll_minus
  end if
end if

if (is_soft .and. is_collinear_plus) then
  if (is_fsr) then
    if ( .not. nearly_equal (this_sqme_rad, sqme_cs, &
      abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
      call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (alr)), COL_RED)
    else
      call msg_print_color (char ("sqme_cs OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_cs = ', this_sqme_rad, sqme_cs
  else
    if ( .not. nearly_equal (this_sqme_rad, sqme_cs_plus, &
      abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then

```



```

        call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (a
    else
        call msg_print_color (char ("sqme_cs_plus OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_cs_plus = ', this_sqme_rad, sqme_cs_plus
end if
end if

if (is_soft .and. is_collinear_minus) then
    if (.not. is_fsr) then
        if ( .not. nearly_equal (this_sqme_rad, sqme_cs_minus, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (a
        else
            call msg_print_color (char ("sqme_cs_minus OK in region " // str (alr)), COL_GREEN)
        end if
        print *, 'this_sqme_rad, sqme_cs_minus = ', this_sqme_rad, sqme_cs_minus
    end if
end if

count_alr (alr) = .true.
if (all (count_alr)) then
    deallocate (count_alr)
    deallocate (sqme_rad_store)
end if
end if
end subroutine real_subtraction_register_debug_sqme

```

For final state radiation, the subtraction remnant cross section is

$$\sigma_{\text{remn}} = (\sigma_{\text{soft}} - \sigma_{\text{soft-coll}}) \log(\xi_{\text{max}}) \cdot \frac{\tilde{\xi}}{\xi_{\text{cut}}}. \quad (27.36)$$

There is only one factor of $\log(\xi_{\text{max}})$ for both limits as ξ_{max} does not depend on y in the case of FSR. We use the already computed `sqme_soft` and `sqme_cs` with a factor of $\tilde{\xi}$ which we have to compensate. We also need a factor $1/\xi_{\text{cut}}$ here to assure that the cross section is independent of this free cutoff parameter. However, it still remains to be motivated analytically.

```

<Real subtraction: real subtraction evaluate region fsr: procedures>≡
function compute_sqme_remnant_fsr (sqme_soft, sqme_cs, xi_max, xi_cut, xi_tilde) result (sqme_re
    real(default) :: sqme_remn
    real(default), intent(in) :: sqme_soft, sqme_cs, xi_max, xi_cut, xi_tilde
    if (debug_on) call msg_debug (D_SUBTRACTION, "compute_sqme_remnant_fsr")
    sqme_remn = (sqme_soft - sqme_cs) * log (xi_max) * xi_tilde / xi_cut
end function compute_sqme_remnant_fsr

```

```

<Real subtraction: real subtraction: TBP>+≡
procedure :: evaluate_region_isr => real_subtraction_evaluate_region_isr

```

```

<Real subtraction: sub interfaces>+≡
module function real_subtraction_evaluate_region_isr (rsub, alr, &
    emitter, i_phs, i_res, alpha_coupling) result (sqme_tot)
    real(default) :: sqme_tot

```

```

class(real_subtraction_t), intent(inout) :: rsub
integer, intent(in) :: alr, emitter, i_phs, i_res
real(default), intent(in) :: alpha_coupling
end function real_subtraction_evaluate_region_isr

<Real subtraction: procedures>+≡
module function real_subtraction_evaluate_region_isr (rsub, alr, &
    emitter, i_phs, i_res, alpha_coupling) result (sqme_tot)
real(default) :: sqme_tot
class(real_subtraction_t), intent(inout) :: rsub
integer, intent(in) :: alr, emitter, i_phs, i_res
real(default), intent(in) :: alpha_coupling
real(default) :: sqme_rad, sqme_soft, sqme_coll_plus, sqme_coll_minus
real(default) :: sqme_cs_plus, sqme_cs_minus
real(default) :: sqme_remn
sqme_rad = zero; sqme_soft = zero;
sqme_coll_plus = zero; sqme_coll_minus = zero
sqme_cs_plus = zero; sqme_cs_minus = zero
sqme_remn = zero
associate (region => rsub%reg_data%regions(alr), template => rsub%settings%fks_template)
    if (rsub%radiation_event) then
        sqme_rad = rsub%sqme_real_non_sub (rsub%reg_data%get_matrix_element_index (alr), i_phs)
        call evaluate_fks_factors (sqme_rad, rsub%reg_data, rsub%real_kinematics, &
            alr, i_phs, emitter, i_res)
        call apply_kinematic_factors_radiation (sqme_rad, rsub%real_kinematics, i_phs)
    end if
    if (rsub%subtraction_event .and. .not. (rsub%subtraction_deactivated &
        .or. region%no_correction_type == "none")) then
        call rsub%evaluate_subtraction_terms_isr (alr, emitter, i_phs, i_res, alpha_coupling, &
            sqme_soft, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
        call apply_kinematic_factors_subtraction_isr (sqme_soft, sqme_coll_plus, &
            sqme_coll_minus, sqme_cs_plus, sqme_cs_minus, rsub%real_kinematics, i_phs)
        associate (symm_factor_fs => rsub%reg_data%born_to_real_symm_factor_fs (alr))
            sqme_soft = sqme_soft * symm_factor_fs
            sqme_coll_plus = sqme_coll_plus * symm_factor_fs
            sqme_coll_minus = sqme_coll_minus * symm_factor_fs
            sqme_cs_plus = sqme_cs_plus * symm_factor_fs
            sqme_cs_minus = sqme_cs_minus * symm_factor_fs
        end associate
        sqme_remn = compute_sqme_remnant_isr (rsub%isr_kinematics%isr_mode, &
            sqme_soft, sqme_cs_plus, sqme_cs_minus, &
            rsub%isr_kinematics, rsub%real_kinematics, i_phs, template%xi_cut)
        sqme_tot = - sqme_soft - sqme_coll_plus - sqme_coll_minus &
            + sqme_cs_plus + sqme_cs_minus + sqme_remn
    else
        sqme_tot = sqme_rad
    end if
end if
end associate
sqme_tot = sqme_tot * rsub%real_kinematics%jac_rand (i_phs)
sqme_tot = sqme_tot * rsub%reg_data%regions(alr)%mult
if (debug_active (D_SUBTRACTION) .and. .not. debug2_active (D_SUBTRACTION)) then
    call real_subtraction_register_debug_sqme (rsub, alr, emitter, i_phs, sqme_rad, &
        sqme_soft, sqme_coll_plus=sqme_coll_plus, sqme_coll_minus=sqme_coll_minus, &
        sqme_cs_plus=sqme_cs_plus, sqme_cs_minus=sqme_cs_minus)
else if (debug2_active (D_SUBTRACTION)) then

```

```

        call write_computation_status_isr ()
    end if
contains
<Real subtraction: evaluate region_isr: procedures>
    subroutine write_computation_status_isr (unit)
        integer, intent(in), optional :: unit
        integer :: i_born
        integer :: u
        real(default) :: xi
        u = given_output_unit (unit); if (u < 0) return
        i_born = rsub%reg_data%regions(alr)%uborn_index
        xi = rsub%real_kinematics%xi_max (i_phs) * rsub%real_kinematics%xi_tilde
        write (u,'(A,I4)') 'alr: ', alr
        write (u,'(A,I2)') 'emitter: ', emitter
        write (u,'(A,F4.2)') 'xi_max: ', rsub%real_kinematics%xi_max (i_phs)
        print *, 'xi: ', xi, 'y: ', rsub%real_kinematics%y (i_phs)
        print *, 'xb1: ', rsub%isr_kinematics%x(1), 'xb2: ', rsub%isr_kinematics%x(2)
        print *, 'random jacobian: ', rsub%real_kinematics%jac_rand (i_phs)
        write (u,'(A,ES16.9)') 'sqme_born: ', rsub%sqme_born(i_born)
        write (u,'(A,ES16.9)') 'sqme_real: ', sqme_rad
        write (u,'(A,ES16.9)') 'sqme_soft: ', sqme_soft
        write (u,'(A,ES16.9)') 'sqme_coll_plus: ', sqme_coll_plus
        write (u,'(A,ES16.9)') 'sqme_coll_minus: ', sqme_coll_minus
        write (u,'(A,ES16.9)') 'sqme_cs_plus: ', sqme_cs_plus
        write (u,'(A,ES16.9)') 'sqme_cs_minus: ', sqme_cs_minus
        write (u,'(A,ES16.9)') 'sqme_remn: ', sqme_remn
        write (u,'(A,ES16.9)') 'sqme_tot: ', sqme_tot
        write (u,'(A,ES16.9)') 'jacobian - real: ', rsub%real_kinematics%jac(i_phs)%jac(1)
        write (u,'(A,ES16.9)') 'jacobian - soft: ', rsub%real_kinematics%jac(i_phs)%jac(2)
        write (u,'(A,ES16.9)') 'jacobian - collplus: ', rsub%real_kinematics%jac(i_phs)%jac(3)
        write (u,'(A,ES16.9)') 'jacobian - collminus: ', rsub%real_kinematics%jac(i_phs)%jac(4)
    end subroutine write_computation_status_isr
end function real_subtraction_evaluate_region_isr

```

Computes the soft remnant for ISR. The formulas can be found in arXiv:1002.2581, eq. 4.21. and arXiv:0709.2092, sec. 5.1.2. This results in

$$\sigma_{\text{remn}}^{\text{ISR}} = \log(\xi_{\text{max}}(y))\sigma_{\text{soft}} - \frac{1}{2}\log(\xi_{\text{max}}(1))\sigma_{\oplus}^{\text{soft-coll}} - \frac{1}{2}\log(\xi_{\text{max}}(-1))\sigma_{\ominus}^{\text{soft-coll}} \quad (27.37)$$

where for ISR, ξ_{max} does explicitly depend on y due to the rescaling of the x values from the Born to the real partonic system according to

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}} \quad (27.38)$$

As ξ_{max} is determined by the fact that the real x_{\oplus}, x_{\ominus} have to stay in a physically

meaningful regime, i.e. $x_{\oplus}, x_{\ominus} < 1$, this leads to

$$\xi_{\max} = 1 - \max \left\{ \frac{2(1+y)\bar{x}_{\oplus}^2}{\sqrt{(1+\bar{x}_{\oplus}^2)^2(1-y)^2 + 16y\bar{x}_{\oplus}^2 + (1-y)(1-\bar{x}_{\oplus}^2)}}, \quad (27.39) \right.$$

$$\left. \frac{2(1-y)\bar{x}_{\oplus}^2}{\sqrt{(1+\bar{x}_{\oplus}^2)^2(1+y)^2 - 16y\bar{x}_{\oplus}^2 + (1+y)(1-\bar{x}_{\oplus}^2)}} \right\} \quad (27.40)$$

and thus

$$\xi_{\max}(y = 1) = 1 - \bar{x}_{\oplus} \quad (27.41)$$

$$\xi_{\max}(y = -1) = 1 - \bar{x}_{\ominus} \quad (27.42)$$

So we need to use the unrescaled $\bar{x}_{\oplus}, \bar{x}_{\ominus}$ here. Factors of $\frac{1}{2}$ and $\frac{1}{\xi}$ are already included in the matrix elements from `apply_kinematic_factors_subtraction_isr`. We keep the former and remove the latter by multiplying with $\tilde{\xi}$. The factor $1/\xi_{\text{cut}}$ is probably needed to assure that the cross section is independent of this free cutoff parameter in analogy to the FSR case. However, it still remains to be motivated analytically and to be validated.

(Real subtraction: evaluate region_isr: procedures)≡

```
function compute_sqme_remnant_isr (isr_mode, sqme_soft, sqme_cs_plus, sqme_cs_minus, &
  isr_kinematics, real_kinematics, i_phs, xi_cut) result (sqme_remn)
  real(default) :: sqme_remn
  integer, intent(in) :: isr_mode
  real(default), intent(in) :: sqme_soft, sqme_cs_plus, sqme_cs_minus
  type(isr_kinematics_t), intent(in) :: isr_kinematics
  type(real_kinematics_t), intent(in) :: real_kinematics
  integer, intent(in) :: i_phs
  real(default), intent(in) :: xi_cut
  real(default) :: xi_tilde, xi_max, xi_max_plus, xi_max_minus, xb_plus, xb_minus
  xi_max = real_kinematics%xi_max (i_phs)
  xi_tilde = real_kinematics%xi_tilde
  select case (isr_mode)
  case (SQRTS_VAR)
    xb_plus = isr_kinematics%x(I_PLUS)
    xb_minus = isr_kinematics%x(I_MINUS)
    xi_max_plus = one - xb_plus
    xi_max_minus = one - xb_minus
  case (SQRTS_FIXED)
    xi_max_plus = real_kinematics%xi_max (i_phs)
    xi_max_minus = real_kinematics%xi_max (i_phs)
  end select
  sqme_remn = log (xi_max) * xi_tilde * sqme_soft &
    - log (xi_max_plus) * xi_tilde * sqme_cs_plus &
    - log (xi_max_minus) * xi_tilde * sqme_cs_minus
  sqme_remn = sqme_remn / xi_cut
end function compute_sqme_remnant_isr
```

(Real subtraction: real subtraction: TBP)+≡

```
procedure :: evaluate_subtraction_terms_fsr => &
  real_subtraction_evaluate_subtraction_terms_fsr
```

<Real subtraction: sub interfaces>+≡

```

module subroutine real_subtraction_evaluate_subtraction_terms_fsr &
  (rsub, alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, &
   sqme_coll, sqme_cs)
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, emitter, i_phs, i_res
  real(default), intent(in) :: alpha_coupling
  real(default), intent(out) :: sqme_soft, sqme_coll, sqme_cs
end subroutine real_subtraction_evaluate_subtraction_terms_fsr

```

<Real subtraction: procedures>+≡

```

module subroutine real_subtraction_evaluate_subtraction_terms_fsr &
  (rsub, alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, &
   sqme_coll, sqme_cs)
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, emitter, i_phs, i_res
  real(default), intent(in) :: alpha_coupling
  real(default), intent(out) :: sqme_soft, sqme_coll, sqme_cs
  if (debug_on) call msg_debug &
    (D_SUBTRACTION, "real_subtraction_evaluate_subtraction_terms_fsr")
  sqme_soft = zero; sqme_coll = zero; sqme_cs = zero
  associate (xi_tilde => rsub%real_kinematics%xi_tilde, &
    y => rsub%real_kinematics%y(i_phs), &
    template => rsub%settings%fks_template)
    if (template%xi_cut > xi_tilde) &
      sqme_soft = rsub%compute_sub_soft &
        (alr, emitter, i_phs, i_res, alpha_coupling)
    if (y - 1 + template%delta_o > 0) &
      sqme_coll = rsub%compute_sub_coll &
        (alr, emitter, i_phs, alpha_coupling)
    if (template%xi_cut > xi_tilde .and. y - 1 + template%delta_o > 0) &
      sqme_cs = rsub%compute_sub_coll_soft &
        (alr, emitter, i_phs, alpha_coupling)
    if (debug2_active (D_SUBTRACTION)) then
      print *, "FSR Cutoff:"
      print *, "sub_soft: ", &
        template%xi_cut > xi_tilde, "(ME: ", sqme_soft, ")"
      print *, "sub_coll: ", &
        (y - 1 + template%delta_o) > 0, "(ME: ", sqme_coll, ")"
      print *, "sub_coll_soft: ", &
        template%xi_cut > xi_tilde .and. (y - 1 + template%delta_o) > 0, &
        "(ME: ", sqme_cs, ")"
    end if
  end associate
end subroutine real_subtraction_evaluate_subtraction_terms_fsr

```

<Real subtraction: procedures>+≡

```

subroutine evaluate_fks_factors (sqme, reg_data, real_kinematics, &
  alr, i_phs, emitter, i_res)
  real(default), intent(inout) :: sqme
  type(region_data_t), intent(inout) :: reg_data
  type(real_kinematics_t), intent(in), target :: real_kinematics
  integer, intent(in) :: alr, i_phs, emitter, i_res
  real(default) :: s_alpha

```

```

type(phs_point_set_t), pointer :: p_real => null ()
if (reg_data%has_pseudo_isr ()) then
  p_real => real_kinematics%p_real_onshell (i_phs)
else
  p_real => real_kinematics%p_real_cms
end if
s_alpha = reg_data%get_svalue (p_real%get_momenta(i_phs), alr, emitter, i_res)
if (debug2_active (D_SUBTRACTION)) call msg_print_color('s_alpha', s_alpha, COL_YELLOW)
if (s_alpha > one + tiny_07) call msg_fatal ("s_alpha > 1!")
sqme = sqme * s_alpha
associate (region => reg_data%regions(alr))
  if (emitter > reg_data%n_in) then
    if (debug2_active (D_SUBTRACTION)) &
      print *, 'Double FSR: ', region%double_fsr_factor (p_real%get_momenta(i_phs))
    sqme = sqme * region%double_fsr_factor (p_real%get_momenta(i_phs))
  end if
end associate
end subroutine evaluate_fks_factors

```

Applies the kinematic dependent part of the Jacobian to the squared matrix element. During integration and when generating fixed order events, the non-kinematic part $\frac{s}{(4\pi)^3}$ is applied in `real_subtraction_compute` via `get_phs_factor`.

The additional factor $\frac{\xi}{\xi}$ comes from eq. (4.19f) in arXiv:1002.2581.

(Real subtraction: procedures) +=

```

subroutine apply_kinematic_factors_radiation (sqme, &
  real_kinematics, i_phs)
  real(default), intent(inout) :: sqme
  type(real_kinematics_t), intent(in) :: real_kinematics
  integer, intent(in) :: i_phs
  real(default) :: xi, xi_tilde, s_b
  xi_tilde = real_kinematics%xi_tilde
  xi = xi_tilde * real_kinematics%xi_max (i_phs)
  sqme = sqme * xi**2 / xi_tilde * real_kinematics%jac(i_phs)%jac(1)
end subroutine apply_kinematic_factors_radiation

```

This routine applies the factors in the integrand of eq. 4.20 in arXiv:1002.2581 to the matrix elements.

(Real subtraction: procedures) +=

```

subroutine apply_kinematic_factors_subtraction_fsr &
  (sqme_soft, sqme_coll, sqme_cs, real_kinematics, i_phs)
  real(default), intent(inout) :: sqme_soft, sqme_coll, sqme_cs
  type(real_kinematics_t), intent(in) :: real_kinematics
  integer, intent(in) :: i_phs
  real(default) :: xi_tilde, onemy
  xi_tilde = real_kinematics%xi_tilde
  onemy = one - real_kinematics%y(i_phs)
  sqme_soft = sqme_soft / onemy / xi_tilde
  sqme_coll = sqme_coll / onemy / xi_tilde
  sqme_cs = sqme_cs / onemy / xi_tilde
  associate (jac => real_kinematics%jac(i_phs)%jac)
    sqme_soft = sqme_soft * jac(2)
    sqme_coll = sqme_coll * jac(3)
  end associate

```

```

      sqme_cs = sqme_cs * jac(2)
    end associate
  end subroutine apply_kinematic_factors_subtraction_fsr

```

This routine applies the factors in the integrand of eq. 4.21 in arXiv:1002.2581 to the matrix elements.

(Real subtraction: procedures)+≡

```

subroutine apply_kinematic_factors_subtraction_isr &
  (sqme_soft, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, &
   sqme_cs_minus, real_kinematics, i_phs)
  real(default), intent(inout) :: sqme_soft, sqme_coll_plus, sqme_coll_minus
  real(default), intent(inout) :: sqme_cs_plus, sqme_cs_minus
  type(real_kinematics_t), intent(in) :: real_kinematics
  integer, intent(in) :: i_phs
  real(default) :: xi_tilde, y, onemy, onepy
  xi_tilde = real_kinematics%xi_tilde
  y = real_kinematics%y (i_phs)
  onemy = one - y; onepy = one + y
  associate (jac => real_kinematics%jac(i_phs)%jac)
    sqme_soft = sqme_soft / (one - y**2) / xi_tilde * jac(2)
    sqme_coll_plus = sqme_coll_plus / onemy / xi_tilde / two * jac(3)
    sqme_coll_minus = sqme_coll_minus / onepy / xi_tilde / two * jac(4)
    sqme_cs_plus = sqme_cs_plus / onemy / xi_tilde / two * jac(2)
    sqme_cs_minus = sqme_cs_minus / onepy / xi_tilde / two * jac(2)
  end associate
end subroutine apply_kinematic_factors_subtraction_isr

```

This subroutine evaluates the soft and collinear subtraction terms for ISR. References:

- arXiv:0709.2092, sec. 2.4.2
- arXiv:0908.4272, sec. 4.2

For the collinear terms, the procedure is as follows:

If the emitter is 0, then a gluon was radiated from one of the incoming partons. Gluon emissions require two counter terms: One for emission in the direction of the first incoming parton \oplus and a second for emission in the direction of the second incoming parton \ominus because in both cases, there are divergent diagrams contributing to the matrix element. So in this case both, `sqme_coll_plus` and `sqme_coll_minus`, are non-zero.

If the emitter is 1 or 2, then a quark was emitted instead of a gluon. This only leads to a divergence collinear to the emitter because for anti-collinear quark emission, there are simply no divergent diagrams in the same region as two collinear quarks that cannot originate in the same splitting are non-divergent. This means that in case the emitter is 1, we need non-zero `sqme_coll_plus` and in case the emitter is 2, we need non-zero `sqme_coll_minus`.

At this point, we want to remind ourselves that in case of initial state divergences, y is just the polar angle, so the `sqme_coll_minus` terms are there to counter emissions in the direction of the second incoming parton \ominus and *not* to counter in general anti-collinear divergences.

(Real subtraction: real subtraction: TBP)+≡

```

procedure :: evaluate_subtraction_terms_isr => &
    real_subtraction_evaluate_subtraction_terms_isr

<Real subtraction: sub interfaces>+=
    module subroutine real_subtraction_evaluate_subtraction_terms_isr (rsub, &
        alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, sqme_coll_plus, &
        sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, emitter, i_phs, i_res
    real(default), intent(in) :: alpha_coupling
    real(default), intent(out) :: sqme_soft
    real(default), intent(out) :: sqme_coll_plus, sqme_coll_minus
    real(default), intent(out) :: sqme_cs_plus, sqme_cs_minus
    end subroutine real_subtraction_evaluate_subtraction_terms_isr

<Real subtraction: procedures>+=
    module subroutine real_subtraction_evaluate_subtraction_terms_isr (rsub, &
        alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, sqme_coll_plus, &
        sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, emitter, i_phs, i_res
    real(default), intent(in) :: alpha_coupling
    real(default), intent(out) :: sqme_soft
    real(default), intent(out) :: sqme_coll_plus, sqme_coll_minus
    real(default), intent(out) :: sqme_cs_plus, sqme_cs_minus
    sqme_coll_plus = zero; sqme_cs_plus = zero
    sqme_coll_minus = zero; sqme_cs_minus = zero
    associate (xi_tilde => rsub%real_kinematics%xi_tilde, &
        y => rsub%real_kinematics%y(i_phs), &
        template => rsub%settings%fks_template)
    if (template%xi_cut > xi_tilde) &
        sqme_soft = rsub%compute_sub_soft &
            (alr, emitter, i_phs, i_res, alpha_coupling)
    if (emitter /= 2) then
        if (y - 1 + template%delta_i > 0) then
            sqme_coll_plus = &
                rsub%compute_sub_coll (alr, 1, i_phs, alpha_coupling)
            if (template%xi_cut > xi_tilde) then
                sqme_cs_plus = &
                    rsub%compute_sub_coll_soft (alr, 1, i_phs, alpha_coupling)
            end if
        end if
    end if
    if (emitter /= 1) then
        if (-y - 1 + template%delta_i > 0) then
            sqme_coll_minus = &
                rsub%compute_sub_coll (alr, 2, i_phs, alpha_coupling)
            if (template%xi_cut > xi_tilde) then
                sqme_cs_minus = &
                    rsub%compute_sub_coll_soft (alr, 2, i_phs, alpha_coupling)
            end if
        end if
    end if
    if (debug2_active (D_SUBTRACTION)) then
        print *, "ISR Cutoff:"
    end if
end if

```



```

print *, "y: ", y
print *, "delta_i: ", template%delta_i
print *, "emitter: ", emitter
print *, "sub_soft: ", &
    template%xi_cut > xi_tilde, "(ME: ", sqme_soft, ")"
print *, "sub_coll_plus: ", &
    (y - 1 + template%delta_i) > 0, "(ME: ", sqme_coll_plus, ")"
print *, "sub_coll_minus: ", &
    (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_coll_minus, ")"
print *, "sub_coll_soft_plus: ", template%xi_cut > xi_tilde .and. &
    (y - 1 + template%delta_i) > 0, "(ME: ", sqme_cs_plus, ")"
print *, "sub_coll_soft_minus: ", template%xi_cut > xi_tilde .and. &
    (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_cs_minus, ")"
end if
end associate
end subroutine real_subtraction_evaluate_subtraction_terms_isr

```

This is basically the global part of the real Jacobian corresponding to

$$\frac{q^2}{8(2\pi)^3}.$$

We interpret it as the additional phase space factor of the real component, to be more consistent with the evaluation of the Born phase space.

We specifically use the Born center-of-mass energy here. The real center-of-mass energy is only different from the Born center-of-mass energy in case of ISR. The missing factor $\frac{1}{1-\xi}$ for this conversion is supplied in `phs_fks_generator_generate_isr`.

```

<Real subtraction: real subtraction: TBP>+≡
  procedure :: get_phs_factor => real_subtraction_get_phs_factor

<Real subtraction: sub interfaces>+≡
  module function real_subtraction_get_phs_factor &
    (rsub, i_con) result (factor)
    real(default) :: factor
    class(real_subtraction_t), intent(in) :: rsub
    integer, intent(in) :: i_con
  end function real_subtraction_get_phs_factor

<Real subtraction: procedures>+≡
  module function real_subtraction_get_phs_factor (rsub, i_con) result (factor)
    real(default) :: factor
    class(real_subtraction_t), intent(in) :: rsub
    integer, intent(in) :: i_con
    real(default) :: s
    s = rsub%real_kinematics%xi_ref_momenta (i_con)**2
    factor = s / (8 * twopi3)
  end function real_subtraction_get_phs_factor

<Real subtraction: real subtraction: TBP>+≡
  procedure :: get_i_contributor => real_subtraction_get_i_contributor

<Real subtraction: sub interfaces>+≡
  module function real_subtraction_get_i_contributor &
    (rsub, alr) result (i_con)

```

```

integer :: i_con
class(real_subtraction_t), intent(in) :: rsub
integer, intent(in) :: alr
end function real_subtraction_get_i_contributor

<Real subtraction: procedures>+≡
module function real_subtraction_get_i_contributor (rsub, alr) result (i_con)
integer :: i_con
class(real_subtraction_t), intent(in) :: rsub
integer, intent(in) :: alr
if (allocated (rsub%reg_data%alr_to_i_contributor)) then
i_con = rsub%reg_data%alr_to_i_contributor (alr)
else
i_con = 1
end if
end function real_subtraction_get_i_contributor

```

Computes the soft subtraction term. If there is an initial state emission having a soft divergence, then a gluon has to have been emitted. A gluon can always be emitted from both IS partons and thus, we can take the `sf_factor` for emitter 0 in this case. Be aware that this approach will not work for *pe* collisions.

```

<Real subtraction: real subtraction: TBP>+≡
procedure :: compute_sub_soft => real_subtraction_compute_sub_soft

<Real subtraction: sub interfaces>+≡
module function real_subtraction_compute_sub_soft (rsub, alr, emitter, &
i_phs, i_res, alpha_coupling) result (sqme_soft)
real(default) :: sqme_soft
class(real_subtraction_t), intent(inout) :: rsub
integer, intent(in) :: alr, emitter, i_phs, i_res
real(default), intent(in) :: alpha_coupling
end function real_subtraction_compute_sub_soft

<Real subtraction: procedures>+≡
module function real_subtraction_compute_sub_soft (rsub, alr, emitter, &
i_phs, i_res, alpha_coupling) result (sqme_soft)
real(default) :: sqme_soft
class(real_subtraction_t), intent(inout) :: rsub
integer, intent(in) :: alr, emitter, i_phs, i_res
real(default), intent(in) :: alpha_coupling
integer :: i_xi_ref, i_born
real(default) :: q2, sf_factor
type(vector4_t), dimension(:), allocatable :: p_born
associate (real_kinematics => rsub%real_kinematics, &
nlo_corr_type => rsub%reg_data%regions(alr)%nlo_correction_type, &
sregion => rsub%reg_data%regions(alr))
sqme_soft = zero
if (sregion%has_soft_divergence ()) then
i_xi_ref = rsub%sub_soft%i_xi_ref (alr, i_phs)
q2 = real_kinematics%xi_ref_momenta (i_xi_ref)**2
allocate (p_born (rsub%reg_data%n_legs_born))
if (rsub%reg_data%has_pseudo_isr ()) then
p_born = real_kinematics%p_born_onshell%get_momenta (1)
else
p_born = real_kinematics%p_born_cms%get_momenta (1)

```

```

end if
if (emitter > rsub%sub_soft%reg_data%n_in) then
  call rsub%sub_soft%create_softvec_fsr &
    (p_born, real_kinematics%y_soft(i_phs), &
     real_kinematics%phi, emitter, &
     real_kinematics%xi_ref_momenta(i_xi_ref))
  sf_factor = one
else
  call rsub%sub_soft%create_softvec_isr &
    (real_kinematics%y_soft(i_phs), real_kinematics%phi)
  sf_factor = rsub%sf_factors(alr, 0)
end if
i_born = sregion%uborn_index
select case (char (nlo_corr_type))
case ("QCD")
  sqme_soft = rsub%sub_soft%compute &
    (p_born, rsub%sqme_born_color_c(:, :, i_born) * &
     sf_factor, real_kinematics%y(i_phs), &
     q2, alpha_coupling, alr, emitter, i_res)
case ("EW")
  sqme_soft = rsub%sub_soft%compute &
    (p_born, rsub%sqme_born_charge_c(:, :, i_born) * &
     sf_factor, real_kinematics%y(i_phs), &
     q2, alpha_coupling, alr, emitter, i_res)
end select
end if
end associate
if (debug2_active (D_SUBTRACTION)) call check_soft_vector ()
contains
subroutine check_soft_vector ()
  !!! p_soft = p_gluon / E_gluon only in the soft limit
  !!! This check only has to be passed for ISR or for FSR if ?test_soft_limit = true is set.
  type(vector4_t) :: p_gluon
  if (debug_on) call msg_debug2 (D_SUBTRACTION, "Compare soft vector: ")
  print *, 'p_soft: ', rsub%sub_soft%p_soft%p
  print *, 'Normalized gluon momentum: '
  if (rsub%reg_data%has_pseudo_isr ()) then
    p_gluon = rsub%real_kinematics%p_real_onshell(thr_leg(emitter))%get_momentum &
      (i_phs, rsub%reg_data%n_legs_real)
  else
    p_gluon = rsub%real_kinematics%p_real_cms%get_momentum &
      (i_phs, rsub%reg_data%n_legs_real)
  end if
  call vector4_write (p_gluon / p_gluon%p(0), show_mass = .true.)
end subroutine check_soft_vector
end function real_subtraction_compute_sub_soft

```

(Real subtraction: real subtraction: TBP)+≡

```

procedure :: get_spin_correlation_term => &
  real_subtraction_get_spin_correlation_term

```

(Real subtraction: sub interfaces)+≡

```

module function real_subtraction_get_spin_correlation_term &
  (rsub, alr, i_born, emitter) result (mom_times_sqme)

```

```

        real(default) :: mom_times_sqme
        class(real_subtraction_t), intent(in) :: rsub
        integer, intent(in) :: alr, i_born, emitter
    end function real_subtraction_get_spin_correlation_term

    <Real subtraction: procedures>+≡
    module function real_subtraction_get_spin_correlation_term &
        (rsub, alr, i_born, emitter) result (mom_times_sqme)
        real(default) :: mom_times_sqme
        class(real_subtraction_t), intent(in) :: rsub
        integer, intent(in) :: alr, i_born, emitter
        real(default), dimension(0:3) :: k_perp
        integer :: mu, nu
        if (rsub%sc_required(alr)) then
            if (debug2_active(D_SUBTRACTION)) call check_me_consistency ()
            associate (real_kin => rsub%real_kinematics)
                if (emitter > rsub%reg_data%n_in) then
                    k_perp = real_subtraction_compute_k_perp_fsr ( &
                        real_kin%p_born_lab%get_momentum(1, emitter), &
                        rsub%real_kinematics%phi)
                else
                    k_perp = real_subtraction_compute_k_perp_isr ( &
                        real_kin%p_born_lab%get_momentum(1, emitter), &
                        rsub%real_kinematics%phi)
                end if
            end associate
            mom_times_sqme = zero
            do mu = 1, 3
                do nu = 1, 3
                    mom_times_sqme = mom_times_sqme + &
                        k_perp(mu) * k_perp(nu) * rsub%sqme_born_spin_c (mu, nu, emitter, i_born)
                end do
            end do
        else
            mom_times_sqme = zero
        end if
    contains
        subroutine check_me_consistency ()
            real(default) :: sqme_sum
            if (debug_on) call msg_debug2 (D_SUBTRACTION, "Spin-correlation: Consistency check")
            sqme_sum = &
                - rsub%sqme_born_spin_c(1,1,emitter,i_born) &
                - rsub%sqme_born_spin_c(2,2,emitter,i_born) &
                - rsub%sqme_born_spin_c(3,3,emitter,i_born)
            if (.not. nearly_equal (sqme_sum, -rsub%sqme_born(i_born))) then
                print *, 'Spin-correlated matrix elements are not consistent: '
                print *, 'emitter: ', emitter
                print *, 'g^{mu,nu} B_{mu,nu}: ', -sqme_sum
                print *, 'all Born matrix elements: ', rsub%sqme_born
                call msg_fatal ("FAIL")
            else
                call msg_print_color ("Success", COL_GREEN)
            end if
        end subroutine check_me_consistency
    end function real_subtraction_get_spin_correlation_term

```

Construct a normalised momentum perpendicular to momentum p and rotate by an arbitrary angle ϕ . The angular conventions we use here are equivalent to those used by POWHEG.

```

<Real subtraction: public>+≡
  public :: real_subtraction_compute_k_perp_fsr
  public :: real_subtraction_compute_k_perp_isr

<Real subtraction: sub interfaces>+≡
  module function real_subtraction_compute_k_perp_fsr &
    (p, phi) result (k_perp_fsr)
    real(default), dimension(0:3) :: k_perp_fsr
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: phi
  end function real_subtraction_compute_k_perp_fsr
  module function real_subtraction_compute_k_perp_isr &
    (p, phi) result (k_perp_isr)
    real(default), dimension(0:3) :: k_perp_isr
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: phi
  end function real_subtraction_compute_k_perp_isr

<Real subtraction: procedures>+≡
  module function real_subtraction_compute_k_perp_fsr &
    (p, phi) result (k_perp_fsr)
    real(default), dimension(0:3) :: k_perp_fsr
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: phi
    type(vector4_t) :: k
    type(vector3_t) :: vec
    type(lorentz_transformation_t) :: rot
    vec = p%p(1:3) / p%p(0)
    k%p(0) = zero
    k%p(1) = p%p(1); k%p(2) = p%p(2)
    k%p(3) = - (p%p(1)**2 + p%p(2)**2) / p%p(3)
    rot = rotation (cos(phi), sin(phi), vec)
    k = rot * k
    k%p(1:3) = k%p(1:3) / space_part_norm (k)
    k_perp_fsr = k%p
  end function real_subtraction_compute_k_perp_fsr

  module function real_subtraction_compute_k_perp_isr &
    (p, phi) result (k_perp_isr)
    real(default), dimension(0:3) :: k_perp_isr
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: phi
    k_perp_isr(0) = zero
    k_perp_isr(1) = sin(phi)
    k_perp_isr(2) = cos(phi)
    k_perp_isr(3) = zero
  end function real_subtraction_compute_k_perp_isr

<Real subtraction: real subtraction: TBP>+≡
  procedure :: compute_sub_coll => real_subtraction_compute_sub_coll

```

(Real subtraction: sub interfaces)+≡

```

module function real_subtraction_compute_sub_coll &
  (rsub, alr, em, i_phs, alpha_coupling) result (sqme_coll)
  real(default) :: sqme_coll
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, em, i_phs
  real(default), intent(in) :: alpha_coupling
end function real_subtraction_compute_sub_coll

```

(Real subtraction: procedures)+≡

```

module function real_subtraction_compute_sub_coll &
  (rsub, alr, em, i_phs, alpha_coupling) result (sqme_coll)
  real(default) :: sqme_coll
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, em, i_phs
  real(default), intent(in) :: alpha_coupling
  real(default) :: xi, xi_max
  real(default) :: mom_times_sqme_spin_c, sqme_born_coll
  real(default) :: N_col
  integer :: i_con, i
  real(default) :: pfr
  associate (sregion => rsub%reg_data%regions(alr))
    sqme_coll = zero
    sqme_born_coll = zero
    N_col = 1
    if (sregion%has_collinear_divergence ()) then
      xi = rsub%real_kinematics%xi_tilde * rsub%real_kinematics%xi_max(i_phs)
      if (rsub%sub_coll%use_resonance_mappings) then
        i_con = rsub%reg_data%alr_to_i_contributor (alr)
      else
        i_con = 1
      end if
      mom_times_sqme_spin_c = &
        rsub%get_spin_correlation_term (alr, sregion%uborn_index, em)
      if (rsub%reg_data%nlo_correction_type == "EW" .and. &
        sregion%nlo_correction_type == "QCD" .and. &
        qcd_ew_interferences (sregion%flst_uborn%flst)) then
        do i = 1, size (sregion%flst_uborn%flst)
          if (is_quark (sregion%flst_uborn%flst (i))) then
            sqme_born_coll = &
              -rsub%sqme_born_color_c (i, i, sregion%uborn_index)/CF
            exit
          end if
        end do
      else
        sqme_born_coll = rsub%sqme_born(sregion%uborn_index)
      end if
      if (em <= rsub%sub_coll%n_in) then
        select case (rsub%isr_kinematics%isr_mode)
          case (SQRTS_FIXED)
            xi_max = rsub%real_kinematics%xi_max(i_phs)
          case (SQRTS_VAR)
            xi_max = one - rsub%isr_kinematics%x(em)
          end select
        xi = rsub%real_kinematics%xi_tilde * xi_max
      end if
    end associate
  end function real_subtraction_compute_sub_coll

```

```

    if (sregion%nlo_correction_type == "QCD") then
        call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
    else if (sregion%nlo_correction_type == "EW") then
        if (is_quark (sregion%flst_real%flst(size(sregion%flst_real%flst)))) N_col = 3
        call rsub%sub_coll%set_parameters (CA = zero, &
            CF = sregion%flst_real%charge(em)**2, &
            TR = N_col*sregion%flst_real%charge(size(sregion%flst_real%flst))**2)
    end if
    sqme_coll = rsub%sub_coll%compute_isr (em, sregion%flst_real%flst, &
        rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
        sqme_born_coll * rsub%sf_factors(alr, em), &
        mom_times_sqme_spin_c * rsub%sf_factors(alr, em), &
        xi, alpha_coupling, rsub%isr_kinematics%isr_mode)
else
    if (sregion%nlo_correction_type == "QCD") then
        call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
    else if (sregion%nlo_correction_type == "EW") then
        if (is_quark (sregion%flst_real%flst(sregion%emitter))) N_col = 3
        call rsub%sub_coll%set_parameters (CA = zero, &
            CF = sregion%flst_real%charge(sregion%emitter)**2, &
            TR = N_col*sregion%flst_real%charge(sregion%emitter)**2)
    end if
    sqme_coll = rsub%sub_coll%compute_fsr (sregion%emitter, &
        sregion%flst_real%flst, &
        rsub%real_kinematics%xi_ref_momenta (i_con), &
        rsub%real_kinematics%p_born_lab%get_momenta(1), &
        sqme_born_coll, &
        mom_times_sqme_spin_c, &
        xi, alpha_coupling, sregion%double_fsr)
    if (rsub%sub_coll%use_resonance_mappings) then
        select type (fks_mapping => rsub%reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            pfr = fks_mapping%get_resonance_weight (alr, &
                rsub%real_kinematics%p_born_cms%get_momenta(1))
        end select
        sqme_coll = sqme_coll * pfr
    end if
end if
end if
end associate
end function real_subtraction_compute_sub_coll

```

Computes the soft-collinear subtraction term. For alpha regions with emitter 0, this routine is called with `em == 1` and `em == 2` separately. To still be able to use the unrescaled pdf factors stored in `sf_factors(alr, 0)` in this case, we need to differentiate between `em` and `em_pdf = 0`.

(Real subtraction: real subtraction: TBP)+≡

```
procedure :: compute_sub_coll_soft => real_subtraction_compute_sub_coll_soft
```

(Real subtraction: sub interfaces)+≡

```

module function real_subtraction_compute_sub_coll_soft &
    (rsub, alr, em, i_phs, alpha_coupling) result (sqme_cs)
    real(default) :: sqme_cs
    class(real_subtraction_t), intent(inout) :: rsub

```

```

integer, intent(in) :: alr, em, i_phs
real(default), intent(in) :: alpha_coupling
end function real_subtraction_compute_sub_coll_soft

(Real subtraction: procedures) +=
module function real_subtraction_compute_sub_coll_soft &
  (rsub, alr, em, i_phs, alpha_coupling) result (sqme_cs)
  real(default) :: sqme_cs
  class(real_subtraction_t), intent(inout) :: rsub
  integer, intent(in) :: alr, em, i_phs
  real(default), intent(in) :: alpha_coupling
  real(default) :: mom_times_sqme_spin_c, sqme_born_coll
  real(default) :: N_col
  integer :: i_con, em_pdf, i
  associate (sregion => rsub%reg_data%regions(alr))
    sqme_cs = zero
    sqme_born_coll = zero
    N_col = 1
    if (sregion%has_collinear_divergence ()) then
      if (rsub%sub_coll%use_resonance_mappings) then
        i_con = rsub%reg_data%alr_to_i_contributor (alr)
      else
        i_con = 1
      end if
      mom_times_sqme_spin_c = rsub%get_spin_correlation_term (alr, sregion%uborn_index, em)
      if (rsub%reg_data%nlo_correction_type == "EW" .and. &
        sregion%nlo_correction_type == "QCD" .and. &
        qcd_ew_interferences (sregion%flst_uborn%flst)) then
        do i = 1, size (sregion%flst_uborn%flst)
          if (is_quark (sregion%flst_uborn%flst (i))) then
            sqme_born_coll = -rsub%sqme_born_color_c (i, i, sregion%uborn_index)/CF
            exit
          end if
        end do
      else
        sqme_born_coll = rsub%sqme_born(sregion%uborn_index)
      end if
      if (em <= rsub%sub_coll%n_in) then
        em_pdf = 0
        if (sregion%nlo_correction_type == "QCD") then
          call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
        else if (sregion%nlo_correction_type == "EW") then
          if (is_quark (sregion%flst_real%flst(size(sregion%flst_real%flst)))) N_col = 3
          call rsub%sub_coll%set_parameters (CA = zero, &
            CF = sregion%flst_real%charge(em)**2, &
            TR = N_col*sregion%flst_real%charge(size(sregion%flst_real%flst))**2)
          end if
        sqme_cs = rsub%sub_coll%compute_isr (em, sregion%flst_real%flst, &
          rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
          sqme_born_coll * rsub%sf_factors(alr, em_pdf), &
          mom_times_sqme_spin_c * rsub%sf_factors(alr, em_pdf), &
          zero, alpha_coupling, rsub%isr_kinematics%isr_mode)
      else
        if (sregion%nlo_correction_type == "QCD") then
          call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)

```



```

else if (sregion%nlo_correction_type == "EW") then
  if (is_quark (sregion%flst_real%flst(sregion%emitter))) N_col = 3
  call rsub%sub_coll%set_parameters (CA = zero, &
    CF = sregion%flst_real%charge(sregion%emitter)**2, &
    TR = N_col*sregion%flst_real%charge(sregion%emitter)**2)
end if
sqme_cs = rsub%sub_coll%compute_fsr (sregion%emitter, sregion%flst_real%flst, &
  rsub%real_kinematics%xi_ref_momenta(i_con), &
  rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
  sqme_born_coll, &
  mom_times_sqme_spin_c, &
  zero, alpha_coupling, sregion%double_fsr)
end if
end if
end associate
end function real_subtraction_compute_sub_coll_soft

```

```

<Real subtraction: real subtraction: TBP>+≡
procedure :: requires_spin_correlations => &
  real_subtraction_requires_spin_correlations

```

```

<Real subtraction: sub interfaces>+≡
module function real_subtraction_requires_spin_correlations &
  (rsub) result (val)
  logical :: val
  class(real_subtraction_t), intent(in) :: rsub
end function real_subtraction_requires_spin_correlations

```

```

<Real subtraction: procedures>+≡
module function real_subtraction_requires_spin_correlations &
  (rsub) result (val)
  logical :: val
  class(real_subtraction_t), intent(in) :: rsub
  val = any (rsub%sc_required)
end function real_subtraction_requires_spin_correlations

```

```

<Real subtraction: real subtraction: TBP>+≡
procedure :: final => real_subtraction_final

```

```

<Real subtraction: sub interfaces>+≡
module subroutine real_subtraction_final (rsub)
  class(real_subtraction_t), intent(inout) :: rsub
end subroutine real_subtraction_final

```

```

<Real subtraction: procedures>+≡
module subroutine real_subtraction_final (rsub)
  class(real_subtraction_t), intent(inout) :: rsub
  call rsub%sub_soft%final ()
  call rsub%sub_coll%final ()
  !!! Finalization of region data is done in pcm_nlo_final
  if (associated (rsub%reg_data)) nullify (rsub%reg_data)
  !!! Finalization of real kinematics is done in pcm_instance_nlo_final
  if (associated (rsub%real_kinematics)) nullify (rsub%real_kinematics)
  if (associated (rsub%isr_kinematics)) nullify (rsub%isr_kinematics)
  if (allocated (rsub%sqme_real_non_sub)) deallocate (rsub%sqme_real_non_sub)

```

```

    if (allocated (rsub%sqme_born)) deallocate (rsub%sqme_born)
    if (allocated (rsub%sf_factors)) deallocate (rsub%sf_factors)
    if (allocated (rsub%sqme_real_arr)) deallocate (rsub%sqme_real_arr)
    if (allocated (rsub%sqme_born_color_c)) deallocate (rsub%sqme_born_color_c)
    if (allocated (rsub%sqme_born_charge_c)) deallocate (rsub%sqme_born_charge_c)
    if (allocated (rsub%sc_required)) deallocate (rsub%sc_required)
    if (allocated (rsub%selected_alr)) deallocate (rsub%selected_alr)
end subroutine real_subtraction_final

```

Partitions of the real matrix element and Powheg damping

```

<Real subtraction: public>+≡
    public :: real_partition_t

<Real subtraction: types>+≡
    type, abstract :: real_partition_t
    contains
    <Real subtraction: real partition: TBP>
    end type real_partition_t

<Real subtraction: real partition: TBP>≡
    procedure (real_partition_init), deferred :: init

<Real subtraction: interfaces>≡
    abstract interface
        subroutine real_partition_init (partition, scale, reg_data)
            import
            class(real_partition_t), intent(out) :: partition
            real(default), intent(in) :: scale
            type(region_data_t), intent(in) :: reg_data
        end subroutine real_partition_init
    end interface

<Real subtraction: real partition: TBP>+≡
    procedure (real_partition_write), deferred :: write

<Real subtraction: interfaces>+≡
    abstract interface
        subroutine real_partition_write (partition, unit)
            import
            class(real_partition_t), intent(in) :: partition
            integer, intent(in), optional :: unit
        end subroutine real_partition_write
    end interface

```

To allow really arbitrary damping functions, `get_f` should get the full real phase space as argument and not just some `pt2` that is extracted higher up.

```

<Real subtraction: real partition: TBP>+≡
    procedure (real_partition_get_f), deferred :: get_f

```

```

<Real subtraction: interfaces>+≡
abstract interface
  function real_partition_get_f (partition, p) result (f)
    import
    real(default) :: f
    class(real_partition_t), intent(in) :: partition
    type(vector4_t), intent(in), dimension(:) :: p
  end function real_partition_get_f
end interface

<Real subtraction: public>+≡
public :: powheg_damping_simple_t

<Real subtraction: types>+≡
type, extends (real_partition_t) :: powheg_damping_simple_t
  real(default) :: h2 = 5._default
  integer :: emitter
contains
  <Real subtraction: powheg damping simple: TBP>
end type powheg_damping_simple_t

<Real subtraction: powheg damping simple: TBP>≡
procedure :: get_f => powheg_damping_simple_get_f

<Real subtraction: sub interfaces>+≡
module function powheg_damping_simple_get_f (partition, p) result (f)
  real(default) :: f
  class(powheg_damping_simple_t), intent(in) :: partition
  type(vector4_t), intent(in), dimension(:) :: p
end function powheg_damping_simple_get_f

<Real subtraction: procedures>+≡
module function powheg_damping_simple_get_f (partition, p) result (f)
  real(default) :: f
  class(powheg_damping_simple_t), intent(in) :: partition
  type(vector4_t), intent(in), dimension(:) :: p
  !!! real(default) :: pt2
  f = 1
  call msg_bug ("Simple damping currently not available")
  !!! TODO (cw-2017-03-01) Compute pt2 from emitter
  !!! f = partition%h2 / (pt2 + partition%h2)
end function powheg_damping_simple_get_f

<Real subtraction: powheg damping simple: TBP>+≡
procedure :: init => powheg_damping_simple_init

<Real subtraction: sub interfaces>+≡
module subroutine powheg_damping_simple_init (partition, scale, reg_data)
  class(powheg_damping_simple_t), intent(out) :: partition
  real(default), intent(in) :: scale
  type(region_data_t), intent(in) :: reg_data
end subroutine powheg_damping_simple_init

```

```

<Real subtraction: procedures>+≡
module subroutine powheg_damping_simple_init (partition, scale, reg_data)
  class(powheg_damping_simple_t), intent(out) :: partition
  real(default), intent(in) :: scale
  type(region_data_t), intent(in) :: reg_data
  partition%h2 = scale**2
end subroutine powheg_damping_simple_init

<Real subtraction: powheg damping simple: TBP>+≡
procedure :: write => powheg_damping_simple_write

<Real subtraction: sub interfaces>+≡
module subroutine powheg_damping_simple_write (partition, unit)
  class(powheg_damping_simple_t), intent(in) :: partition
  integer, intent(in), optional :: unit
end subroutine powheg_damping_simple_write

<Real subtraction: procedures>+≡
module subroutine powheg_damping_simple_write (partition, unit)
  class(powheg_damping_simple_t), intent(in) :: partition
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "Powheg damping simple: "
  write (u, "(1x,A, "// FMT_15 // ")") "scale h2: ", partition%h2
end subroutine powheg_damping_simple_write

<Real subtraction: public>+≡
public :: real_partition_fixed_order_t

<Real subtraction: types>+≡
type, extends (real_partition_t) :: real_partition_fixed_order_t
  real(default) :: scale
  type(ftuple_t), dimension(:), allocatable :: fks_pairs
contains
  <Real subtraction: real partition fixed order: TBP>
end type real_partition_fixed_order_t

<Real subtraction: real partition fixed order: TBP>≡
procedure :: init => real_partition_fixed_order_init

<Real subtraction: sub interfaces>+≡
module subroutine real_partition_fixed_order_init &
  (partition, scale, reg_data)
  class(real_partition_fixed_order_t), intent(out) :: partition
  real(default), intent(in) :: scale
  type(region_data_t), intent(in) :: reg_data
end subroutine real_partition_fixed_order_init

<Real subtraction: procedures>+≡
module subroutine real_partition_fixed_order_init (partition, scale, reg_data)
  class(real_partition_fixed_order_t), intent(out) :: partition
  real(default), intent(in) :: scale
  type(region_data_t), intent(in) :: reg_data
end subroutine real_partition_fixed_order_init

```

```

<Real subtraction: real partition fixed order: TBP>+≡
  procedure :: write => real_partition_fixed_order_write

<Real subtraction: sub interfaces>+≡
  module subroutine real_partition_fixed_order_write (partition, unit)
    class(real_partition_fixed_order_t), intent(in) :: partition
    integer, intent(in), optional :: unit
  end subroutine real_partition_fixed_order_write

<Real subtraction: procedures>+≡
  module subroutine real_partition_fixed_order_write (partition, unit)
    class(real_partition_fixed_order_t), intent(in) :: partition
    integer, intent(in), optional :: unit
  end subroutine real_partition_fixed_order_write

```

Implements the suppression factor

$$F(\Phi_{n+1}) = 1 - \prod_{(i,j) \in P_{FKS}} \theta \left[m_i + m_j + h - \sqrt{(p_j + p_j)^2} \right] \quad (27.43)$$

to split the real matrix element into singular and finite part.

```

<Real subtraction: real partition fixed order: TBP>+≡
  procedure :: get_f => real_partition_fixed_order_get_f

<Real subtraction: sub interfaces>+≡
  module function real_partition_fixed_order_get_f (partition, p) result (f)
    real(default) :: f
    class(real_partition_fixed_order_t), intent(in) :: partition
    type(vector4_t), intent(in), dimension(:) :: p
  end function real_partition_fixed_order_get_f

<Real subtraction: procedures>+≡
  module function real_partition_fixed_order_get_f (partition, p) result (f)
    real(default) :: f
    class(real_partition_fixed_order_t), intent(in) :: partition
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: i, em
    f = zero
    PAIRS: do i = 1, size (partition%fks_pairs)
      associate (ii => partition%fks_pairs(i)%ireg)
        if (ii(1) == 0) then
          IS: do em = 1, 2
            if ((p(em) + p(ii(2)))**1 < p(em)**1 + p(ii(2))**1 + &
              partition%scale) then
              f = one
              exit PAIRS
            end if
          end do IS
        else
          if ((p(ii(1)) + p(ii(2)))**1 < p(ii(1))**1 + p(ii(2))**1 + &
            partition%scale) then
            f = one
            exit PAIRS
          end if
        end if
      end if
    end if
  end function

```

```

        end associate
    end do PAIRS
end function real_partition_fixed_order_get_f

```

27.6.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<real_subtraction_ut.f90>≡
  <File header>

```

```

  module real_subtraction_ut
    use unit_tests
    use real_subtraction_util

```

```

  <Standard module head>

```

```

  <Real subtraction: public test>

```

```

  contains

```

```

  <Real subtraction: test driver>

```

```

  end module real_subtraction_ut

```

```

<real_subtraction_util.f90>≡
  <File header>

```

```

  module real_subtraction_util
    <Use kinds>

```

```

    use physics_defs
    use lorentz
    use numeric_utils
    use real_subtraction

```

```

  <Standard module head>

```

```

  <Real subtraction: test declarations>

```

```

  contains

```

```

  <Real subtraction: tests>

```

```

  end module real_subtraction_util

```

API: driver for the unit tests below.

```

<Real subtraction: public test>≡
  public :: real_subtraction_test

```

```

<Real subtraction: test driver>≡
  subroutine real_subtraction_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Real subtraction: execute tests>

```

```
end subroutine real_subtraction_test
```

Test the final-state collinear subtraction.

```
<Real subtraction: execute tests>≡
```

```
call test (real_subtraction_1, "real_subtraction_1", &
  "final-state collinear subtraction", &
  u, results)
```

```
<Real subtraction: test declarations>≡
```

```
public :: real_subtraction_1
```

```
<Real subtraction: tests>≡
```

```
subroutine real_subtraction_1 (u)
  integer, intent(in) :: u
```

```

  type(coll_subtraction_t) :: coll_sub
  real(default) :: sqme_coll
  type(vector4_t) :: p_res
  type(vector4_t), dimension(5) :: p_born
  real(default), dimension(4) :: k_perp
  real(default), dimension(4,4) :: b_munu
  integer :: mu, nu
  real(default) :: born, born_c
  integer, dimension(6) :: flst
```

```

  p_born(1)%p = [500, 0, 0, 500]
  p_born(2)%p = [500, 0, 0, -500]
  p_born(3)%p = [3.7755E+02, 2.2716E+02, -95.4172, 2.8608E+02]
  p_born(4)%p = [4.9529E+02, -2.739E+02, 84.8535, -4.0385E+02]
  p_born(5)%p = [1.2715E+02, 46.7375, 10.5637, 1.1778E+02]
  p_res = p_born(1) + p_born(2)
  flst = [11, -11, -2, 2, -2, 2]
```

```

  b_munu(1, :) = [0., 0., 0., 0.]
  b_munu(2, :) = [0., 1., 1., 1.]
  b_munu(3, :) = [0., 1., 1., 1.]
  b_munu(4, :) = [0., 1., 1., 1.]
```

```

  k_perp = real_subtraction_compute_k_perp_fsr (p = p_born(5), phi = 0.5_default)
  born = - b_munu(1, 1) + b_munu(2, 2) + b_munu(3, 3) + b_munu(4, 4)
  born_c = 0.
  do mu = 1, 4
    do nu = 1, 4
      born_c = born_c + k_perp(mu) * k_perp(nu) * b_munu(mu, nu)
    end do
  end do
```

```

  write (u, "(A)") "*" Test output: real_subtraction_1"
  write (u, "(A)") "*" Purpose: final-state collinear subtraction"
  write (u, "(A)")
```

```

  write (u, "(A, L1)") "*" vanishing scalar-product of 3-momenta k_perp and p_born(emitter): ", &
    nearly_equal (dot_product (p_born(5)%p(1:3), k_perp(2:4)), 0._default)
```

```
call coll_sub%init (n_alr = 1, n_in = 2)
```

```

call coll_sub%set_parameters (CA, CF, TR)

write (u, "(A)")
write (u, "(A)") "* g -> qq splitting"
write (u, "(A)")

sqme_coll = coll_sub%compute_fsr(5, flst, p_res, p_born, &
    born, born_c, 0.5_default, 0.25_default, .false.)

write (u, "(A,F15.12)") "ME: ", sqme_coll

write (u, "(A)")
write (u, "(A)") "* g -> gg splitting"
write (u, "(A)")

b_munu(1, :) = [0., 0., 0., 0.]
b_munu(2, :) = [0., 0., 0., 1.]
b_munu(3, :) = [0., 0., 1., 1.]
b_munu(4, :) = [0., 0., 1., 1.]

k_perp = real_subtraction_compute_k_perp_fsr (p = p_born(5), phi = 0.5_default)
born = - b_munu(1, 1) + b_munu(2, 2) + b_munu(3, 3) + b_munu(4, 4)
born_c = 0.
do mu = 1, 4
    do nu = 1, 4
        born_c = born_c + k_perp(mu) * k_perp(nu) * b_munu(mu, nu)
    end do
end do

flst = [11, -11, 2, -2, 21, 21]
sqme_coll = coll_sub%compute_fsr(5, flst, p_res, p_born, &
    born, born_c, 0.5_default, 0.25_default, .true.)

write (u, "(A,F15.12)") "ME: ", sqme_coll

write (u, "(A)")
write (u, "(A)") "* Test output end: real_subtraction_1"
write (u, "(A)")
end subroutine real_subtraction_1

```


27.7 Contribution of divergencies due to PDF Evolution

References:

- arXiv:hep-ph/9512328, (2.1)-(2.5), (4.29)-(4.53)
- arXiv:0709.2092, (2.102)-(2.106)

The parton distribution densities have to be evaluated at NLO, too. The NLO PDF evolution is given by

$$f(\bar{x}) = \int_0^1 \int_0^1 dx dz f(x) \Gamma(z) \delta(\bar{x} - xz), \quad (27.44)$$

where Γ are the DGLAP evolution kernels for an $a \rightarrow d$ splitting,

$$\Gamma_a^{(d)} = \delta_{ad} \delta(1-x) - \frac{\alpha_s}{2\pi} \left(\frac{1}{\epsilon} P_{ad}(x, 0) - K_{ad}(x) \right) + \mathcal{O}(\alpha_s^2). \quad (27.45)$$

K_{ad} is a renormalization scheme matching factor, which is exactly zero in $\overline{\text{MS}}$. Let the leading-order hadronic cross section be given by

$$d\sigma^{(0)}(s) = \int dx_{\oplus} dx_{\ominus} f_{\oplus}(x_{\oplus}) f_{\ominus}(x_{\ominus}) d\tilde{\sigma}^{(0)}(x_{\oplus} x_{\ominus} s), \quad (27.46)$$

then the NLO hadronic cross section is

$$d\sigma^{(1)}(s) = \int dx_{\oplus} dx_{\ominus} dz_{\oplus} dz_{\ominus} f_{\oplus}(x_{\oplus}) f_{\ominus}(x_{\ominus}) \underbrace{\Gamma_{\oplus}(z_{\oplus}) \Gamma_{\ominus}(z_{\ominus}) d\tilde{\sigma}^{(1)}(z_{\oplus} z_{\ominus} s)}_{d\hat{\sigma}^{(1)}}. \quad (27.47)$$

$d\hat{\sigma}$ is called the subtracted partonic cross section. Expanding in α_s we find

$$d\hat{\sigma}_{ab}^{(0)}(k_1, k_2) = d\tilde{\sigma}_{ab}^{(0)}(k_1, k_2), \quad (27.48)$$

$$d\hat{\sigma}_{ab}^{(1)}(k_1, k_2) = d\tilde{\sigma}_{ab}^{(1)}(k_1, k_2) \quad (27.49)$$

$$+ \frac{\alpha_s}{2\pi} \sum_d \int dx \left(\frac{1}{\epsilon} P_{da}(x, 0) - K_{da}(x) \right) d\tilde{\sigma}_{db}^{(0)}(xk_1, k_2) \quad (27.50)$$

$$+ \frac{\alpha_s}{2\pi} \sum_d \int \left(\frac{1}{\epsilon} P_{db}(x, 0) - K_{db}(x) \right) d\tilde{\sigma}_{ad}^{(0)}(k_1, xk_2). \quad (27.51)$$

$$= d\tilde{\sigma}_{ab}^{(1)} + d\tilde{\sigma}_{ab}^{(cnt,+)} + d\tilde{\sigma}_{ab}^{(cnt,-)} \quad (27.52)$$

Let us now turn to the soft-subtracted real part of the cross section. For ease of notation, it is constrained to one singular region,

$$d\sigma_{\alpha}^{(in)} = \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] (1-y^2) \xi^2 \mathcal{R}_{\alpha} \mathcal{S}_{\alpha} \\ \times \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} (1-y^2)^{-1-\epsilon} d\phi d\xi dy d\Omega^{2-2\epsilon},$$

where we regularize collinear divergencies using the identity

$$(1 - y^2)^{-1-\epsilon} = -\frac{2^{-\epsilon}}{2\epsilon} (\delta(1 - y) + \delta(1 + y)) + \underbrace{\frac{1}{2} \left[\left(\frac{1}{1 - y} \right)_c + \left(\frac{1}{1 + y} \right)_c \right]}_{\mathcal{P}(y)}.$$

This enables us to split the cross section into a finite and a singular part. The latter can further be separated into a contribution of the incoming and of the outgoing particles,

$$d\sigma_\alpha^{(in)} = d\sigma_\alpha^{(in,+)} + d\sigma_\alpha^{(in,-)} + d\sigma_\alpha^{(in,f)}.$$

They are given by

$$d\sigma_\alpha^{(in,f)} = \mathcal{P}(y) \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} \times (1 - y^2) \xi^2 \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy d\Omega^{2-2\epsilon} \quad (27.53)$$

and

$$d\sigma_\alpha^{(in,\pm)} = -\frac{2^{-\epsilon}}{2\epsilon} \delta(1 \mp y) \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] \times \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} (1 - y^2) \xi^2 \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy d\Omega^{2-2\epsilon}. \quad (27.54)$$

Equation 27.53 is the contribution to the real cross section which is computed in `evaluate_region_isr`. It is regularized both in the soft and collinear limit via the plus distributions. Equation 27.54 is a different contribution. It is only present exactly in the collinear limit, due to the delta function. The divergences present in this term do not completely cancel out divergences in the virtual matrix element, because the beam axis is distinguished. Thus, the conditions in which the KLN theorem applies are not met. To see this, we carry out the collinear limit, obtaining

$$\lim_{y \rightarrow 1} (1 - y^2) \xi^2 \mathcal{R}_\alpha = 8\pi\alpha_s \mu^{2\epsilon} \left(\frac{2}{\sqrt{s}} \right)^2 \xi P^<(1 - \xi, \epsilon) \mathcal{R}_\alpha,$$

with the Altarelli-Parisi splitting kernel for $z < 1$, $P^<(z, \epsilon)$. Moreover, $\lim_{\vec{k} \parallel \vec{k}_1} d\phi = d\phi_3$ violates spatial averaging. The integration over the spherical angle $d\Omega$ can be carried out easily, yielding a factor of $2\pi^{1-\epsilon}/\Gamma(1 - \epsilon)$. This allows us to redefine ϵ ,

$$\frac{1}{\epsilon} - \gamma_E + \log(4\pi) \rightarrow \frac{1}{\epsilon}. \quad (27.55)$$

Coming back to $d\tilde{\sigma}_{ab}^{(cnt,+)}$ in order to make a connection to $d\sigma_\alpha^{(in,+)}$, we relate $P_{ab}(z, 0)$ to $P_{ab}^<(z, 0)$ via the equation

$$P_{ab}(z, 0) = (1 - z) P_{ab}^<(z, 0) \left(\frac{1}{1 - z} \right)_+ + \gamma(a) \delta_{ab} \delta(1 - z),$$

which yields

$$d\tilde{\sigma}_\alpha^{(cnt,+)} = \frac{\alpha_s}{2\pi} \sum_d \left\{ -K_{da}(1 - \xi) + \frac{1}{\epsilon} \left[\left(\frac{1}{\xi} \right)_+ \xi P_{da}^<(1 - \xi, 0) + \delta_{da} \delta(\xi) \gamma(d) \right] \right\} \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy. \quad (27.56)$$

This term has the same pole structure as eqn. 27.54. This makes clear that the quantity

$$d\hat{\sigma}^{(in,+)} = d\tilde{\sigma}^{(in,+)} + d\tilde{\sigma}^{(cnt,+)} \quad (27.57)$$

has no collinear poles. Therefore, our task is to add up eqns. 27.54 and 27.56 in order to compute the finite remainder. This is the integrand which is evaluated in the `dglap_remnant` component.

So, we have to perform an expansion of $d\hat{\sigma}^{(in,+)}$ in ϵ . Hereby, we must not neglect the implicit ϵ -dependence of $P^<$, which leads to additional terms involving the first derivative,

$$P_{ab}^<(z, \epsilon) = P_{ab}^<(z, 0) + \epsilon \frac{\partial P_{ab}^<(z, \epsilon)}{\partial \epsilon} \Big|_{\epsilon=0} + \mathcal{O}(\alpha_s^2).$$

This finally gives us the equation for the collinear remnant. Note that there is still one soft $1/\epsilon$ -pole, which cancels out with the corresponding expression in the soft-virtual terms.

$$\begin{aligned} d\hat{\sigma}^{(in,+)} &= \frac{\alpha_s}{2\pi} \frac{1}{\epsilon} \gamma(a) \mathcal{R}_\alpha \mathcal{S}_\alpha \\ &+ \frac{\alpha_s}{2\pi} \sum_d \left\{ (1-z) P_{da}^<(z, 0) \left[\left(\frac{1}{1-z} \right)_c \log \frac{s\delta_I}{2\mu^2} + 2 \left(\frac{\log(1-z)}{1-z} \right)_c \right] \right. \\ &\quad \left. - (1-z) \frac{\partial P_{da}^<(z, \epsilon)}{\partial \epsilon} \left(\frac{1}{1-z} \right)_c - K_{da}(z) \right\} \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy \end{aligned} \quad (27.58)$$

```

<dglap_remnant.f90>≡
  <File header>

  module dglap_remnant

    <Use kinds with double>
    <Use strings>
    use phs_fks, only: isr_kinematics_t
    use fks_regions, only: region_data_t

    use nlo_data

    <Standard module head>

    <DGLAP remnant: public>

    <DGLAP remnant: types>

    interface
    <DGLAP remnant: sub interfaces>
    end interface

  end module dglap_remnant

<dglap_remnant_sub.f90>≡
  <File header>

  submodule (dglap_remnant) dglap_remnant_s

```

```

    use numeric_utils
    use diagnostics
    use constants
    use physics_defs
    use pdg_arrays

    implicit none

contains

<DGLAP remnant: procedures>

end submodule dglap_remnant_s

<DGLAP remnant: public>≡
    public :: dglap_remnant_t

<DGLAP remnant: types>≡
    type :: dglap_remnant_t
        type(nlo_settings_t), pointer :: settings => null ()
        type(region_data_t), pointer :: reg_data => null ()
        type(isr_kinematics_t), pointer :: isr_kinematics => null ()
        real(default) :: CA = 0, CF = 0, TR = 0
        real(default), dimension(:), allocatable :: sqme_born
        real(default), dimension(:,:), allocatable :: sf_factors
        real(default), dimension(:,:,:), allocatable :: sqme_color_c_extra
    contains
        <DGLAP remnant: dglap remnant: TBP>
    end type dglap_remnant_t

<DGLAP remnant: dglap remnant: TBP>≡
    procedure :: init => dglap_remnant_init

<DGLAP remnant: sub interfaces>≡
    module subroutine dglap_remnant_init &
        (dglap, settings, reg_data, isr_kinematics)
        class(dglap_remnant_t), intent(inout) :: dglap
        type(nlo_settings_t), intent(in), target :: settings
        type(region_data_t), intent(in), target :: reg_data
        type(isr_kinematics_t), intent(in), target :: isr_kinematics
    end subroutine dglap_remnant_init

<DGLAP remnant: procedures>≡
    module subroutine dglap_remnant_init &
        (dglap, settings, reg_data, isr_kinematics)
        class(dglap_remnant_t), intent(inout) :: dglap
        type(nlo_settings_t), intent(in), target :: settings
        type(region_data_t), intent(in), target :: reg_data
        integer :: n_flv_born
        type(isr_kinematics_t), intent(in), target :: isr_kinematics
        dglap%reg_data => reg_data
        n_flv_born = reg_data%get_n_flv_born ()
        allocate (dglap%sf_factors (reg_data%n_regions, 0:reg_data%n_in))
        dglap%sf_factors = zero

```

```

dglap%settings => settings
allocate (dglap%sqme_born(n_flv_born))
dglap%sqme_born = zero
allocate (dglap%sqme_color_c_extra (reg_data%n_legs_born, &
    reg_data%n_legs_born, reg_data%n_flv_born))
dglap%sqme_color_c_extra = zero
dglap%isr_kinematics => isr_kinematics
end subroutine dglap_remnant_init

```

```

⟨DGLAP remnant: dglap remnant: TBP⟩+≡
  procedure :: set_parameters => dglap_remnant_set_parameters

⟨DGLAP remnant: sub interfaces⟩+≡
  module subroutine dglap_remnant_set_parameters (dglap, CA, CF, TR)
    class(dglap_remnant_t), intent(inout) :: dglap
    real(default), intent(in) :: CA, CF, TR
  end subroutine dglap_remnant_set_parameters

⟨DGLAP remnant: procedures⟩+≡
  module subroutine dglap_remnant_set_parameters (dglap, CA, CF, TR)
    class(dglap_remnant_t), intent(inout) :: dglap
    real(default), intent(in) :: CA, CF, TR
    dglap%CA = CA
    dglap%CF = CF
    dglap%TR = TR
  end subroutine dglap_remnant_set_parameters

```

Evaluates formula 27.58. Note that, as also in the case for the real subtraction, we have to take into account an additional term, occuring because the integral the plus distribution is evaluated over is not constrained on the interval $[0, 1]$. Explicitly, this means (see JHEP 06(2010)043, (4.11)-(4.12))

$$\int_{\bar{x}_{\oplus}}^1 dz \left(\frac{1}{1-z} \right)_{\xi_{\text{cut}}} = \log \frac{1-\bar{x}_{\oplus}}{\xi_{\text{cut}}} f(1) + \int_{\bar{x}_{\oplus}}^1 \frac{f(z) - f(1)}{1-z}, \quad (27.59)$$

$$\int_{\bar{x}_{\oplus}}^1 dz \left(\frac{\log(1-z)}{1-z} \right)_{\xi_{\text{cut}}} f(z) = \frac{1}{2} (\log^2(1-\bar{x}_{\oplus}) - \log^2(\xi_{\text{cut}})) f(1) + \int_{\bar{x}_{\oplus}}^1 \frac{\log(1-z)[f(z) - f(1)]}{1-z}, \quad (27.60)$$

and the same of course for \bar{x}_{\ominus} . These two terms are stored in the `plus_dist_remnant` variable below.

The option `separate_uborns` allows to compute the contribution of the DGLAP remnant separately for each underlying Born flavor structure. We need this option during event generation to generate counter events with a specific Born flavor structure.

```

⟨DGLAP remnant: dglap remnant: TBP⟩+≡
  procedure :: evaluate => dglap_remnant_evaluate

⟨DGLAP remnant: sub interfaces⟩+≡
  module subroutine dglap_remnant_evaluate &
    (dglap, alpha_coupling, separate_uborns, sqme_dglap)
    class(dglap_remnant_t), intent(inout) :: dglap
    real(default), dimension(2), intent(in) :: alpha_coupling
    logical, intent(in) :: separate_uborns

```

```

        real(default), intent(inout), dimension(:) :: sqme_dglap
    end subroutine dglap_remnant_evaluate

    (DGLAP remnant: procedures)+≡
    module subroutine dglap_remnant_evaluate &
        (dglap, alpha_coupling, separate_uborns, sqme_dglap)
        class(dglap_remnant_t), intent(inout) :: dglap
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns
        real(default), intent(inout), dimension(:) :: sqme_dglap
        integer :: alr, emitter, i_corr
        real(default) :: sqme_alr
        logical, dimension(:,:,:), allocatable :: evaluated
        real(default) :: sb, fac_scale2
        sb = dglap%isr_kinematics%sqrts_born**2
        fac_scale2 = dglap%isr_kinematics%fac_scale**2
        allocate (evaluated(dglap%reg_data%get_n_flv_born (), &
            dglap%reg_data%get_n_flv_real (), dglap%reg_data%n_in))
        evaluated = .false.
        do alr = 1, dglap%reg_data%n_regions
            i_corr = 0
            if (dglap%reg_data%regions(alr)%nlo_correction_type == "QCD") then
                i_corr = 1
            else if (dglap%reg_data%regions(alr)%nlo_correction_type == "EW") then
                i_corr = 2
            end if
            if (allocated (dglap%settings%selected_alr)) then
                if (.not. any (dglap%settings%selected_alr == alr)) cycle
            end if
            sqme_alr = zero
            emitter = dglap%reg_data%regions(alr)%emitter
            if (emitter > dglap%reg_data%n_in .or. i_corr == 0) cycle
            associate (i_flv_born => dglap%reg_data%regions(alr)%uborn_index, &
                i_flv_real => dglap%reg_data%regions(alr)%real_index)
                if (emitter == 0) then
                    do emitter = 1, 2
                        if (evaluated(i_flv_born, i_flv_real, emitter)) cycle
                        call evaluate_alr (alr, emitter, i_flv_born, &
                            i_flv_real, sqme_alr, evaluated)
                    end do
                else if (emitter > 0) then
                    if (evaluated(i_flv_born, i_flv_real, emitter)) cycle
                    call evaluate_alr (alr, emitter, i_flv_born, &
                        i_flv_real, sqme_alr, evaluated)
                end if
            end associate
            if (separate_uborns) then
                sqme_dglap(i_flv_born) = sqme_dglap(i_flv_born) &
                    + alpha_coupling (i_corr)/ twopi * sqme_alr
            else
                sqme_dglap(1) = sqme_dglap(1) &
                    + alpha_coupling (i_corr) / twopi * sqme_alr
            end if
            end associate
        end do
    end module

```

```
contains
⟨DGLAP remnant: dglap remnant evaluate: procedures⟩
end subroutine dglap_remnant_evaluate
```

We introduce $\hat{P}(z, \epsilon) = (1 - z)P(z, \epsilon)$ and have

$$\hat{P}_{g \rightarrow gg}(z) = 2C_A \left[z + \frac{(1 - z)^2}{z} + z(1 - z)^2 \right], \quad (27.61)$$

$$\hat{P}_{g \rightarrow qq}(z) = C_F(1 - z) \frac{1 + (1 - z)^2}{z}, \quad (27.62)$$

$$\hat{P}_{q \rightarrow qq}(z) = T_F(1 - z - 2z(1 - z)^2), \quad (27.63)$$

$$\hat{P}_{q \rightarrow qg}(z) = C_F(1 + z^2). \quad (27.64)$$

```
⟨DGLAP remnant: dglap remnant evaluate: procedures⟩≡
function p_hat_gtogg (z)
  real(default) :: p_hat_gtogg
  ⟨p variables⟩
  p_hat_gtogg = two * dglap%CA * (z + onemz**2 / z + z * onemz**2)
end function p_hat_gtogg

function p_hat_gtoqq (z)
  real(default) :: p_hat_gtoqq
  ⟨p variables⟩
  p_hat_gtoqq = dglap%CF * onemz / z * (one + onemz**2)
end function p_hat_gtoqq

function p_hat_qtogq (z)
  real(default) :: p_hat_qtogq
  ⟨p variables⟩
  p_hat_qtogq = dglap%TR * (onemz - two * z * onemz**2)
end function p_hat_qtogq

function p_hat_qtoqg (z)
  real(default) :: p_hat_qtoqg
  real(default), intent(in) :: z
  p_hat_qtoqg = dglap%CF * (one + z**2)
end function p_hat_qtoqg
```

$$\left. \frac{\partial P_{g \rightarrow gg}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = 0, \quad (27.65)$$

$$\left. \frac{\partial P_{g \rightarrow qq}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -C_F z, \quad (27.66)$$

$$\left. \frac{\partial P_{q \rightarrow qq}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -2T_F z(1 - z), \quad (27.67)$$

$$\left. \frac{\partial P_{q \rightarrow qg}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -C_F(1 - z). \quad (27.68)$$

$$(27.69)$$

```
⟨DGLAP remnant: dglap remnant evaluate: procedures⟩+≡
function p_derived_gtogg (z)
```

```

    real(default) :: p_derived_gtogg
    real(default), intent(in) :: z
    p_derived_gtogg = zero
end function p_derived_gtogg

function p_derived_gtoqq (z)
    real(default) :: p_derived_gtoqq
    real(default), intent(in) :: z
    p_derived_gtoqq = -dglap%CF * z
end function p_derived_gtoqq

function p_derived_qtogq (z)
    real(default) :: p_derived_qtogq
    <p variables>
    p_derived_qtogq = -two * dglap%TR * z * onemz
end function p_derived_qtogq

function p_derived_qtoqg (z)
    real(default) :: p_derived_qtoqg
    <p variables>
    p_derived_qtoqg = -dglap%CF * onemz
end function p_derived_qtoqg

```

<DGLAP remnant: dglap remnant evaluate: procedures>+≡

```

subroutine evaluate_alr (alr, emitter, i_flv_born, i_flv_real, sqme_alr, evaluated)
    integer, intent(in) :: alr, emitter, i_flv_born, i_flv_real
    real(default), intent(inout) :: sqme_alr
    logical, intent(inout), dimension(:, :, :) :: evaluated
    real(default) :: z, jac
    real(default) :: factor, factor_soft, plus_dist_remnant
    real(default) :: xb, onemz
    real(default) :: sqme_scaled, sqme_born_dglap
    real(default) :: charge_rad2, charge_em2
    integer :: flv_em, flv_rad, N_col, i
    N_col = 1
    sqme_born_dglap = zero
    associate (template => dglap%settings%fks_template)
        z = dglap%isr_kinematics%z(emitter)
        flv_rad = dglap%reg_data%regions(alr)%flst_real%flst(dglap%reg_data%n_legs_real)
        flv_em = dglap%reg_data%regions(alr)%flst_real%flst(emitter)
        charge_rad2 = dglap%reg_data%regions(alr)%flst_real%charge(dglap%reg_data%n_legs_real)**2
        charge_em2 = dglap%reg_data%regions(alr)%flst_real%charge(emitter)**2
        if (dglap%reg_data%regions(alr)%nlo_correction_type == "QCD") then
            call dglap%set_parameters (CA = CA, CF = CF, TR = TR)
        else if (dglap%reg_data%regions(alr)%nlo_correction_type == "EW") then
            if (is_quark(flvrad)) N_col = NC
            call dglap%set_parameters (CA = zero, CF = charge_em2, TR = N_col*charge_rad2)
        end if
        jac = dglap%isr_kinematics%jacobian(emitter)
        onemz = one - z
        factor = log (sb * template%delta_i / two / z / fac_scale2) / &
            onemz + two * log (onemz) / onemz
        factor_soft = log (sb * template%delta_i / two / fac_scale2) / &
            onemz + two * log (onemz) / onemz
    end associate

```



```

        xb = dglap%isr_kinematics%x(emitter)
        plus_dist_remnant = log ((one - xb) / template%xi_cut) * log (sb * template%delta_i / &
            two / fac_scale2) + (log (one - xb)**2 - log (template%xi_cut)**2)
    end associate
    if (dglap%reg_data%nlo_correction_type == "EW" .and. &
        dglap%reg_data%regions(alr)%nlo_correction_type == "QCD" .and. &
        qcd_ew_interferences (dglap%reg_data%regions(alr)%flst_uborn%flst)) then
        do i = 1, size (dglap%reg_data%regions(alr)%flst_uborn%flst)
            if (is_quark (dglap%reg_data%regions(alr)%flst_uborn%flst (i))) then
                sqme_born_dglap = -dglap%sqme_color_c_extra (i, i, i_flv_born)/CF
                exit
            end if
        end do
    else
        sqme_born_dglap = dglap%sqme_born(i_flv_born)
    end if
    sqme_scaled = sqme_born_dglap * dglap%sf_factors(alr, emitter)
    if (is_massless_vector (flv_em) .and. is_massless_vector (flv_rad)) then
        sqme_alr = sqme_alr + p_hat_gtogg(z) * factor / z * sqme_scaled * jac &
            - p_hat_gtogg(one) * factor_soft * sqme_born_dglap * jac &
            + p_hat_gtogg(one) * plus_dist_remnant * sqme_born_dglap
    else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
        sqme_alr = sqme_alr + p_hat_qtoqg(z) * factor / z * sqme_scaled * jac &
            - p_derived_qtoqg(z) / z * sqme_scaled * jac &
            - p_hat_qtoqg(one) * factor_soft * sqme_born_dglap * jac &
            + p_hat_qtoqg(one) * plus_dist_remnant * sqme_born_dglap
    else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
        sqme_alr = sqme_alr + (p_hat_gtoqq(z) * factor - p_derived_gtoqq(z)) / z * jac * &
            sqme_scaled
    else if (is_massless_vector (flv_em) .and. is_fermion (flv_rad)) then
        sqme_alr = sqme_alr + (p_hat_qtogq(z) * factor - p_derived_qtogq(z)) / z * sqme_scaled * jac
    else
        sqme_alr = sqme_alr + zero
    end if
    evaluated(i_flv_born, i_flv_real, emitter) = .true.
end subroutine evaluate_alr

<p variables>≡
    real(default), intent(in) :: z
    real(default) :: onemz
    onemz = one - z

<DGLAP remnant: dglap remnant: TBP>+≡
    procedure :: final => dglap_remnant_final

<DGLAP remnant: sub interfaces>+≡
    module subroutine dglap_remnant_final (dglap)
        class(dglap_remnant_t), intent(inout) :: dglap
    end subroutine dglap_remnant_final

<DGLAP remnant: procedures>+≡
    module subroutine dglap_remnant_final (dglap)
        class(dglap_remnant_t), intent(inout) :: dglap
        if (associated (dglap%isr_kinematics)) nullify (dglap%isr_kinematics)
        if (associated (dglap%reg_data)) nullify (dglap%reg_data)

```

```

    if (associated (dglap%settings)) nullify (dglap%settings)
    if (allocated (dglap%sqme_born)) deallocate (dglap%sqme_born)
    if (allocated (dglap%sf_factors)) deallocate (dglap%sf_factors)
end subroutine dglap_remnant_final

```

27.8 Dispatch

```

(dispatch_fks.f90)≡
  <File header>

  module dispatch_fks

    <Use kinds>
    <Use strings>
    use variables, only: var_list_t
    use nlo_data, only: fks_template_t, FKS_DEFAULT, FKS_RESONANCES

    <Standard module head>

    <Dispatch fks: public>

    interface
    <Dispatch fks: sub interfaces>
    end interface

  end module dispatch_fks

(dispatch_fks_sub.f90)≡
  <File header>

  submodule (dispatch_fks) dispatch_fks_s

    use string_utils, only: split_string

    implicit none

  contains

    <Dispatch fks: procedures>

  end submodule dispatch_fks_s

```

Initialize parameters used to optimize FKS calculations.

```

<Dispatch fks: public>≡
  public :: dispatch_fks_setup

<Dispatch fks: sub interfaces>≡
  module subroutine dispatch_fks_setup (fks_template, var_list)
    type(fks_template_t), intent(inout) :: fks_template
    type(var_list_t), intent(in) :: var_list
  end subroutine dispatch_fks_setup

```

```

<Dispatch fks: procedures>≡
module subroutine dispatch_fks_setup (fks_template, var_list)
  type(fks_template_t), intent(inout) :: fks_template
  type(var_list_t), intent(in) :: var_list
  real(default) :: fks_dij_exp1, fks_dij_exp2
  type(string_t) :: fks_mapping_type
  logical :: subtraction_disabled
  type(string_t) :: exclude_from_resonance
  fks_dij_exp1 = &
    var_list%get_rval (var_str ("fks_dij_exp1"))
  fks_dij_exp2 = &
    var_list%get_rval (var_str ("fks_dij_exp2"))
  fks_mapping_type = &
    var_list%get_sval (var_str ("fks_mapping_type"))
  subtraction_disabled = &
    var_list%get_lval (var_str ("?disable_subtraction"))
  exclude_from_resonance = &
    var_list%get_sval (var_str ("fks_resonances_exclude_particles"))
  if (exclude_from_resonance /= var_str ("default")) &
    call split_string (exclude_from_resonance, var_str (":"), &
      fks_template%excluded_resonances)
  call fks_template%set_parameters ( &
    exp1 = fks_dij_exp1, exp2 = fks_dij_exp2, &
    xi_min = var_list%get_rval (var_str ("fks_xi_min")), &
    y_max = var_list%get_rval (var_str ("fks_y_max")), &
    xi_cut = var_list%get_rval (var_str ("fks_xi_cut")), &
    delta_o = var_list%get_rval (var_str ("fks_delta_o")), &
    delta_i = var_list%get_rval (var_str ("fks_delta_i")))
  select case (char (fks_mapping_type))
  case ("default")
    call fks_template%set_mapping_type (FKS_DEFAULT)
  case ("resonances")
    call fks_template%set_mapping_type (FKS_RESONANCES)
  end select
  fks_template%subtraction_disabled = subtraction_disabled
  fks_template%n_f = var_list%get_ival (var_str ("alphas_nf"))
end subroutine dispatch_fks_setup

```

Chapter 28

Model Handling and Features

These modules deal with process definitions and physics models.

These modules use the `model_data` methods to automatically generate process definitions.

auto_components Generic process-definition generator. We can specify a basic process or initial particle(s) and some rules to extend this process, given a model definition with particle names and vertex structures.

radiation_generator Applies the generic generator to the specific problem of generating NLO corrections in a restricted setup.

Model construction:

eval_trees Implementation of the generic `expr_t` type for the concrete evaluation of expressions that access user variables.

This module is actually part of the Sindarin language implementation, and should be moved elsewhere. Currently, the `models` module relies on it.

models Extends the `model_data_t` structure by user-variable objects for easy access, and provides the means to read a model definition from file.

slha_interface Read/write a SUSY model in the standardized SLHA format. The format defines fields and parameters, but no vertices.

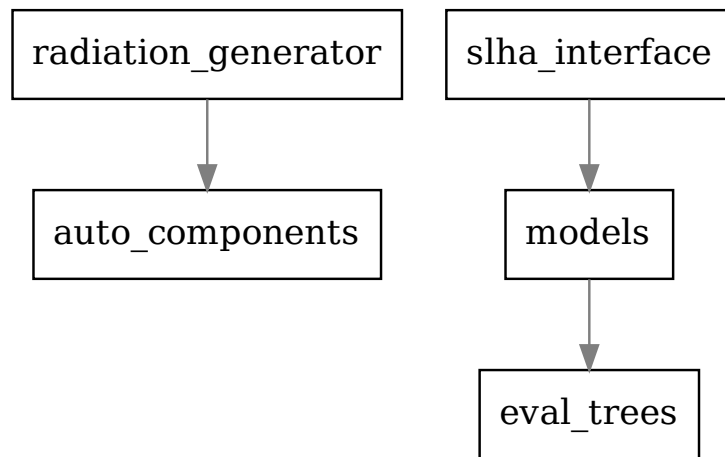


Figure 28.1: Module dependencies in `src/model_features`.

28.1 Automatic generation of process components

This module provides the functionality for automatically generating radiation corrections or decays, provided as lists of PDG codes.

```
<auto_components.f90>≡  
  <File header>  
  
  module auto_components  
  
    <Use kinds>  
    <Use strings>  
    use model_data  
    use pdg_arrays  
  
    <Standard module head>  
  
    <Auto components: public>  
  
    <Auto components: types>  
  
    <Auto components: interfaces>  
  
    interface  
    <Auto components: sub interfaces>  
    end interface  
  
    contains  
  
    <Auto components: main procedures>  
  
  end module auto_components  
<auto_components_sub.f90>≡  
  <File header>  
  
  submodule (auto_components) auto_components_s  
  
    use io_units  
    use diagnostics  
    use physics_defs, only: PHOTON, GLUON, Z_BOSON, W_BOSON  
    use numeric_utils, only: extend_integer_array  
  
    implicit none  
  
    <Auto components: parameters>  
  
    contains  
  
    <Auto components: procedures>  
  
  end submodule auto_components_s
```

28.1.1 Constraints: Abstract types

An abstract type that denotes a constraint on the automatically generated states. The concrete objects are applied as visitor objects at certain hooks during the splitting algorithm.

```
<Auto components: types>≡
    type, abstract :: split_constraint_t
    contains
    <Auto components: split constraint: TBP>
end type split_constraint_t
```

By default, all checks return true.

```
<Auto components: split constraint: TBP>≡
    procedure :: check_before_split => split_constraint_check_before_split
    procedure :: check_before_insert => split_constraint_check_before_insert
    procedure :: check_before_record => split_constraint_check_before_record

<Auto components: sub interfaces>≡
    module subroutine split_constraint_check_before_split (c, table, pl, k, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: k
        logical, intent(out) :: passed
    end subroutine split_constraint_check_before_split
    module subroutine split_constraint_check_before_insert (c, table, pa, pl, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_array_t), intent(in) :: pa
        type(pdg_list_t), intent(inout) :: pl
        logical, intent(out) :: passed
    end subroutine split_constraint_check_before_insert
    module subroutine split_constraint_check_before_record (c, table, pl, n_loop, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
    end subroutine split_constraint_check_before_record

<Auto components: procedures>≡
    module subroutine split_constraint_check_before_split (c, table, pl, k, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: k
        logical, intent(out) :: passed
        passed = .true.
    end subroutine split_constraint_check_before_split

    module subroutine split_constraint_check_before_insert (c, table, pa, pl, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_array_t), intent(in) :: pa
        type(pdg_list_t), intent(inout) :: pl
```

```

        logical, intent(out) :: passed
        passed = .true.
    end subroutine split_constraint_check_before_insert

    module subroutine split_constraint_check_before_record (c, table, pl, n_loop, passed)
        class(split_constraint_t), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
        passed = .true.
    end subroutine split_constraint_check_before_record

```

A transparent wrapper, so we can collect constraints of different type.

```

<Auto components: types>+≡
    type :: split_constraint_wrap_t
        class(split_constraint_t), allocatable :: c
    end type split_constraint_wrap_t

```

A collection of constraints.

```

<Auto components: public>≡
    public :: split_constraints_t

<Auto components: types>+≡
    type :: split_constraints_t
        class(split_constraint_wrap_t), dimension(:), allocatable :: cc
        contains
        <Auto components: split constraints: TBP>
    end type split_constraints_t

```

Gfortran 7/8/9 bug: has to remain in the main module. Initialize the constraints set with a specific number of elements.

```

<Auto components: split constraints: TBP>≡
    procedure :: init => split_constraints_init

<Auto components: main procedures>≡
    subroutine split_constraints_init (constraints, n)
        class(split_constraints_t), intent(out) :: constraints
        integer, intent(in) :: n
        allocate (constraints%cc (n))
    end subroutine split_constraints_init

```

Set a constraint.

```

<Auto components: split constraints: TBP>+≡
    procedure :: set => split_constraints_set

<Auto components: sub interfaces>+≡
    module subroutine split_constraints_set (constraints, i, c)
        class(split_constraints_t), intent(inout) :: constraints
        integer, intent(in) :: i
        class(split_constraint_t), intent(in) :: c
    end subroutine split_constraints_set

```



```

<Auto components: procedures>+≡
module subroutine split_constraints_set (constraints, i, c)
  class(split_constraints_t), intent(inout) :: constraints
  integer, intent(in) :: i
  class(split_constraint_t), intent(in) :: c
  allocate (constraints%cc(i)%c, source = c)
end subroutine split_constraints_set

```

Apply checks.

`check_before_split` is applied to the particle list that we want to split.

`check_before_insert` is applied to the particle list `pl` that is to replace the particle `pa` that is split. This check may transform the particle list.

`check_before_record` is applied to the complete new particle list that results from splitting before it is recorded.

```

<Auto components: split constraints: TBP>+≡
procedure :: check_before_split => split_constraints_check_before_split
procedure :: check_before_insert => split_constraints_check_before_insert
procedure :: check_before_record => split_constraints_check_before_record

```

```

<Auto components: sub interfaces>+≡
module subroutine split_constraints_check_before_split &
  (constraints, table, pl, k, passed)
  class(split_constraints_t), intent(in) :: constraints
  class(ps_table_t), intent(in) :: table
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: k
  logical, intent(out) :: passed
end subroutine split_constraints_check_before_split
module subroutine split_constraints_check_before_insert &
  (constraints, table, pa, pl, passed)
  class(split_constraints_t), intent(in) :: constraints
  class(ps_table_t), intent(in) :: table
  type(pdg_array_t), intent(in) :: pa
  type(pdg_list_t), intent(inout) :: pl
  logical, intent(out) :: passed
end subroutine split_constraints_check_before_insert
module subroutine split_constraints_check_before_record &
  (constraints, table, pl, n_loop, passed)
  class(split_constraints_t), intent(in) :: constraints
  class(ps_table_t), intent(in) :: table
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n_loop
  logical, intent(out) :: passed
end subroutine split_constraints_check_before_record

```

```

<Auto components: procedures>+≡
module subroutine split_constraints_check_before_split &
  (constraints, table, pl, k, passed)
  class(split_constraints_t), intent(in) :: constraints
  class(ps_table_t), intent(in) :: table
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: k
  logical, intent(out) :: passed
  integer :: i

```

```

    passed = .true.
    do i = 1, size (constraints%cc)
        call constraints%cc(i)%c%check_before_split (table, pl, k, passed)
        if (.not. passed) return
    end do
end subroutine split_constraints_check_before_split

module subroutine split_constraints_check_before_insert &
    (constraints, table, pa, pl, passed)
    class(split_constraints_t), intent(in) :: constraints
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    integer :: i
    passed = .true.
    do i = 1, size (constraints%cc)
        call constraints%cc(i)%c%check_before_insert (table, pa, pl, passed)
        if (.not. passed) return
    end do
end subroutine split_constraints_check_before_insert

module subroutine split_constraints_check_before_record &
    (constraints, table, pl, n_loop, passed)
    class(split_constraints_t), intent(in) :: constraints
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    integer :: i
    passed = .true.
    do i = 1, size (constraints%cc)
        call constraints%cc(i)%c%check_before_record (table, pl, n_loop, passed)
        if (.not. passed) return
    end do
end subroutine split_constraints_check_before_record

```

28.1.2 Specific constraints

Number of particles

Specific constraint: The number of particles plus the number of loops, if any, must remain less than the given limit. Note that the number of loops is defined only when we are recording the entry.

(Auto components: types)+≡

```

type, extends (split_constraint_t) :: constraint_n_tot
private
integer :: n_max = 0
contains
    procedure :: check_before_split => constraint_n_tot_check_before_split
    procedure :: check_before_record => constraint_n_tot_check_before_record
end type constraint_n_tot

```

```

<Auto components: public>+≡
    public :: constrain_n_tot

<Auto components: sub interfaces>+≡
    module function constrain_n_tot (n_max) result (c)
        integer, intent(in) :: n_max
        type(constraint_n_tot) :: c
    end function constrain_n_tot

    module subroutine constraint_n_tot_check_before_split (c, table, pl, k, passed)
        class(constraint_n_tot), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: k
        logical, intent(out) :: passed
    end subroutine constraint_n_tot_check_before_split

    module subroutine constraint_n_tot_check_before_record (c, table, pl, n_loop, passed)
        class(constraint_n_tot), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
    end subroutine constraint_n_tot_check_before_record

<Auto components: procedures>+≡
    module function constrain_n_tot (n_max) result (c)
        integer, intent(in) :: n_max
        type(constraint_n_tot) :: c
        c%n_max = n_max
    end function constrain_n_tot

    module subroutine constraint_n_tot_check_before_split (c, table, pl, k, passed)
        class(constraint_n_tot), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: k
        logical, intent(out) :: passed
        passed = pl%get_size () < c%n_max
    end subroutine constraint_n_tot_check_before_split

    module subroutine constraint_n_tot_check_before_record (c, table, pl, n_loop, passed)
        class(constraint_n_tot), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
        passed = pl%get_size () + n_loop <= c%n_max
    end subroutine constraint_n_tot_check_before_record

```

Number of loops

Specific constraint: The number of loops is limited, independent of the total number of particles.

```

<Auto components: types>+≡

```

```

type, extends (split_constraint_t) :: constraint_n_loop
  private
    integer :: n_loop_max = 0
  contains
    procedure :: check_before_record => constraint_n_loop_check_before_record
end type constraint_n_loop

<Auto components: public>+≡
  public :: constrain_n_loop

<Auto components: sub interfaces>+≡
  module function constrain_n_loop (n_loop_max) result (c)
    integer, intent(in) :: n_loop_max
    type(constraint_n_loop) :: c
  end function constrain_n_loop
  module subroutine constraint_n_loop_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_n_loop), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
  end subroutine constraint_n_loop_check_before_record

<Auto components: procedures>+≡
  module function constrain_n_loop (n_loop_max) result (c)
    integer, intent(in) :: n_loop_max
    type(constraint_n_loop) :: c
    c%n_loop_max = n_loop_max
  end function constrain_n_loop

  module subroutine constraint_n_loop_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_n_loop), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    passed = n_loop <= c%n_loop_max
  end subroutine constraint_n_loop_check_before_record

```

Particles allowed in splitting

Specific constraint: The entries in the particle list ready for insertion are matched to a given list of particle patterns. If a match occurs, the entry is replaced by the corresponding pattern. If there is no match, the check fails. If a massless gauge boson splitting is detected, the splitting partners are checked against a list of excluded particles. If a match occurs, the check fails.

```

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_splittings
  private
    type(pdg_list_t) :: pl_match, pl_excluded_gauge_splittings
  contains

```

```

        procedure :: check_before_insert => constraintSplittings_check_before_insert
    end type constraintSplittings

    <Auto components: public>+≡
        public :: constrainSplittings

    <Auto components: sub interfaces>+≡
        module function constrainSplittings &
            (pl_match, pl_excluded_gaugeSplittings) result (c)
            type(pdg_list_t), intent(in) :: pl_match
            type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
            type(constraintSplittings) :: c
        end function constrainSplittings

        module subroutine constraintSplittings_check_before_insert &
            (c, table, pa, pl, passed)
            class(constraintSplittings), intent(in) :: c
            class(ps_table_t), intent(in) :: table
            type(pdg_array_t), intent(in) :: pa
            type(pdg_list_t), intent(inout) :: pl
            logical, intent(out) :: passed
        end subroutine constraintSplittings_check_before_insert

    <Auto components: procedures>+≡
        module function constrainSplittings &
            (pl_match, pl_excluded_gaugeSplittings) result (c)
            type(pdg_list_t), intent(in) :: pl_match
            type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
            type(constraintSplittings) :: c
            c%pl_match = pl_match
            c%pl_excluded_gaugeSplittings = pl_excluded_gaugeSplittings
        end function constrainSplittings

        module subroutine constraintSplittings_check_before_insert &
            (c, table, pa, pl, passed)
            class(constraintSplittings), intent(in) :: c
            class(ps_table_t), intent(in) :: table
            type(pdg_array_t), intent(in) :: pa
            type(pdg_list_t), intent(inout) :: pl
            logical, intent(out) :: passed
            logical :: has_massless_vector
            integer :: i
            has_massless_vector = .false.
            do i = 1, pa%get_length ()
                if (is_massless_vector(pa%get(i))) then
                    has_massless_vector = .true.
                    exit
                end if
            end do
            passed = .false.
            if (has_massless_vector .and. count (is_fermion(pl%a%get ())) == 2) then
                do i = 1, c%pl_excluded_gaugeSplittings%get_size ()
                    if (pl .match. c%pl_excluded_gaugeSplittings%a(i)) return
                end do
                call pl%match_replace (c%pl_match, passed)
                passed = .true.
            end if
        end subroutine constraintSplittings_check_before_insert

```

```

else
  call pl%match_replace (c%pl_match, passed)
end if
end subroutine constraint_splittings_check_before_insert

```

Specific constraint: The entries in the particle list ready for insertion are matched to a given list of particle patterns. If a match occurs, the entry is replaced by the corresponding pattern. If there is no match, the check fails.

```

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_insert
  private
  type(pdg_list_t) :: pl_match
  contains
  procedure :: check_before_insert => constraint_insert_check_before_insert
end type constraint_insert

<Auto components: public>+≡
  public :: constrain_insert

<Auto components: sub interfaces>+≡
  module function constrain_insert (pl_match) result (c)
    type(pdg_list_t), intent(in) :: pl_match
    type(constraint_insert) :: c
  end function constrain_insert
  module subroutine constraint_insert_check_before_insert (c, table, pa, pl, passed)
    class(constraint_insert), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
  end subroutine constraint_insert_check_before_insert

<Auto components: procedures>+≡
  module function constrain_insert (pl_match) result (c)
    type(pdg_list_t), intent(in) :: pl_match
    type(constraint_insert) :: c
    c%pl_match = pl_match
  end function constrain_insert

  module subroutine constraint_insert_check_before_insert (c, table, pa, pl, passed)
    class(constraint_insert), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    call pl%match_replace (c%pl_match, passed)
  end subroutine constraint_insert_check_before_insert

```

Particles required in final state

Specific constraint: The entries in the recorded state must be a superset of the entries in the given list (for instance, the lowest-order state).

```

<Auto components: types>+≡

```

```

type, extends (split_constraint_t) :: constraint_require
  private
  type(pdg_list_t) :: pl
  contains
    procedure :: check_before_record => constraint_require_check_before_record
  end type constraint_require

```

We check the current state by matching all particle entries against the stored particle list, and crossing out the particles in the latter list when a match is found. The constraint passed if all entries have been crossed out.

For an `if_table` in particular, we check the final state only.

```

<Auto components: public>+≡
  public :: constrain_require

<Auto components: sub interfaces>+≡
  module function constrain_require (pl) result (c)
    type(pdg_list_t), intent(in) :: pl
    type(constraint_require) :: c
  end function constrain_require
  module subroutine constraint_require_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_require), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
  end subroutine constraint_require_check_before_record

<Auto components: procedures>+≡
  module function constrain_require (pl) result (c)
    type(pdg_list_t), intent(in) :: pl
    type(constraint_require) :: c
    c%pl = pl
  end function constrain_require

  module subroutine constraint_require_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_require), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    logical, dimension(:), allocatable :: mask
    integer :: i, k, n_in
    select type (table)
    type is (if_table_t)
      if (table%proc_type > 0) then
        select case (table%proc_type)
        case (PROC_DECAY)
          n_in = 1
        case (PROC_SCATTER)
          n_in = 2
        end select
      else

```

```

        call msg_fatal ("Neither a decay nor a scattering process")
    end if
    class default
        n_in = 0
    end select
    allocate (mask (c%pl%get_size ()), source = .true.)
    do i = n_in + 1, pl%get_size ()
        k = c%pl%find_match (pl%get (i), mask)
        if (k /= 0) mask(k) = .false.
    end do
    passed = .not. any (mask)
end subroutine constraint_require_check_before_record

```

Radiation

Specific constraint: We have radiation pattern if the original particle matches an entry in the list of particles that should replace it. The constraint prohibits this situation.

```

<Auto components: public>+≡
    public :: constrain_radiation

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_radiation
    private
    contains
        procedure :: check_before_insert => &
            constraint_radiation_check_before_insert
    end type constraint_radiation

<Auto components: sub interfaces>+≡
    module function constrain_radiation () result (c)
        type(constraint_radiation) :: c
    end function constrain_radiation
    module subroutine constraint_radiation_check_before_insert &
        (c, table, pa, pl, passed)
        class(constraint_radiation), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_array_t), intent(in) :: pa
        type(pdg_list_t), intent(inout) :: pl
        logical, intent(out) :: passed
    end subroutine constraint_radiation_check_before_insert

<Auto components: procedures>+≡
    module function constrain_radiation () result (c)
        type(constraint_radiation) :: c
    end function constrain_radiation

    module subroutine constraint_radiation_check_before_insert &
        (c, table, pa, pl, passed)
        class(constraint_radiation), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_array_t), intent(in) :: pa
        type(pdg_list_t), intent(inout) :: pl

```



```

    logical, intent(out) :: passed
    passed = .not. (pl .match. pa)
end subroutine constraint_radiation_check_before_insert

```

Mass sum

Specific constraint: The sum of masses within the particle list must be smaller than a given limit. For in/out state combinations, we check initial and final state separately.

If we specify `margin` in the initialization, the sum must be strictly less than the limit minus the given margin (which may be zero). If not, equality is allowed.

```

<Auto components: public>+≡
    public :: constrain_mass_sum

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_mass_sum
    private
    real(default) :: mass_limit = 0
    logical :: strictly_less = .false.
    real(default) :: margin = 0
    contains
    procedure :: check_before_record => constraint_mass_sum_check_before_record
end type constraint_mass_sum

<Auto components: sub interfaces>+≡
    module function constrain_mass_sum (mass_limit, margin) result (c)
    real(default), intent(in) :: mass_limit
    real(default), intent(in), optional :: margin
    type(constraint_mass_sum) :: c
    end function constrain_mass_sum
    module subroutine constraint_mass_sum_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_mass_sum), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    end subroutine constraint_mass_sum_check_before_record

<Auto components: procedures>+≡
    module function constrain_mass_sum (mass_limit, margin) result (c)
    real(default), intent(in) :: mass_limit
    real(default), intent(in), optional :: margin
    type(constraint_mass_sum) :: c
    c%mass_limit = mass_limit
    if (present (margin)) then
        c%strictly_less = .true.
        c%margin = margin
    end if
    end function constrain_mass_sum

    module subroutine constraint_mass_sum_check_before_record &
    (c, table, pl, n_loop, passed)

```

```

class(constraint_mass_sum), intent(in) :: c
class(ps_table_t), intent(in) :: table
type(pdg_list_t), intent(in) :: pl
integer, intent(in) :: n_loop
logical, intent(out) :: passed
real(default) :: limit
if (c%strictly_less) then
  limit = c%mass_limit - c%margin
  select type (table)
  type is (if_table_t)
    passed = mass_sum (pl, 1, 2, table%model) < limit &
      .and. mass_sum (pl, 3, pl%get_size (), table%model) < limit
  class default
    passed = mass_sum (pl, 1, pl%get_size (), table%model) < limit
  end select
else
  limit = c%mass_limit
  select type (table)
  type is (if_table_t)
    passed = mass_sum (pl, 1, 2, table%model) <= limit &
      .and. mass_sum (pl, 3, pl%get_size (), table%model) <= limit
  class default
    passed = mass_sum (pl, 1, pl%get_size (), table%model) <= limit
  end select
end if
end subroutine constraint_mass_sum_check_before_record

```

Initial state particles

Specific constraint: The two incoming particles must both match the given particle list. This is checked for the generated particle list, just before it is recorded.

```

<Auto components: public>+≡
  public :: constrain_in_state

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_in_state
  private
  type(pdg_list_t) :: pl
  contains
  procedure :: check_before_record => constraint_in_state_check_before_record
end type constraint_in_state

<Auto components: sub interfaces>+≡
  module function constrain_in_state (pl) result (c)
    type(pdg_list_t), intent(in) :: pl
    type(constraint_in_state) :: c
  end function constrain_in_state
  module subroutine constraint_in_state_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_in_state), intent(in) :: c
    class(ps_table_t), intent(in) :: table
  end subroutine

```

```

        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
    end subroutine constraint_in_state_check_before_record

    <Auto components: procedures>+≡
    module function constrain_in_state (pl) result (c)
        type(pdg_list_t), intent(in) :: pl
        type(constraint_in_state) :: c
        c%pl = pl
    end function constrain_in_state

    module subroutine constraint_in_state_check_before_record &
        (c, table, pl, n_loop, passed)
        class(constraint_in_state), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
        integer :: i
        select type (table)
        type is (if_table_t)
            passed = .false.
            do i = 1, 2
                if (.not. (c%pl .match. pl%get (i))) return
            end do
        end select
        passed = .true.
    end subroutine constraint_in_state_check_before_record

```

Photon induced processes

If set, filter out photon induced processes.

```

    <Auto components: public>+≡
    public :: constrain_photon_induced_processes

    <Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_photon_induced_processes
    private
    integer :: n_in
    contains
    procedure :: check_before_record => &
        constrain_photon_induced_processes_check_before_record
    end type constraint_photon_induced_processes

    <Auto components: sub interfaces>+≡
    module function constrain_photon_induced_processes (n_in) result (c)
        integer, intent(in) :: n_in
        type(constraint_photon_induced_processes) :: c
    end function constrain_photon_induced_processes

    module subroutine constraint_photon_induced_processes_check_before_record &
        (c, table, pl, n_loop, passed)
        class(constraint_photon_induced_processes), intent(in) :: c

```

```

        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
    end subroutine constraint_photon_induced_processes_check_before_record
<Auto components: procedures>+≡
    module function constrain_photon_induced_processes (n_in) result (c)
        integer, intent(in) :: n_in
        type(constraint_photon_induced_processes) :: c
        c%n_in = n_in
    end function constrain_photon_induced_processes

    module subroutine constraint_photon_induced_processes_check_before_record &
        (c, table, pl, n_loop, passed)
        class(constraint_photon_induced_processes), intent(in) :: c
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop
        logical, intent(out) :: passed
        integer :: i
        select type (table)
        type is (if_table_t)
            passed = .false.
            do i = 1, c%n_in
                if (pl%a(i)%get () == 22) return
            end do
        end select
        passed = .true.
    end subroutine constraint_photon_induced_processes_check_before_record

```

Coupling constraint

Filters vertices which do not match the desired NLO pattern.

```

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_coupling_t
    private
        logical :: qed = .false.
        logical :: qcd = .true.
        logical :: ew = .false.
        integer :: n_nlo_correction_types
    contains
    <Auto components: constraint coupling: TBP>
    end type constraint_coupling_t

<Auto components: public>+≡
    public :: constrain_couplings

<Auto components: sub interfaces>+≡
    module function constrain_couplings (qcd, qed, n_nlo_correction_types) result (c)
        type(constraint_coupling_t) :: c
        logical, intent(in) :: qcd, qed
        integer, intent(in) :: n_nlo_correction_types
    end function constrain_couplings

```

```

<Auto components: procedures>+≡
  module function constrain_couplings (qcd, qed, n_nlo_correction_types) result (c)
    type(constraint_coupling_t) :: c
    logical, intent(in) :: qcd, qed
    integer, intent(in) :: n_nlo_correction_types
    c%qcd = qcd; c%qed = qed
    c%n_nlo_correction_types = n_nlo_correction_types
  end function constrain_couplings

<Auto components: constraint coupling: TBP>≡
  procedure :: check_before_insert => constraint_coupling_check_before_insert

<Auto components: sub interfaces>+≡
  module subroutine constraint_coupling_check_before_insert (c, table, pa, pl, passed)
    class(constraint_coupling_t), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
  end subroutine constraint_coupling_check_before_insert

<Auto components: procedures>+≡
  module subroutine constraint_coupling_check_before_insert (c, table, pa, pl, passed)
    class(constraint_coupling_t), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    type(pdg_list_t) :: pl_vertex
    type(pdg_array_t) :: pdg_gluon, pdg_photon, pdg_W_Z, pdg_gauge_bosons
    integer :: i, j
    pdg_gluon = GLUON; pdg_photon = PHOTON
    pdg_W_Z = [W_BOSON, -W_BOSON, Z_BOSON]
    if (c%qcd) pdg_gauge_bosons = pdg_gauge_bosons // pdg_gluon
    if (c%qed) pdg_gauge_bosons = pdg_gauge_bosons // pdg_photon
    if (c%ew) pdg_gauge_bosons = pdg_gauge_bosons // pdg_W_Z
    do j = 1, pa%get_length ()
      call pl_vertex%init (pl%get_size () + 1)
      call pl_vertex%set (1, pa%get(j))
      do i = 1, pl%get_size ()
        call pl_vertex%set (i + 1, pl%get(i))
      end do
      if (pl_vertex%get_size () > 3) then
        passed = .false.
        cycle
      end if
      if (is_massless_vector(pa%get(j))) then
        if (.not. table%model%check_vertex &
          (pl_vertex%a(1)%get (), pl_vertex%a(2)%get (), pl_vertex%a(3)%get ())) then
          passed = .false.
          cycle
        end if
      end if
      if (.not. table%model%check_vertex &
        (- pl_vertex%a(1)%get (), pl_vertex%a(2)%get (), pl_vertex%a(3)%get ())) then
        passed = .false.
      end if
    end do
  end subroutine

```

```

        cycle
    end if
    if (.not. (pl_vertex .match. pdg_gauge_bosons)) then
        passed = .false.
        cycle
    end if
    passed = .true.
    exit
end do
end subroutine constraint_coupling_check_before_insert

```

28.1.3 Tables of states

Automatically generate a list of possible process components for a given initial set (a single massive particle or a preset list of states).

The set of process components are generated by recursive splitting, applying constraints on the fly that control and limit the process. The generated states are accumulated in a table that we can read out after completion.

```

⟨Auto components: types⟩+≡
    type, extends (pdg_list_t) :: ps_entry_t
        integer :: n_loop = 0
        integer :: n_rad = 0
        type(ps_entry_t), pointer :: previous => null ()
        type(ps_entry_t), pointer :: next => null ()
    end type ps_entry_t

```

```

⟨Auto components: parameters⟩≡
    integer, parameter :: PROC_UNDEFINED = 0
    integer, parameter :: PROC_DECAY = 1
    integer, parameter :: PROC_SCATTER = 2

```

This is the wrapper type for the decay tree for the list of final states and the final array. First, an abstract base type:

```

⟨Auto components: public⟩+≡
    public :: ps_table_t

⟨Auto components: types⟩+≡
    type, abstract :: ps_table_t
        private
        class(model_data_t), pointer :: model => null ()
        logical :: loops = .false.
        type(ps_entry_t), pointer :: first => null ()
        type(ps_entry_t), pointer :: last => null ()
        integer :: proc_type
    contains
        ⟨Auto components: ps table: TBP⟩
    end type ps_table_t

```

The extensions: one for decay, one for generic final states. The decay-state table stores the initial particle. The final-state table is indifferent, and the initial/final state table treats the first two particles in its list as incoming antiparticles.

```

<Auto components: public>+≡
  public :: ds_table_t
  public :: fs_table_t
  public :: if_table_t

<Auto components: types>+≡
  type, extends (ps_table_t) :: ds_table_t
    private
      integer :: pdg_in = 0
    contains
      <Auto components: ds table: TBP>
  end type ds_table_t

  type, extends (ps_table_t) :: fs_table_t
    contains
      <Auto components: fs table: TBP>
  end type fs_table_t

  type, extends (fs_table_t) :: if_table_t
    contains
      <Auto components: if table: TBP>
  end type if_table_t

```

Finalizer: we must deallocate the embedded list.

```

<Auto components: ps table: TBP>≡
  procedure :: final => ps_table_final

<Auto components: sub interfaces>+≡
  module subroutine ps_table_final (object)
    class(ps_table_t), intent(inout) :: object
  end subroutine ps_table_final

<Auto components: procedures>+≡
  module subroutine ps_table_final (object)
    class(ps_table_t), intent(inout) :: object
    type(ps_entry_t), pointer :: current
    do while (associated (object%first))
      current => object%first
      object%first => current%next
      deallocate (current)
    end do
    nullify (object%last)
  end subroutine ps_table_final

```

Write the table. A base writer for the body and specific writers for the headers.

```

<Auto components: ps table: TBP>+≡
  procedure :: base_write => ps_table_base_write
  procedure (ps_table_write), deferred :: write

<Auto components: interfaces>≡
  interface

```

```

subroutine ps_table_write (object, unit)
  import
  class(ps_table_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine ps_table_write
end interface

<Auto components: ds table: TBP>≡
  procedure :: write => ds_table_write

<Auto components: fs table: TBP>≡
  procedure :: write => fs_table_write

<Auto components: if table: TBP>≡
  procedure :: write => if_table_write

```

The first `n_in` particles will be replaced by antiparticles in the output, and we write an arrow if `n_in` is present.

```

<Auto components: sub interfaces>+≡
  module subroutine ps_table_base_write (object, unit, n_in)
    class(ps_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: n_in
  end subroutine ps_table_base_write
  module subroutine ds_table_write (object, unit)
    class(ds_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine ds_table_write
  module subroutine fs_table_write (object, unit)
    class(fs_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine fs_table_write
  module subroutine if_table_write (object, unit)
    class(if_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine if_table_write

<Auto components: procedures>+≡
  module subroutine ps_table_base_write (object, unit, n_in)
    class(ps_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: n_in
    integer, dimension(:), allocatable :: pdg
    type(ps_entry_t), pointer :: entry
    type(field_data_t), pointer :: prt
    integer :: u, i, j, n0
    u = given_output_unit (unit)
    entry => object%first
    do while (associated (entry))
      write (u, "(2x)", advance = "no")
      if (present (n_in)) then
        do i = 1, n_in
          write (u, "(1x)", advance = "no")
          pdg = entry%get (i)
          do j = 1, size (pdg)
            prt => object%model%get_field_ptr (pdg(j))
            if (j > 1) write (u, "(::)", advance = "no")

```



```

        write (u, "(A)", advance = "no") &
        char (prt%get_name (pdg(j) >= 0))
    end do
end do
write (u, "(1x,A)", advance = "no")  "=>"
n0 = n_in + 1
else
    n0 = 1
end if
do i = n0, entry%get_size ()
    write (u, "(1x)", advance = "no")
    pdg = entry%get (i)
    do j = 1, size (pdg)
        prt => object%model%get_field_ptr (pdg(j))
        if (j > 1) write (u, "(:')", advance = "no")
        write (u, "(A)", advance = "no") &
        char (prt%get_name (pdg(j) < 0))
    end do
end do
if (object%loops) then
    write (u, "(2x,['',I0,',',',I0,']')") entry%n_loop, entry%n_rad
else
    write (u, "(A)")
end if
entry => entry%next
end do
end subroutine ps_table_base_write

module subroutine ds_table_write (object, unit)
    class(ds_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: prt
    integer :: u
    u = given_output_unit (unit)
    prt => object%model%get_field_ptr (object%pdg_in)
    write (u, "(1x,A,1x,A)") "Decays for particle:", &
    char (prt%get_name (object%pdg_in < 0))
    call object%base_write (u)
end subroutine ds_table_write

module subroutine fs_table_write (object, unit)
    class(fs_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Table of final states:"
    call object%base_write (u)
end subroutine fs_table_write

module subroutine if_table_write (object, unit)
    class(if_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)

```

```

write (u, "(1x,A)") "Table of in/out states:"
select case (object%proc_type)
case (PROC_DECAY)
    call object%base_write (u, n_in = 1)
case (PROC_SCATTER)
    call object%base_write (u, n_in = 2)
end select
end subroutine if_table_write

```

Obtain a particle string for a given index in the pdg list

(Auto components: ps_table: TBP)+≡

```

procedure :: get_particle_string => ps_table_get_particle_string

```

(Auto components: sub interfaces)+≡

```

module subroutine ps_table_get_particle_string (object, index, prt_in, prt_out)
    class(ps_table_t), intent(in) :: object
    integer, intent(in) :: index
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
end subroutine ps_table_get_particle_string

```

(Auto components: procedures)+≡

```

module subroutine ps_table_get_particle_string (object, index, prt_in, prt_out)
    class(ps_table_t), intent(in) :: object
    integer, intent(in) :: index
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
    integer :: n_in
    type(field_data_t), pointer :: prt
    type(ps_entry_t), pointer :: entry
    integer, dimension(:), allocatable :: pdg
    integer :: n0
    integer :: i, j
    entry => object%first
    i = 1
    do while (i < index)
        if (associated (entry%next)) then
            entry => entry%next
            i = i + 1
        else
            call msg_fatal ("ps_table: entry with requested index does not exist!")
        end if
    end do

    if (object%proc_type > 0) then
        select case (object%proc_type)
        case (PROC_DECAY)
            n_in = 1
        case (PROC_SCATTER)
            n_in = 2
        end select
    else
        call msg_fatal ("Neither decay nor scattering process")
    end if

    n0 = n_in + 1
    allocate (prt_in (n_in), prt_out (entry%get_size () - n_in))

```

```

do i = 1, n_in
  prt_in(i) = ""
  pdg = entry%get(i)
  do j = 1, size (pdg)
    prt => object%model%get_field_ptr (pdg(j))
    prt_in(i) = prt_in(i) // prt%get_name (pdg(j) >= 0)
    if (j /= size (pdg)) prt_in(i) = prt_in(i) // ":"
  end do
end do
do i = n0, entry%get_size ()
  prt_out(i-n_in) = ""
  pdg = entry%get(i)
  do j = 1, size (pdg)
    prt => object%model%get_field_ptr (pdg(j))
    prt_out(i-n_in) = prt_out(i-n_in) // prt%get_name (pdg(j) < 0)
    if (j /= size (pdg)) prt_out(i-n_in) = prt_out(i-n_in) // ":"
  end do
end do
end subroutine ps_table_get_particle_string

```

Initialize with a predefined set of final states, or in/out state lists.

```

<Auto components: ps table: TBP>+≡
  generic :: init => ps_table_init
  procedure, private :: ps_table_init

<Auto components: if table: TBP>+≡
  generic :: init => if_table_init
  procedure, private :: if_table_init

<Auto components: sub interfaces>+≡
  module subroutine ps_table_init &
    (table, model, pl, constraints, n_in, do_not_check_regular)
    class(ps_table_t), intent(out) :: table
    class(model_data_t), intent(in), target :: model
    type(pdg_list_t), dimension(:), intent(in) :: pl
    type(split_constraints_t), intent(in) :: constraints
    integer, intent(in), optional :: n_in
    logical, intent(in), optional :: do_not_check_regular
  end subroutine ps_table_init
  module subroutine if_table_init (table, model, pl_in, pl_out, constraints)
    class(if_table_t), intent(out) :: table
    class(model_data_t), intent(in), target :: model
    type(pdg_list_t), dimension(:), intent(in) :: pl_in, pl_out
    type(split_constraints_t), intent(in) :: constraints
  end subroutine if_table_init

<Auto components: procedures>+≡
  module subroutine ps_table_init &
    (table, model, pl, constraints, n_in, do_not_check_regular)
    class(ps_table_t), intent(out) :: table
    class(model_data_t), intent(in), target :: model
    type(pdg_list_t), dimension(:), intent(in) :: pl
    type(split_constraints_t), intent(in) :: constraints
    integer, intent(in), optional :: n_in
    logical, intent(in), optional :: do_not_check_regular

```

```

logical :: passed
integer :: i
table%model => model

if (present (n_in)) then
  select case (n_in)
    case (1)
      table%proc_type = PROC_DECAY
    case (2)
      table%proc_type = PROC_SCATTER
    case default
      table%proc_type = PROC_UNDEFINED
  end select
else
  table%proc_type = PROC_UNDEFINED
end if

do i = 1, size (pl)
  call table%record (pl(i), 0, 0, constraints, &
    do_not_check_regular, passed)
  if (.not. passed) then
    call msg_fatal ("ps_table: Registering process components failed")
  end if
end do
end subroutine ps_table_init

module subroutine if_table_init (table, model, pl_in, pl_out, constraints)
  class(if_table_t), intent(out) :: table
  class(model_data_t), intent(in), target :: model
  type(pdg_list_t), dimension(:), intent(in) :: pl_in, pl_out
  type(split_constraints_t), intent(in) :: constraints
  integer :: i, j, k, p, n_in, n_out
  type(pdg_array_t), dimension(:), allocatable :: pa_in
  type(pdg_list_t), dimension(:), allocatable :: pl
  allocate (pl (size (pl_in) * size (pl_out)))
  k = 0
  do i = 1, size (pl_in)
    n_in = pl_in(i)%get_size ()
    allocate (pa_in (n_in))
    do p = 1, n_in
      pa_in(p) = pl_in(i)%get (p)
    end do
    do j = 1, size (pl_out)
      n_out = pl_out(j)%get_size ()
      k = k + 1
      call pl(k)%init (n_in + n_out)
      do p = 1, n_in
        call pl(k)%set (p, invert_pdg_array (pa_in(p), model))
      end do
      do p = 1, n_out
        call pl(k)%set (n_in + p, pl_out(j)%get (p))
      end do
    end do
    deallocate (pa_in)
  end do
end subroutine if_table_init

```

```

end do
n_in = size (pl_in(1)%a)
call table%init (model, pl, constraints, n_in, do_not_check_regular = .true.)
end subroutine if_table_init

```

Enable loops for the table. This affects both splitting and output.

```

<Auto components: ps table: TBP>+≡
  procedure :: enable_loops => ps_table_enable_loops

<Auto components: sub interfaces>+≡
  module subroutine ps_table_enable_loops (table)
    class(ps_table_t), intent(inout) :: table
  end subroutine ps_table_enable_loops

<Auto components: procedures>+≡
  module subroutine ps_table_enable_loops (table)
    class(ps_table_t), intent(inout) :: table
    table%loops = .true.
  end subroutine ps_table_enable_loops

```

28.1.4 Top-level methods

Create a table for a single-particle decay. Construct all possible final states from a single particle with PDG code `pdg_in`. The construction is limited by the given `constraints`.

```

<Auto components: ds table: TBP>+≡
  procedure :: make => ds_table_make

<Auto components: sub interfaces>+≡
  module subroutine ds_table_make (table, model, pdg_in, constraints)
    class(ds_table_t), intent(out) :: table
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: pdg_in
    type(split_constraints_t), intent(in) :: constraints
  end subroutine ds_table_make

<Auto components: procedures>+≡
  module subroutine ds_table_make (table, model, pdg_in, constraints)
    class(ds_table_t), intent(out) :: table
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: pdg_in
    type(split_constraints_t), intent(in) :: constraints
    type(pdg_list_t) :: pl_in
    type(pdg_list_t), dimension(0) :: pl
    call table%init (model, pl, constraints)
    table%pdg_in = pdg_in
    call pl_in%init (1)
    call pl_in%set (1, [pdg_in])
    call table%split (pl_in, 0, constraints)
  end subroutine ds_table_make

```

Split all entries in a growing table, starting from a table that may already contain states. Add and record split states on the fly.

```

<Auto components: fs table: TBP>+≡
  procedure :: radiate => fs_table_radiate

<Auto components: sub interfaces>+≡
  module subroutine fs_table_radiate (table, constraints, do_not_check_regular)
    class(fs_table_t), intent(inout) :: table
    type(split_constraints_t) :: constraints
    logical, intent(in), optional :: do_not_check_regular
  end subroutine fs_table_radiate

<Auto components: procedures>+≡
  module subroutine fs_table_radiate (table, constraints, do_not_check_regular)
    class(fs_table_t), intent(inout) :: table
    type(split_constraints_t) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    type(ps_entry_t), pointer :: current
    current => table%first
    do while (associated (current))
      call table%split (current, 0, constraints, record = .true., &
        do_not_check_regular = do_not_check_regular)
      current => current%next
    end do
  end subroutine fs_table_radiate

```

28.1.5 Splitting algorithm

Recursive splitting. First of all, we record the current `pdg_list` in the table, subject to `constraints`, if requested. We also record copies of the list marked as loop corrections.

When we record a particle list, we sort it first.

If there is room for splitting, We take a PDG array list and the index of an element, and split this element in all possible ways. The split entry is inserted into the list, which we split further.

The recursion terminates whenever the split array would have a length greater than n_{\max} .

```

<Auto components: ps table: TBP>+≡
  procedure :: split => ps_table_split

<Auto components: sub interfaces>+≡
  recursive module subroutine ps_table_split (table, pl, n_rad, constraints, &
    record, do_not_check_regular)
    class(ps_table_t), intent(inout) :: table
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: record, do_not_check_regular
  end subroutine ps_table_split

<Auto components: procedures>+≡
  recursive module subroutine ps_table_split (table, pl, n_rad, constraints, &
    record, do_not_check_regular)

```

```

class(ps_table_t), intent(inout) :: table
class(pdg_list_t), intent(in) :: pl
integer, intent(in) :: n_rad
type(split_constraints_t), intent(in) :: constraints
logical, intent(in), optional :: record, do_not_check_regular
integer :: n_loop, i
logical :: passed, save_pdg_index
type(vertex_iterator_t) :: vit
integer, dimension(:), allocatable :: pdg1
integer, dimension(:), allocatable :: pdg2
if (present (record)) then
  if (record) then
    n_loop = 0
    INCR_LOOPS: do
      call table%record_sorted (pl, n_loop, n_rad, constraints, &
        do_not_check_regular, passed)
      if (.not. passed) exit INCR_LOOPS
      if (.not. table%loops) exit INCR_LOOPS
      n_loop = n_loop + 1
    end do INCR_LOOPS
  end if
end if
select type (table)
type is (if_table_t)
  save_pdg_index = .true.
class default
  save_pdg_index = .false.
end select
do i = 1, pl%get_size ()
  call constraints%check_before_split (table, pl, i, passed)
  if (passed) then
    pdg1 = pl%get (i)
    call vit%init (table%model, pdg1, save_pdg_index)
    SCAN_VERTICES: do
      call vit%get_next_match (pdg2)
      if (allocated (pdg2)) then
        call table%insert (pl, n_rad, i, pdg2, constraints, &
          do_not_check_regular = do_not_check_regular)
      else
        exit SCAN_VERTICES
      end if
    end do SCAN_VERTICES
  end if
end do
end subroutine ps_table_split

```

The worker part: insert the list of particles found by vertex matching in place of entry *i* in the PDG list. Then split/record further.

The *n_in* parameter tells the replacement routine to insert the new particles after entry *n_in*. Otherwise, they follow index *i*.

<Auto components: ps table: TBP>+≡

procedure :: insert => ps_table_insert

<Auto components: sub interfaces>+≡

```

recursive module subroutine ps_table_insert &
  (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
  class(ps_table_t), intent(inout) :: table
  class(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n_rad, i
  integer, dimension(:), intent(in) :: pdg
  type(split_constraints_t), intent(in) :: constraints
  integer, intent(in), optional :: n_in
  logical, intent(in), optional :: do_not_check_regular
end subroutine ps_table_insert

```

(Auto components: procedures)+≡

```

recursive module subroutine ps_table_insert &
  (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
  class(ps_table_t), intent(inout) :: table
  class(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n_rad, i
  integer, dimension(:), intent(in) :: pdg
  type(split_constraints_t), intent(in) :: constraints
  integer, intent(in), optional :: n_in
  logical, intent(in), optional :: do_not_check_regular
  type(pdg_list_t) :: pl_insert
  logical :: passed
  integer :: k, s
  s = size (pdg)
  call pl_insert%init (s)
  do k = 1, s
    call pl_insert%set (k, pdg(k))
  end do
  call constraints%check_before_insert (table, pl%get (i), pl_insert, passed)
  if (passed) then
    if (.not. is_colored_isr ()) return
    call table%split (pl%replace (i, pl_insert, n_in), n_rad + s - 1, &
      constraints, record = .true., do_not_check_regular = .true.)
  end if
contains
  logical function is_colored_isr () result (ok)
    type(pdg_list_t) :: pl_replaced
    ok = .true.
    if (present (n_in)) then
      if (i <= n_in) then
        ok = pl_insert%contains_colored_particles ()
        if (.not. ok) then
          pl_replaced = pl%replace (i, pl_insert, n_in)
          associate (size_replaced => pl_replaced%get_pdg_sizes (), &
            size => pl%get_pdg_sizes ())
            ok = all (size_replaced(:n_in) == size(:n_in))
          end associate
        end if
      end if
    end if
  end function is_colored_isr
end subroutine ps_table_insert

```


Special case: If we are splitting an initial particle, there is slightly more to do. We loop over the particles from the vertex match and replace the initial particle by each of them in turn. The remaining particles must be appended after the second initial particle, so they will end up in the out state. This is done by providing the `n_in` argument to the base method as an optional argument.

Note that we must call the base-method procedure explicitly, so the `table` argument keeps its dynamic type as `if_table` inside this procedure.

```

<Auto components: if table: TBP>+≡
  procedure :: insert => if_table_insert

<Auto components: sub interfaces>+≡
  recursive module subroutine if_table_insert &
    (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
    class(if_table_t), intent(inout) :: table
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_rad, i
    integer, dimension(:), intent(in) :: pdg
    type(split_constraints_t), intent(in) :: constraints
    integer, intent(in), optional :: n_in
    logical, intent(in), optional :: do_not_check_regular
  end subroutine if_table_insert

<Auto components: procedures>+≡
  recursive module subroutine if_table_insert &
    (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
    class(if_table_t), intent(inout) :: table
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_rad, i
    integer, dimension(:), intent(in) :: pdg
    type(split_constraints_t), intent(in) :: constraints
    integer, intent(in), optional :: n_in
    logical, intent(in), optional :: do_not_check_regular
    integer, dimension(:), allocatable :: pdg_work
    integer :: p
    if (i > 2) then
      call ps_table_insert (table, pl, n_rad, i, pdg, constraints, &
        do_not_check_regular = do_not_check_regular)
    else
      allocate (pdg_work (size (pdg)))
      do p = 1, size (pdg)
        pdg_work(1) = pdg(p)
        pdg_work(2:p) = pdg(1:p-1)
        pdg_work(p+1:) = pdg(p+1:)
        select case (table%proc_type)
          case (PROC_DECAY)
            call ps_table_insert (table, &
              pl, n_rad, i, pdg_work, constraints, n_in = 1, &
              do_not_check_regular = do_not_check_regular)
          case (PROC_SCATTER)
            call ps_table_insert (table, &
              pl, n_rad, i, pdg_work, constraints, n_in = 2, &
              do_not_check_regular = do_not_check_regular)
        end select
      end do
    end if
  end if

```

```
end subroutine if_table_insert
```

Sort before recording. In the case of the `if_table`, we do not sort the first `n_in` particle entries. Instead, we check whether they are allowed in the `pl_beam` PDG list, if that is provided.

```
<Auto components: ps table: TBP>+≡
  procedure :: record_sorted => ps_table_record_sorted

<Auto components: if table: TBP>+≡
  procedure :: record_sorted => if_table_record_sorted

<Auto components: sub interfaces>+≡
  module subroutine ps_table_record_sorted &
    (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
    class(ps_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
  end subroutine ps_table_record_sorted
  module subroutine if_table_record_sorted &
    (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
    class(if_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
  end subroutine if_table_record_sorted

<Auto components: procedures>+≡
  module subroutine ps_table_record_sorted &
    (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
    class(ps_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
    call table%record (pl%sort_abs (), n_loop, n_rad, constraints, &
      do_not_check_regular, passed)
  end subroutine ps_table_record_sorted

  module subroutine if_table_record_sorted &
    (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
    class(if_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
    call table%record (pl%sort_abs (2), n_loop, n_rad, constraints, &
      do_not_check_regular, passed)
  end subroutine if_table_record_sorted
```

Record an entry: insert into the list. Check the ordering and insert it at the correct place, unless it is already there.

We record an array only if its mass sum is less than the total available energy. This restriction is removed by setting `constrained` to false.

<Auto components: ps table: TBP>+≡

```
procedure :: record => ps_table_record
```

<Auto components: sub interfaces>+≡

```
module subroutine ps_table_record (table, pl, n_loop, n_rad, constraints, &
    do_not_check_regular, passed)
    class(ps_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
end subroutine ps_table_record
```

<Auto components: procedures>+≡

```
module subroutine ps_table_record (table, pl, n_loop, n_rad, constraints, &
    do_not_check_regular, passed)
    class(ps_table_t), intent(inout) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop, n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: do_not_check_regular
    logical, intent(out) :: passed
    type(ps_entry_t), pointer :: current
    logical :: needs_check
    passed = .false.
    needs_check = .true.
    if (present (do_not_check_regular)) needs_check = .not. do_not_check_regular
    if (needs_check .and. .not. pl%is_regular ()) then
        call msg_warning ("Record ps_table entry: Irregular pdg-list encountered!")
        return
    end if
    call constraints%check_before_record (table, pl, n_loop, passed)
    if (.not. passed) then
        return
    end if
    current => table%first
    do while (associated (current))
        if (pl == current) then
            if (n_loop == current%n_loop) return
        else if (pl < current) then
            call record_insert ()
            return
        end if
        current => current%next
    end do
    call record_insert ()
contains
    subroutine record_insert ()
```

```

type(ps_entry_t), pointer :: entry
allocate (entry)
entry%pdg_list_t = pl
entry%n_loop = n_loop
entry%n_rad = n_rad
if (associated (current)) then
  if (associated (current%previous)) then
    current%previous%next => entry
    entry%previous => current%previous
  else
    table%first => entry
  end if
  entry%next => current
  current%previous => entry
else
  if (associated (table%last)) then
    table%last%next => entry
    entry%previous => table%last
  else
    table%first => entry
  end if
  table%last => entry
end if
end subroutine record_insert
end subroutine ps_table_record

```

28.1.6 Tools

Compute the mass sum for a PDG list object, counting the entries with indices between (including) `n1` and `n2`. Rely on the requirement that if an entry is a PDG array, this array must be degenerate in mass.

(Auto components: procedures)+≡

```

function mass_sum (pl, n1, n2, model) result (m)
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n1, n2
  class(model_data_t), intent(in), target :: model
  integer, dimension(:), allocatable :: pdg
  real(default) :: m
  type(field_data_t), pointer :: prt
  integer :: i
  m = 0
  do i = n1, n2
    pdg = pl%get (i)
    prt => model%get_field_ptr (pdg(1))
    m = m + prt%get_mass ()
  end do
end function mass_sum

```

Invert a PDG array, replacing particles by antiparticles. This depends on the model.

(Auto components: procedures)+≡

```

function invert_pdg_array (pa, model) result (pa_inv)
  type(pdg_array_t), intent(in) :: pa
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t) :: pa_inv
  type(field_data_t), pointer :: prt
  integer :: i, pdg
  pa_inv = pa
  do i = 1, pa_inv%get_length ()
    pdg = pa_inv%get (i)
    prt => model%get_field_ptr (pdg)
    if (prt%has_antiparticle ()) call pa_inv%set (i, -pdg)
  end do
end function invert_pdg_array

```

28.1.7 Access results

Return the number of generated decays.

```

<Auto components: ps table: TBP>+≡
  procedure :: get_length => ps_table_get_length

<Auto components: sub interfaces>+≡
  module function ps_table_get_length (ps_table) result (n)
    class(ps_table_t), intent(in) :: ps_table
    integer :: n
  end function ps_table_get_length

<Auto components: procedures>+≡
  module function ps_table_get_length (ps_table) result (n)
    class(ps_table_t), intent(in) :: ps_table
    integer :: n
    type(ps_entry_t), pointer :: entry
    n = 0
    entry => ps_table%first
    do while (associated (entry))
      n = n + 1
      entry => entry%next
    end do
  end function ps_table_get_length

<Auto components: ps table: TBP>+≡
  procedure :: get_emitters => ps_table_get_emitters

<Auto components: sub interfaces>+≡
  module subroutine ps_table_get_emitters (table, constraints, emitters)
    class(ps_table_t), intent(in) :: table
    type(split_constraints_t), intent(in) :: constraints
    integer, dimension(:), allocatable, intent(out) :: emitters
  end subroutine ps_table_get_emitters

<Auto components: procedures>+≡
  module subroutine ps_table_get_emitters (table, constraints, emitters)
    class(ps_table_t), intent(in) :: table
    type(split_constraints_t), intent(in) :: constraints
    integer, dimension(:), allocatable, intent(out) :: emitters

```

```

class(pdg_list_t), pointer :: pl
integer :: i
logical :: passed
type(vertex_iterator_t) :: vit
integer, dimension(:), allocatable :: pdg1, pdg2
integer :: n_emitters
integer, dimension(:), allocatable :: emitters_tmp
integer, parameter :: buf0 = 6
n_emitters = 0
pl => table%first
allocate (emitters_tmp (buf0))
do i = 1, pl%get_size ()
  call constraints%check_before_split (table, pl, i, passed)
  if (passed) then
    pdg1 = pl%get(i)
    call vit%init (table%model, pdg1, .false.)
    do
      call vit%get_next_match(pdg2)
      if (allocated (pdg2)) then
        if (n_emitters + 1 > size (emitters_tmp)) &
          call extend_integer_array (emitters_tmp, 10)
        emitters_tmp (n_emitters + 1) = pdg1(1)
        n_emitters = n_emitters + 1
      else
        exit
      end if
    end do
  end if
end do
allocate (emitters (n_emitters))
emitters = emitters_tmp (1:n_emitters)
deallocate (emitters_tmp)
end subroutine ps_table_get_emitters

```

Return an allocated array of decay products (PDG codes). If requested, return also the loop and radiation order count.

<Auto components: ps table: TBP>+≡

```

procedure :: get_pdg_out => ps_table_get_pdg_out

```

<Auto components: sub interfaces>+≡

```

module subroutine ps_table_get_pdg_out (ps_table, i, pa_out, n_loop, n_rad)
  class(ps_table_t), intent(in) :: ps_table
  integer, intent(in) :: i
  type(pdg_array_t), dimension(:), allocatable, intent(out) :: pa_out
  integer, intent(out), optional :: n_loop, n_rad
end subroutine ps_table_get_pdg_out

```

<Auto components: procedures>+≡

```

module subroutine ps_table_get_pdg_out (ps_table, i, pa_out, n_loop, n_rad)
  class(ps_table_t), intent(in) :: ps_table
  integer, intent(in) :: i
  type(pdg_array_t), dimension(:), allocatable, intent(out) :: pa_out
  integer, intent(out), optional :: n_loop, n_rad
  type(ps_entry_t), pointer :: entry
  integer :: n, j

```

```

n = 0
entry => ps_table%first
FIND_ENTRY: do while (associated (entry))
  n = n + 1
  if (n == i) then
    allocate (pa_out (entry%get_size ()))
    do j = 1, entry%get_size ()
      pa_out(j) = entry%get (j)
      if (present (n_loop)) n_loop = entry%n_loop
      if (present (n_rad)) n_rad = entry%n_rad
    end do
    exit FIND_ENTRY
  end if
  entry => entry%next
end do FIND_ENTRY
end subroutine ps_table_get_pdg_out

```

28.1.8 Unit tests

Test module, followed by the corresponding implementation module.

```

(auto_components_ut.f90)≡
  <File header>

```

```

module auto_components_ut
  use unit_tests
  use auto_components_uti

```

```

  <Standard module head>

```

```

  <Auto components: public test>

```

```

contains

```

```

  <Auto components: test driver>

```

```

end module auto_components_ut

```

```

(auto_components_uti.f90)≡
  <File header>

```

```

module auto_components_uti

```

```

  <Use kinds>

```

```

  <Use strings>

```

```

  use pdg_arrays

```

```

  use model_data

```

```

  use model_testbed, only: prepare_model, cleanup_model

```

```

  use auto_components

```

```

  <Standard module head>

```

```

  <Auto components: test declarations>

```

contains

<Auto components: tests>

end module auto_components_util

API: driver for the unit tests below.

<Auto components: public test>≡

public :: auto_components_test

<Auto components: test driver>≡

subroutine auto_components_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Auto components: execute tests>

end subroutine auto_components_test

Generate Decay Table

Determine all kinematically allowed decay channels for a Higgs boson, using default parameter values.

<Auto components: execute tests>≡

call test (auto_components_1, "auto_components_1", &
"generate decay table", &
u, results)

<Auto components: test declarations>≡

public :: auto_components_1

<Auto components: tests>≡

subroutine auto_components_1 (u)

integer, intent(in) :: u

class(model_data_t), pointer :: model

type(field_data_t), pointer :: prt

type(ds_table_t) :: ds_table

type(split_constraints_t) :: constraints

write (u, "(A)") "* Test output: auto_components_1"

write (u, "(A)") "* Purpose: determine Higgs decay table"

write (u, *)

write (u, "(A)") "* Read Standard Model"

model => null ()

call prepare_model (model, var_str ("SM"))

prt => model%get_field_ptr (25)

write (u, *)

write (u, "(A)") "* Higgs decays n = 2"

write (u, *)

call constraints%init (2)


```

call constraints%set (1, constrain_n_tot (2))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "** Higgs decays n = 3 (w/o radiative)"
write (u, *)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))
call constraints%set (3, constrain_radiation ())

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "** Higgs decays n = 3 (w/ radiative)"
write (u, *)

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "** Cleanup"

call cleanup_model (model)
deallocate (model)

write (u, *)
write (u, "(A)")  "** Test output end: auto_components_1"

end subroutine auto_components_1

```

Generate radiation

Given a final state, add radiation (NLO and NNLO). We provide a list of particles that is allowed to occur in the generated final states.

```

(Auto components: execute tests)+≡
call test (auto_components_2, "auto_components_2", &
  "generate NLO corrections, final state", &
  u, results)

```

```

<Auto components: test declarations>+≡
    public :: auto_components_2

<Auto components: tests>+≡
    subroutine auto_components_2 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: model
        type(pdg_list_t), dimension(:), allocatable :: pl, pl_zzh
        type(pdg_list_t) :: pl_match
        type(fs_table_t) :: fs_table
        type(split_constraints_t) :: constraints
        real(default) :: sqrts
        integer :: i

        write (u, "(A)")  "* Test output: auto_components_2"
        write (u, "(A)")  "*   Purpose: generate radiation (NLO)"
        write (u, *)

        write (u, "(A)")  "* Read Standard Model"

        model => null ()
        call prepare_model (model, var_str ("SM"))

        write (u, *)
        write (u, "(A)")  "* LO final state"
        write (u, *)

        allocate (pl (2))
        call pl(1)%init (2)
        call pl(1)%set (1, 1)
        call pl(1)%set (2, -1)
        call pl(2)%init (2)
        call pl(2)%set (1, 21)
        call pl(2)%set (2, 21)
        do i = 1, 2
            call pl(i)%write (u); write (u, *)
        end do

        write (u, *)
        write (u, "(A)")  "* Initialize FS table"
        write (u, *)

        call constraints%init (1)
        call constraints%set (1, constrain_n_tot (3))

        call fs_table%init (model, pl, constraints)
        call fs_table%write (u)

        write (u, *)
        write (u, "(A)")  "* Generate NLO corrections, unconstrained"
        write (u, *)

        call fs_table%radiate (constraints)
        call fs_table%write (u)

```

```

call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &complete but mass-constrained"
write (u, *)

sqrts = 50

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (sqrts))

call fs_table%init (model, pl, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, restricted"
write (u, *)

call pl_match%init ([1, -1, 21])

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NNLO corrections, restricted, with one loop"
write (u, *)

call pl_match%init ([1, -1, 21])

call constraints%init (3)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_n_loop (1))
call constraints%set (3, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%enable_loops ()
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NNLO corrections, restricted, with loops"
write (u, *)

```

```

call constraints%init (2)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%enable_loops ()
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NNLO corrections, restricted, to Z Z H, &
    &no loops"
write (u, *)

allocate (pl_zzh (1))
call pl_zzh(1)%init (3)
call pl_zzh(1)%set (1, 23)
call pl_zzh(1)%set (2, 23)
call pl_zzh(1)%set (3, 25)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (5))
call constraints%set (2, constrain_mass_sum (500._default))
call constraints%set (3, constrain_require (pl_zzh(1)))

call fs_table%init (model, pl_zzh, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

call cleanup_model (model)
deallocate (model)

write (u, *)
write (u, "(A)")  "* Test output end: auto_components_2"

end subroutine auto_components_2

```

Generate radiation from initial and final state

Given a process, add radiation (NLO and NNLO). We provide a list of particles that is allowed to occur in the generated final states.

```

<Auto components: execute tests>+≡
    call test (auto_components_3, "auto_components_3", &
        "generate NLO corrections, in and out", &
        u, results)

<Auto components: test declarations>+≡
    public :: auto_components_3

<Auto components: tests>+≡
    subroutine auto_components_3 (u)

```

```

integer, intent(in) :: u
class(model_data_t), pointer :: model
type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out
type(pdg_list_t) :: pl_match, pl_beam
type(if_table_t) :: if_table
type(split_constraints_t) :: constraints
real(default) :: sqrts
integer :: i

write (u, "(A)")  "* Test output: auto_components_3"
write (u, "(A)")  "* Purpose: generate radiation (NLO)"
write (u, *)

write (u, "(A)")  "* Read Standard Model"

model => null ()
call prepare_model (model, var_str ("SM"))

write (u, *)
write (u, "(A)")  "* LO initial state"
write (u, *)

allocate (pl_in (2))
call pl_in(1)%init (2)
call pl_in(1)%set (1, 1)
call pl_in(1)%set (2, -1)
call pl_in(2)%init (2)
call pl_in(2)%set (1, -1)
call pl_in(2)%set (2, 1)
do i = 1, 2
    call pl_in(i)%write (u); write (u, *)
end do

write (u, *)
write (u, "(A)")  "* LO final state"
write (u, *)

allocate (pl_out (1))
call pl_out(1)%init (1)
call pl_out(1)%set (1, 23)
call pl_out(1)%write (u); write (u, *)

write (u, *)
write (u, "(A)")  "* Initialize FS table"
write (u, *)

call constraints%init (1)
call constraints%set (1, constrain_n_tot (4))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%write (u)

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, unconstrained"

```

```

write (u, *)

call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &complete but mass-constrained"
write (u, *)

sqrts = 100
call constraints%init (2)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_mass_sum (sqrts))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &mass-constrained, restricted beams"
write (u, *)

call pl_beam%init (3)
call pl_beam%set (1, 1)
call pl_beam%set (2, -1)
call pl_beam%set (3, 21)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, restricted"
write (u, *)

call pl_match%init ([1, -1, 21])

call constraints%init (4)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))
call constraints%set (4, constrain_insert (pl_match))

call if_table%init (model, pl_in, pl_out, constraints)

```

```

call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "** Generate NNLO corrections, restricted, Z preserved, &
                  &with loops"
write (u, *)

call constraints%init (5)
call constraints%set (1, constrain_n_tot (5))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))
call constraints%set (4, constrain_insert (pl_match))
call constraints%set (5, constrain_require (pl_out(1)))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%enable_loops ()
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

call cleanup_model (model)
deallocate (model)

write (u, *)
write (u, "(A)")  "** Test output end: auto_components_3"

end subroutine auto_components_3

```

28.2 Creating the real flavor structure

```

<radiation_generator.f90>≡
<File header>

module radiation_generator

  <Use kinds>
  <Use strings>
  use sorting, only: sort_abs
  use pdg_arrays
  use model_data
  use auto_components

  implicit none
  private

  <Radiation generator: public>

  <Radiation generator: types>

  interface

```

```

    <Radiation generator: sub interfaces>
    end interface

end module radiation_generator

<radiation_generator_sub.f90>≡
<File header>

submodule (radiation_generator) radiation_generator_s

    use io_units
    use diagnostics
    use physics_defs, only: PHOTON, GLUON
    use string_utils, only: split_string, string_contains_word
    use flavors

    implicit none

contains

    <Radiation generator: procedures>

end submodule radiation_generator_s

<Radiation generator: types>≡
type :: pdg_sorter_t
    integer :: pdg
    logical :: checked = .false.
    integer :: associated_born = 0
end type pdg_sorter_t

<Radiation generator: types>+≡
type :: pdg_states_t
    type(pdg_array_t), dimension(:), allocatable :: pdg
    type(pdg_states_t), pointer :: next
    integer :: n_particles
contains
    <Radiation generator: pdg states: TBP>
end type pdg_states_t

<Radiation generator: pdg states: TBP>≡
procedure :: init => pdg_states_init

<Radiation generator: sub interfaces>≡
module subroutine pdg_states_init (states)
    class(pdg_states_t), intent(inout) :: states
end subroutine pdg_states_init

<Radiation generator: procedures>≡
module subroutine pdg_states_init (states)
    class(pdg_states_t), intent(inout) :: states
    nullify (states%next)
end subroutine pdg_states_init

```



```

<Radiation generator: pdg states: TBP>+≡
  procedure :: add => pdg_states_add

<Radiation generator: sub interfaces>+≡
  module subroutine pdg_states_add (states, pdg)
    class(pdg_states_t), intent(inout), target :: states
    type(pdg_array_t), dimension(:), intent(in) :: pdg
  end subroutine pdg_states_add

<Radiation generator: procedures>+≡
  module subroutine pdg_states_add (states, pdg)
    class(pdg_states_t), intent(inout), target :: states
    type(pdg_array_t), dimension(:), intent(in) :: pdg
    type(pdg_states_t), pointer :: current_state
    select type (states)
    type is (pdg_states_t)
      current_state => states
    do
      if (associated (current_state%next)) then
        current_state => current_state%next
      else
        allocate (current_state%next)
        nullify(current_state%next%next)
        current_state%pdg = pdg
        exit
      end if
    end do
  end select
end subroutine pdg_states_add

<Radiation generator: pdg states: TBP>+≡
  procedure :: get_n_states => pdg_states_get_n_states

<Radiation generator: sub interfaces>+≡
  module function pdg_states_get_n_states (states) result (n)
    class(pdg_states_t), intent(in), target :: states
    integer :: n
  end function pdg_states_get_n_states

<Radiation generator: procedures>+≡
  module function pdg_states_get_n_states (states) result (n)
    class(pdg_states_t), intent(in), target :: states
    integer :: n
    type(pdg_states_t), pointer :: current_state
    n = 0
    select type(states)
    type is (pdg_states_t)
      current_state => states
    do
      if (associated (current_state%next)) then
        n = n+1
        current_state => current_state%next
      else
        exit
      end if
    end do
  end function

```

```

        end select
    end function pdg_states_get_n_states

<Radiation generator: types>+≡
type :: prt_queue_t
    type(string_t), dimension(:), allocatable :: prt_string
    type(prt_queue_t), pointer :: next => null ()
    type(prt_queue_t), pointer :: previous => null ()
    type(prt_queue_t), pointer :: front => null ()
    type(prt_queue_t), pointer :: current_prt => null ()
    type(prt_queue_t), pointer :: back => null ()
    integer :: n_lists = 0
contains
<Radiation generator: prt queue: TBP>
end type prt_queue_t

<Radiation generator: prt queue: TBP>≡
procedure :: null => prt_queue_null

<Radiation generator: sub interfaces>+≡
module subroutine prt_queue_null (queue)
    class(prt_queue_t), intent(out) :: queue
end subroutine prt_queue_null

<Radiation generator: procedures>+≡
module subroutine prt_queue_null (queue)
    class(prt_queue_t), intent(out) :: queue
    queue%next => null ()
    queue%previous => null ()
    queue%front => null ()
    queue%current_prt => null ()
    queue%back => null ()
    queue%n_lists = 0
    if (allocated (queue%prt_string)) deallocate (queue%prt_string)
end subroutine prt_queue_null

<Radiation generator: prt queue: TBP>+≡
procedure :: append => prt_queue_append

<Radiation generator: sub interfaces>+≡
module subroutine prt_queue_append (queue, prt_string)
    class(prt_queue_t), intent(inout) :: queue
    type(string_t), intent(in), dimension(:) :: prt_string
end subroutine prt_queue_append

<Radiation generator: procedures>+≡
module subroutine prt_queue_append (queue, prt_string)
    class(prt_queue_t), intent(inout) :: queue
    type(string_t), intent(in), dimension(:) :: prt_string
    type(prt_queue_t), pointer :: new_element => null ()
    type(prt_queue_t), pointer :: current_back => null ()
    allocate (new_element)
    allocate (new_element%prt_string(size (prt_string)))
    new_element%prt_string = prt_string
    if (associated (queue%back)) then

```

```

        current_back => queue%back
        current_back%next => new_element
        new_element%previous => current_back
        queue%back => new_element
    else
        !!! Initial entry
        queue%front => new_element
        queue%back => queue%front
        queue%current_prt => queue%front
    end if
    queue%n_lists = queue%n_lists + 1
end subroutine prt_queue_append

```

<Radiation generator: prt queue: TBP>+≡
 procedure :: get => prt_queue_get

<Radiation generator: sub interfaces>+≡
 module subroutine prt_queue_get (queue, prt_string)
 class(prt_queue_t), intent(inout) :: queue
 type(string_t), dimension(:), allocatable, intent(out) :: prt_string
 end subroutine prt_queue_get

<Radiation generator: procedures>+≡
 module subroutine prt_queue_get (queue, prt_string)
 class(prt_queue_t), intent(inout) :: queue
 type(string_t), dimension(:), allocatable, intent(out) :: prt_string
 if (associated (queue%current_prt)) then
 prt_string = queue%current_prt%prt_string
 if (associated (queue%current_prt%next)) &
 queue%current_prt => queue%current_prt%next
 else
 prt_string = " "
 end if
 end subroutine prt_queue_get

As above.

<Radiation generator: prt queue: TBP>+≡
 procedure :: get_last => prt_queue_get_last

<Radiation generator: sub interfaces>+≡
 module subroutine prt_queue_get_last (queue, prt_string)
 class(prt_queue_t), intent(in) :: queue
 type(string_t), dimension(:), allocatable, intent(out) :: prt_string
 end subroutine prt_queue_get_last

<Radiation generator: procedures>+≡
 module subroutine prt_queue_get_last (queue, prt_string)
 class(prt_queue_t), intent(in) :: queue
 type(string_t), dimension(:), allocatable, intent(out) :: prt_string
 if (associated (queue%back)) then
 allocate (prt_string(size (queue%back%prt_string)))
 prt_string = queue%back%prt_string
 else
 prt_string = " "
 end if

```

end subroutine prt_queue_get_last

<Radiation generator: prt queue: TBP>+≡
  procedure :: reset => prt_queue_reset

<Radiation generator: sub interfaces>+≡
  module subroutine prt_queue_reset (queue)
    class(prt_queue_t), intent(inout) :: queue
  end subroutine prt_queue_reset

<Radiation generator: procedures>+≡
  module subroutine prt_queue_reset (queue)
    class(prt_queue_t), intent(inout) :: queue
    queue%current_prt => queue%front
  end subroutine prt_queue_reset

<Radiation generator: prt queue: TBP>+≡
  procedure :: check_for_same_prt_strings => prt_queue_check_for_same_prt_strings

<Radiation generator: sub interfaces>+≡
  module function prt_queue_check_for_same_prt_strings (queue) result (val)
    class(prt_queue_t), intent(inout) :: queue
    logical :: val
  end function prt_queue_check_for_same_prt_strings

<Radiation generator: procedures>+≡
  module function prt_queue_check_for_same_prt_strings (queue) result (val)
    class(prt_queue_t), intent(inout) :: queue
    logical :: val
    type(string_t), dimension(:), allocatable :: prt_string
    integer, dimension(:,:), allocatable :: i_particle
    integer :: n_d, n_dbar, n_u, n_ubar, n_s, n_sbar, n_gl, n_e, n_ep, n_mu, n_mup, n_A
    integer :: i, j
    call queue%reset ()
    allocate (i_particle (queue%n_lists, 12))
    do i = 1, queue%n_lists
      call queue%get (prt_string)
      n_d = count_particle (prt_string, 1)
      n_dbar = count_particle (prt_string, -1)
      n_u = count_particle (prt_string, 2)
      n_ubar = count_particle (prt_string, -2)
      n_s = count_particle (prt_string, 3)
      n_sbar = count_particle (prt_string, -3)
      n_gl = count_particle (prt_string, 21)
      n_e = count_particle (prt_string, 11)
      n_ep = count_particle (prt_string, -11)
      n_mu = count_particle (prt_string, 13)
      n_mup = count_particle (prt_string, -13)
      n_A = count_particle (prt_string, 22)
      i_particle (i, 1) = n_d
      i_particle (i, 2) = n_dbar
      i_particle (i, 3) = n_u
      i_particle (i, 4) = n_ubar
      i_particle (i, 5) = n_s
      i_particle (i, 6) = n_sbar
    end do
  end function prt_queue_check_for_same_prt_strings

```

```

        i_particle (i, 7) = n_gl
        i_particle (i, 8) = n_e
        i_particle (i, 9) = n_ep
        i_particle (i, 10) = n_mu
        i_particle (i, 11) = n_mup
        i_particle (i, 12) = n_A
    end do
    val = .false.
    do i = 1, queue%n_lists
        do j = 1, queue%n_lists
            if (i == j) cycle
            val = val .or. all (i_particle (i,:) == i_particle(j,:))
        end do
    end do
contains
function count_particle (prt_string, pdg) result (n)
    type(string_t), dimension(:), intent(in) :: prt_string
    integer, intent(in) :: pdg
    integer :: n
    integer :: i
    type(string_t) :: prt_ref
    n = 0
    select case (pdg)
    case (1)
        prt_ref = "d"
    case (-1)
        prt_ref = "dbar"
    case (2)
        prt_ref = "u"
    case (-2)
        prt_ref = "ubar"
    case (3)
        prt_ref = "s"
    case (-3)
        prt_ref = "sbar"
    case (21)
        prt_ref = "gl"
    case (11)
        prt_ref = "e-"
    case (-11)
        prt_ref = "e+"
    case (13)
        prt_ref = "mu-"
    case (-13)
        prt_ref = "mu+"
    case (22)
        prt_ref = "A"
    end select
    do i = 1, size (prt_string)
        if (prt_string(i) == prt_ref) n = n+1
    end do
end function count_particle

end function prt_queue_check_for_same_prt_strings

```

```

<Radiation generator: prt queue: TBP>+≡
    procedure :: contains => prt_queue_contains

<Radiation generator: sub interfaces>+≡
    module function prt_queue_contains (queue, prt_string) result (val)
        class(prt_queue_t), intent(in) :: queue
        type(string_t), intent(in), dimension(:) :: prt_string
        logical :: val
    end function prt_queue_contains

<Radiation generator: procedures>+≡
    module function prt_queue_contains (queue, prt_string) result (val)
        class(prt_queue_t), intent(in) :: queue
        type(string_t), intent(in), dimension(:) :: prt_string
        logical :: val
        type(prt_queue_t), pointer :: current => null()
        if (associated (queue%front)) then
            current => queue%front
        else
            call msg_fatal ("Trying to access empty particle queue")
        end if
        val = .false.
        do
            if (size (current%prt_string) == size (prt_string)) then
                if (all (current%prt_string == prt_string)) then
                    val = .true.
                    exit
                end if
            end if
            if (associated (current%next)) then
                current => current%next
            else
                exit
            end if
        end do
    end function prt_queue_contains

<Radiation generator: prt queue: TBP>+≡
    procedure :: write => prt_queue_write

<Radiation generator: sub interfaces>+≡
    module subroutine prt_queue_write (queue, unit)
        class(prt_queue_t), intent(in) :: queue
        integer, optional :: unit
    end subroutine prt_queue_write

<Radiation generator: procedures>+≡
    module subroutine prt_queue_write (queue, unit)
        class(prt_queue_t), intent(in) :: queue
        integer, optional :: unit
        type(prt_queue_t), pointer :: current => null ()
        integer :: i, j, u
        u = given_output_unit (unit)
        if (associated (queue%front)) then

```

```

        current => queue%front
    else
        write (u, "(A)") "[Particle queue is empty]"
        return
    end if
    j = 1
    do
        write (u, "(I2,A,1X)", advance = 'no') j , ":"
        do i = 1, size (current%prt_string)
            write (u, "(A,1X)", advance = 'no') char (current%prt_string(i))
        end do
        write (u, "(A)")
        if (associated (current%next)) then
            current => current%next
            j = j+1
        else
            exit
        end if
    end do
end subroutine prt_queue_write

```

(Radiation generator: procedures)+≡

```

subroutine sort_prt (prt, model)
    type(string_t), dimension(:), intent(inout) :: prt
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(:), allocatable :: pdg
    type(flavor_t) :: flv
    integer :: i
    call create_pdg_array (prt, model, pdg)
    call sort_pdg (pdg)
    do i = 1, size (pdg)
        call flv%init (pdg(i)%get(), model)
        prt(i) = flv%get_name ()
    end do
end subroutine sort_prt

subroutine sort_pdg (pdg)
    type(pdg_array_t), dimension(:), intent(inout) :: pdg
    integer, dimension(:), allocatable :: i_pdg
    integer :: i
    allocate (i_pdg (size (pdg)))
    do i = 1, size (pdg)
        i_pdg(i) = pdg(i)%get ()
    end do
    i_pdg = sort_abs (i_pdg)
    do i = 1, size (pdg)
        call pdg(i)%set (1, i_pdg(i))
    end do
end subroutine sort_pdg

subroutine create_pdg_array (prt, model, pdg)
    type (string_t), dimension(:), intent(in) :: prt
    class (model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(:), allocatable, intent(out) :: pdg

```

```

type(flavor_t) :: flv
integer :: i
allocate (pdg (size (prt)))
do i = 1, size (prt)
    call flv%init (prt(i), model)
    pdg(i) = flv%get_pdg ()
end do
end subroutine create_pdg_array

```

This is used in unit tests:

```

<Radiation generator: test auxiliary>≡
subroutine write_pdg_array (pdg, u)
    use pdg_arrays
    type(pdg_array_t), dimension(:), intent(in) :: pdg
    integer, intent(in) :: u
    integer :: i
    do i = 1, size (pdg)
        call pdg(i)%write (u)
    end do
    write (u, "(A)")
end subroutine write_pdg_array

subroutine write_particle_string (prt, u)
    <Use strings>
    type(string_t), dimension(:), intent(in) :: prt
    integer, intent(in) :: u
    integer :: i
    do i = 1, size (prt)
        write (u, "(A,1X)", advance = "no") char (prt(i))
    end do
    write (u, "(A)")
end subroutine write_particle_string

```

```

<Radiation generator: types>+≡
type :: reshuffle_list_t
    integer, dimension(:), allocatable :: ii
    type(reshuffle_list_t), pointer :: next => null ()
contains
    <Radiation generator: reshuffle list: TBP>
end type reshuffle_list_t

```

```

<Radiation generator: reshuffle list: TBP>≡
procedure :: write => reshuffle_list_write

```

```

<Radiation generator: sub interfaces>+≡
module subroutine reshuffle_list_write (rlist)
    class(reshuffle_list_t), intent(in) :: rlist
end subroutine reshuffle_list_write

```

```

<Radiation generator: procedures>+≡
module subroutine reshuffle_list_write (rlist)
    class(reshuffle_list_t), intent(in) :: rlist
    type(reshuffle_list_t), pointer :: current => null ()
    integer :: i

```



```

print *, 'Content of reshuffling list: '
if (associated (rlist%next)) then
    current => rlist%next
    i = 1
    do
        print *, 'i: ', i, 'list: ', current%ii
        i = i + 1
        if (associated (current%next)) then
            current => current%next
        else
            exit
        end if
    end do
else
    print *, '[EMPTY]'
end if
end subroutine reshuffle_list_write

```

<Radiation generator: reshuffle list: TBP>+≡
 procedure :: append => reshuffle_list_append

<Radiation generator: sub interfaces>+≡
 module subroutine reshuffle_list_append (rlist, ii)
 class(reshuffle_list_t), intent(inout) :: rlist
 integer, dimension(:), allocatable, intent(in) :: ii
 end subroutine reshuffle_list_append

<Radiation generator: procedures>+≡
 module subroutine reshuffle_list_append (rlist, ii)
 class(reshuffle_list_t), intent(inout) :: rlist
 integer, dimension(:), allocatable, intent(in) :: ii
 type(reshuffle_list_t), pointer :: current
 if (associated (rlist%next)) then
 current => rlist%next
 do
 if (associated (current%next)) then
 current => current%next
 else
 allocate (current%next)
 allocate (current%next%ii (size (ii)))
 current%next%ii = ii
 exit
 end if
 end do
 else
 allocate (rlist%next)
 allocate (rlist%next%ii (size (ii)))
 rlist%next%ii = ii
 end if
 end subroutine reshuffle_list_append

<Radiation generator: reshuffle list: TBP>+≡
 procedure :: is_empty => reshuffle_list_is_empty

```

<Radiation generator: sub interfaces>+≡
    elemental module function reshuffle_list_is_empty (rlist) result (is_empty)
        logical :: is_empty
        class(reshuffle_list_t), intent(in) :: rlist
    end function reshuffle_list_is_empty

<Radiation generator: procedures>+≡
    elemental module function reshuffle_list_is_empty (rlist) result (is_empty)
        logical :: is_empty
        class(reshuffle_list_t), intent(in) :: rlist
        is_empty = .not. associated (rlist%next)
    end function reshuffle_list_is_empty

<Radiation generator: reshuffle list: TBP>+≡
    procedure :: get => reshuffle_list_get

<Radiation generator: sub interfaces>+≡
    module function reshuffle_list_get (rlist, index) result (ii)
        integer, dimension(:), allocatable :: ii
        class(reshuffle_list_t), intent(inout) :: rlist
        integer, intent(in) :: index
    end function reshuffle_list_get

<Radiation generator: procedures>+≡
    module function reshuffle_list_get (rlist, index) result (ii)
        integer, dimension(:), allocatable :: ii
        class(reshuffle_list_t), intent(inout) :: rlist
        integer, intent(in) :: index
        type(reshuffle_list_t), pointer :: current => null ()
        integer :: i
        current => rlist%next
        do i = 1, index - 1
            if (associated (current%next)) then
                current => current%next
            else
                call msg_fatal ("Index exceeds size of reshuffling list")
            end if
        end do
        allocate (ii (size (current%ii)))
        ii = current%ii
    end function reshuffle_list_get

```

We need to reset the `reshuffle_list` in order to deal with subsequent usages of the `radiation_generator`. Below is obviously the lazy and dirty solution. Otherwise, we would have to equip this auxiliary type with additional information about `last` and `previous` pointers. Considering that at most n_{legs} integers are saved in the lists, and that the subroutine is only called during the initialization phase (more precisely: at the moment only in the `radiation_generator` unit tests), I think this quick fix is justified.

```

<Radiation generator: reshuffle list: TBP>+≡
    procedure :: reset => reshuffle_list_reset

<Radiation generator: sub interfaces>+≡
    module subroutine reshuffle_list_reset (rlist)

```

```

        class(reshuffle_list_t), intent(inout) :: rlist
    end subroutine reshuffle_list_reset

<Radiation generator: procedures>+≡
    module subroutine reshuffle_list_reset (rlist)
        class(reshuffle_list_t), intent(inout) :: rlist
        rlist%next => null ()
    end subroutine reshuffle_list_reset

<Radiation generator: public>≡
    public :: radiation_generator_t

<Radiation generator: types>+≡
    type :: radiation_generator_t
        logical :: qcd_enabled = .false.
        logical :: qed_enabled = .false.
        logical :: is_gluon = .false.
        logical :: fs_gluon = .false.
        logical :: is_photon = .false.
        logical :: fs_photon = .false.
        logical :: only_final_state = .true.
        type(pdg_list_t) :: pl_in, pl_out
        type(pdg_list_t) :: pl_excluded_gaugeSplittings
        type(split_constraints_t) :: constraints
        integer :: n_tot
        integer :: n_in, n_out
        integer :: n_loops
        integer :: n_light_quarks
        real(default) :: mass_sum
        type(prt_queue_t) :: prt_queue
        type(pdg_states_t) :: pdg_raw
        type(pdg_array_t), dimension(:), allocatable :: pdg_in_born, pdg_out_born
        type(if_table_t) :: if_table
        type(reshuffle_list_t) :: reshuffle_list
    contains
    <Radiation generator: radiation generator: TBP>
    end type radiation_generator_t

```

These are infrastructure types needed in some of the routines.

```

<Radiation generator: types>+≡
    type :: prt_array_t
        type(string_t), dimension(:), allocatable :: prt
    end type prt_array_t

<Radiation generator: types>+≡
    type :: prt_table_t
        type(string_t), dimension(:), allocatable :: prt
    end type prt_table_t

<Radiation generator: radiation generator: TBP>≡
    generic :: init => init_pdg_list, init_pdg_array
    procedure :: init_pdg_list => radiation_generator_init_pdg_list
    procedure :: init_pdg_array => radiation_generator_init_pdg_array

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_init_pdg_list &
  (generator, pl_in, pl_out, pl_excluded_gaugeSplittings, qcd, qed)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_list_t), intent(in) :: pl_in, pl_out
  type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
  logical, intent(in), optional :: qcd, qed
end subroutine radiation_generator_init_pdg_list
module subroutine radiation_generator_init_pdg_array &
  (generator, pdg_in, pdg_out, pdg_excluded_gaugeSplittings, qcd, qed)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), intent(in), dimension(:) :: pdg_in, pdg_out
  type(pdg_array_t), intent(in), dimension(:) :: pdg_excluded_gaugeSplittings
  logical, intent(in), optional :: qcd, qed
end subroutine radiation_generator_init_pdg_array

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_init_pdg_list &
  (generator, pl_in, pl_out, pl_excluded_gaugeSplittings, qcd, qed)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_list_t), intent(in) :: pl_in, pl_out
  type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
  logical, intent(in), optional :: qcd, qed
  if (present (qcd)) generator%qcd_enabled = qcd
  if (present (qed)) generator%qed_enabled = qed
  generator%pl_in = pl_in
  generator%pl_out = pl_out
  generator%pl_excluded_gaugeSplittings = pl_excluded_gaugeSplittings
  generator%is_gluon = pl_in%search_for_particle (GLUON)
  generator%fs_gluon = pl_out%search_for_particle (GLUON)
  generator%is_photon = pl_in%search_for_particle (PHOTON)
  generator%fs_photon = pl_out%search_for_particle (PHOTON)
  generator%mass_sum = 0._default
  call generator%pdg_raw%init ()
end subroutine radiation_generator_init_pdg_list

module subroutine radiation_generator_init_pdg_array &
  (generator, pdg_in, pdg_out, pdg_excluded_gaugeSplittings, qcd, qed)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), intent(in), dimension(:) :: pdg_in, pdg_out
  type(pdg_array_t), intent(in), dimension(:) :: pdg_excluded_gaugeSplittings
  logical, intent(in), optional :: qcd, qed
  type(pdg_list_t) :: pl_in, pl_out
  type(pdg_list_t) :: pl_excluded_gaugeSplittings
  integer :: i
  call pl_in%init(size (pdg_in))
  call pl_out%init(size (pdg_out))
  do i = 1, size (pdg_in)
    call pl_in%set (i, pdg_in(i))
  end do
  do i = 1, size (pdg_out)
    call pl_out%set (i, pdg_out(i))
  end do
  call pl_excluded_gaugeSplittings%init(size (pdg_excluded_gaugeSplittings))
  do i = 1, size (pdg_excluded_gaugeSplittings)

```

```

        call pl_excluded_gaugeSplittings%set &
            (i, pdg_excluded_gaugeSplittings(i))
    end do
    call generator%init (pl_in, pl_out, pl_excluded_gaugeSplittings, qcd, qed)
end subroutine radiation_generator_init_pdg_array

<Radiation generator: radiation generator: TBP>+≡
    procedure :: set_initial_state_emissions => &
        radiation_generator_set_initial_state_emissions

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_set_initial_state_emissions (generator)
        class(radiation_generator_t), intent(inout) :: generator
    end subroutine radiation_generator_set_initial_state_emissions

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_set_initial_state_emissions (generator)
        class(radiation_generator_t), intent(inout) :: generator
        generator%only_final_state = .false.
    end subroutine radiation_generator_set_initial_state_emissions

<Radiation generator: radiation generator: TBP>+≡
    procedure :: setup_if_table => radiation_generator_setup_if_table

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_setup_if_table (generator, model)
        class(radiation_generator_t), intent(inout) :: generator
        class(model_data_t), intent(in), target :: model
    end subroutine radiation_generator_setup_if_table

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_setup_if_table (generator, model)
        class(radiation_generator_t), intent(inout) :: generator
        class(model_data_t), intent(in), target :: model
        type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out

        allocate (pl_in(1), pl_out(1))

        pl_in(1) = generator%pl_in
        pl_out(1) = generator%pl_out

        call generator%if_table%init &
            (model, pl_in, pl_out, generator%constraints)
    end subroutine radiation_generator_setup_if_table

<Radiation generator: radiation generator: TBP>+≡
    generic :: reset_particle_content => reset_particle_content_pdg_array, &
        reset_particle_content_pdg_list

    procedure :: reset_particle_content_pdg_list => &
        radiation_generator_reset_particle_content_pdg_list
    procedure :: reset_particle_content_pdg_array => &
        radiation_generator_reset_particle_content_pdg_array

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_reset_particle_content_pdg_list (generator, pl)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_list_t), intent(in) :: pl
end subroutine radiation_generator_reset_particle_content_pdg_list
module subroutine radiation_generator_reset_particle_content_pdg_array (generator, pdg)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), intent(in), dimension(:) :: pdg
end subroutine radiation_generator_reset_particle_content_pdg_array

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_reset_particle_content_pdg_list (generator, pl)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_list_t), intent(in) :: pl
  generator%pl_out = pl
  generator%fs_gluon = pl%search_for_particle (GLUON)
  generator%fs_photon = pl%search_for_particle (PHOTON)
end subroutine radiation_generator_reset_particle_content_pdg_list

module subroutine radiation_generator_reset_particle_content_pdg_array (generator, pdg)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), intent(in), dimension(:) :: pdg
  type(pdg_list_t) :: pl
  integer :: i
  call pl%init (size (pdg))
  do i = 1, size (pdg)
    call pl%set (i, pdg(i))
  end do
  call generator%reset_particle_content (pl)
end subroutine radiation_generator_reset_particle_content_pdg_array

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: reset_reshuffle_list=> radiation_generator_reset_reshuffle_list

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_reset_reshuffle_list (generator)
  class(radiation_generator_t), intent(inout) :: generator
end subroutine radiation_generator_reset_reshuffle_list

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_reset_reshuffle_list (generator)
  class(radiation_generator_t), intent(inout) :: generator
  call generator%reshuffle_list%reset ()
end subroutine radiation_generator_reset_reshuffle_list

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: set_n => radiation_generator_set_n

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_set_n (generator, n_in, n_out, n_loops)
  class(radiation_generator_t), intent(inout) :: generator
  integer, intent(in) :: n_in, n_out, n_loops
end subroutine radiation_generator_set_n

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_set_n (generator, n_in, n_out, n_loops)
  class(radiation_generator_t), intent(inout) :: generator
  integer, intent(in) :: n_in, n_out, n_loops
  generator%n_tot = n_in + n_out + 1
  generator%n_in = n_in
  generator%n_out = n_out
  generator%n_loops = n_loops
end subroutine radiation_generator_set_n

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: set_constraints => radiation_generator_set_constraints

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_set_constraints &
  (generator, set_n_loop, set_mass_sum, &
   set_selected_particles, set_required_particles)
  class(radiation_generator_t), intent(inout), target :: generator
  logical, intent(in) :: set_n_loop
  logical, intent(in) :: set_mass_sum
  logical, intent(in) :: set_selected_particles
  logical, intent(in) :: set_required_particles
end subroutine radiation_generator_set_constraints

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_set_constraints &
  (generator, set_n_loop, set_mass_sum, &
   set_selected_particles, set_required_particles)
  class(radiation_generator_t), intent(inout), target :: generator
  logical, intent(in) :: set_n_loop
  logical, intent(in) :: set_mass_sum
  logical, intent(in) :: set_selected_particles
  logical, intent(in) :: set_required_particles
  logical :: set_no_photon_induced = .true.
  integer :: i, j, n, n_constraints
  type(pdg_list_t) :: pl_req, pl_insert
  type(pdg_list_t) :: pl_antiparticles
  type(pdg_array_t) :: pdg_gluon, pdg_photon
  type(pdg_array_t) :: pdg_add, pdg_tmp
  integer :: last_index
  integer :: n_new_particles, n_skip
  integer, dimension(:), allocatable :: i_skip
  integer :: n_nlo_correction_types

  n_nlo_correction_types = count ([generator%qcd_enabled, generator%qed_enabled])
  if (generator%is_photon) set_no_photon_induced = .false.

  allocate (i_skip (generator%n_tot))
  i_skip = -1

  n_constraints = 2 + count([set_n_loop, set_mass_sum, &
    set_selected_particles, set_required_particles, set_no_photon_induced])
  associate (constraints => generator%constraints)
    n = 1
    call constraints%init (n_constraints)
  end associate

```

```

call constraints%set (n, constrain_n_tot (generator%n_tot))
n = 2
call constraints%set (n, constrain_couplings (generator%qcd_enabled, &
generator%qed_enabled, n_nlo_correction_types))
n = n + 1
if (set_no_photon_induced) then
    call constraints%set (n, constrain_photon_induced_processes (generator%n_in))
    n = n + 1
end if
if (set_n_loop) then
    call constraints%set (n, constrain_n_loop(generator%n_loops))
    n = n + 1
end if
if (set_mass_sum) then
    call constraints%set (n, constrain_mass_sum(generator%mass_sum))
    n = n + 1
end if
if (set_required_particles) then
    if (generator%fs_gluon .or. generator%fs_photon) then
        do i = 1, generator%n_out
            pdg_tmp = generator%pl_out%get(i)
            if (pdg_tmp%search_for_particle (GLUON) &
                .or. pdg_tmp%search_for_particle (PHOTON)) then
                i_skip(i) = i
            end if
        end do

        n_skip = count (i_skip > 0)
        call pl_req%init (generator%n_out-n_skip)
    else
        call pl_req%init (generator%n_out)
    end if
    j = 1
    do i = 1, generator%n_out
        if (any (i == i_skip)) cycle
        call pl_req%set (j, generator%pl_out%get(i))
        j = j + 1
    end do
    call constraints%set (n, constrain_require (pl_req))
    n = n + 1
end if
if (set_selected_particles) then
    if (generator%only_final_state ) then
        call pl_insert%init (generator%n_out + n_nlo_correction_types)
        do i = 1, generator%n_out
            call pl_insert%set(i, generator%pl_out%get(i))
        end do
        last_index = generator%n_out + 1
    else
        call generator%pl_in%create_antiparticles (pl_antiparticles, n_new_particles)
        call pl_insert%init (generator%n_tot + n_new_particles &
            + n_nlo_correction_types)
        do i = 1, generator%n_in
            call pl_insert%set(i, generator%pl_in%get(i))
        end do
    end if
end if

```



```

end do
do i = 1, generator%n_out
  j = i + generator%n_in
  call pl_insert%set(j, generator%pl_out%get(i))
end do
do i = 1, n_new_particles
  j = i + generator%n_in + generator%n_out
  call pl_insert%set(j, pl_antiparticles%get(i))
end do
last_index = generator%n_tot + n_new_particles + 1
end if
pdg_gluon = GLUON; pdg_photon = PHOTON
if (generator%qcd_enabled) then
  pdg_add = pdg_gluon
  call pl_insert%set (last_index, pdg_add)
  last_index = last_index + 1
end if
if (generator%qed_enabled) then
  pdg_add = pdg_photon
  call pl_insert%set (last_index, pdg_add)
end if
call constraints%set (n, constrainSplittings (pl_insert, &
  generator%pl_excluded_gaugeSplittings))
end if
end associate
end subroutine radiation_generator_set_constraints

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: findSplittings => radiation_generator_findSplittings

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_findSplittings (generator)
  class(radiation_generator_t), intent(inout) :: generator
end subroutine radiation_generator_findSplittings

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_findSplittings (generator)
  class(radiation_generator_t), intent(inout) :: generator
  integer :: i
  type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out, pdg_tmp
  integer, dimension(:), allocatable :: reshuffle_list

  call generator%pl_in%create_pdg_array (pdg_in)
  call generator%pl_out%create_pdg_array (pdg_out)

  associate (if_table => generator%if_table)
    call if_table%radiate (generator%constraints, do_not_check_regular = .true.)

    do i = 1, if_table%get_length ()
      call if_table%get_pdg_out (i, pdg_tmp)
      if (size (pdg_tmp) == generator%n_tot) then
        call pdg_reshuffle (pdg_out, pdg_tmp, reshuffle_list)
        call generator%reshuffle_list%append (reshuffle_list)
      end if
    end do
  end associate
end subroutine radiation_generator_findSplittings

```

```

end associate

contains

subroutine pdg_reshuffle (pdg_born, pdg_real, list)
  type(pdg_array_t), intent(in), dimension(:) :: pdg_born, pdg_real
  integer, intent(out), dimension(:), allocatable :: list
  type(pdg_sorter_t), dimension(:), allocatable :: sort_born
  type(pdg_sorter_t), dimension(:), allocatable :: sort_real
  integer :: i_min, n_in, n_born, n_real
  integer :: ib, ir

  n_in = generator%n_in
  n_born = size (pdg_born)
  n_real = size (pdg_real)
  allocate (list (n_real - n_in))
  allocate (sort_born (n_born))
  allocate (sort_real (n_real - n_in))
  sort_born%pdg = pdg_born%get ( )
  sort_real%pdg = pdg_real(n_in + 1 : n_real)%get()
  do ib = 1, n_born
    if (any (sort_born(ib)%pdg == sort_real%pdg)) &
      call associate_born_indices (sort_born(ib), sort_real, ib, n_real)
  end do
  i_min = maxval (sort_real%associated_born) + 1
  do ir = 1, n_real - n_in
    if (sort_real(ir)%associated_born == 0) then
      sort_real(ir)%associated_born = i_min
      i_min = i_min + 1
    end if
  end do
  list = sort_real%associated_born
end subroutine pdg_reshuffle

subroutine associate_born_indices (sort_born, sort_real, ib, n_real)
  type(pdg_sorter_t), intent(in) :: sort_born
  type(pdg_sorter_t), intent(inout), dimension(:) :: sort_real
  integer, intent(in) :: ib, n_real
  integer :: ir
  do ir = 1, n_real - generator%n_in
    if (sort_born%pdg == sort_real(ir)%pdg &
      .and..not. sort_real(ir)%checked) then
      sort_real(ir)%associated_born = ib
      sort_real(ir)%checked = .true.
    exit
  end if
end do
end subroutine associate_born_indices
end subroutine radiation_generator_findSplittings

```

(Radiation generator: radiation generator: TBP)+≡
 procedure :: generate_real_particle_strings &
 => radiation_generator_generate_real_particle_strings

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_generate_real_particle_strings &
  (generator, prt_tot_in, prt_tot_out)
  class(radiation_generator_t), intent(inout) :: generator
  type(string_t), intent(out), dimension(:), allocatable :: prt_tot_in, prt_tot_out
end subroutine radiation_generator_generate_real_particle_strings

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_generate_real_particle_strings &
  (generator, prt_tot_in, prt_tot_out)
  class(radiation_generator_t), intent(inout) :: generator
  type(string_t), intent(out), dimension(:), allocatable :: prt_tot_in, prt_tot_out
  type(prt_array_t), dimension(:), allocatable :: prt_in, prt_out
  type(prt_array_t), dimension(:), allocatable :: prt_out0, prt_in0
  type(pdg_array_t), dimension(:), allocatable :: pdg_tmp, pdg_out, pdg_in
  type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out
  type(prt_array_t) :: prt_out0_tmp, prt_in0_tmp
  integer :: i, j
  integer, dimension(:), allocatable :: reshuffle_list_local
  type(reshuffle_list_t) :: reshuffle_list
  integer :: flv
  type(string_t), dimension(:), allocatable :: buf
  integer :: i_buf

  flv = 0
  allocate (prt_in0(0), prt_out0(0))
  associate (if_table => generator%if_table)
    do i = 1, if_table%get_length ()
      call if_table%get_pdg_out (i, pdg_tmp)
      if (size (pdg_tmp) == generator%n_tot) then
        call if_table%get_particle_string (i, &
          prt_in0_tmp%prt, prt_out0_tmp%prt)
        prt_in0 = [prt_in0, prt_in0_tmp]
        prt_out0 = [prt_out0, prt_out0_tmp]
        flv = flv + 1
      end if
    end do
  end associate

  allocate (prt_in(size (prt_in0)), prt_out(size (prt_out0)))
  do i = 1, flv
    allocate (prt_in(i)%prt (generator%n_in))
    allocate (prt_out(i)%prt (generator%n_tot - generator%n_in))
  end do
  allocate (prt_tot_in (generator%n_in))
  allocate (prt_tot_out (generator%n_tot - generator%n_in))
  allocate (buf (generator%n_tot))
  buf = ""

  do j = 1, flv
    do i = 1, generator%n_in
      prt_in(j)%prt(i) = prt_in0(j)%prt(i)
      call fill_buffer (buf(i), prt_in0(j)%prt(i))
    end do
  end do

```

```

prt_tot_in = buf(1 : generator%n_in)

do j = 1, flv
  allocate (reshuffle_list_local (size (generator%reshuffle_list%get(j))))
  reshuffle_list_local = generator%reshuffle_list%get(j)
  do i = 1, size (reshuffle_list_local)
    prt_out(j)%prt(reshuffle_list_local(i)) = prt_out0(j)%prt(i)
    i_buf = reshuffle_list_local(i) + generator%n_in
    call fill_buffer (buf(i_buf), &
      prt_out(j)%prt(reshuffle_list_local(i)))
  end do
  !!! Need to deallocate here because in the next iteration the reshuffling
  !!! list can have a different size
  deallocate (reshuffle_list_local)
end do
prt_tot_out = buf(generator%n_in + 1 : generator%n_tot)
if (debug2_active (D_CORE)) then
  print *, 'Generated initial state: '
  do i = 1, size (prt_tot_in)
    print *, char (prt_tot_in(i))
  end do
  print *, 'Generated final state: '
  do i = 1, size (prt_tot_out)
    print *, char (prt_tot_out(i))
  end do
end if
end if

```

contains

```

subroutine fill_buffer (buffer, particle)
  type(string_t), intent(inout) :: buffer
  type(string_t), intent(in) :: particle
  logical :: particle_present
  if (len (buffer) > 0) then
    particle_present = check_for_substring (char(buffer), particle)
    if (.not. particle_present) buffer = buffer // ":" // particle
  else
    buffer = buffer // particle
  end if
end subroutine fill_buffer

function check_for_substring (buffer, substring) result (exist)
  character(len=*), intent(in) :: buffer
  type(string_t), intent(in) :: substring
  character(len=50) :: buffer_internal
  logical :: exist
  integer :: i_first, i_last
  exist = .false.
  i_first = 1; i_last = 1
  do
    if (buffer(i_last:i_last) == ":") then
      buffer_internal = buffer (i_first : i_last - 1)
      if (buffer_internal == char (substring)) then

```

```

        exist = .true.
        exit
    end if
    i_first = i_last + 1; i_last = i_first + 1
    if (i_last > len(buffer)) exit
else if (i_last == len(buffer)) then
    buffer_internal = buffer (i_first : i_last)
    exist = buffer_internal == char (substring)
    exit
else
    i_last = i_last + 1
    if (i_last > len(buffer)) exit
end if
end do
end function check_for_substring
end subroutine radiation_generator_generate_real_particle_strings

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: contains_emissions => radiation_generator_contains_emissions

```

<Radiation generator: sub interfaces>+≡

```

module function radiation_generator_contains_emissions (generator) result (has_em)
    logical :: has_em
    class(radiation_generator_t), intent(in) :: generator
end function radiation_generator_contains_emissions

```

<Radiation generator: procedures>+≡

```

module function radiation_generator_contains_emissions (generator) result (has_em)
    logical :: has_em
    class(radiation_generator_t), intent(in) :: generator
    has_em = .not. generator%reshuffle_list%is_empty ()
end function radiation_generator_contains_emissions

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: generate => radiation_generator_generate

```

<Radiation generator: sub interfaces>+≡

```

module subroutine radiation_generator_generate (generator, prt_in, prt_out)
    class(radiation_generator_t), intent(inout) :: generator
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
end subroutine radiation_generator_generate

```

<Radiation generator: procedures>+≡

```

module subroutine radiation_generator_generate (generator, prt_in, prt_out)
    class(radiation_generator_t), intent(inout) :: generator
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
    call generator%findSplittings ()
    call generator%generate_real_particle_strings (prt_in, prt_out)
end subroutine radiation_generator_generate

```

<Radiation generator: radiation generator: TBP>+≡

```

procedure :: generate_multiple => radiation_generator_generate_multiple

```

```

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_generate_multiple &
        (generator, max_multiplicity, model)
        class(radiation_generator_t), intent(inout) :: generator
        integer, intent(in) :: max_multiplicity
        class(model_data_t), intent(in), target :: model
    end subroutine radiation_generator_generate_multiple

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_generate_multiple &
        (generator, max_multiplicity, model)
        class(radiation_generator_t), intent(inout) :: generator
        integer, intent(in) :: max_multiplicity
        class(model_data_t), intent(in), target :: model
        if (max_multiplicity <= generator%n_out) &
            call msg_fatal ("GKS states: Multiplicity is not large enough!")
        call generator%first_emission (model)
        call generator%reset_resuffle_list ()
        if (max_multiplicity - generator%n_out > 1) &
            call generator%append_emissions (max_multiplicity, model)
    end subroutine radiation_generator_generate_multiple

<Radiation generator: radiation generator: TBP>+≡
    procedure :: first_emission => radiation_generator_first_emission

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_first_emission (generator, model)
        class(radiation_generator_t), intent(inout) :: generator
        class(model_data_t), intent(in), target :: model
    end subroutine radiation_generator_first_emission

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_first_emission (generator, model)
        class(radiation_generator_t), intent(inout) :: generator
        class(model_data_t), intent(in), target :: model
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        call generator%setup_if_table (model)
        call generator%generate (prt_in, prt_out)
        call generator%prt_queue%null ()
        call generator%prt_queue%append (prt_out)
    end subroutine radiation_generator_first_emission

<Radiation generator: radiation generator: TBP>+≡
    procedure :: append_emissions => radiation_generator_append_emissions

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_append_emissions &
        (generator, max_multiplicity, model)
        class(radiation_generator_t), intent(inout) :: generator
        integer, intent(in) :: max_multiplicity
        class(model_data_t), intent(in), target :: model
    end subroutine radiation_generator_append_emissions

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_append_emissions &
        (generator, max_multiplicity, model)

```

```

class(radiation_generator_t), intent(inout) :: generator
integer, intent(in) :: max_multiplicity
class(model_data_t), intent(in), target :: model
type(string_t), dimension(:), allocatable :: prt_fetched
type(string_t), dimension(:), allocatable :: prt_in
type(string_t), dimension(:), allocatable :: prt_out
type(pdg_array_t), dimension(:), allocatable :: pdg_new_out
integer :: current_multiplicity, i, j, n_longest_length
type(prt_table_t), dimension(:), allocatable :: prt_table_out
do
    call generator%prt_queue%get (prt_fetched)
    current_multiplicity = size (prt_fetched)
    if (current_multiplicity == max_multiplicity) exit
    call create_pdg_array (prt_fetched, model, &
        pdg_new_out)
    call generator%reset_particle_content (pdg_new_out)
    call generator%set_n (2, current_multiplicity, 0)
    call generator%set_constraints (.false., .false., .true., .true.)
    call generator%setup_if_table (model)
    call generator%generate (prt_in, prt_out)
    n_longest_length = get_length_of_longest_tuple (prt_out)
    call separate_particles (prt_out, prt_table_out)
    do i = 1, n_longest_length
        if (.not. any (prt_table_out(i)%prt == " ")) then
            call sort_prt (prt_table_out(i)%prt, model)
            if (.not. generator%prt_queue%contains (prt_table_out(i)%prt)) then
                call generator%prt_queue%append (prt_table_out(i)%prt)
            end if
        end if
    end do
    call generator%reset_resuffle_list ()
end do

contains
subroutine separate_particles (prt, prt_table)
    type(string_t), intent(in), dimension(:) :: prt
    type(string_t), dimension(:), allocatable :: prt_tmp
    type(prt_table_t), intent(out), dimension(:), allocatable :: prt_table
    integer :: i, j
    logical, dimension(:), allocatable :: tuples_occured
    allocate (prt_table (n_longest_length))
    do i = 1, n_longest_length
        allocate (prt_table(i)%prt (size (prt)))
    end do
    allocate (tuples_occured (size (prt)))
    do j = 1, size (prt)
        call split_string (prt(j), var_str (":"), prt_tmp)
        do i = 1, n_longest_length
            if (i <= size (prt_tmp)) then
                prt_table(i)%prt(j) = prt_tmp(i)
            else
                prt_table(i)%prt(j) = " "
            end if
        end do
    end do
end do

```

```

        if (n_longest_length > 1) &
            tuples_occured(j) = prt_table(1)%prt(j) /= " " &
            .and. prt_table(2)%prt(j) /= " "
    end do
    if (any (tuples_occured)) then
        do j = 1, size (tuples_occured)
            if (.not. tuples_occured(j)) then
                do i = 2, n_longest_length
                    prt_table(i)%prt(j) = prt_table(1)%prt(j)
                end do
            end if
        end do
    end if
end subroutine separate_particles

function get_length_of_longest_tuple (prt) result (longest_length)
    type(string_t), intent(in), dimension(:) :: prt
    integer :: longest_length, i
    type(prt_table_t), dimension(:), allocatable :: prt_table
    allocate (prt_table (size (prt)))
    longest_length = 0
    do i = 1, size (prt)
        call split_string (prt(i), var_str (":"), prt_table(i)%prt)
        if (size (prt_table(i)%prt) > longest_length) &
            longest_length = size (prt_table(i)%prt)
    end do
end function get_length_of_longest_tuple
end subroutine radiation_generator_append_emissions

<Radiation generator: radiation generator: TBP>+≡
    procedure :: reset_queue => radiation_generator_reset_queue

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_reset_queue (generator)
        class(radiation_generator_t), intent(inout) :: generator
    end subroutine radiation_generator_reset_queue

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_reset_queue (generator)
        class(radiation_generator_t), intent(inout) :: generator
        call generator%prt_queue%reset ()
    end subroutine radiation_generator_reset_queue

<Radiation generator: radiation generator: TBP>+≡
    procedure :: get_n_gks_states => radiation_generator_get_n_gks_states

<Radiation generator: sub interfaces>+≡
    module function radiation_generator_get_n_gks_states (generator) result (n)
        class(radiation_generator_t), intent(in) :: generator
        integer :: n
    end function radiation_generator_get_n_gks_states

<Radiation generator: procedures>+≡
    module function radiation_generator_get_n_gks_states (generator) result (n)
        class(radiation_generator_t), intent(in) :: generator
        integer :: n

```



```

        n = generator%prt_queue%n_lists
    end function radiation_generator_get_n_gks_states

<Radiation generator: radiation generator: TBP>+≡
    procedure :: get_next_state => radiation_generator_get_next_state

<Radiation generator: sub interfaces>+≡
    module function radiation_generator_get_next_state (generator) result (prt_string)
        class(radiation_generator_t), intent(inout) :: generator
        type(string_t), dimension(:), allocatable :: prt_string
    end function radiation_generator_get_next_state

<Radiation generator: procedures>+≡
    module function radiation_generator_get_next_state (generator) result (prt_string)
        class(radiation_generator_t), intent(inout) :: generator
        type(string_t), dimension(:), allocatable :: prt_string
        call generator%prt_queue%get (prt_string)
    end function radiation_generator_get_next_state

<Radiation generator: radiation generator: TBP>+≡
    procedure :: get_emitter_indices => radiation_generator_get_emitter_indices

<Radiation generator: sub interfaces>+≡
    module subroutine radiation_generator_get_emitter_indices (generator, indices)
        class(radiation_generator_t), intent(in) :: generator
        integer, dimension(:), allocatable, intent(out) :: indices
    end subroutine radiation_generator_get_emitter_indices

<Radiation generator: procedures>+≡
    module subroutine radiation_generator_get_emitter_indices (generator, indices)
        class(radiation_generator_t), intent(in) :: generator
        integer, dimension(:), allocatable, intent(out) :: indices
        type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
        integer, dimension(:), allocatable :: flv_in, flv_out
        integer, dimension(:), allocatable :: emitters
        integer :: i, j
        integer :: n_in, n_out

        call generator%pl_in%create_pdg_array (pdg_in)
        call generator%pl_out%create_pdg_array (pdg_out)

        n_in = size (pdg_in); n_out = size (pdg_out)
        allocate (flv_in (n_in), flv_out (n_out))
        forall (i=1:n_in) flv_in(i) = pdg_in(i)%get()
        forall (i=1:n_out) flv_out(i) = pdg_out(i)%get()

        call generator%if_table%get_emitters (generator%constraints, emitters)
        allocate (indices (size (emitters)))

        j = 1
        do i = 1, n_in + n_out
            if (i <= n_in) then
                if (any (flv_in(i) == emitters)) then
                    indices (j) = i
                    j = j + 1
                end if
            end if
        end do
    end subroutine radiation_generator_get_emitter_indices

```

```

        end if
    else
        if (any (flv_out(i-n_in) == emitters)) then
            indices (j) = i
            j = j + 1
        end if
    end if
end do
end subroutine radiation_generator_get_emitter_indices

```

<Radiation generator: radiation generator: TBP>+≡

```

    procedure :: get_raw_states => radiation_generator_get_raw_states

```

<Radiation generator: sub interfaces>+≡

```

    module function radiation_generator_get_raw_states (generator) result (raw_states)
        class(radiation_generator_t), intent(in), target :: generator
        integer, dimension(:,:), allocatable :: raw_states
    end function radiation_generator_get_raw_states

```

<Radiation generator: procedures>+≡

```

    module function radiation_generator_get_raw_states (generator) result (raw_states)
        class(radiation_generator_t), intent(in), target :: generator
        integer, dimension(:,:), allocatable :: raw_states
        type(pdg_states_t), pointer :: state
        integer :: n_states, n_particles
        integer :: i_state
        integer :: j
        state => generator%pdg_raw
        n_states = generator%pdg_raw%get_n_states ()
        n_particles = size (generator%pdg_raw%pdg)
        allocate (raw_states (n_particles, n_states))
        do i_state = 1, n_states
            do j = 1, n_particles
                raw_states (j, i_state) = state%pdg(j)%get ()
            end do
            state => state%next
        end do
    end function radiation_generator_get_raw_states

```

<Radiation generator: radiation generator: TBP>+≡

```

    procedure :: save_born_raw => radiation_generator_save_born_raw

```

<Radiation generator: sub interfaces>+≡

```

    module subroutine radiation_generator_save_born_raw (generator, pdg_in, pdg_out)
        class(radiation_generator_t), intent(inout) :: generator
        type(pdg_array_t), dimension(:), allocatable, intent(in) :: pdg_in, pdg_out
    end subroutine radiation_generator_save_born_raw

```

<Radiation generator: procedures>+≡

```

    module subroutine radiation_generator_save_born_raw (generator, pdg_in, pdg_out)
        class(radiation_generator_t), intent(inout) :: generator
        type(pdg_array_t), dimension(:), allocatable, intent(in) :: pdg_in, pdg_out
        generator%pdg_in_born = pdg_in
        generator%pdg_out_born = pdg_out
    end subroutine radiation_generator_save_born_raw

```

```

<Radiation generator: radiation generator: TBP>+≡
  procedure :: get_born_raw => radiation_generator_get_born_raw

<Radiation generator: sub interfaces>+≡
  module function radiation_generator_get_born_raw (generator) result (flv_born)
    class(radiation_generator_t), intent(in) :: generator
    integer, dimension(:,:), allocatable :: flv_born
  end function radiation_generator_get_born_raw

<Radiation generator: procedures>+≡
  module function radiation_generator_get_born_raw (generator) result (flv_born)
    class(radiation_generator_t), intent(in) :: generator
    integer, dimension(:,:), allocatable :: flv_born
    integer :: i_part, n_particles
    n_particles = size (generator%pdg_in_born) + size (generator%pdg_out_born)
    allocate (flv_born (n_particles, 1))
    flv_born(1,1) = generator%pdg_in_born(1)%get ()
    flv_born(2,1) = generator%pdg_in_born(2)%get ()
    do i_part = 3, n_particles
      flv_born(i_part, 1) = generator%pdg_out_born(i_part-2)%get ()
    end do
  end function radiation_generator_get_born_raw

```

28.2.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<radiation_generator_ut.f90>≡
  <File header>

  module radiation_generator_ut
    use unit_tests
    use radiation_generator_uti

    <Standard module head>

    <Radiation generator: public test>

    contains

    <Radiation generator: test driver>

  end module radiation_generator_ut

<radiation_generator_uti.f90>≡
  <File header>

  module radiation_generator_uti

    <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use pdg_arrays
    use models
    use kinds, only: default

```

```

    use radiation_generator

    <Standard module head>

    <Radiation generator: test declarations>

contains

    <Radiation generator: tests>

    <Radiation generator: test auxiliary>

end module radiation_generator_util

API: driver for the unit tests below.
<Radiation generator: public test>≡
    public :: radiation_generator_test

<Radiation generator: test driver>≡
    subroutine radiation_generator_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        call test(radiation_generator_1, "radiation_generator_1", &
            "Test the generator of N+1-particle flavor structures in QCD", &
            u, results)
        call test(radiation_generator_2, "radiation_generator_2", &
            "Test multiple splittings in QCD", &
            u, results)
        call test(radiation_generator_3, "radiation_generator_3", &
            "Test the generator of N+1-particle flavor structures in QED", &
            u, results)
        call test(radiation_generator_4, "radiation_generator_4", &
            "Test multiple splittings in QED", &
            u, results)
    end subroutine radiation_generator_test

<Radiation generator: test declarations>≡
    public :: radiation_generator_1

<Radiation generator: tests>≡
    subroutine radiation_generator_1 (u)
        integer, intent(in) :: u
        type(radiation_generator_t) :: generator
        type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(model_t), pointer :: model => null ()

        write (u, "(A)") "* Test output: radiation_generator_1"
        write (u, "(A)") "* Purpose: Create N+1-particle flavor structures &
            &from predefined N-particle flavor structures"
        write (u, "(A)") "* One additional strong coupling, no additional electroweak coupling"
        write (u, "(A)")
        write (u, "(A)") "* Loading radiation model: SM.mdl"

```

```

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)
write (u, "(A)") "* Success"

allocate (pdg_in (2))
pdg_in(1) = 11; pdg_in(2) = -11

write (u, "(A)") "* Start checking processes"
call write_separator (u)

write (u, "(A)") "* Process 1: Top pair-production with additional gluon"
allocate (pdg_out(3))
pdg_out(1) = 6; pdg_out(2) = -6; pdg_out(3) = 21
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 2: Top pair-production with additional jet"
allocate (pdg_out(3))
pdg_out(1) = 6; pdg_out(2) = -6; pdg_out(3) = [-1,1,-2,2,-3,3,-4,4,-5,5,21]
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 3: Quark-antiquark production"
allocate (pdg_out(2))
pdg_out(1) = 2; pdg_out(2) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 4: Quark-antiquark production with additional gluon"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 21
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 5: Z + jets"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 23
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 6: Top Decay"
allocate (pdg_out(4))
pdg_out(1) = 24; pdg_out(2) = -24
pdg_out(3) = 5; pdg_out(4) = -5
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 7: Production of four quarks"
allocate (pdg_out(4))
pdg_out(1) = 2; pdg_out(2) = -2;

```

```

pdg_out(3) = 2; pdg_out(4) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 8: Drell-Yan lepto-production"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 2; pdg_in(2) = -2
pdg_out(1) = 11; pdg_out(2) = -11
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 9: WZ production at hadron-colliders"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 1; pdg_in(2) = -2
pdg_out(1) = -24; pdg_out(2) = 23
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

contains
subroutine test_process (generator, pdg_in, pdg_out, u, include_initial_state)
  type(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), dimension(:), intent(in) :: pdg_in, pdg_out
  integer, intent(in) :: u
  logical, intent(in), optional :: include_initial_state
  type(string_t), dimension(:), allocatable :: prt_strings_in
  type(string_t), dimension(:), allocatable :: prt_strings_out
  type(pdg_array_t), dimension(10) :: pdg_excluded
  logical :: yorn
  yorn = .false.
  pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]
  if (present (include_initial_state)) yorn = include_initial_state
  write (u, "(A)") "* Leading order: "
  write (u, "(A)", advance = 'no') '* Incoming: '
  call write_pdg_array (pdg_in, u)
  write (u, "(A)", advance = 'no') '* Outgoing: '
  call write_pdg_array (pdg_out, u)

  call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .true., qed = .false.)
  call generator%set_n (2, size(pdg_out), 0)
  if (yorn) call generator%set_initial_state_emissions ()
  call generator%set_constraints (.false., .false., .true., .true.)
  call generator%setup_if_table (model)
  call generator%generate (prt_strings_in, prt_strings_out)
  write (u, "(A)") "* Additional radiation: "
  write (u, "(A)") "* Incoming: "
  call write_particle_string (prt_strings_in, u)
  write (u, "(A)") "* Outgoing: "
  call write_particle_string (prt_strings_out, u)
  call write_separator(u)
  call generator%reset_resuffle_list ()
end subroutine test_process

end subroutine radiation_generator_1

```

```

<Radiation generator: test declarations>+≡
    public :: radiation_generator_2

<Radiation generator: tests>+≡
    subroutine radiation_generator_2 (u)
        integer, intent(in) :: u
        type(radiation_generator_t) :: generator
        type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
        type(pdg_array_t), dimension(:), allocatable :: pdg_excluded
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(model_t), pointer :: model => null ()
        integer, parameter :: max_multiplicity = 10
        type(string_t), dimension(:), allocatable :: prt_last

        write (u, "(A)") "* Test output: radiation_generator_2"
        write (u, "(A)") "* Purpose: Test the repeated application of &
            &a radiation generator splitting in QCD"
        write (u, "(A)") "* Only Final state emissions! "
        write (u, "(A)")
        write (u, "(A)") "* Loading radiation model: SM.mdl"

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM"), var_str ("SM.mdl"), &
            os_data, model)
        write (u, "(A)") "* Success"

        allocate (pdg_in (2))
        pdg_in(1) = 11; pdg_in(2) = -11
        allocate (pdg_out(2))
        pdg_out(1) = 2; pdg_out(2) = -2
        allocate (pdg_excluded (10))
        pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]

        write (u, "(A)") "* Leading order"
        write (u, "(A)", advance = 'no') "* Incoming: "
        call write_pdg_array (pdg_in, u)
        write (u, "(A)", advance = 'no') "* Outgoing: "
        call write_pdg_array (pdg_out, u)

        call generator%init (pdg_in, pdg_out, &
            pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .true., qed = .false.)
        call generator%set_n (2, 2, 0)
        call generator%set_constraints (.false., .false., .true., .true.)

        call write_separator (u)
        write (u, "(A)") "Generate higher-multiplicity states"
        write (u, "(A,IO)") "Desired multiplicity: ", max_multiplicity
        call generator%generate_multiple (max_multiplicity, model)
        call generator%prt_queue%write (u)
        call write_separator (u)

```

```

write (u, "(A,IO)") "Number of higher-multiplicity states: ", generator%prt_queue%n_lists

write (u, "(A)") "Check that no particle state occurs twice or more"
if (.not. generator%prt_queue%check_for_same_prt_strings()) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
call write_separator (u)
write (u, "(A,IO,A)") "Check that there are ", max_multiplicity, " particles in the last entry"
call generator%prt_queue%get_last (prt_last)
if (size (prt_last) == max_multiplicity) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
end subroutine radiation_generator_2

```

<Radiation generator: test declarations>+≡

```
public :: radiation_generator_3
```

<Radiation generator: tests>+≡

```

subroutine radiation_generator_3 (u)
    integer, intent(in) :: u
    type(radiation_generator_t) :: generator
    type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model => null ()

    write (u, "(A)") "* Test output: radiation_generator_3"
    write (u, "(A)") "* Purpose: Create N+1-particle flavor structures &
        &from predefined N-particle flavor structures"
    write (u, "(A)") "* One additional electroweak coupling, no additional strong coupling"
    write (u, "(A)")
    write (u, "(A)") "* Loading radiation model: SM.mdl"

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
        (var_str ("SM"), var_str ("SM.mdl"), &
        os_data, model)
    write (u, "(A)") "* Success"

    allocate (pdg_in (2))
    pdg_in(1) = 11; pdg_in(2) = -11

    write (u, "(A)") "* Start checking processes"
    call write_separator (u)

    write (u, "(A)") "* Process 1: Tau pair-production with additional photon"
    allocate (pdg_out(3))
    pdg_out(1) = 15; pdg_out(2) = -15; pdg_out(3) = 22
    call test_process (generator, pdg_in, pdg_out, u)

```



```

deallocate (pdg_out)

write (u, "(A)") "* Process 2: Tau pair-production with additional leptons or photon"
allocate (pdg_out(3))
pdg_out(1) = 15; pdg_out(2) = -15; pdg_out(3) = [-13, 13, 22]
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 3: Electron-positron production"
allocate (pdg_out(2))
pdg_out(1) = 11; pdg_out(2) = -11
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 4: Quark-antiquark production with additional photon"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 22
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 5: Z + jets "
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 23
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 6: W + jets"
allocate (pdg_out(3))
pdg_out(1) = 1; pdg_out(2) = -2; pdg_out(3) = -24
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 7: Top Decay"
allocate (pdg_out(4))
pdg_out(1) = 24; pdg_out(2) = -24
pdg_out(3) = 5; pdg_out(4) = -5
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 8: Production of four quarks"
allocate (pdg_out(4))
pdg_out(1) = 2; pdg_out(2) = -2;
pdg_out(3) = 2; pdg_out(4) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 9: Neutrino pair-production"
allocate (pdg_out(2))
pdg_out(1) = 12; pdg_out(2) = -12
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 10: Drell-Yan lepto-production"
allocate (pdg_in (2)); allocate (pdg_out (2))

```

```

pdg_in(1) = 2; pdg_in(2) = -2
pdg_out(1) = 11; pdg_out(2) = -11
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 11: WZ production at hadron-colliders"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 1; pdg_in(2) = -2
pdg_out(1) = -24; pdg_out(2) = 23
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 12: Positron-neutrino production"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = -1; pdg_in(2) = 2
pdg_out(1) = -11; pdg_out(2) = 12
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out); deallocate (pdg_in)

contains
subroutine test_process (generator, pdg_in, pdg_out, u, include_initial_state)
  type(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), dimension(:), intent(in) :: pdg_in, pdg_out
  integer, intent(in) :: u
  logical, intent(in), optional :: include_initial_state
  type(string_t), dimension(:), allocatable :: prt_strings_in
  type(string_t), dimension(:), allocatable :: prt_strings_out
  type(pdg_array_t), dimension(10) :: pdg_excluded
  logical :: yorn
  yorn = .false.
  pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]
  if (present (include_initial_state)) yorn = include_initial_state
  write (u, "(A)") "* Leading order: "
  write (u, "(A)", advance = 'no') '* Incoming: '
  call write_pdg_array (pdg_in, u)
  write (u, "(A)", advance = 'no') '* Outgoing: '
  call write_pdg_array (pdg_out, u)

  call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .false., qed = .true.)
  call generator%set_n (2, size(pdg_out), 0)
  if (yorn) call generator%set_initial_state_emissions ()
  call generator%set_constraints (.false., .false., .true., .true.)
  call generator%setup_if_table (model)
  call generator%generate (prt_strings_in, prt_strings_out)
  write (u, "(A)") "* Additional radiation: "
  write (u, "(A)") "* Incoming: "
  call write_particle_string (prt_strings_in, u)
  write (u, "(A)") "* Outgoing: "
  call write_particle_string (prt_strings_out, u)
  call write_separator(u)
  call generator%reset_resuffle_list ()
end subroutine test_process

```

```
end subroutine radiation_generator_3
```

```
<Radiation generator: test declarations>+≡
```

```
public :: radiation_generator_4
```

```
<Radiation generator: tests>+≡
```

```
subroutine radiation_generator_4 (u)
  integer, intent(in) :: u
  type(radiation_generator_t) :: generator
  type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
  type(pdg_array_t), dimension(:), allocatable :: pdg_excluded
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(model_t), pointer :: model => null ()
  integer, parameter :: max_multiplicity = 10
  type(string_t), dimension(:), allocatable :: prt_last

  write (u, "(A)") "* Test output: radiation_generator_4"
  write (u, "(A)") "* Purpose: Test the repeated application of &
    &a radiation generator splitting in QED"
  write (u, "(A)") "* Only Final state emissions! "
  write (u, "(A)")
  write (u, "(A)") "* Loading radiation model: SM.mdl"

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
     os_data, model)
  write (u, "(A)") "* Success"

  allocate (pdg_in (2))
  pdg_in(1) = 2; pdg_in(2) = -2
  allocate (pdg_out(2))
  pdg_out(1) = 11; pdg_out(2) = -11
  allocate ( pdg_excluded (14))
  pdg_excluded = [1, -1, 2, -2, 3, -3, 4, -4, 5, -5, 6, -6, 15, -15]

  write (u, "(A)") "* Leading order"
  write (u, "(A)", advance = 'no') "* Incoming: "
  call write_pdg_array (pdg_in, u)
  write (u, "(A)", advance = 'no') "* Outgoing: "
  call write_pdg_array (pdg_out, u)

  call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .false., qed = .true.)
  call generator%set_n (2, 2, 0)
  call generator%set_constraints (.false., .false., .true., .true.)

  call write_separator (u)
  write (u, "(A)") "Generate higher-multiplicity states"
  write (u, "(A,I0)") "Desired multiplicity: ", max_multiplicity
  call generator%generate_multiple (max_multiplicity, model)
  call generator%prt_queue%write (u)
```

```

call write_separator (u)
write (u, "(A,IO)") "Number of higher-multiplicity states: ", generator%prt_queue%n_lists

write (u, "(A)") "Check that no particle state occurs twice or more"
if (.not. generator%prt_queue%check_for_same_prt_strings()) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
call write_separator (u)
write (u, "(A,IO,A)") "Check that there are ", max_multiplicity, " particles in the last entry"
call generator%prt_queue%get_last (prt_last)
if (size (prt_last) == max_multiplicity) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
end subroutine radiation_generator_4

```

28.3 Sindarin Expression Implementation

This module defines expressions of all kinds, represented in a tree structure, for repeated evaluation. This provides an implementation of the `expr_base` abstract type.

We have two flavors of expressions: one with particles and one without particles. The latter version is used for defining cut/selection criteria and for online analysis.

```
(eval_trees.f90)≡
  <File header>

  module eval_trees

    use, intrinsic :: iso_c_binding !NODEP!
    <Use kinds>
    <Use strings>
    use ifiles
    use lexers
    use syntax_rules
    use parser
    use pdg_arrays
    use subevents
    use var_base
    use expr_base
    use variables

    <Standard module head>

    <Eval trees: public>

    <Eval trees: types>

    <Eval trees: interfaces>

    <Eval trees: variables>

    interface
    <Eval trees: sub interfaces>
    end interface

    contains

    <Eval trees: main procedures>

  end module eval_trees

(eval_trees_sub.f90)≡
  <File header>

  submodule (eval_trees) eval_trees_s

    use io_units
    use constants, only: DEGREE, IMAGO, PI
    use format_defs, only: FMT_19
```



```

type(string_t) :: tag
integer :: type = EN_UNKNOWN
integer :: result_type = V_NONE
type(var_list_t), pointer :: var_list => null ()
type(string_t) :: var_name
logical, pointer :: value_is_known => null ()
logical,          pointer :: lval => null ()
integer,          pointer :: ival => null ()
real(default),    pointer :: rval => null ()
complex(default), pointer :: cval => null ()
type(subevt_t),   pointer :: pval => null ()
type(pdg_array_t), pointer :: aval => null ()
type(string_t),   pointer :: sval => null ()
type(eval_node_t), pointer :: arg0 => null ()
type(eval_node_t), pointer :: arg1 => null ()
type(eval_node_t), pointer :: arg2 => null ()
type(eval_node_t), pointer :: arg3 => null ()
type(eval_node_t), pointer :: arg4 => null ()
procedure(obs_unary_int),  nopass, pointer :: obs1_int  => null ()
procedure(obs_unary_real), nopass, pointer :: obs1_real => null ()
procedure(obs_binary_int), nopass, pointer :: obs2_int  => null ()
procedure(obs_binary_real), nopass, pointer :: obs2_real => null ()
procedure(obs_sev_int),   nopass, pointer :: obsev_int  => null ()
procedure(obs_sev_real),  nopass, pointer :: obsev_real => null ()
integer, pointer :: prt_type => null ()
integer, pointer :: index => null ()
real(default), pointer :: tolerance => null ()
integer, pointer :: jet_algorithm => null ()
real(default), pointer :: jet_r => null ()
real(default), pointer :: jet_p => null ()
real(default), pointer :: jet_ycut => null ()
real(default), pointer :: jet_dcut => null ()
real(default), pointer :: photon_iso_eps => null ()
real(default), pointer :: photon_iso_n => null ()
real(default), pointer :: photon_iso_r0 => null ()
real(default), pointer :: photon_rec_r0 => null ()
type(prt_t), pointer :: prt1 => null ()
type(prt_t), pointer :: prt2 => null ()
procedure(unary_log),  nopass, pointer :: op1_log  => null ()
procedure(unary_int),  nopass, pointer :: op1_int  => null ()
procedure(unary_real), nopass, pointer :: op1_real => null ()
procedure(unary_cmplx), nopass, pointer :: op1_cmplx => null ()
procedure(unary_pdg),  nopass, pointer :: op1_pdg  => null ()
procedure(unary_sev),  nopass, pointer :: op1_sev  => null ()
procedure(unary_str),  nopass, pointer :: op1_str  => null ()
procedure(unary_cut),  nopass, pointer :: op1_cut  => null ()
procedure(unary_evi),  nopass, pointer :: op1_evi  => null ()
procedure(unary_evr),  nopass, pointer :: op1_evr  => null ()
procedure(binary_log),  nopass, pointer :: op2_log  => null ()
procedure(binary_int),  nopass, pointer :: op2_int  => null ()
procedure(binary_real), nopass, pointer :: op2_real => null ()
procedure(binary_cmplx), nopass, pointer :: op2_cmplx => null ()
procedure(binary_pdg),  nopass, pointer :: op2_pdg  => null ()
procedure(binary_sev),  nopass, pointer :: op2_sev  => null ()

```

```

    procedure(binary_str), nopass, pointer :: op2_str => null ()
    procedure(binary_cut), nopass, pointer :: op2_cut => null ()
    procedure(binary_evi), nopass, pointer :: op2_evi => null ()
    procedure(binary_evr), nopass, pointer :: op2_evr => null ()
    procedure(cum_evi), nopass, pointer :: opcum_evi => null ()
    procedure(cum_evr), nopass, pointer :: opcum_evr => null ()
contains
  <Eval trees: eval node: TBP>
end type eval_node_t

```

Finalize a node recursively. Allocated constants are deleted, pointers are ignored.

```

<Eval trees: eval node: TBP>≡
  procedure :: final_rec => eval_node_final_rec

<Eval trees: sub interfaces>≡
  recursive module subroutine eval_node_final_rec (node)
    class(eval_node_t), intent(inout) :: node
  end subroutine eval_node_final_rec

<Eval trees: procedures>≡
  recursive module subroutine eval_node_final_rec (node)
    class(eval_node_t), intent(inout) :: node
    select case (node%type)
    case (EN_UNARY)
      call eval_node_final_rec (node%arg1)
    case (EN_BINARY)
      call eval_node_final_rec (node%arg1)
      call eval_node_final_rec (node%arg2)
    case (EN_CONDITIONAL)
      call eval_node_final_rec (node%arg0)
      call eval_node_final_rec (node%arg1)
      call eval_node_final_rec (node%arg2)
    case (EN_BLOCK)
      call eval_node_final_rec (node%arg0)
      call eval_node_final_rec (node%arg1)
    case (EN_PRT_FUN_UNARY, EN_EVAL_FUN_UNARY, &
          EN_LOG_FUN_UNARY, EN_INT_FUN_UNARY, EN_REAL_FUN_UNARY)
      if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
      call eval_node_final_rec (node%arg1)
      deallocate (node%index)
      deallocate (node%prt1)
    case (EN_REAL_FUN_CUM)
      if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
      call eval_node_final_rec (node%arg1)
      deallocate (node%index)
      deallocate (node%prt1)
    case (EN_PRT_FUN_BINARY, EN_EVAL_FUN_BINARY, &
          EN_LOG_FUN_BINARY, EN_INT_FUN_BINARY, EN_REAL_FUN_BINARY)
      if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
      call eval_node_final_rec (node%arg1)
      call eval_node_final_rec (node%arg2)
      deallocate (node%index)
      deallocate (node%prt1)
      deallocate (node%prt2)

```



```

case (EN_FORMAT_STR)
  if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
  if (associated (node%arg1)) call eval_node_final_rec (node%arg1)
  deallocate (node%ival)
case (EN_RECORD_CMD)
  if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
  if (associated (node%arg1)) call eval_node_final_rec (node%arg1)
  if (associated (node%arg2)) call eval_node_final_rec (node%arg2)
  if (associated (node%arg3)) call eval_node_final_rec (node%arg3)
  if (associated (node%arg4)) call eval_node_final_rec (node%arg4)
end select
select case (node%type)
case (EN_UNARY, EN_BINARY, EN_CONDITIONAL, EN_CONSTANT, EN_BLOCK, &
      EN_PRT_FUN_UNARY, EN_PRT_FUN_BINARY, &
      EN_EVAL_FUN_UNARY, EN_EVAL_FUN_BINARY, &
      EN_LOG_FUN_UNARY, EN_LOG_FUN_BINARY, &
      EN_INT_FUN_UNARY, EN_INT_FUN_BINARY, &
      EN_REAL_FUN_UNARY, EN_REAL_FUN_BINARY, &
      EN_REAL_FUN_CUM, &
      EN_FORMAT_STR, EN_RECORD_CMD)
  select case (node%result_type)
  case (V_LOG); deallocate (node%lval)
  case (V_INT); deallocate (node%ival)
  case (V_REAL); deallocate (node%rval)
  case (V_CMLX); deallocate (node%cval)
  case (V_SEV); deallocate (node%pval)
  case (V_PDG); deallocate (node%aval)
  case (V_STR); deallocate (node%sval)
  end select
  deallocate (node%value_is_known)
end select
end subroutine eval_node_final_rec

```

Leaf nodes

Initialize a leaf node with a literal constant.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_log (node, lval)
  type(eval_node_t), intent(out) :: node
  logical, intent(in) :: lval
  node%type = EN_CONSTANT
  node%result_type = V_LOG
  allocate (node%lval, node%value_is_known)
  node%lval = lval
  node%value_is_known = .true.
end subroutine eval_node_init_log

subroutine eval_node_init_int (node, ival)
  type(eval_node_t), intent(out) :: node
  integer, intent(in) :: ival
  node%type = EN_CONSTANT
  node%result_type = V_INT

```

```

        allocate (node%ival, node%value_is_known)
        node%ival = ival
        node%value_is_known = .true.
    end subroutine eval_node_init_int

subroutine eval_node_init_real (node, rval)
    type(eval_node_t), intent(out) :: node
    real(default), intent(in) :: rval
    node%type = EN_CONSTANT
    node%result_type = V_REAL
    allocate (node%rval, node%value_is_known)
    node%rval = rval
    node%value_is_known = .true.
end subroutine eval_node_init_real

subroutine eval_node_init_cmplx (node, cval)
    type(eval_node_t), intent(out) :: node
    complex(default), intent(in) :: cval
    node%type = EN_CONSTANT
    node%result_type = V_CMPLX
    allocate (node%cval, node%value_is_known)
    node%cval = cval
    node%value_is_known = .true.
end subroutine eval_node_init_cmplx

subroutine eval_node_init_subevt (node, pval)
    type(eval_node_t), intent(out) :: node
    type(subevt_t), intent(in) :: pval
    node%type = EN_CONSTANT
    node%result_type = V_SEV
    allocate (node%pval, node%value_is_known)
    node%pval = pval
    node%value_is_known = .true.
end subroutine eval_node_init_subevt

subroutine eval_node_init_pdg_array (node, aval)
    type(eval_node_t), intent(out) :: node
    type(pdg_array_t), intent(in) :: aval
    node%type = EN_CONSTANT
    node%result_type = V_PDG
    allocate (node%aval, node%value_is_known)
    node%aval = aval
    node%value_is_known = .true.
end subroutine eval_node_init_pdg_array

subroutine eval_node_init_string (node, sval)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: sval
    node%type = EN_CONSTANT
    node%result_type = V_STR
    allocate (node%sval, node%value_is_known)
    node%sval = sval
    node%value_is_known = .true.
end subroutine eval_node_init_string

```

Initialize a leaf node with a pointer to a named parameter

(Eval trees: procedures)+≡

```

subroutine eval_node_init_log_ptr (node, name, lval, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  logical, intent(in), target :: lval
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_LOG
  node%lval => lval
  node%value_is_known => is_known
end subroutine eval_node_init_log_ptr

subroutine eval_node_init_int_ptr (node, name, ival, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  integer, intent(in), target :: ival
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_INT
  node%ival => ival
  node%value_is_known => is_known
end subroutine eval_node_init_int_ptr

subroutine eval_node_init_real_ptr (node, name, rval, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  real(default), intent(in), target :: rval
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_REAL
  node%rval => rval
  node%value_is_known => is_known
end subroutine eval_node_init_real_ptr

subroutine eval_node_init_cmplx_ptr (node, name, cval, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  complex(default), intent(in), target :: cval
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_CMPLX
  node%cval => cval
  node%value_is_known => is_known
end subroutine eval_node_init_cmplx_ptr

subroutine eval_node_init_subevt_ptr (node, name, pval, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name

```

```

    type(subevt_t), intent(in), target :: pval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_SEV
    node%pval => pval
    node%value_is_known => is_known
end subroutine eval_node_init_subevt_ptr

subroutine eval_node_init_pdg_array_ptr (node, name, aval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    type(pdg_array_t), intent(in), target :: aval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_PDG
    node%aval => aval
    node%value_is_known => is_known
end subroutine eval_node_init_pdg_array_ptr

subroutine eval_node_init_string_ptr (node, name, sval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    type(string_t), intent(in), target :: sval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_STR
    node%sval => sval
    node%value_is_known => is_known
end subroutine eval_node_init_string_ptr

```

The procedure-pointer cases:

(Eval trees: procedures)+≡

```

subroutine eval_node_init_obs1_int_ptr (node, name, obs1_iptr, p1)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    procedure(obs_unary_int), intent(in), pointer :: obs1_iptr
    type(prt_t), intent(in), target :: p1
    node%type = EN_OBS1_INT
    node%tag = name
    node%result_type = V_INT
    node%obs1_int => obs1_iptr
    node%prt1 => p1
    allocate (node%ival, node%value_is_known)
    node%value_is_known = .false.
end subroutine eval_node_init_obs1_int_ptr

subroutine eval_node_init_obs2_int_ptr (node, name, obs2_iptr, p1, p2)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    procedure(obs_binary_int), intent(in), pointer :: obs2_iptr
    type(prt_t), intent(in), target :: p1, p2

```

```

node%type = EN_OBS2_INT
node%tag = name
node%result_type = V_INT
node%obs2_int => obs2_iptr
node%prt1 => p1
node%prt2 => p2
allocate (node%ival, node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_init_obs2_int_ptr

subroutine eval_node_init_obsev_int_ptr (node, name, obsev_iptr, pval)
type(eval_node_t), intent(out) :: node
type(string_t), intent(in) :: name
procedure(obs_sev_int), intent(in), pointer :: obsev_iptr
type(subevt_t), intent(in), target :: pval
node%type = EN_OBSEV_INT
node%tag = name
node%result_type = V_INT
node%obsev_int => obsev_iptr
node%pval => pval
allocate (node%rval, node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_init_obsev_int_ptr

subroutine eval_node_init_obs1_real_ptr (node, name, obs1_rptr, p1)
type(eval_node_t), intent(out) :: node
type(string_t), intent(in) :: name
procedure(obs_unary_real), intent(in), pointer :: obs1_rptr
type(prt_t), intent(in), target :: p1
node%type = EN_OBS1_REAL
node%tag = name
node%result_type = V_REAL
node%obs1_real => obs1_rptr
node%prt1 => p1
allocate (node%rval, node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_init_obs1_real_ptr

subroutine eval_node_init_obs2_real_ptr (node, name, obs2_rptr, p1, p2)
type(eval_node_t), intent(out) :: node
type(string_t), intent(in) :: name
procedure(obs_binary_real), intent(in), pointer :: obs2_rptr
type(prt_t), intent(in), target :: p1, p2
node%type = EN_OBS2_REAL
node%tag = name
node%result_type = V_REAL
node%obs2_real => obs2_rptr
node%prt1 => p1
node%prt2 => p2
allocate (node%rval, node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_init_obs2_real_ptr

subroutine eval_node_init_obsev_real_ptr (node, name, obsev_rptr, pval)

```

```

type(eval_node_t), intent(out) :: node
type(string_t), intent(in) :: name
procedure(obs_sev_real), intent(in), pointer :: obsev_rptr
type(subevt_t), intent(in), target :: pval
node%type = EN_OBSEV_REAL
node%tag = name
node%result_type = V_REAL
node%obsev_real => obsev_rptr
node%pval => pval
allocate (node%rval, node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_init_obsev_real_ptr

```

Branch nodes

Initialize a branch node, sub-nodes are given.

```

<Eval trees: procedures>+≡
subroutine eval_node_init_branch (node, tag, result_type, arg1, arg2)
type(eval_node_t), intent(out) :: node
type(string_t), intent(in) :: tag
integer, intent(in) :: result_type
type(eval_node_t), intent(in), target :: arg1
type(eval_node_t), intent(in), target, optional :: arg2
if (present (arg2)) then
    node%type = EN_BINARY
else
    node%type = EN_UNARY
end if
node%tag = tag
node%result_type = result_type
call eval_node_allocate_value (node)
node%arg1 => arg1
if (present (arg2)) node%arg2 => arg2
end subroutine eval_node_init_branch

```

Allocate the node value according to the result type.

```

<Eval trees: procedures>+≡
subroutine eval_node_allocate_value (node)
type(eval_node_t), intent(inout) :: node
select case (node%result_type)
case (V_LOG); allocate (node%lval)
case (V_INT); allocate (node%ival)
case (V_REAL); allocate (node%rval)
case (V_CMPLX); allocate (node%cval)
case (V_PDG); allocate (node%aval)
case (V_SEV); allocate (node%pval)
    call subevt_init (node%pval)
case (V_STR); allocate (node%sval)
end select
allocate (node%value_is_known)
node%value_is_known = .false.
end subroutine eval_node_allocate_value

```

Initialize a block node which contains, in addition to the expression to be evaluated, a variable definition. The result type is not yet assigned, because we can compile the enclosed expression only after the var list is set up.

Note that the node always allocates a new variable list and appends it to the current one. Thus, if the variable redefines an existing one, it only shadows it but does not reset it. Any side-effects are therefore absent and need not be undone outside the block.

If the flag **new** is set, a variable is (re)declared. This must not be done for intrinsic variables. Vice versa, if the variable is not existent, the **new** flag is required.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_block (node, name, type, var_def, var_list)
  type(eval_node_t), intent(out), target :: node
  type(string_t), intent(in) :: name
  integer, intent(in) :: type
  type(eval_node_t), intent(in), target :: var_def
  type(var_list_t), intent(in), target :: var_list
  node%type = EN_BLOCK
  node%tag = "var_def"
  node%var_name = name
  node%arg1 => var_def
  allocate (node%var_list)
  call node%var_list%link (var_list)
  if (var_def%type == EN_CONSTANT) then
    select case (type)
      case (V_LOG)
        call node%var_list%append_log (name, var_def%lval)
      case (V_INT)
        call node%var_list%append_int (name, var_def%ival)
      case (V_REAL)
        call node%var_list%append_real (name, var_def%rval)
      case (V_CMPLX)
        call node%var_list%append_cmplx (name, var_def%cval)
      case (V_PDG)
        call node%var_list%append_pdg_array (name, var_def%aval)
      case (V_SEV)
        call node%var_list%append_subevt (name, var_def%pval)
      case (V_STR)
        call node%var_list%append_string (name, var_def%sval)
    end select
  else
    select case (type)
      case (V_LOG); call node%var_list%append_log_ptr &
        (name, var_def%lval, var_def%value_is_known)
      case (V_INT); call node%var_list%append_int_ptr &
        (name, var_def%ival, var_def%value_is_known)
      case (V_REAL); call node%var_list%append_real_ptr &
        (name, var_def%rval, var_def%value_is_known)
      case (V_CMPLX); call node%var_list%append_cmplx_ptr &
        (name, var_def%cval, var_def%value_is_known)
      case (V_PDG); call node%var_list%append_pdg_array_ptr &
        (name, var_def%aval, var_def%value_is_known)
    end select
  end if
end subroutine

```

```

        case (V_SEV); call node%var_list%append_subevt_ptr &
            (name, var_def%pval, var_def%value_is_known)
        case (V_STR); call node%var_list%append_string_ptr &
            (name, var_def%sval, var_def%value_is_known)
        end select
    end if
end subroutine eval_node_init_block

```

Complete block initialization by assigning the expression to evaluate to `arg0`.

(Eval trees: procedures)+≡

```

subroutine eval_node_set_expr (node, arg, result_type)
    type(eval_node_t), intent(inout) :: node
    type(eval_node_t), intent(in), target :: arg
    integer, intent(in), optional :: result_type
    if (present (result_type)) then
        node%result_type = result_type
    else
        node%result_type = arg%result_type
    end if
    call eval_node_allocate_value (node)
    node%arg0 => arg
end subroutine eval_node_set_expr

```

Initialize a conditional. There are three branches: the condition (evaluates to logical) and the two alternatives (evaluate both to the same arbitrary type).

(Eval trees: procedures)+≡

```

subroutine eval_node_init_conditional (node, result_type, cond, arg1, arg2)
    type(eval_node_t), intent(out) :: node
    integer, intent(in) :: result_type
    type(eval_node_t), intent(in), target :: cond, arg1, arg2
    node%type = EN_CONDITIONAL
    node%tag = "cond"
    node%result_type = result_type
    call eval_node_allocate_value (node)
    node%arg0 => cond
    node%arg1 => arg1
    node%arg2 => arg2
end subroutine eval_node_init_conditional

```

Initialize a recording command (which evaluates to a logical constant). The first branch is the ID of the analysis object to be filled, the optional branches 1 to 4 are the values to be recorded.

If the event-weight pointer is null, we record values with unit weight. Otherwise, we use the value pointed to as event weight.

There can be up to four arguments which represent x , y , Δy , Δx . Therefore, this is the only node type that may fill four sub-nodes.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_record_cmd &
    (node, event_weight, id, arg1, arg2, arg3, arg4)
    type(eval_node_t), intent(out) :: node
    real(default), pointer :: event_weight
    type(eval_node_t), intent(in), target :: id

```



```

type(eval_node_t), intent(in), optional, target :: arg1, arg2, arg3, arg4
call eval_node_init_log (node, .true.)
node%type = EN_RECORD_CMD
node%rval => event_weight
node%tag = "record_cmd"
node%arg0 => id
if (present (arg1)) then
  node%arg1 => arg1
  if (present (arg2)) then
    node%arg2 => arg2
    if (present (arg3)) then
      node%arg3 => arg3
      if (present (arg4)) then
        node%arg4 => arg4
      end if
    end if
  end if
end if
end if
end subroutine eval_node_init_record_cmd

```

Initialize a node for operations on subevents. The particle lists (one or two) are inserted as **arg1** and **arg2**. We allocated particle pointers as temporaries for iterating over particle lists. The procedure pointer which holds the function to evaluate for the subevents (e.g., combine, select) is also initialized.

(*Eval trees: procedures*)+≡

```

subroutine eval_node_init_prt_fun_unary (node, arg1, name, proc)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1
  type(string_t), intent(in) :: name
  procedure(unary_sev) :: proc
  node%type = EN_PRT_FUN_UNARY
  node%tag = name
  node%result_type = V_SEV
  call eval_node_allocate_value (node)
  node%arg1 => arg1
  allocate (node%index, source = 0)
  allocate (node%prt1)
  node%op1_sev => proc
end subroutine eval_node_init_prt_fun_unary

subroutine eval_node_init_prt_fun_binary (node, arg1, arg2, name, proc)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1, arg2
  type(string_t), intent(in) :: name
  procedure(binary_sev) :: proc
  node%type = EN_PRT_FUN_BINARY
  node%tag = name
  node%result_type = V_SEV
  call eval_node_allocate_value (node)
  node%arg1 => arg1
  node%arg2 => arg2
  allocate (node%index, source = 0)
  allocate (node%prt1)

```

```

        allocate (node%prt2)
        node%op2_sev => proc
    end subroutine eval_node_init_prt_fun_binary

```

Similar, but for particle-list functions that evaluate to a real value.

<Eval trees: procedures>+≡

```

subroutine eval_node_init_eval_fun_unary (node, arg1, name)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), intent(in), target :: arg1
    type(string_t), intent(in) :: name
    node%type = EN_EVAL_FUN_UNARY
    node%tag = name
    node%result_type = V_REAL
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    allocate (node%index, source = 0)
    allocate (node%prt1)
end subroutine eval_node_init_eval_fun_unary

subroutine eval_node_init_eval_fun_binary (node, arg1, arg2, name)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), intent(in), target :: arg1, arg2
    type(string_t), intent(in) :: name
    node%type = EN_EVAL_FUN_BINARY
    node%tag = name
    node%result_type = V_REAL
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    node%arg2 => arg2
    allocate (node%index, source = 0)
    allocate (node%prt1)
    allocate (node%prt2)
end subroutine eval_node_init_eval_fun_binary

```

These are for particle-list functions that evaluate to a logical value.

<Eval trees: procedures>+≡

```

subroutine eval_node_init_log_fun_unary (node, arg1, name, proc)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), intent(in), target :: arg1
    type(string_t), intent(in) :: name
    procedure(unary_cut) :: proc
    node%type = EN_LOG_FUN_UNARY
    node%tag = name
    node%result_type = V_LOG
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    allocate (node%index, source = 0)
    allocate (node%prt1)
    node%op1_cut => proc
end subroutine eval_node_init_log_fun_unary

subroutine eval_node_init_log_fun_binary (node, arg1, arg2, name, proc)
    type(eval_node_t), intent(out) :: node

```

```

type(eval_node_t), intent(in), target :: arg1, arg2
type(string_t), intent(in) :: name
procedure(binary_cut) :: proc
node%type = EN_LOG_FUN_BINARY
node%tag = name
node%result_type = V_LOG
call eval_node_allocate_value (node)
node%arg1 => arg1
node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
node%op2_cut => proc
end subroutine eval_node_init_log_fun_binary

```

These are for particle-list functions that evaluate to an integer value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_int_fun_unary (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1
type(string_t), intent(in) :: name
procedure(unary_evi) :: proc
node%type = EN_INT_FUN_UNARY
node%tag = name
node%result_type = V_INT
call eval_node_allocate_value (node)
node%arg1 => arg1
allocate (node%index, source = 0)
allocate (node%prt1)
node%op1_evi => proc
end subroutine eval_node_init_int_fun_unary

subroutine eval_node_init_int_fun_binary (node, arg1, arg2, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1, arg2
type(string_t), intent(in) :: name
procedure(binary_evi) :: proc
node%type = EN_INT_FUN_BINARY
node%tag = name
node%result_type = V_INT
call eval_node_allocate_value (node)
node%arg1 => arg1
node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
node%op2_evi => proc
end subroutine eval_node_init_int_fun_binary

```

These are for particle-list functions that evaluate to a real value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_real_fun_unary (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node

```

```

    type(eval_node_t), intent(in), target :: arg1
    type(string_t), intent(in) :: name
    procedure(unary_evr) :: proc
    node%type = EN_REAL_FUN_UNARY
    node%tag = name
    node%result_type = V_REAL
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    allocate (node%index, source = 0)
    allocate (node%prt1)
    node%op1_evr => proc
end subroutine eval_node_init_real_fun_unary

subroutine eval_node_init_real_fun_binary (node, arg1, arg2, name, proc)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), intent(in), target :: arg1, arg2
    type(string_t), intent(in) :: name
    procedure(binary_evr) :: proc
    node%type = EN_REAL_FUN_BINARY
    node%tag = name
    node%result_type = V_REAL
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    node%arg2 => arg2
    allocate (node%index, source = 0)
    allocate (node%prt1)
    allocate (node%prt2)
    node%op2_evr => proc
end subroutine eval_node_init_real_fun_binary

subroutine eval_node_init_real_fun_cum (node, arg1, name, proc)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), intent(in), target :: arg1
    type(string_t), intent(in) :: name
    procedure(cum_evr) :: proc
    node%type = EN_REAL_FUN_CUM
    node%tag = name
    node%result_type = V_REAL
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    allocate (node%index, source = 0)
    allocate (node%prt1)
    node%opcum_evr => proc
end subroutine eval_node_init_real_fun_cum

```

Initialize a node for a string formatting function (sprintf).

<Eval trees: procedures>+≡

```

subroutine eval_node_init_format_string (node, fmt, arg, name, n_args)
    type(eval_node_t), intent(out) :: node
    type(eval_node_t), pointer :: fmt, arg
    type(string_t), intent(in) :: name
    integer, intent(in) :: n_args
    node%type = EN_FORMAT_STR
    node%tag = name

```

```

node%result_type = V_STR
call eval_node_allocate_value (node)
node%arg0 => fmt
node%arg1 => arg
allocate (node%ival)
node%ival = n_args
end subroutine eval_node_init_format_string

```

If particle functions depend upon a condition (or an expression is evaluated), the observables that can be evaluated for the given particles have to be thrown on the local variable stack. This is done here. Each observable is initialized with the particle pointers which have been allocated for the node.

The integer variable that is referred to by the `Index` pseudo-observable is always known when it is referred to.

```

<Eval trees: procedures>+≡
subroutine eval_node_set_observables (node, var_list)
  type(eval_node_t), intent(inout) :: node
  type(var_list_t), intent(in), target :: var_list
  logical, save, target :: known = .true.
  allocate (node%var_list)
  call node%var_list%link (var_list)
  allocate (node%index, source = 0)
  call node%var_list%append_int_ptr &
    (var_str ("Index"), node%index, known, intrinsic=.true.)
  if (.not. associated (node%prt2)) then
    call var_list_set_observables_unary &
      (node%var_list, node%prt1)
    if (associated (node%pval)) then
      call var_list_set_observables_sev &
        (node%var_list, node%pval)
    end if
  else
    call var_list_set_observables_binary &
      (node%var_list, node%prt1, node%prt2)
  end if
end subroutine eval_node_set_observables

```

Output

```

<Eval trees: eval node: TBP>+≡
procedure :: write => eval_node_write

<Eval trees: sub interfaces>+≡
module subroutine eval_node_write (node, unit, indent)
  class(eval_node_t), intent(in) :: node
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: indent
end subroutine eval_node_write

<Eval trees: procedures>+≡
module subroutine eval_node_write (node, unit, indent)
  class(eval_node_t), intent(in) :: node
  integer, intent(in), optional :: unit

```

```

integer, intent(in), optional :: indent
integer :: u, ind
u = given_output_unit (unit); if (u < 0) return
ind = 0; if (present (indent)) ind = indent
write (u, "(A)", advance="no") repeat ("| ", ind) // "o "
select case (node%type)
case (EN_UNARY, EN_BINARY, EN_CONDITIONAL, &
      EN_PRT_FUN_UNARY, EN_PRT_FUN_BINARY, &
      EN_EVAL_FUN_UNARY, EN_EVAL_FUN_BINARY, &
      EN_LOG_FUN_UNARY, EN_LOG_FUN_BINARY, &
      EN_INT_FUN_UNARY, EN_INT_FUN_BINARY, &
      EN_REAL_FUN_UNARY, EN_REAL_FUN_BINARY, &
      EN_REAL_FUN_CUM)
  write (u, "(A)", advance="no") "[" // char (node%tag) // "]" = "
case (EN_CONSTANT)
  write (u, "(A)", advance="no") "[const] ="
case (EN_VARIABLE)
  write (u, "(A)", advance="no") char (node%tag) // " =>"
case (EN_OBS1_INT, EN_OBS2_INT, EN_OBS1_REAL, EN_OBS2_REAL)
  write (u, "(A)", advance="no") char (node%tag) // " ="
case (EN_BLOCK)
  write (u, "(A)", advance="no") "[" // char (node%tag) // "]" // &
    char (node%var_name) // " [expr] ="
case default
  write (u, "(A)", advance="no") "[???] ="
end select
select case (node%result_type)
case (V_LOG)
  if (node%value_is_known) then
    if (node%lval) then
      write (u, "(1x,A)") "true"
    else
      write (u, "(1x,A)") "false"
    end if
  else
    write (u, "(1x,A)") "[unknown logical]"
  end if
case (V_INT)
  if (node%value_is_known) then
    write (u, "(1x,I0)") node%ival
  else
    write (u, "(1x,A)") "[unknown integer]"
  end if
case (V_REAL)
  if (node%value_is_known) then
    write (u, "(1x," // FMT_19 // ")") node%rval
  else
    write (u, "(1x,A)") "[unknown real]"
  end if
case (V_CMPLX)
  if (node%value_is_known) then
    write (u, "(1x,'('," // FMT_19 // ",','," // &
      FMT_19 // ",')')") node%cval
  else

```

```

        write (u, "(1x,A)") "[unknown complex]"
    end if
case (V_SEV)
    if (char (node%tag) == "@evt") then
        write (u, "(1x,A)") "[event subevent]"
    else if (node%value_is_known) then
        call node%pval%write (unit, prefix = repeat ("| ", ind + 1))
    else
        write (u, "(1x,A)") "[unknown subevent]"
    end if
case (V_PDG)
    write (u, "(1x)", advance="no")
    call node%aval%write (u); write (u, *)
case (V_STR)
    if (node%value_is_known) then
        write (u, "(A)") ''' // char (node%sval) // '''
    else
        write (u, "(1x,A)") "[unknown string]"
    end if
case default
    write (u, "(1x,A)") "[empty]"
end select
select case (node%type)
case (EN_OBS1_INT, EN_OBS1_REAL)
    write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt1 ="
    call prt_write (node%prt1, unit)
case (EN_OBS2_INT, EN_OBS2_REAL)
    write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt1 ="
    call prt_write (node%prt1, unit)
    write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt2 ="
    call prt_write (node%prt2, unit)
end select
end subroutine eval_node_write

recursive subroutine eval_node_write_rec (node, unit, indent)
    type(eval_node_t), intent(in) :: node
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind
    u = given_output_unit (unit); if (u < 0) return
    ind = 0; if (present (indent)) ind = indent
    call eval_node_write (node, unit, indent)
    select case (node%type)
    case (EN_UNARY)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
    case (EN_BINARY)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
        call eval_node_write_rec (node%arg2, unit, ind+1)
    case (EN_BLOCK)
        call eval_node_write_rec (node%arg1, unit, ind+1)

```

```

        call eval_node_write_rec (node%arg0, unit, ind+1)
case (EN_CONDITIONAL)
    call eval_node_write_rec (node%arg0, unit, ind+1)
    call eval_node_write_rec (node%arg1, unit, ind+1)
    call eval_node_write_rec (node%arg2, unit, ind+1)
case (EN_PRT_FUN_UNARY, EN_EVAL_FUN_UNARY, &
      EN_LOG_FUN_UNARY, EN_INT_FUN_UNARY, EN_REAL_FUN_UNARY, &
      EN_REAL_FUN_CUM)
    if (associated (node%arg0)) &
        call eval_node_write_rec (node%arg0, unit, ind+1)
    call eval_node_write_rec (node%arg1, unit, ind+1)
case (EN_PRT_FUN_BINARY, EN_EVAL_FUN_BINARY, &
      EN_LOG_FUN_BINARY, EN_INT_FUN_BINARY, EN_REAL_FUN_BINARY)
    if (associated (node%arg0)) &
        call eval_node_write_rec (node%arg0, unit, ind+1)
    call eval_node_write_rec (node%arg1, unit, ind+1)
    call eval_node_write_rec (node%arg2, unit, ind+1)
case (EN_RECORD_CMD)
    if (associated (node%arg1)) then
        call eval_node_write_rec (node%arg1, unit, ind+1)
    if (associated (node%arg2)) then
        call eval_node_write_rec (node%arg2, unit, ind+1)
    if (associated (node%arg3)) then
        call eval_node_write_rec (node%arg3, unit, ind+1)
    if (associated (node%arg4)) then
        call eval_node_write_rec (node%arg4, unit, ind+1)
    end if
    end if
    end if
    end if
end select
end subroutine eval_node_write_rec

```

28.3.2 Operation types

For the operations associated to evaluation tree nodes, we define abstract interfaces for all cases.

Particles/subevents are transferred by-reference, to avoid unnecessary copying. Therefore, subroutines instead of functions.

(Eval trees: interfaces)≡

```

abstract interface
    logical function unary_log (arg)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_log
end interface
abstract interface
    integer function unary_int (arg)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_int
end interface

```



```

abstract interface
  real(default) function unary_real (arg)
    import default
    import eval_node_t
    type(eval_node_t), intent(in) :: arg
  end function unary_real
end interface
abstract interface
  complex(default) function unary_cmplx (arg)
    import default
    import eval_node_t
    type(eval_node_t), intent(in) :: arg
  end function unary_cmplx
end interface
abstract interface
  subroutine unary_pdg (pdg_array, arg)
    import pdg_array_t
    import eval_node_t
    type(pdg_array_t), intent(out) :: pdg_array
    type(eval_node_t), intent(in) :: arg
  end subroutine unary_pdg
end interface
abstract interface
  subroutine unary_sev (subevt, arg, arg0)
    import subevt_t
    import eval_node_t
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: arg
    type(eval_node_t), intent(inout), optional :: arg0
  end subroutine unary_sev
end interface
abstract interface
  subroutine unary_str (string, arg)
    import string_t
    import eval_node_t
    type(string_t), intent(out) :: string
    type(eval_node_t), intent(in) :: arg
  end subroutine unary_str
end interface
abstract interface
  logical function unary_cut (arg1, arg0)
    import eval_node_t
    type(eval_node_t), intent(in) :: arg1
    type(eval_node_t), intent(inout) :: arg0
  end function unary_cut
end interface
abstract interface
  subroutine unary_evi (ival, arg1, arg0)
    import eval_node_t
    integer, intent(out) :: ival
    type(eval_node_t), intent(in) :: arg1
    type(eval_node_t), intent(inout), optional :: arg0
  end subroutine unary_evi
end interface

```

```

abstract interface
  subroutine unary_evr (rval, arg1, arg0)
    import eval_node_t, default
    real(default), intent(out) :: rval
    type(eval_node_t), intent(in) :: arg1
    type(eval_node_t), intent(inout), optional :: arg0
  end subroutine unary_evr
end interface
abstract interface
  logical function binary_log (arg1, arg2)
    import eval_node_t
    type(eval_node_t), intent(in) :: arg1, arg2
  end function binary_log
end interface
abstract interface
  integer function binary_int (arg1, arg2)
    import eval_node_t
    type(eval_node_t), intent(in) :: arg1, arg2
  end function binary_int
end interface
abstract interface
  real(default) function binary_real (arg1, arg2)
    import default
    import eval_node_t
    type(eval_node_t), intent(in) :: arg1, arg2
  end function binary_real
end interface
abstract interface
  complex(default) function binary_cmplx (arg1, arg2)
    import default
    import eval_node_t
    type(eval_node_t), intent(in) :: arg1, arg2
  end function binary_cmplx
end interface
abstract interface
  subroutine binary_pdg (pdg_array, arg1, arg2)
    import pdg_array_t
    import eval_node_t
    type(pdg_array_t), intent(out) :: pdg_array
    type(eval_node_t), intent(in) :: arg1, arg2
  end subroutine binary_pdg
end interface
abstract interface
  subroutine binary_sev (subevt, arg1, arg2, arg0)
    import subevt_t
    import eval_node_t
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: arg1, arg2
    type(eval_node_t), intent(inout), optional :: arg0
  end subroutine binary_sev
end interface
abstract interface
  subroutine binary_str (string, arg1, arg2)
    import string_t

```

```

        import eval_node_t
        type(string_t), intent(out) :: string
        type(eval_node_t), intent(in) :: arg1, arg2
    end subroutine binary_str
end interface
abstract interface
    logical function binary_cut (arg1, arg2, arg0)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout) :: arg0
    end function binary_cut
end interface
abstract interface
    subroutine binary_evi (ival, arg1, arg2, arg0)
        import eval_node_t
        integer, intent(out) :: ival
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine binary_evi
end interface
abstract interface
    subroutine binary_evr (rval, arg1, arg2, arg0)
        import eval_node_t, default
        real(default), intent(out) :: rval
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine binary_evr
end interface
abstract interface
    integer function cum_evi (arg1, arg0)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg1
        type(eval_node_t), intent(inout) :: arg0
    end function cum_evi
end interface
abstract interface
    real(default) function cum_evr (arg1, arg0)
        import eval_node_t, default
        type(eval_node_t), intent(in) :: arg1
        type(eval_node_t), intent(inout) :: arg0
    end function cum_evr
end interface

```

The following subroutines set the procedure pointer:

(Eval trees: procedures)+≡

```

subroutine eval_node_set_op1_log (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(unary_log) :: op
    en%op1_log => op
end subroutine eval_node_set_op1_log

subroutine eval_node_set_op1_int (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(unary_int) :: op

```

```

        en%op1_int => op
    end subroutine eval_node_set_op1_int

    subroutine eval_node_set_op1_real (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(unary_real) :: op
        en%op1_real => op
    end subroutine eval_node_set_op1_real

    subroutine eval_node_set_op1_cmplx (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(unary_cmplx) :: op
        en%op1_cmplx => op
    end subroutine eval_node_set_op1_cmplx

    subroutine eval_node_set_op1_pdg (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(unary_pdg) :: op
        en%op1_pdg => op
    end subroutine eval_node_set_op1_pdg

    subroutine eval_node_set_op1_sev (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(unary_sev) :: op
        en%op1_sev => op
    end subroutine eval_node_set_op1_sev

    subroutine eval_node_set_op1_str (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(unary_str) :: op
        en%op1_str => op
    end subroutine eval_node_set_op1_str

    subroutine eval_node_set_op2_log (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_log) :: op
        en%op2_log => op
    end subroutine eval_node_set_op2_log

    subroutine eval_node_set_op2_int (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_int) :: op
        en%op2_int => op
    end subroutine eval_node_set_op2_int

    subroutine eval_node_set_op2_real (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_real) :: op
        en%op2_real => op
    end subroutine eval_node_set_op2_real

    subroutine eval_node_set_op2_cmplx (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_cmplx) :: op

```

```

        en%op2_cmplx => op
    end subroutine eval_node_set_op2_cmplx

    subroutine eval_node_set_op2_pdg (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_pdg) :: op
        en%op2_pdg => op
    end subroutine eval_node_set_op2_pdg

    subroutine eval_node_set_op2_sev (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_sev) :: op
        en%op2_sev => op
    end subroutine eval_node_set_op2_sev

    subroutine eval_node_set_op2_str (en, op)
        type(eval_node_t), intent(inout) :: en
        procedure(binary_str) :: op
        en%op2_str => op
    end subroutine eval_node_set_op2_str

```

28.3.3 Specific operators

Our expression syntax contains all Fortran functions that make sense. These functions have to be provided in a form that they can be used in procedures pointers, and have the abstract interfaces above. For some intrinsic functions, we could use specific versions provided by Fortran directly. However, this has two drawbacks: (i) We should work with the values instead of the eval-nodes as argument, which complicates the interface; (ii) more importantly, the **default** real type need not be equivalent to double precision. This would, at least, introduce system dependencies. Finally, for operators there are no specific versions.

Therefore, we write wrappers for all possible functions, at the expense of some overhead.

Binary numerical functions

```

<Eval trees: procedures>+≡
    integer function add_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival + en2%ival
    end function add_ii
    real(default) function add_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival + en2%rval
    end function add_ir
    complex(default) function add_ic (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival + en2%cval
    end function add_ic
    real(default) function add_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval + en2%ival

```

```

end function add_ri
complex(default) function add_ci (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%ival
end function add_ci
complex(default) function add_cr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%rval
end function add_cr
complex(default) function add_rc (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval + en2%cval
end function add_rc
real(default) function add_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval + en2%rval
end function add_rr
complex(default) function add_cc (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%cval
end function add_cc

integer function sub_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival - en2%ival
end function sub_ii
real(default) function sub_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival - en2%rval
end function sub_ir
real(default) function sub_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval - en2%ival
end function sub_ri
complex(default) function sub_ic (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival - en2%cval
end function sub_ic
complex(default) function sub_ci (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval - en2%ival
end function sub_ci
complex(default) function sub_cr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval - en2%rval
end function sub_cr
complex(default) function sub_rc (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval - en2%cval
end function sub_rc
real(default) function sub_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval - en2%rval
end function sub_rr

```

```

complex(default) function sub_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval - en2%cval
end function sub_cc

integer function mul_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%ival
end function mul_ii
real(default) function mul_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%rval
end function mul_ir
real(default) function mul_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%ival
end function mul_ri
complex(default) function mul_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%cval
end function mul_ic
complex(default) function mul_ci (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%ival
end function mul_ci
complex(default) function mul_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%cval
end function mul_rc
complex(default) function mul_cr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%rval
end function mul_cr
real(default) function mul_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%rval
end function mul_rr
complex(default) function mul_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%cval
end function mul_cc

integer function div_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (en2%ival == 0) then
        if (en1%ival >= 0) then
            call msg_warning ("division by zero: " // int2char (en1%ival) // &
                " / 0 ; result set to 0")
        else
            call msg_warning ("division by zero: (" // int2char (en1%ival) // &
                ") / 0 ; result set to 0")
        end if
        y = 0
    return

```

```

        end if
        y = en1%ival / en2%ival
    end function div_ii
    real(default) function div_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival / en2%rval
    end function div_ir
    real(default) function div_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval / en2%ival
    end function div_ri
    complex(default) function div_ic (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival / en2%cval
    end function div_ic
    complex(default) function div_ci (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval / en2%ival
    end function div_ci
    complex(default) function div_rc (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval / en2%cval
    end function div_rc
    complex(default) function div_cr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval / en2%rval
    end function div_cr
    real(default) function div_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval / en2%rval
    end function div_rr
    complex(default) function div_cc (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval / en2%cval
    end function div_cc

    integer function pow_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        integer :: a, b
        real(default) :: rres
        a = en1%ival
        b = en2%ival
        if ((a == 0) .and. (b < 0)) then
            call msg_warning ("division by zero: " // int2char (a) // &
                " ^ (" // int2char (b) // ") ; result set to 0")
            y = 0
            return
        end if
        rres = real(a, default) ** b
        y = rres
        if (real(y, default) /= rres) then
            if (b < 0) then
                call msg_warning ("result of all-integer operation " // &
                    int2char (a) // " ^ (" // int2char (b) // &

```



```

        ") has been truncated to "// int2char (y), &
    [ var_str ("Chances are that you want to use " // &
        "reals instead of integers at this point.") ])
    else
        call msg_warning ("integer overflow in " // int2char (a) // &
            " ^ " // int2char (b) // " ; result is " // int2char (y), &
        [ var_str ("Using reals instead of integers might help.") ])
    end if
end if
end if
end function pow_ii
real(default) function pow_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval ** en2%ival
end function pow_ri
complex(default) function pow_ci (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval ** en2%ival
end function pow_ci
real(default) function pow_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival ** en2%rval
end function pow_ir
real(default) function pow_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval ** en2%rval
end function pow_rr
complex(default) function pow_cr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval ** en2%rval
end function pow_cr
complex(default) function pow_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival ** en2%cval
end function pow_ic
complex(default) function pow_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval ** en2%cval
end function pow_rc
complex(default) function pow_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval ** en2%cval
end function pow_cc

integer function max_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (en1%ival, en2%ival)
end function max_ii
real(default) function max_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (real (en1%ival, default), en2%rval)
end function max_ir
real(default) function max_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (en1%rval, real (en2%ival, default))

```

```

end function max_ri
real(default) function max_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = max (en1%rval, en2%rval)
end function max_rr
integer function min_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = min (en1%ival, en2%ival)
end function min_ii
real(default) function min_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = min (real (en1%ival, default), en2%rval)
end function min_ir
real(default) function min_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = min (en1%rval, real (en2%ival, default))
end function min_ri
real(default) function min_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = min (en1%rval, en2%rval)
end function min_rr

integer function mod_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = mod (en1%ival, en2%ival)
end function mod_ii
real(default) function mod_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = mod (real (en1%ival, default), en2%rval)
end function mod_ir
real(default) function mod_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = mod (en1%rval, real (en2%ival, default))
end function mod_ri
real(default) function mod_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = mod (en1%rval, en2%rval)
end function mod_rr
integer function modulo_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = modulo (en1%ival, en2%ival)
end function modulo_ii
real(default) function modulo_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = modulo (real (en1%ival, default), en2%rval)
end function modulo_ir
real(default) function modulo_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = modulo (en1%rval, real (en2%ival, default))
end function modulo_ri
real(default) function modulo_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = modulo (en1%rval, en2%rval)
end function modulo_rr

```

Unary numeric functions

(Eval trees: procedures)+≡

```
real(default) function real_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%ival
end function real_i
real(default) function real_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%cval
end function real_c
integer function int_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%rval
end function int_r
complex(default) function cmplx_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%ival
end function cmplx_i
integer function int_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%cval
end function int_c
complex(default) function cmplx_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%rval
end function cmplx_r
integer function nint_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = nint (en%rval)
end function nint_r
integer function floor_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = floor (en%rval)
end function floor_r
integer function ceiling_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = ceiling (en%rval)
end function ceiling_r

integer function neg_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = - en%ival
end function neg_i
real(default) function neg_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = - en%rval
end function neg_r
complex(default) function neg_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = - en%cval
end function neg_c
```

```

integer function abs_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = abs (en%ival)
end function abs_i
real(default) function abs_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = abs (en%rval)
end function abs_r
real(default) function abs_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = abs (en%cval)
end function abs_c
integer function conjg_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%ival
end function conjg_i
real(default) function conjg_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = en%rval
end function conjg_r
complex(default) function conjg_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = conjg (en%cval)
end function conjg_c
integer function sgn_i (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sign (1, en%ival)
end function sgn_i
real(default) function sgn_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sign (1._default, en%rval)
end function sgn_r

real(default) function sqrt_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sqrt (en%rval)
end function sqrt_r
real(default) function exp_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = exp (en%rval)
end function exp_r
real(default) function log_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = log (en%rval)
end function log_r
real(default) function log10_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = log10 (en%rval)
end function log10_r

complex(default) function sqrt_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sqrt (en%cval)
end function sqrt_c

```

```

complex(default) function exp_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = exp (en%cval)
end function exp_c
complex(default) function log_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = log (en%cval)
end function log_c

real(default) function sin_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sin (en%rval)
end function sin_r
real(default) function cos_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = cos (en%rval)
end function cos_r
real(default) function tan_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = tan (en%rval)
end function tan_r
real(default) function asin_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = asin (en%rval)
end function asin_r
real(default) function acos_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = acos (en%rval)
end function acos_r
real(default) function atan_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = atan (en%rval)
end function atan_r

complex(default) function sin_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sin (en%cval)
end function sin_c
complex(default) function cos_c (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = cos (en%cval)
end function cos_c

real(default) function sinh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = sinh (en%rval)
end function sinh_r
real(default) function cosh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = cosh (en%rval)
end function cosh_r
real(default) function tanh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = tanh (en%rval)

```

```

end function tanh_r
real(default) function asinh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = asinh (en%rval)
end function asinh_r
real(default) function acosh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = acosh (en%rval)
end function acosh_r
real(default) function atanh_r (en) result (y)
  type(eval_node_t), intent(in) :: en
  y = atanh (en%rval)
end function atanh_r

```

Binary logical functions

Logical expressions:

```

<Eval trees: procedures>+≡
logical function ignore_first_ll (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en2%lval
end function ignore_first_ll
logical function or_ll (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%lval .or. en2%lval
end function or_ll
logical function and_ll (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%lval .and. en2%lval
end function and_ll

```

Comparisons:

```

<Eval trees: procedures>+≡
logical function comp_lt_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival < en2%ival
end function comp_lt_ii
logical function comp_lt_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival < en2%rval
end function comp_lt_ir
logical function comp_lt_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval < en2%ival
end function comp_lt_ri
logical function comp_lt_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval < en2%rval
end function comp_lt_rr

logical function comp_gt_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2

```

```

        y = en1%ival > en2%ival
    end function comp_gt_ii
    logical function comp_gt_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival > en2%rval
    end function comp_gt_ir
    logical function comp_gt_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval > en2%ival
    end function comp_gt_ri
    logical function comp_gt_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval > en2%rval
    end function comp_gt_rr

    logical function comp_le_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival <= en2%ival
    end function comp_le_ii
    logical function comp_le_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival <= en2%rval
    end function comp_le_ir
    logical function comp_le_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval <= en2%ival
    end function comp_le_ri
    logical function comp_le_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval <= en2%rval
    end function comp_le_rr

    logical function comp_ge_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival >= en2%ival
    end function comp_ge_ii
    logical function comp_ge_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival >= en2%rval
    end function comp_ge_ir
    logical function comp_ge_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval >= en2%ival
    end function comp_ge_ri
    logical function comp_ge_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval >= en2%rval
    end function comp_ge_rr

    logical function comp_eq_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival == en2%ival
    end function comp_eq_ii
    logical function comp_eq_ir (en1, en2) result (y)

```

```

        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival == en2%rval
    end function comp_eq_ir
    logical function comp_eq_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval == en2%ival
    end function comp_eq_ri
    logical function comp_eq_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval == en2%rval
    end function comp_eq_rr
    logical function comp_eq_ss (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%sval == en2%sval
    end function comp_eq_ss

    logical function comp_ne_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival /= en2%ival
    end function comp_ne_ii
    logical function comp_ne_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival /= en2%rval
    end function comp_ne_ir
    logical function comp_ne_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval /= en2%ival
    end function comp_ne_ri
    logical function comp_ne_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval /= en2%rval
    end function comp_ne_rr
    logical function comp_ne_ss (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%sval /= en2%sval
    end function comp_ne_ss

```

Comparisons with tolerance:

(Eval trees: procedures)+≡

```

    logical function comp_se_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        if (associated (en1%tolerance)) then
            y = abs (en1%ival - en2%ival) <= en1%tolerance
        else
            y = en1%ival == en2%ival
        end if
    end function comp_se_ii
    logical function comp_se_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        if (associated (en1%tolerance)) then
            y = abs (en1%rval - en2%ival) <= en1%tolerance
        else
            y = en1%rval == en2%ival
        end if

```



```

end function comp_se_ri
logical function comp_se_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%ival - en2%rval) <= en1%tolerance
  else
    y = en1%ival == en2%rval
  end if
end function comp_se_ir
logical function comp_se_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%rval - en2%rval) <= en1%tolerance
  else
    y = en1%rval == en2%rval
  end if
end function comp_se_rr
logical function comp_ns_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%ival - en2%ival) > en1%tolerance
  else
    y = en1%ival /= en2%ival
  end if
end function comp_ns_ii
logical function comp_ns_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%rval - en2%ival) > en1%tolerance
  else
    y = en1%rval /= en2%ival
  end if
end function comp_ns_ri
logical function comp_ns_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%ival - en2%rval) > en1%tolerance
  else
    y = en1%ival /= en2%rval
  end if
end function comp_ns_ir
logical function comp_ns_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = abs (en1%rval - en2%rval) > en1%tolerance
  else
    y = en1%rval /= en2%rval
  end if
end function comp_ns_rr

logical function comp_ls_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%ival <= en2%ival + en1%tolerance

```

```

else
    y = en1%ival <= en2%ival
end if
end function comp_ls_ii
logical function comp_ls_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval <= en2%ival + en1%tolerance
    else
        y = en1%rval <= en2%ival
    end if
end function comp_ls_ri
logical function comp_ls_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival <= en2%rval + en1%tolerance
    else
        y = en1%ival <= en2%rval
    end if
end function comp_ls_ir
logical function comp_ls_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval <= en2%rval + en1%tolerance
    else
        y = en1%rval <= en2%rval
    end if
end function comp_ls_rr

logical function comp_ll_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival < en2%ival - en1%tolerance
    else
        y = en1%ival < en2%ival
    end if
end function comp_ll_ii
logical function comp_ll_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval < en2%ival - en1%tolerance
    else
        y = en1%rval < en2%ival
    end if
end function comp_ll_ri
logical function comp_ll_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival < en2%rval - en1%tolerance
    else
        y = en1%ival < en2%rval
    end if
end function comp_ll_ir
logical function comp_ll_rr (en1, en2) result (y)

```

```

    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval < en2%rval - en1%tolerance
    else
        y = en1%rval < en2%rval
    end if
end function comp_ll_rr

logical function comp_gs_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival >= en2%ival - en1%tolerance
    else
        y = en1%ival >= en2%ival
    end if
end function comp_gs_ii

logical function comp_gs_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval >= en2%ival - en1%tolerance
    else
        y = en1%rval >= en2%ival
    end if
end function comp_gs_ri

logical function comp_gs_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival >= en2%rval - en1%tolerance
    else
        y = en1%ival >= en2%rval
    end if
end function comp_gs_ir

logical function comp_gs_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval >= en2%rval - en1%tolerance
    else
        y = en1%rval >= en2%rval
    end if
end function comp_gs_rr

logical function comp_gg_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival > en2%ival + en1%tolerance
    else
        y = en1%ival > en2%ival
    end if
end function comp_gg_ii

logical function comp_gg_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval > en2%ival + en1%tolerance
    else

```

```

        y = en1%rval > en2%ival
    end if
end function comp_gg_ri
logical function comp_gg_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival > en2%rval + en1%tolerance
    else
        y = en1%ival > en2%rval
    end if
end function comp_gg_ir
logical function comp_gg_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval > en2%rval + en1%tolerance
    else
        y = en1%rval > en2%rval
    end if
end function comp_gg_rr

```

Unary logical functions

<Eval trees: procedures>+≡

```

logical function not_l (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = .not. en%lval
end function not_l

```

Unary PDG-array functions

Make a PDG-array object from an integer.

<Eval trees: procedures>+≡

```

subroutine pdg_i (pdg_array, en)
    type(pdg_array_t), intent(out) :: pdg_array
    type(eval_node_t), intent(in) :: en
    pdg_array = en%ival
end subroutine pdg_i

```

Binary PDG-array functions

Concatenate two PDG-array objects.

<Eval trees: procedures>+≡

```

subroutine concat_cc (pdg_array, en1, en2)
    type(pdg_array_t), intent(out) :: pdg_array
    type(eval_node_t), intent(in) :: en1, en2
    pdg_array = en1%aval // en2%aval
end subroutine concat_cc

```

Unary particle-list functions

Combine all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

(Eval trees: procedures)+≡

```
subroutine collect_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:), allocatable :: mask1
  integer :: n, i
  n = en1%pval%get_length ()
  allocate (mask1 (n))
  if (present (en0)) then
    do i = 1, n
      en0%index = i
      en0%prt1 = en1%pval%get_prt (i)
      call eval_node_evaluate (en0)
      mask1(i) = en0%lval
    end do
  else
    mask1 = .true.
  end if
  call subevt_collect (subevt, en1%pval, mask1)
end subroutine collect_p
```

Cluster the particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

(Eval trees: procedures)+≡

```
subroutine cluster_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:), allocatable :: mask1
  integer :: n, i
  !!! Should not be initialized for every event
  type(jet_definition_t) :: jet_def
  logical :: keep_jets, exclusive
  call jet_def%init (en1%jet_algorithm, en1%jet_r, en1%jet_p, en1%jet_ycut)
  n = en1%pval%get_length ()
  allocate (mask1 (n))
  if (present (en0)) then
    do i = 1, n
      en0%index = i
      en0%prt1 = en1%pval%get_prt (i)
      call eval_node_evaluate (en0)
      mask1(i) = en0%lval
    end do
  else
    mask1 = .true.
  end if
  if (associated (en1%var_list)) then
    keep_jets = en1%var_list%get_lval (var_str("?keep_flavors_when_clustering"))
  end if
```

```

else
    keep_jets = .false.
end if
exclusive = .false.
select case (en1%jet_algorithm)
case (ee_kt_algorithm)
    exclusive = .true.
case (ee_genkt_algorithm)
    if (en1%jet_r > Pi) exclusive = .true.
end select
call subevt_cluster (subevt, en1%pval, en1%jet_dcut, mask1, &
    jet_def, keep_jets, exclusive)
call jet_def%final ()
end subroutine cluster_p

```

Recombine photons with other particles (usually charged leptons and maybe quarks) given in the same subevent. If `en0` is present, create a mask which is true only for those particles that pass the test.

(Eval trees: procedures)+≡

```

subroutine photon_recombination_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    type(prt_t), dimension(:), allocatable :: prt
    integer :: n, i
    real(default) :: reco_r0
    logical :: keep_flg
    reco_r0 = en1%photon_rec_r0
    n = en1%pval%get_length ()
    allocate (prt (n))
    do i = 1, n
        prt(i) = en1%pval%get_prt (i)
        if (.not. prt_is_recombinable (prt (i))) then
            call msg_fatal ("Only charged leptons, quarks, and " // &
                "photons can be included in photon recombination.")
        end if
    end do
    if (count (prt_is_photon (prt)) > 1) &
        call msg_fatal ("Photon recombination is supported " // &
            "only for single photons.")
    allocate (mask1 (n))
    if (present (en0)) then
        do i = 1, n
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval
        end do
    else
        mask1 = .true.
    end if
    if (associated (en1%var_list)) then

```

```

        keep_flg = en1%var_list%get_lval &
            (var_str("?keep_flavors_when_recombining"))
    else
        keep_flg = .false.
    end if
    call subevt_recombine &
        (subevt, en1%pval, mask1, reco_r0, keep_flg)
end subroutine photon_recombination_p

```

Select all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

(Eval trees: procedures)+≡

```

subroutine select_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = en1%pval%get_length ()
    allocate (mask1 (n))
    if (present (en0)) then
        do i = 1, n
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval
        end do
    else
        mask1 = .true.
    end if
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_p

```

`select_b_jet_p`, `select_non_b_jet_p`, `select_c_jet_p`, and `select_light_jet_p` are special selection function acting on a subevent of combined particles (jets) and result in a list of *b* jets, non-*b* jets (i.e. *c* and light jets), *c* jets, and light jets, respectively.

(Eval trees: procedures)+≡

```

subroutine select_b_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = en1%pval%get_length ()
    allocate (mask1 (n))
    do i = 1, n
        mask1(i) = prt_is_b_jet (en1%pval%get_prt (i))
        if (present (en0)) then
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval .and. mask1(i)
        end if
    end do
end subroutine select_b_jet_p

```

```

        end if
    end do
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_b_jet_p

```

<Eval trees: procedures>+≡

```

subroutine select_non_b_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = en1%pval%get_length ()
    allocate (mask1 (n))
    do i = 1, n
        mask1(i) = .not. prt_is_b_jet (en1%pval%get_prt (i))
        if (present (en0)) then
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval .and. mask1(i)
        end if
    end do
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_non_b_jet_p

```

<Eval trees: procedures>+≡

```

subroutine select_c_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = en1%pval%get_length ()
    allocate (mask1 (n))
    do i = 1, n
        mask1(i) = .not. prt_is_b_jet (en1%pval%get_prt (i)) &
            .and. prt_is_c_jet (en1%pval%get_prt (i))
        if (present (en0)) then
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval .and. mask1(i)
        end if
    end do
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_c_jet_p

```

<Eval trees: procedures>+≡

```

subroutine select_light_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0

```



```

logical, dimension(:), allocatable :: mask1
integer :: n, i
n = en1%pval%get_length ()
allocate (mask1 (n))
do i = 1, n
  mask1(i) = .not. prt_is_b_jet (en1%pval%get_prt (i)) &
    .and. .not. prt_is_c_jet (en1%pval%get_prt (i))
  if (present (en0)) then
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    call eval_node_evaluate (en0)
    mask1(i) = en0%lval .and. mask1(i)
  end if
end do
call subevt_select (subevt, en1%pval, mask1)
end subroutine select_light_jet_p

```

Extract the particle with index given by `en0` from the argument list. Negative indices count from the end. If `en0` is absent, extract the first particle. The result is a list with a single entry, or no entries if the original list was empty or if the index is out of range.

This function has no counterpart with two arguments.

```

<Eval trees: procedures>+≡
subroutine extract_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  integer :: index
  if (present (en0)) then
    call eval_node_evaluate (en0)
    select case (en0%result_type)
    case (V_INT); index = en0%ival
    case default
      call eval_node_write (en0)
      call msg_fatal (" Index parameter of 'extract' must be integer.")
    end select
  else
    index = 1
  end if
  call subevt_extract (subevt, en1%pval, index)
end subroutine extract_p

```

Sort the subevent according to the result of evaluating `en0`. If `en0` is absent, sort by default method (PDG code, particles before antiparticles).

```

<Eval trees: procedures>+≡
subroutine sort_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  integer, dimension(:), allocatable :: ival
  real(default), dimension(:), allocatable :: rval
  integer :: i, n

```

```

n = en1%pval%get_length ()
if (present (en0)) then
  select case (en0%result_type)
  case (V_INT); allocate (ival (n))
  case (V_REAL); allocate (rval (n))
  end select
  do i = 1, n
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    call eval_node_evaluate (en0)
    select case (en0%result_type)
    case (V_INT); ival(i) = en0%ival
    case (V_REAL); rval(i) = en0%rval
    end select
  end do
  select case (en0%result_type)
  case (V_INT); call subevt_sort (subevt, en1%pval, ival)
  case (V_REAL); call subevt_sort (subevt, en1%pval, rval)
  end select
else
  call subevt_sort (subevt, en1%pval)
end if
end subroutine sort_p

```

The following functions return a logical value. `all` evaluates to true if the condition `en0` is true for all elements of the subevent. `any` and `no` are analogous.

(Eval trees: procedures)+≡

```

function all_p (en1, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout) :: en0
  integer :: i, n
  n = en1%pval%get_length ()
  lval = .true.
  do i = 1, n
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    call eval_node_evaluate (en0)
    lval = en0%lval
    if (.not. lval) exit
  end do
end function all_p

function any_p (en1, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout) :: en0
  integer :: i, n
  n = en1%pval%get_length ()
  lval = .false.
  do i = 1, n
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)

```

```

        call eval_node_evaluate (en0)
        lval = en0%lval
        if (lval) exit
    end do
end function any_p

function no_p (en1, en0) result (lval)
    logical :: lval
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout) :: en0
    integer :: i, n
    n = en1%pval%get_length ()
    lval = .true.
    do i = 1, n
        en0%index = i
        en0%prt1 = en1%pval%get_prt (i)
        call eval_node_evaluate (en0)
        lval = .not. en0%lval
        if (lval) exit
    end do
end function no_p

```

The following function returns an integer value, namely the number of particles for which the condition is true. If there is no condition, it returns simply the length of the subevent.

(Eval trees: procedures)+≡

```

subroutine count_a (ival, en1, en0)
    integer, intent(out) :: ival
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    integer :: i, n, count
    n = en1%pval%get_length ()
    if (present (en0)) then
        count = 0
        do i = 1, n
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            call eval_node_evaluate (en0)
            if (en0%lval) count = count + 1
        end do
        ival = count
    else
        ival = n
    end if
end subroutine count_a

```

The following functions return either an integer or a real value, namely the sum or the product of the values of the corresponding expression.

(Eval trees: procedures)+≡

```

function sum_a (en1, en0) result (rval)
    real(default) :: rval
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout) :: en0

```

```

integer :: i, n
n = en1%pval%get_length ()
rval = 0._default
do i = 1, n
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    call eval_node_evaluate (en0)
    rval = rval + en0%rval
end do
end function sum_a

function prod_a (en1, en0) result (rval)
real(default) :: rval
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout) :: en0
integer :: i, n
n = en1%pval%get_length ()
rval = 1._default
do i = 1, n
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    call eval_node_evaluate (en0)
    rval = rval * en0%rval
end do
end function prod_a

```

Binary particle-list functions

This joins two subevents, stored in the evaluation nodes `en1` and `en2`. If `en0` is also present, it amounts to a logical test returning true or false for every pair of particles. A particle of the second list gets a mask entry only if it passes the test for all particles of the first list.

(Eval trees: procedures)+≡

```

subroutine join_pp (subevt, en1, en2, en0)
type(subevt_t), intent(inout) :: subevt
type(eval_node_t), intent(in) :: en1, en2
type(eval_node_t), intent(inout), optional :: en0
logical, dimension(:), allocatable :: mask2
integer :: i, j, n1, n2
n1 = en1%pval%get_length ()
n2 = en2%pval%get_length ()
allocate (mask2 (n2))
mask2 = .true.
if (present (en0)) then
do i = 1, n1
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
do j = 1, n2
    en0%prt2 = en2%pval%get_prt (j)
    call eval_node_evaluate (en0)
    mask2(j) = mask2(j) .and. en0%lval
end do
end if
end subroutine join_pp

```

```

        end do
    end if
    call subevt_join (subevt, en1%pval, en2%pval, mask2)
end subroutine join_pp

```

Combine two subevents, i.e., make a list of composite particles built from all possible particle pairs from the two lists. If `en0` is present, create a mask which is true only for those pairs that pass the test.

```

<Eval trees: procedures>+≡
subroutine combine_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:,:), allocatable :: mask12
    integer :: i, j, n1, n2
    n1 = en1%pval%get_length ()
    n2 = en2%pval%get_length ()
    if (present (en0)) then
        allocate (mask12 (n1, n2))
        do i = 1, n1
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            do j = 1, n2
                en0%prt2 = en2%pval%get_prt (j)
                call eval_node_evaluate (en0)
                mask12(i,j) = en0%lval
            end do
        end do
        call subevt_combine (subevt, en1%pval, en2%pval, mask12)
    else
        call subevt_combine (subevt, en1%pval, en2%pval)
    end if
end subroutine combine_pp

```

Combine all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test w.r.t. all particles in the second argument. If `en0` is absent, the second argument is ignored.

```

<Eval trees: procedures>+≡
subroutine collect_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: i, j, n1, n2
    n1 = en1%pval%get_length ()
    n2 = en2%pval%get_length ()
    allocate (mask1 (n1))
    mask1 = .true.
    if (present (en0)) then
        do i = 1, n1
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            do j = 1, n2

```

```

        en0%prt2 = en2%pval%get_prt (j)
        call eval_node_evaluate (en0)
        mask1(i) = mask1(i) .and. en0%lval
    end do
end do
end if
call subevt_collect (subevt, en1%pval, mask1)
end subroutine collect_pp

```

Select all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test w.r.t. all particles in the second argument. If `en0` is absent, the second argument is ignored, and the first argument is transferred unchanged. (This case is not very useful, of course.)

(Eval trees: procedures)+≡

```

subroutine select_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: i, j, n1, n2
    n1 = en1%pval%get_length ()
    n2 = en2%pval%get_length ()
    allocate (mask1 (n1))
    mask1 = .true.
    if (present (en0)) then
        do i = 1, n1
            en0%index = i
            en0%prt1 = en1%pval%get_prt (i)
            do j = 1, n2
                en0%prt2 = en2%pval%get_prt (j)
                call eval_node_evaluate (en0)
                mask1(i) = mask1(i) .and. en0%lval
            end do
        end do
    end if
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_pp

```

Sort the first subevent according to the result of evaluating `en0`. From the second subevent, only the first element is taken as reference. If `en0` is absent, we sort by default method (PDG code, particles before antiparticles).

(Eval trees: procedures)+≡

```

subroutine sort_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    integer, dimension(:), allocatable :: ival
    real(default), dimension(:), allocatable :: rval
    integer :: i, n1
    n1 = en1%pval%get_length ()
    if (present (en0)) then
        select case (en0%result_type)
            case (V_INT); allocate (ival (n1))

```

```

        case (V_REAL); allocate (rval (n1))
    end select
    do i = 1, n1
        en0%index = i
        en0%prt1 = en1%pval%get_prt (i)
        en0%prt2 = en2%pval%get_prt (1)
        call eval_node_evaluate (en0)
        select case (en0%result_type)
            case (V_INT); ival(i) = en0%ival
            case (V_REAL); rval(i) = en0%rval
        end select
    end do
    select case (en0%result_type)
        case (V_INT); call subevt_sort (subevt, en1%pval, ival)
        case (V_REAL); call subevt_sort (subevt, en1%pval, rval)
    end select
else
    call subevt_sort (subevt, en1%pval)
end if
end subroutine sort_pp

```

The following functions return a logical value. `all` evaluates to true if the condition `en0` is true for all valid element pairs of both subevents. Invalid pairs (with common `src` entry) are ignored.

`any` and `no` are analogous.

(Eval trees: procedures)+≡

```

function all_pp (en1, en2, en0) result (lval)
    logical :: lval
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout) :: en0
    integer :: i, j, n1, n2
    n1 = en1%pval%get_length ()
    n2 = en2%pval%get_length ()
    lval = .true.
    LOOP1: do i = 1, n1
        en0%index = i
        en0%prt1 = en1%pval%get_prt (i)
        do j = 1, n2
            en0%prt2 = en2%pval%get_prt (j)
            if (are_disjoint (en0%prt1, en0%prt2)) then
                call eval_node_evaluate (en0)
                lval = en0%lval
                if (.not. lval) exit LOOP1
            end if
        end do
    end do LOOP1
end function all_pp

function any_pp (en1, en2, en0) result (lval)
    logical :: lval
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout) :: en0
    integer :: i, j, n1, n2

```

```

n1 = en1%pval%get_length ()
n2 = en2%pval%get_length ()
lval = .false.
LOOP1: do i = 1, n1
  en0%index = i
  en0%prt1 = en1%pval%get_prt (i)
  do j = 1, n2
    en0%prt2 = en2%pval%get_prt (j)
    if (are_disjoint (en0%prt1, en0%prt2)) then
      call eval_node_evaluate (en0)
      lval = en0%lval
      if (lval) exit LOOP1
    end if
  end do
end do LOOP1
end function any_pp

function no_pp (en1, en2, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  integer :: i, j, n1, n2
  n1 = en1%pval%get_length ()
  n2 = en2%pval%get_length ()
  lval = .true.
  LOOP1: do i = 1, n1
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    do j = 1, n2
      en0%prt2 = en2%pval%get_prt (j)
      if (are_disjoint (en0%prt1, en0%prt2)) then
        call eval_node_evaluate (en0)
        lval = .not. en0%lval
        if (lval) exit LOOP1
      end if
    end do
  end do LOOP1
end function no_pp

```

The conditional restriction encoded in the `eval_node_t en_0` is applied only to the photons from `en1`, not to the objects being isolated from in `en2`.

(Eval trees: procedures)+≡

```

function photon_isolation_pp (en1, en2, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  type(prt_t) :: prt
  type(prt_t), dimension(:), allocatable :: prt_gam0, prt_lep
  type(vector4_t), dimension(:), allocatable :: &
    p_gam0, p_lep0, p_lep, p_par
  integer :: i, j, n1, n2, n_par, n_lep, n_gam, n_delta
  real(default), dimension(:), allocatable :: delta_r, et_sum
  integer, dimension(:), allocatable :: index

```



```

real(default) :: eps, iso_n, r0, pt_gam
logical, dimension(:,:), allocatable :: photon_mask
n1 = en1%pval%get_length ()
n2 = en2%pval%get_length ()
allocate (p_gam0 (n1), prt_gam0 (n1))
eps = en1%photon_iso_eps
iso_n = en1%photon_iso_n
r0 = en1%photon_iso_r0
lval = .true.
do i = 1, n1
    en0%index = i
    prt = en1%pval%get_prt (i)
    prt_gam0(i) = prt
    if (.not. prt_is_photon (prt_gam0(i))) &
        call msg_fatal ("Photon isolation can only " // &
            "be applied to photons.")
    p_gam0(i) = prt_get_momentum (prt_gam0(i))
    en0%prt1 = prt
    call eval_node_evaluate (en0)
    lval = en0%lval
    if (.not. lval) return
end do
if (n1 == 0) then
    call msg_fatal ("Photon isolation applied on empty photon sample.")
end if
n_par = 0
n_lep = 0
n_gam = 0
do i = 1, n2
    prt = en2%pval%get_prt (i)
    if (prt_is_parton (prt) .or. prt_is_clustered (prt)) then
        n_par = n_par + 1
    end if
    if (prt_is_lepton (prt)) then
        n_lep = n_lep + 1
    end if
    if (prt_is_photon (prt)) then
        n_gam = n_gam + 1
    end if
end do
if (n_lep > 0 .and. n_gam == 0) then
    call msg_fatal ("Photon isolation from EM energy: photons " // &
        "have to be included.")
end if
if (n_lep > 0 .and. n_gam /= n1) then
    call msg_fatal ("Photon isolation: photon samples do not match.")
end if
allocate (p_par (n_par))
allocate (p_lep0 (n_gam+n_lep), prt_lep(n_gam+n_lep))
n_par = 0
n_lep = 0
do i = 1, n2
    prt = en2%pval%get_prt (i)
    if (prt_is_parton (prt) .or. prt_is_clustered (prt)) then

```

```

        n_par = n_par + 1
        p_par(n_par) = prt_get_momentum (prt)
    end if
    if (prt_is_lepton (prt) .or. prt_is_photon(prt)) then
        n_lep = n_lep + 1
        prt_lep(n_lep) = prt
        p_lep0(n_lep) = prt_get_momentum (prt_lep(n_lep))
    end if
end do
if (n_par > 0) then
    allocate (delta_r (n_par), index (n_par))
    HADRON_ISOLATION: do i = 1, n1
        pt_gam = transverse_part (p_gam0(i))
        delta_r(1:n_par) = sort (eta_phi_distance (p_gam0(i), p_par(1:n_par)))
        index(1:n_par) = order (eta_phi_distance (p_gam0(i), p_par(1:n_par)))
        n_delta = count (delta_r < r0)
        allocate (et_sum(n_delta))
        do j = 1, n_delta
            et_sum(j) = sum (transverse_part (p_par (index (1:j))))
            if (.not. et_sum(j) <= &
                iso_chi_gamma (delta_r(j), r0, iso_n, eps, pt_gam)) then
                lval = .false.
                return
            end if
        end do
        deallocate (et_sum)
    end do HADRON_ISOLATION
    deallocate (delta_r)
    deallocate (index)
end if
if (n_lep > 0) then
    allocate (photon_mask(n1,n_lep))
    do i = 1, n1
        photon_mask(i,:) = .not. (prt_gam0(i) .match. prt_lep(:))
    end do
    allocate (delta_r (n_lep-1), index (n_lep-1), p_lep(n_lep-1))
    EM_ISOLATION: do i = 1, n1
        pt_gam = transverse_part (p_gam0(i))
        p_lep = pack (p_lep0, photon_mask(i,:))
        delta_r(1:n_lep-1) = sort (eta_phi_distance (p_gam0(i), p_lep(1:n_lep-1)))
        index(1:n_lep-1) = order (eta_phi_distance (p_gam0(i), p_lep(1:n_lep-1)))
        n_delta = count (delta_r < r0)
        allocate (et_sum(n_delta))
        do j = 1, n_delta
            et_sum(j) = sum (transverse_part (p_lep (index(1:j))))
            if (.not. et_sum(j) <= &
                iso_chi_gamma (delta_r(j), r0, iso_n, eps, pt_gam)) then
                lval = .false.
                return
            end if
        end do
        deallocate (et_sum)
    end do EM_ISOLATION
    deallocate (delta_r)

```

```

        deallocate (index)
    end if
contains
    function iso_chi_gamma (dr, r0_gam, n_gam, eps_gam, pt_gam) result (iso)
        real(default) :: iso
        real(default), intent(in) :: dr, r0_gam, n_gam, eps_gam, pt_gam
        iso = eps_gam * pt_gam
        if (.not. nearly_equal (abs(n_gam), 0._default)) then
            iso = iso * ((1._default - cos(dr)) / &
                (1._default - cos(r0_gam)))*abs(n_gam)
        end if
    end function iso_chi_gamma
end function photon_isolation_pp

```

This function evaluates an observable for a pair of particles. From the two particle lists, we take the first pair without `src` overlap. If there is no valid pair, we revert the status of the value to unknown.

(Eval trees: procedures) +≡

```

subroutine eval_pp (en1, en2, en0, rval, is_known)
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout) :: en0
    real(default), intent(out) :: rval
    logical, intent(out) :: is_known
    integer :: i, j, n1, n2
    n1 = en1%pval%get_length ()
    n2 = en2%pval%get_length ()
    rval = 0
    is_known = .false.
    LOOP1: do i = 1, n1
        en0%index = i
        en0%prt1 = en1%pval%get_prt (i)
        do j = 1, n2
            en0%prt2 = en2%pval%get_prt (j)
            if (are_disjoint (en0%prt1, en0%prt2)) then
                call eval_node_evaluate (en0)
                rval = en0%rval
                is_known = .true.
                exit LOOP1
            end if
        end do
    end do LOOP1
end subroutine eval_pp

```

The following function returns an integer value, namely the number of valid particle-pairs from both lists for which the condition is true. Invalid pairs (with common `src` entry) are ignored. If there is no condition, it returns the number of valid particle pairs.

(Eval trees: procedures) +≡

```

subroutine count_pp (ival, en1, en2, en0)
    integer, intent(out) :: ival
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    integer :: i, j, n1, n2, count

```

```

n1 = en1%pval%get_length ()
n2 = en2%pval%get_length ()
if (present (en0)) then
  count = 0
  do i = 1, n1
    en0%index = i
    en0%prt1 = en1%pval%get_prt (i)
    do j = 1, n2
      en0%prt2 = en2%pval%get_prt (j)
      if (are_disjoint (en0%prt1, en0%prt2)) then
        call eval_node_evaluate (en0)
        if (en0%lval) count = count + 1
      end if
    end do
  end do
else
  count = 0
  do i = 1, n1
    do j = 1, n2
      if (are_disjoint (en1%pval%get_prt (i), &
                        en2%pval%get_prt (j))) then
        count = count + 1
      end if
    end do
  end do
end if
ival = count
end subroutine count_pp

```

This function makes up a subevent from the second argument which consists only of particles which match the PDG code array (first argument).

(Eval trees: procedures)+≡

```

subroutine select_pdg_ca (subevt, en1, en2, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  if (present (en0)) then
    call subevt_select_pdg_code (subevt, en1%aval, en2%pval, en0%ival)
  else
    call subevt_select_pdg_code (subevt, en1%aval, en2%pval)
  end if
end subroutine select_pdg_ca

```

Binary string functions

Currently, the only string operation is concatenation.

(Eval trees: procedures)+≡

```

subroutine concat_ss (string, en1, en2)
  type(string_t), intent(out) :: string
  type(eval_node_t), intent(in) :: en1, en2
  string = en1%sval // en2%sval
end subroutine concat_ss

```

28.3.4 Compiling the parse tree

The evaluation tree is built recursively by following a parse tree. Evaluate an expression. The requested type is given as an optional argument; default is numeric (integer or real).

(Eval trees: procedures)+≡

```
recursive subroutine eval_node_compile_genexpr &
    (en, pn, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(in), optional :: result_type
    if (debug_active (D_MODEL_F)) then
        print *, "read genexpr"; call parse_node_write (pn)
    end if
    if (present (result_type)) then
        select case (result_type)
            case (V_INT, V_REAL, V_CMPLX)
                call eval_node_compile_expr (en, pn, var_list)
            case (V_LOG)
                call eval_node_compile_lexpr (en, pn, var_list)
            case (V_SEV)
                call eval_node_compile_pexpr (en, pn, var_list)
            case (V_PDG)
                call eval_node_compile_cexpr (en, pn, var_list)
            case (V_STR)
                call eval_node_compile_sexpr (en, pn, var_list)
        end select
    else
        call eval_node_compile_expr (en, pn, var_list)
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done genexpr"
    end if
end subroutine eval_node_compile_genexpr
```

Numeric expressions

This procedure compiles a numerical expression. This is a single term or a sum or difference of terms. We have to account for all combinations of integer and real arguments. If both are constant, we immediately do the calculation and allocate a constant node.

(Eval trees: procedures)+≡

```
recursive subroutine eval_node_compile_expr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_term, pn_addition, pn_op, pn_arg
```

```

type(eval_node_t), pointer :: en1, en2
type(string_t) :: key
integer :: t1, t2, t
if (debug_active (D_MODEL_F)) then
    print *, "read expr"; call parse_node_write (pn)
end if
pn_term => parse_node_get_sub_ptr (pn)
select case (char (parse_node_get_rule_key (pn_term)))
case ("term")
    call eval_node_compile_term (en, pn_term, var_list)
    pn_addition => parse_node_get_next_ptr (pn_term, tag="addition")
case ("addition")
    en => null ()
    pn_addition => pn_term
case default
    call parse_node_mismatch ("term|addition", pn)
end select
do while (associated (pn_addition))
    pn_op => parse_node_get_sub_ptr (pn_addition)
    pn_arg => parse_node_get_next_ptr (pn_op, tag="term")
    call eval_node_compile_term (en2, pn_arg, var_list)
    t2 = en2%result_type
    if (associated (en)) then
        en1 => en
        t1 = en1%result_type
    else
        allocate (en1)
        select case (t2)
        case (V_INT); call eval_node_init_int (en1, 0)
        case (V_REAL); call eval_node_init_real (en1, 0._default)
        case (V_CMPLX); call eval_node_init_cmplx (en1, cmplx &
            (0._default, 0._default, kind=default))
        end select
        t1 = t2
    end if
    t = numeric_result_type (t1, t2)
    allocate (en)
    key = parse_node_get_key (pn_op)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        select case (char (key))
        case ("+")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_init_int (en, add_ii (en1, en2))
                case (V_REAL); call eval_node_init_real (en, add_ir (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_ic (en1, en2))
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_init_real (en, add_ri (en1, en2))
                case (V_REAL); call eval_node_init_real (en, add_rr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_rc (en1, en2))
                end select
        end select
    end if
end while

```

```

        case (V_CMPLX)
            select case (t2)
                case (V_INT); call eval_node_init_cmplx (en, add_ci (en1, en2))
                case (V_REAL); call eval_node_init_cmplx (en, add_cr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_cc (en1, en2))
            end select
        end select
    case ("-")
        select case (t1)
            case (V_INT)
                select case (t2)
                    case (V_INT); call eval_node_init_int (en, sub_ii (en1, en2))
                    case (V_REAL); call eval_node_init_real (en, sub_ir (en1, en2))
                    case (V_CMPLX); call eval_node_init_cmplx (en, sub_ic (en1, en2))
                end select
            case (V_REAL)
                select case (t2)
                    case (V_INT); call eval_node_init_real (en, sub_ri (en1, en2))
                    case (V_REAL); call eval_node_init_real (en, sub_rr (en1, en2))
                    case (V_CMPLX); call eval_node_init_cmplx (en, sub_rc (en1, en2))
                end select
            case (V_CMPLX)
                select case (t2)
                    case (V_INT); call eval_node_init_cmplx (en, sub_ci (en1, en2))
                    case (V_REAL); call eval_node_init_cmplx (en, sub_cr (en1, en2))
                    case (V_CMPLX); call eval_node_init_cmplx (en, sub_cc (en1, en2))
                end select
            end select
        end select
    call eval_node_final_rec (en1)
    call eval_node_final_rec (en2)
    deallocate (en1, en2)
else
    call eval_node_init_branch (en, key, t, en1, en2)
    select case (char (key))
        case ("+")
            select case (t1)
                case (V_INT)
                    select case (t2)
                        case (V_INT); call eval_node_set_op2_int (en, add_ii)
                        case (V_REAL); call eval_node_set_op2_real (en, add_ir)
                        case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_ic)
                    end select
                case (V_REAL)
                    select case (t2)
                        case (V_INT); call eval_node_set_op2_real (en, add_ri)
                        case (V_REAL); call eval_node_set_op2_real (en, add_rr)
                        case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_rc)
                    end select
                case (V_CMPLX)
                    select case (t2)
                        case (V_INT); call eval_node_set_op2_cmplx (en, add_ci)
                        case (V_REAL); call eval_node_set_op2_cmplx (en, add_cr)
                        case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_cc)
                    end select
            end select
        end select
    end select

```

```

        end select
    end select
case ("-")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, sub_ii)
        case (V_REAL); call eval_node_set_op2_real (en, sub_ir)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_ic)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, sub_ri)
        case (V_REAL); call eval_node_set_op2_real (en, sub_rr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_rc)
        end select
    case (V_CMPLX)
        select case (t2)
        case (V_INT); call eval_node_set_op2_cmplx (en, sub_ci)
        case (V_REAL); call eval_node_set_op2_cmplx (en, sub_cr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_cc)
        end select
    end select
end select
end if
pn_addition => parse_node_get_next_ptr (pn_addition)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done expr"
end if
end subroutine eval_node_compile_expr

```

<Eval trees: procedures>+≡

```

recursive subroutine eval_node_compile_term (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_factor, pn_multiplication, pn_op, pn_arg
    type(eval_node_t), pointer :: en1, en2
    type(string_t) :: key
    integer :: t1, t2, t
    if (debug_active (D_MODEL_F)) then
        print *, "read term"; call parse_node_write (pn)
    end if
    pn_factor => parse_node_get_sub_ptr (pn, tag="factor")
    call eval_node_compile_factor (en, pn_factor, var_list)
    pn_multiplication => &
        parse_node_get_next_ptr (pn_factor, tag="multiplication")
    do while (associated (pn_multiplication))
        pn_op => parse_node_get_sub_ptr (pn_multiplication)
        pn_arg => parse_node_get_next_ptr (pn_op, tag="factor")
        en1 => en
        call eval_node_compile_factor (en2, pn_arg, var_list)
    end do

```



```

t1 = en1%result_type
t2 = en2%result_type
t = numeric_result_type (t1, t2)
allocate (en)
key = parse_node_get_key (pn_op)
if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
  select case (char (key))
  case ("*")
    select case (t1)
    case (V_INT)
      select case (t2)
      case (V_INT); call eval_node_init_int (en, mul_ii (en1, en2))
      case (V_REAL); call eval_node_init_real (en, mul_ir (en1, en2))
      case (V_CMPLX); call eval_node_init_cmplx (en, mul_ic (en1, en2))
      end select
    case (V_REAL)
      select case (t2)
      case (V_INT); call eval_node_init_real (en, mul_ri (en1, en2))
      case (V_REAL); call eval_node_init_real (en, mul_rr (en1, en2))
      case (V_CMPLX); call eval_node_init_cmplx (en, mul_rc (en1, en2))
      end select
    case (V_CMPLX)
      select case (t2)
      case (V_INT); call eval_node_init_cmplx (en, mul_ci (en1, en2))
      case (V_REAL); call eval_node_init_cmplx (en, mul_cr (en1, en2))
      case (V_CMPLX); call eval_node_init_cmplx (en, mul_cc (en1, en2))
      end select
    end select
  case ("/")
    select case (t1)
    case (V_INT)
      select case (t2)
      case (V_INT); call eval_node_init_int (en, div_ii (en1, en2))
      case (V_REAL); call eval_node_init_real (en, div_ir (en1, en2))
      case (V_CMPLX); call eval_node_init_real (en, div_ir (en1, en2))
      end select
    case (V_REAL)
      select case (t2)
      case (V_INT); call eval_node_init_real (en, div_ri (en1, en2))
      case (V_REAL); call eval_node_init_real (en, div_rr (en1, en2))
      case (V_CMPLX); call eval_node_init_cmplx (en, div_rc (en1, en2))
      end select
    case (V_CMPLX)
      select case (t2)
      case (V_INT); call eval_node_init_cmplx (en, div_ci (en1, en2))
      case (V_REAL); call eval_node_init_cmplx (en, div_cr (en1, en2))
      case (V_CMPLX); call eval_node_init_cmplx (en, div_cc (en1, en2))
      end select
    end select
  end select
  call eval_node_final_rec (en1)
  call eval_node_final_rec (en2)
  deallocate (en1, en2)
else

```

```

call eval_node_init_branch (en, key, t, en1, en2)
select case (char (key))
case ("*")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, mul_ii)
        case (V_REAL); call eval_node_set_op2_real (en, mul_ir)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_ic)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, mul_ri)
        case (V_REAL); call eval_node_set_op2_real (en, mul_rr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_rc)
        end select
    case (V_CMPLX)
        select case (t2)
        case (V_INT); call eval_node_set_op2_cmplx (en, mul_ci)
        case (V_REAL); call eval_node_set_op2_cmplx (en, mul_cr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_cc)
        end select
    end select
case ("/")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, div_ii)
        case (V_REAL); call eval_node_set_op2_real (en, div_ir)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, div_ic)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, div_ri)
        case (V_REAL); call eval_node_set_op2_real (en, div_rr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, div_rc)
        end select
    case (V_CMPLX)
        select case (t2)
        case (V_INT); call eval_node_set_op2_cmplx (en, div_ci)
        case (V_REAL); call eval_node_set_op2_cmplx (en, div_cr)
        case (V_CMPLX); call eval_node_set_op2_cmplx (en, div_cc)
        end select
    end select
    end select
end if
pn_multiplication => parse_node_get_next_ptr (pn_multiplication)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done term"
end if
end subroutine eval_node_compile_term

```

<Eval trees: procedures>+≡

```

recursive subroutine eval_node_compile_factor (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_value, pn_exponentiation, pn_op, pn_arg
  type(eval_node_t), pointer :: en1, en2
  type(string_t) :: key
  integer :: t1, t2, t
  if (debug_active (D_MODEL_F)) then
    print *, "read factor"; call parse_node_write (pn)
  end if
  pn_value => parse_node_get_sub_ptr (pn)
  call eval_node_compile_signed_value (en, pn_value, var_list)
  pn_exponentiation => &
    parse_node_get_next_ptr (pn_value, tag="exponentiation")
  if (associated (pn_exponentiation)) then
    pn_op => parse_node_get_sub_ptr (pn_exponentiation)
    pn_arg => parse_node_get_next_ptr (pn_op)
    en1 => en
    call eval_node_compile_signed_value (en2, pn_arg, var_list)
    t1 = en1%result_type
    t2 = en2%result_type
    t = numeric_result_type (t1, t2)
    allocate (en)
    key = parse_node_get_key (pn_op)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
      select case (t1)
        case (V_INT)
          select case (t2)
            case (V_INT); call eval_node_init_int (en, pow_ii (en1, en2))
            case (V_REAL); call eval_node_init_real (en, pow_ir (en1, en2))
            case (V_CMPLX); call eval_node_init_cmplx (en, pow_ic (en1, en2))
          end select
        case (V_REAL)
          select case (t2)
            case (V_INT); call eval_node_init_real (en, pow_ri (en1, en2))
            case (V_REAL); call eval_node_init_real (en, pow_rr (en1, en2))
            case (V_CMPLX); call eval_node_init_cmplx (en, pow_rc (en1, en2))
          end select
        case (V_CMPLX)
          select case (t2)
            case (V_INT); call eval_node_init_cmplx (en, pow_ci (en1, en2))
            case (V_REAL); call eval_node_init_cmplx (en, pow_cr (en1, en2))
            case (V_CMPLX); call eval_node_init_cmplx (en, pow_cc (en1, en2))
          end select
      end select
      call eval_node_final_rec (en1)
      call eval_node_final_rec (en2)
      deallocate (en1, en2)
    else
      call eval_node_init_branch (en, key, t, en1, en2)
      select case (t1)
        case (V_INT)

```

```

        select case (t2)
        case (V_INT);    call eval_node_set_op2_int  (en, pow_ii)
        case (V_REAL,V_CMPLX); call eval_type_error (pn, "exponentiation", t1)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT);    call eval_node_set_op2_real (en, pow_ri)
        case (V_REAL);   call eval_node_set_op2_real (en, pow_rr)
        case (V_CMPLX);  call eval_type_error (pn, "exponentiation", t1)
        end select
    case (V_CMPLX)
        select case (t2)
        case (V_INT);    call eval_node_set_op2_cmplx (en, pow_ci)
        case (V_REAL);   call eval_node_set_op2_cmplx (en, pow_cr)
        case (V_CMPLX);  call eval_node_set_op2_cmplx (en, pow_cc)
        end select
    end select
end if
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done factor"
end if
end subroutine eval_node_compile_factor

```

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_signed_value (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_arg
    type(eval_node_t), pointer :: en1
    integer :: t
    if (debug_active (D_MODEL_F)) then
        print *, "read signed value"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("signed_value")
        pn_arg => parse_node_get_sub_ptr (pn, 2)
        call eval_node_compile_value (en1, pn_arg, var_list)
        t = en1%result_type
        allocate (en)
        if (en1%type == EN_CONSTANT) then
            select case (t)
            case (V_INT); call eval_node_init_int  (en, neg_i (en1))
            case (V_REAL); call eval_node_init_real (en, neg_r (en1))
            case (V_CMPLX); call eval_node_init_cmplx (en, neg_c (en1))
            end select
            call eval_node_final_rec (en1)
            deallocate (en1)
        else
            call eval_node_init_branch (en, var_str ("-"), t, en1)
            select case (t)
            case (V_INT); call eval_node_set_op1_int  (en, neg_i)

```

```

        case (V_REAL); call eval_node_set_op1_real (en, neg_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, neg_c)
    end select
end if
case default
    call eval_node_compile_value (en, pn, var_list)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done signed value"
end if
end subroutine eval_node_compile_signed_value

```

Integer, real and complex values have an optional unit. The unit is extracted and applied immediately. An integer with unit evaluates to a real constant.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_value (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read value"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("integer_value", "real_value", "complex_value")
        call eval_node_compile_numeric_value (en, pn)
    case ("pi")
        call eval_node_compile_constant (en, pn)
    case ("I")
        call eval_node_compile_constant (en, pn)
    case ("variable")
        call eval_node_compile_variable (en, pn, var_list)
    case ("result")
        call eval_node_compile_result (en, pn, var_list)
    case ("expr")
        call eval_node_compile_expr (en, pn, var_list)
    case ("block_expr")
        call eval_node_compile_block_expr (en, pn, var_list)
    case ("conditional_expr")
        call eval_node_compile_conditional (en, pn, var_list)
    case ("unary_function")
        call eval_node_compile_unary_function (en, pn, var_list)
    case ("binary_function")
        call eval_node_compile_binary_function (en, pn, var_list)
    case ("eval_fun")
        call eval_node_compile_eval_function (en, pn, var_list)
    case ("count_fun")
        call eval_node_compile_count_function (en, pn, var_list)
    case ("sum_fun", "prod_fun")
        call eval_node_compile_numeric_function (en, pn, var_list)
    case default
        call parse_node_mismatch &
            ("integer|real|complex|constant|variable|" // &

```

```

        "expr|block_expr|conditional_expr|" // &
        "unary_function|binary_function|numeric_pexpr", pn)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done value"
end if
end subroutine eval_node_compile_value

```

Real, complex and integer values are numeric literals with an optional unit attached. In case of an integer, the unit actually makes it a real value in disguise. The signed version of real values is not possible in generic expressions; it is a special case for numeric constants in model files (see below). We do not introduce signed versions of complex values.

(*Eval trees: procedures*) \equiv

```

subroutine eval_node_compile_numeric_value (en, pn)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(parse_node_t), pointer :: pn_val, pn_unit
    allocate (en)
    pn_val => parse_node_get_sub_ptr (pn)
    pn_unit => parse_node_get_next_ptr (pn_val)
    select case (char (parse_node_get_rule_key (pn)))
    case ("integer_value")
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                parse_node_get_integer (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_int (en, parse_node_get_integer (pn_val))
        end if
    case ("real_value")
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_real (en, parse_node_get_real (pn_val))
        end if
    case ("complex_value")
        if (associated (pn_unit)) then
            call eval_node_init_cmplx (en, &
                parse_node_get_cmplx (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_cmplx (en, parse_node_get_cmplx (pn_val))
        end if
    case ("neg_real_value")
        pn_val => parse_node_get_sub_ptr (parse_node_get_sub_ptr (pn, 2))
        pn_unit => parse_node_get_next_ptr (pn_val)
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                - parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_real (en, - parse_node_get_real (pn_val))
        end if
    end select
end subroutine

```

```

case ("pos_real_value")
  pn_val => parse_node_get_sub_ptr (parse_node_get_sub_ptr (pn, 2))
  pn_unit => parse_node_get_next_ptr (pn_val)
  if (associated (pn_unit)) then
    call eval_node_init_real (en, &
      parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
  else
    call eval_node_init_real (en, parse_node_get_real (pn_val))
  end if
case default
  call parse_node_mismatch &
    ("integer_value|real_value|complex_value|neg_real_value|pos_real_value", pn)
end select
end subroutine eval_node_compile_numeric_value

```

These are the units, predefined and hardcoded. The default energy unit is GeV, the default angular unit is radians. We include units for observables of dimension energy squared. Luminosities are normalized in inverse femtobarns.

(Eval trees: procedures)+≡

```

function parse_node_get_unit (pn) result (factor)
  real(default) :: factor
  real(default) :: unit
  type(parse_node_t), intent(in) :: pn
  type(parse_node_t), pointer :: pn_unit, pn_unit_power
  type(parse_node_t), pointer :: pn_frac, pn_num, pn_int, pn_div, pn_den
  integer :: num, den
  pn_unit => parse_node_get_sub_ptr (pn)
  select case (char (parse_node_get_key (pn_unit)))
    case ("TeV"); unit = 1.e3_default
    case ("GeV"); unit = 1
    case ("MeV"); unit = 1.e-3_default
    case ("keV"); unit = 1.e-6_default
    case ("eV"); unit = 1.e-9_default
    case ("meV"); unit = 1.e-12_default
    case ("nbarn"); unit = 1.e6_default
    case ("pbarn"); unit = 1.e3_default
    case ("fbarn"); unit = 1
    case ("abarn"); unit = 1.e-3_default
    case ("rad"); unit = 1
    case ("mrad"); unit = 1.e-3_default
    case ("degree"); unit = degree
    case ("%"); unit = 1.e-2_default
    case default
      call msg_bug (" Unit '" // &
        char (parse_node_get_key (pn)) // "' is undefined.")
  end select
  pn_unit_power => parse_node_get_next_ptr (pn_unit)
  if (associated (pn_unit_power)) then
    pn_frac => parse_node_get_sub_ptr (pn_unit_power, 2)
    pn_num => parse_node_get_sub_ptr (pn_frac)
    select case (char (parse_node_get_rule_key (pn_num)))
      case ("neg_int")
        pn_int => parse_node_get_sub_ptr (pn_num, 2)
    end select
  end if
end function

```

```

        num = - parse_node_get_integer (pn_int)
    case ("pos_int")
        pn_int => parse_node_get_sub_ptr (pn_num, 2)
        num = parse_node_get_integer (pn_int)
    case ("integer_literal")
        num = parse_node_get_integer (pn_num)
    case default
        call parse_node_mismatch ("neg_int|pos_int|integer_literal", pn_num)
    end select
    pn_div => parse_node_get_next_ptr (pn_num)
    if (associated (pn_div)) then
        pn_den => parse_node_get_sub_ptr (pn_div, 2)
        den = parse_node_get_integer (pn_den)
    else
        den = 1
    end if
else
    num = 1
    den = 1
end if
factor = unit ** (real (num, default) / den)
end function parse_node_get_unit

```

There are only two predefined constants, but more can be added easily.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_constant (en, pn)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    if (debug_active (D_MODEL_F)) then
        print *, "read constant"; call parse_node_write (pn)
    end if
    allocate (en)
    select case (char (parse_node_get_key (pn)))
    case ("pi"); call eval_node_init_real (en, pi)
    case ("I"); call eval_node_init_cmplx (en, imago)
    case default
        call parse_node_mismatch ("pi or I", pn)
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done constant"
    end if
end subroutine eval_node_compile_constant

```

Compile a variable, with or without a specified type. Take the list of variables, look for the name and make a node with a pointer to the value. If no type is provided, the variable is numeric, and the stored value determines whether it is real or integer.

We explicitly demand that the variable is defined, so we do not accidentally point to variables that are declared only later in the script but have come into existence in a previous compilation pass.

Variables may actually be anonymous, these are expressions in disguise. In that case, the expression replaces the variable name in the parse tree, and we

allocate an ordinary expression node in the eval tree.

Variables of type V_PDG (pdg-code array) are not treated here. They are handled by eval_node_compile_cvariable.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_variable (en, pn, var_list, var_type)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in), target :: pn
  type(var_list_t), intent(in), target :: var_list
  integer, intent(in), optional :: var_type
  type(parse_node_t), pointer :: pn_name
  type(string_t) :: var_name
  logical, target, save :: no_lval
  real(default), target, save :: no_rval
  type(subevt_t), target, save :: no_pval
  type(string_t), target, save :: no_sval
  logical, target, save :: unknown = .false.
  integer :: type
  logical :: defined
  logical, pointer :: known
  logical, pointer :: lptr
  integer, pointer :: iptr
  real(default), pointer :: rptr
  complex(default), pointer :: cptr
  type(subevt_t), pointer :: pptr
  type(string_t), pointer :: sptr
  procedure(obs_unary_int), pointer :: obs1_iptr
  procedure(obs_unary_real), pointer :: obs1_rptr
  procedure(obs_binary_int), pointer :: obs2_iptr
  procedure(obs_binary_real), pointer :: obs2_rptr
  procedure(obs_sev_int), pointer :: obsev_iptr
  procedure(obs_sev_real), pointer :: obsev_rptr
  type(prt_t), pointer :: p1, p2
  if (debug_active (D_MODEL_F)) then
    print *, "read variable"; call parse_node_write (pn)
  end if
  if (present (var_type)) then
    select case (var_type)
      case (V_REAL, V_OBS1_REAL, V_OBS2_REAL, V_INT, V_OBS1_INT, &
            V_OBS2_INT, V_CMPLX)
        pn_name => pn
      case default
        pn_name => parse_node_get_sub_ptr (pn, 2)
    end select
  else
    pn_name => pn
  end if
  select case (char (parse_node_get_rule_key (pn_name)))
  case ("expr")
    call eval_node_compile_expr (en, pn_name, var_list)
  case ("lexpr")
    call eval_node_compile_lexpr (en, pn_name, var_list)
  case ("sexpr")
    call eval_node_compile_sexpr (en, pn_name, var_list)
  case ("pexpr")

```

```

    call eval_node_compile_pexpr (en, pn_name, var_list)
case ("variable")
    var_name = parse_node_get_string (pn_name)
    if (present (var_type)) then
        select case (var_type)
        case (V_LOG);   var_name = "?" // var_name
        case (V_SEV);   var_name = "@" // var_name
        case (V_STR);   var_name = "$" // var_name    ! $ sign
        end select
    end if
    call var_list%get_var_properties &
        (var_name, req_type=var_type, type=type, is_defined=defined)
    allocate (en)
    if (defined) then
        select case (type)
        case (V_LOG)
            call var_list%get_lptr (var_name, lptr, known)
            call eval_node_init_log_ptr (en, var_name, lptr, known)
        case (V_INT)
            call var_list%get_iptr (var_name, iptr, known)
            call eval_node_init_int_ptr (en, var_name, iptr, known)
        case (V_REAL)
            call var_list%get_rptr (var_name, rptr, known)
            call eval_node_init_real_ptr (en, var_name, rptr, known)
        case (V_CMPLX)
            call var_list%get_cptr (var_name, cptr, known)
            call eval_node_init_cmplx_ptr (en, var_name, cptr, known)
        case (V_SEV)
            call var_list%get_pptr (var_name, pptr, known)
            call eval_node_init_subevt_ptr (en, var_name, pptr, known)
        case (V_STR)
            call var_list%get_sptr (var_name, sptr, known)
            call eval_node_init_string_ptr (en, var_name, sptr, known)
        case (V_OBS1_INT)
            call var_list%get_obs1_iptr (var_name, obs1_iptr, p1)
            call eval_node_init_obs1_int_ptr (en, var_name, obs1_iptr, p1)
        case (V_OBS2_INT)
            call var_list%get_obs2_iptr (var_name, obs2_iptr, p1, p2)
            call eval_node_init_obs2_int_ptr (en, var_name, obs2_iptr, p1, p2)
        case (V_OBSEV_INT)
            call var_list%get_obsev_iptr (var_name, obsev_iptr, pptr)
            call eval_node_init_obsev_int_ptr (en, var_name, obsev_iptr, pptr)
        case (V_OBS1_REAL)
            call var_list%get_obs1_rptr (var_name, obs1_rptr, p1)
            call eval_node_init_obs1_real_ptr (en, var_name, obs1_rptr, p1)
        case (V_OBS2_REAL)
            call var_list%get_obs2_rptr (var_name, obs2_rptr, p1, p2)
            call eval_node_init_obs2_real_ptr (en, var_name, obs2_rptr, p1, p2)
        case (V_OBSEV_REAL)
            call var_list%get_obsev_rptr (var_name, obsev_rptr, pptr)
            call eval_node_init_obsev_real_ptr (en, var_name, obsev_rptr, pptr)
        case default
            call parse_node_write (pn)
            call msg_fatal ("Variable of this type " // &

```

```

        "is not allowed in the present context")
    if (present (var_type)) then
        select case (var_type)
        case (V_LOG)
            call eval_node_init_log_ptr (en, var_name, no_lval, unknown)
        case (V_SEV)
            call eval_node_init_subevt_ptr &
                (en, var_name, no_pval, unknown)
        case (V_STR)
            call eval_node_init_string_ptr &
                (en, var_name, no_sval, unknown)
        end select
    else
        call eval_node_init_real_ptr (en, var_name, no_rval, unknown)
    end if
end select
else
    call parse_node_write (pn)
    call msg_error ("This variable is undefined at this point")
    if (present (var_type)) then
        select case (var_type)
        case (V_LOG)
            call eval_node_init_log_ptr (en, var_name, no_lval, unknown)
        case (V_SEV)
            call eval_node_init_subevt_ptr &
                (en, var_name, no_pval, unknown)
        case (V_STR)
            call eval_node_init_string_ptr (en, var_name, no_sval, unknown)
        end select
    else
        call eval_node_init_real_ptr (en, var_name, no_rval, unknown)
    end if
end if
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done variable"
end if
end subroutine eval_node_compile_variable

```

In a given context, a variable has to have a certain type.

(Eval trees: procedures)+≡

```

subroutine check_var_type (pn, ok, type_actual, type_requested)
    type(parse_node_t), intent(in) :: pn
    logical, intent(out) :: ok
    integer, intent(in) :: type_actual
    integer, intent(in), optional :: type_requested
    if (present (type_requested)) then
        select case (type_requested)
        case (V_LOG)
            select case (type_actual)
            case (V_LOG)
            case default
                call parse_node_write (pn)

```

```

        call msg_fatal ("Variable type is invalid (should be logical)")
        ok = .false.
    end select
case (V_SEV)
    select case (type_actual)
    case (V_SEV)
    case default
        call parse_node_write (pn)
        call msg_fatal &
            ("Variable type is invalid (should be particle set)")
        ok = .false.
    end select
case (V_PDG)
    select case (type_actual)
    case (V_PDG)
    case default
        call parse_node_write (pn)
        call msg_fatal &
            ("Variable type is invalid (should be PDG array)")
        ok = .false.
    end select
case (V_STR)
    select case (type_actual)
    case (V_STR)
    case default
        call parse_node_write (pn)
        call msg_fatal &
            ("Variable type is invalid (should be string)")
        ok = .false.
    end select
case default
    call parse_node_write (pn)
    call msg_bug ("Variable type is unknown")
end select
else
    select case (type_actual)
    case (V_REAL, V_OBS1_REAL, V_OBS2_REAL, V_INT, V_OBS1_INT, &
        V_OBS2_INT, V_CMPLX)
    case default
        call parse_node_write (pn)
        call msg_fatal ("Variable type is invalid (should be numeric)")
        ok = .false.
    end select
end if
ok = .true.
end subroutine check_var_type

```

Retrieve the result of an integration. If the requested process has been integrated, the results are available as special variables. (The variables cannot be accessed in the usual way since they contain brackets in their names.)

Since this compilation step may occur before the processes have been loaded, we have to initialize the required variables before they are used.

<Eval trees: procedures>+≡

```

subroutine eval_node_compile_result (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in), target :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_key, pn_prc_id
  type(string_t) :: key, prc_id, var_name
  integer, pointer :: iptr
  real(default), pointer :: rptr
  logical, pointer :: known
  if (debug_active (D_MODEL_F)) then
    print *, "read result"; call parse_node_write (pn)
  end if
  pn_key => parse_node_get_sub_ptr (pn)
  pn_prc_id => parse_node_get_next_ptr (pn_key)
  key = parse_node_get_key (pn_key)
  prc_id = parse_node_get_string (pn_prc_id)
  var_name = key // "(" // prc_id // ")"
  if (var_list%contains (var_name)) then
    allocate (en)
    select case (char(key))
      case ("num_id", "n_calls")
        call var_list%get_iptr (var_name, iptr, known)
        call eval_node_init_int_ptr (en, var_name, iptr, known)
      case ("integral", "error")
        call var_list%get_rptr (var_name, rptr, known)
        call eval_node_init_real_ptr (en, var_name, rptr, known)
    end select
  else
    call msg_fatal ("Result variable '" // char (var_name) &
      // "' is undefined (call 'integrate' before use)")
  end if
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done result"
  end if
end subroutine eval_node_compile_result

```

Functions with a single argument. For non-constant arguments, watch for functions which convert their argument to a different type.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_unary_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_fname, pn_arg
  type(eval_node_t), pointer :: en1
  type(string_t) :: key
  integer :: t
  if (debug_active (D_MODEL_F)) then
    print *, "read unary function"; call parse_node_write (pn)
  end if
  pn_fname => parse_node_get_sub_ptr (pn)
  pn_arg => parse_node_get_next_ptr (pn_fname, tag="function_arg1")

```

```

call eval_node_compile_expr &
    (en1, parse_node_get_sub_ptr (pn_arg, tag="expr"), var_list)
t = en1%result_type
allocate (en)
key = parse_node_get_key (pn_fname)
if (en1%type == EN_CONSTANT) then
    select case (char (key))
    case ("complex")
        select case (t)
        case (V_INT); call eval_node_init_cmplx (en, cmplx_i (en1))
        case (V_REAL); call eval_node_init_cmplx (en, cmplx_r (en1))
        case (V_CMPLX); deallocate (en); en => en1; en1 => null ()
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("real")
        select case (t)
        case (V_INT); call eval_node_init_real (en, real_i (en1))
        case (V_REAL); deallocate (en); en => en1; en1 => null ()
        case (V_CMPLX); call eval_node_init_real (en, real_c (en1))
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("int")
        select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, int_r (en1))
        case (V_CMPLX); call eval_node_init_int (en, int_c (en1))
        end select
    case ("nint")
        select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, nint_r (en1))
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("floor")
        select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, floor_r (en1))
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("ceiling")
        select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, ceiling_r (en1))
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("abs")
        select case (t)
        case (V_INT); call eval_node_init_int (en, abs_i (en1))
        case (V_REAL); call eval_node_init_real (en, abs_r (en1))
        case (V_CMPLX); call eval_node_init_real (en, abs_c (en1))
        end select
    case ("conjg")
        select case (t)
        case (V_INT); call eval_node_init_int (en, conjg_i (en1))

```

```

        case (V_REAL); call eval_node_init_real (en, conjg_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, conjg_c (en1))
    end select
case ("sgn")
    select case (t)
        case (V_INT); call eval_node_init_int (en, sgn_i (en1))
        case (V_REAL); call eval_node_init_real (en, sgn_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("sqrt")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, sqrt_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, sqrt_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("exp")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, exp_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, exp_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, log_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, log_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log10")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, log10_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("sin")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, sin_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, sin_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("cos")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, cos_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, cos_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("tan")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, tan_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("asin")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, asin_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select

```

```

case ("acos")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, acos_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atan")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, atan_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("sinh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, sinh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cosh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, cosh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tanh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, tanh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asinh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, asinh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acosh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, acosh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atanh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, atanh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case default
  call parse_node_mismatch ("function name", pn_fname)
end select
if (associated (en1)) then
  call eval_node_final_rec (en1)
  deallocate (en1)
end if
else
  select case (char (key))
    case ("complex")
      call eval_node_init_branch (en, key, V_CMPLX, en1)
    case ("real")
      call eval_node_init_branch (en, key, V_REAL, en1)
    case ("int", "nint", "floor", "ceiling")

```



```

        call eval_node_init_branch (en, key, V_INT, en1)
case default
    call eval_node_init_branch (en, key, t, en1)
end select
select case (char (key))
case ("complex")
    select case (t)
    case (V_INT); call eval_node_set_op1_cmplx (en, cmplx_i)
    case (V_REAL); call eval_node_set_op1_cmplx (en, cmplx_r)
    case (V_CMPLX); deallocate (en); en => en1
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("real")
    select case (t)
    case (V_INT); call eval_node_set_op1_real (en, real_i)
    case (V_REAL); deallocate (en); en => en1
    case (V_CMPLX); call eval_node_set_op1_real (en, real_c)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("int")
    select case (t)
    case (V_INT); deallocate (en); en => en1
    case (V_REAL); call eval_node_set_op1_int (en, int_r)
    case (V_CMPLX); call eval_node_set_op1_int (en, int_c)
    end select
case ("nint")
    select case (t)
    case (V_INT); deallocate (en); en => en1
    case (V_REAL); call eval_node_set_op1_int (en, nint_r)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("floor")
    select case (t)
    case (V_INT); deallocate (en); en => en1
    case (V_REAL); call eval_node_set_op1_int (en, floor_r)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("ceiling")
    select case (t)
    case (V_INT); deallocate (en); en => en1
    case (V_REAL); call eval_node_set_op1_int (en, ceiling_r)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("abs")
    select case (t)
    case (V_INT); call eval_node_set_op1_int (en, abs_i)
    case (V_REAL); call eval_node_set_op1_real (en, abs_r)
    case (V_CMPLX);
        call eval_node_init_branch (en, key, V_REAL, en1)
        call eval_node_set_op1_real (en, abs_c)
    end select
case ("conj")
    select case (t)
    case (V_INT); call eval_node_set_op1_int (en, conjg_i)

```

```

        case (V_REAL); call eval_node_set_op1_real (en, conjg_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, conjg_c)
    end select
case ("sgn")
    select case (t)
        case (V_INT); call eval_node_set_op1_int (en, sgn_i)
        case (V_REAL); call eval_node_set_op1_real (en, sgn_r)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("sqrt")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, sqrt_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, sqrt_c)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("exp")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, exp_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, exp_c)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, log_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, log_c)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log10")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, log10_r)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("sin")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, sin_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, sin_c)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("cos")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, cos_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, cos_c)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("tan")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, tan_r)
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("asin")
    select case (t)
        case (V_REAL); call eval_node_set_op1_real (en, asin_r)
        case default; call eval_type_error (pn, char (key), t)
    end select

```

```

case ("acos")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, acos_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atan")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, atan_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("sinh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, sinh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cosh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, cosh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tanh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, tanh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asinh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, asinh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acosh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, acosh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atanh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, atanh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case default
  call parse_node_mismatch ("function name", pn_fname)
end select
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done function"
end if
end subroutine eval_node_compile_unary_function

```

Functions with two arguments.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_binary_function (en, pn, var_list)
  type(eval_node_t), pointer :: en

```

```

type(parse_node_t), intent(in) :: pn
type(var_list_t), intent(in), target :: var_list
type(parse_node_t), pointer :: pn_fname, pn_arg, pn_arg1, pn_arg2
type(eval_node_t), pointer :: en1, en2
type(string_t) :: key
integer :: t1, t2
if (debug_active (D_MODEL_F)) then
    print *, "read binary function"; call parse_node_write (pn)
end if
pn_fname => parse_node_get_sub_ptr (pn)
pn_arg => parse_node_get_next_ptr (pn_fname, tag="function_arg2")
pn_arg1 => parse_node_get_sub_ptr (pn_arg, tag="expr")
pn_arg2 => parse_node_get_next_ptr (pn_arg1, tag="expr")
call eval_node_compile_expr (en1, pn_arg1, var_list)
call eval_node_compile_expr (en2, pn_arg2, var_list)
t1 = en1%result_type
t2 = en2%result_type
allocate (en)
key = parse_node_get_key (pn_fname)
if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
    select case (char (key))
    case ("max")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_init_int (en, max_ii (en1, en2))
            case (V_REAL); call eval_node_init_real (en, max_ir (en1, en2))
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_init_real (en, max_ri (en1, en2))
            case (V_REAL); call eval_node_init_real (en, max_rr (en1, en2))
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case default; call eval_type_error (pn, char (key), t1)
        end select
    case ("min")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_init_int (en, min_ii (en1, en2))
            case (V_REAL); call eval_node_init_real (en, min_ir (en1, en2))
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_init_real (en, min_ri (en1, en2))
            case (V_REAL); call eval_node_init_real (en, min_rr (en1, en2))
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case default; call eval_type_error (pn, char (key), t1)
        end select
    case ("mod")

```

```

select case (t1)
case (V_INT)
  select case (t2)
    case (V_INT); call eval_node_init_int (en, mod_ii (en1, en2))
    case (V_REAL); call eval_node_init_real (en, mod_ir (en1, en2))
    case default; call eval_type_error (pn, char (key), t2)
  end select
case (V_REAL)
  select case (t2)
    case (V_INT); call eval_node_init_real (en, mod_ri (en1, en2))
    case (V_REAL); call eval_node_init_real (en, mod_rr (en1, en2))
    case default; call eval_type_error (pn, char (key), t2)
  end select
case default; call eval_type_error (pn, char (key), t1)
end select
case ("modulo")
  select case (t1)
  case (V_INT)
    select case (t2)
      case (V_INT); call eval_node_init_int (en, modulo_ii (en1, en2))
      case (V_REAL); call eval_node_init_real (en, modulo_ir (en1, en2))
      case default; call eval_type_error (pn, char (key), t2)
    end select
  case (V_REAL)
    select case (t2)
      case (V_INT); call eval_node_init_real (en, modulo_ri (en1, en2))
      case (V_REAL); call eval_node_init_real (en, modulo_rr (en1, en2))
      case default; call eval_type_error (pn, char (key), t2)
    end select
  case default; call eval_type_error (pn, char (key), t2)
end select
case default
  call parse_node_mismatch ("function name", pn_fname)
end select
call eval_node_final_rec (en1)
deallocate (en1)
else
  call eval_node_init_branch (en, key, t1, en1, en2)
  select case (char (key))
  case ("max")
    select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, max_ii)
        case (V_REAL); call eval_node_set_op2_real (en, max_ir)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, max_ri)
        case (V_REAL); call eval_node_set_op2_real (en, max_rr)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case default; call eval_type_error (pn, char (key), t2)
  end select

```

```

end select
case ("min")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, min_ii)
        case (V_REAL); call eval_node_set_op2_real (en, min_ir)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, min_ri)
        case (V_REAL); call eval_node_set_op2_real (en, min_rr)
        case default; call eval_type_error (pn, char (key), t2)
      end select
      case default; call eval_type_error (pn, char (key), t2)
    end select
  end select
case ("mod")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, mod_ii)
        case (V_REAL); call eval_node_set_op2_real (en, mod_ir)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, mod_ri)
        case (V_REAL); call eval_node_set_op2_real (en, mod_rr)
        case default; call eval_type_error (pn, char (key), t2)
      end select
      case default; call eval_type_error (pn, char (key), t2)
    end select
  end select
case ("modulo")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, modulo_ii)
        case (V_REAL); call eval_node_set_op2_real (en, modulo_ir)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, modulo_ri)
        case (V_REAL); call eval_node_set_op2_real (en, modulo_rr)
        case default; call eval_type_error (pn, char (key), t2)
      end select
      case default; call eval_type_error (pn, char (key), t2)
    end select
  end select
case default
  call parse_node_mismatch ("function name", pn_fname)
end select
end if
if (debug_active (D_MODEL_F)) then

```

```

        call eval_node_write (en)
        print *, "done function"
    end if
end subroutine eval_node_compile_binary_function

```

Variable definition

A block expression contains a variable definition (first argument) and an expression where the definition can be used (second argument). The `result_type` decides which type of expression is expected for the second argument. For numeric variables, if there is a mismatch between real and integer type, insert an extra node for type conversion.

(*Eval trees: procedures*) +=

```

recursive subroutine eval_node_compile_block_expr &
    (en, pn, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(in), optional :: result_type
    type(parse_node_t), pointer :: pn_var_spec, pn_var_subspec
    type(parse_node_t), pointer :: pn_var_type, pn_var_name, pn_var_expr
    type(parse_node_t), pointer :: pn_expr
    type(string_t) :: var_name
    type(eval_node_t), pointer :: en1, en2
    integer :: var_type
    logical :: new
    if (debug_active (D_MODEL_F)) then
        print *, "read block expr"; call parse_node_write (pn)
    end if
    new = .false.
    pn_var_spec => parse_node_get_sub_ptr (pn, 2)
    select case (char (parse_node_get_rule_key (pn_var_spec)))
    case ("var_num");      var_type = V_NONE
        pn_var_name => parse_node_get_sub_ptr (pn_var_spec)
    case ("var_int");      var_type = V_INT
        new = .true.
        pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
    case ("var_real");     var_type = V_REAL
        new = .true.
        pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
    case ("var_cmplx");    var_type = V_CMPLX
        new = .true.
        pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
    case ("var_logical_new"); var_type = V_LOG
        new = .true.
        pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)
        pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
    case ("var_logical_spec"); var_type = V_LOG
        pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
    case ("var_plist_new"); var_type = V_SEV
        new = .true.
        pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)

```

```

        pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
case ("var_plist_spec");    var_type = V_SEV
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_alias");    var_type = V_PDG
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_string_new");    var_type = V_STR
    new = .true.
    pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)
    pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
case ("var_string_spec");    var_type = V_STR
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case default
    call parse_node_mismatch &
        ("logical|int|real|plist|alias", pn_var_type)
end select
pn_var_expr => parse_node_get_next_ptr (pn_var_name, 2)
pn_expr => parse_node_get_next_ptr (pn_var_spec, 2)
var_name = parse_node_get_string (pn_var_name)
select case (var_type)
case (V_LOG);    var_name = "?" // var_name
case (V_SEV);    var_name = "@" // var_name
case (V_STR);    var_name = "$" // var_name    ! $ sign
end select
call var_list%check_user_var (var_name, var_type, new)
call eval_node_compile_genexpr (en1, pn_var_expr, var_list, var_type)
call insert_conversion_node (en1, var_type)
allocate (en)
call eval_node_init_block (en, var_name, var_type, en1, var_list)
call eval_node_compile_genexpr (en2, pn_expr, en%var_list, result_type)
call eval_node_set_expr (en, en2)
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done block expr"
end if
end subroutine eval_node_compile_block_expr

```

Insert a conversion node for integer/real/complex transformation if necessary.

What shall we do for the complex to integer/real conversion?

<Eval trees: procedures>+≡

```

subroutine insert_conversion_node (en, result_type)
    type(eval_node_t), pointer :: en
    integer, intent(in) :: result_type
    type(eval_node_t), pointer :: en_conv
    select case (en%result_type)
    case (V_INT)
        select case (result_type)
        case (V_REAL)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("real"), V_REAL, en)
            call eval_node_set_op1_real (en_conv, real_i)
            en => en_conv

```



```

        case (V_CMPLX)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("complex"), V_CMPLX, en)
            call eval_node_set_op1_cmplx (en_conv, cmplx_i)
            en => en_conv
        end select
    case (V_REAL)
        select case (result_type)
        case (V_INT)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("int"), V_INT, en)
            call eval_node_set_op1_int (en_conv, int_r)
            en => en_conv
        case (V_CMPLX)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("complex"), V_CMPLX, en)
            call eval_node_set_op1_cmplx (en_conv, cmplx_r)
            en => en_conv
        end select
    case (V_CMPLX)
        select case (result_type)
        case (V_INT)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("int"), V_INT, en)
            call eval_node_set_op1_int (en_conv, int_c)
            en => en_conv
        case (V_REAL)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("real"), V_REAL, en)
            call eval_node_set_op1_real (en_conv, real_c)
            en => en_conv
        end select
    case default
    end select
end subroutine insert_conversion_node

```

Conditionals

A conditional has the structure `if lexpr then expr else expr`. So we first evaluate the logical expression, then depending on the result the first or second expression. Note that the second expression is mandatory.

The `result_type`, if present, defines the requested type of the **then** and **else** clauses. Default is numeric (int/real). If there is a mismatch between real and integer result types, insert conversion nodes.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_conditional &
    (en, pn, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(in), optional :: result_type
    type(parse_node_t), pointer :: pn_condition, pn_expr

```

```

type(parse_node_t), pointer :: pn_maybe_elseif, pn_elseif_branch
type(parse_node_t), pointer :: pn_maybe_else, pn_else_branch, pn_else_expr
type(eval_node_t), pointer :: en0, en1, en2
integer :: restype
if (debug_active (D_MODEL_F)) then
    print *, "read conditional"; call parse_node_write (pn)
end if
pn_condition => parse_node_get_sub_ptr (pn, 2, tag="lexpr")
pn_expr => parse_node_get_next_ptr (pn_condition, 2)
call eval_node_compile_lexpr (en0, pn_condition, var_list)
call eval_node_compile_genexpr (en1, pn_expr, var_list, result_type)
if (present (result_type)) then
    restype = major_result_type (result_type, en1%result_type)
else
    restype = en1%result_type
end if
pn_maybe_elseif => parse_node_get_next_ptr (pn_expr)
select case (char (parse_node_get_rule_key (pn_maybe_elseif)))
case ("maybe_elseif_expr", &
    "maybe_elseif_lexpr", &
    "maybe_elseif_pexpr", &
    "maybe_elseif_cexpr", &
    "maybe_elseif_sexpr")
    pn_elseif_branch => parse_node_get_sub_ptr (pn_maybe_elseif)
    pn_maybe_else => parse_node_get_next_ptr (pn_maybe_elseif)
    select case (char (parse_node_get_rule_key (pn_maybe_else)))
    case ("maybe_else_expr", &
        "maybe_else_lexpr", &
        "maybe_else_pexpr", &
        "maybe_else_cexpr", &
        "maybe_else_sexpr")
        pn_else_branch => parse_node_get_sub_ptr (pn_maybe_else)
        pn_else_expr => parse_node_get_sub_ptr (pn_else_branch, 2)
    case default
        pn_else_expr => null ()
    end select
    call eval_node_compile_elseif &
        (en2, pn_elseif_branch, pn_else_expr, var_list, restype)
case ("maybe_else_expr", &
    "maybe_else_lexpr", &
    "maybe_else_pexpr", &
    "maybe_else_cexpr", &
    "maybe_else_sexpr")
    pn_maybe_else => pn_maybe_elseif
    pn_maybe_elseif => null ()
    pn_else_branch => parse_node_get_sub_ptr (pn_maybe_else)
    pn_else_expr => parse_node_get_sub_ptr (pn_else_branch, 2)
    call eval_node_compile_genexpr &
        (en2, pn_else_expr, var_list, restype)
case ("endif")
    call eval_node_compile_default_else (en2, restype)
case default
    call msg_bug ("Broken conditional: unexpected " &
        // char (parse_node_get_rule_key (pn_maybe_elseif)))

```

```

end select
call eval_node_create_conditional (en, en0, en1, en2, restype)
call conditional_insert_conversion_nodes (en, restype)
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done conditional"
end if
end subroutine eval_node_compile_conditional

```

This recursively generates 'elsif' conditionals as a chain of sub-nodes of the main conditional.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_elsif &
    (en, pn, pn_elsif_expr, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(parse_node_t), pointer :: pn_elsif_expr
    type(var_list_t), intent(in), target :: var_list
    integer, intent(inout) :: result_type
    type(parse_node_t), pointer :: pn_next, pn_condition, pn_expr
    type(eval_node_t), pointer :: en0, en1, en2
    pn_condition => parse_node_get_sub_ptr (pn, 2, tag="lexpr")
    pn_expr => parse_node_get_next_ptr (pn_condition, 2)
    call eval_node_compile_lexpr (en0, pn_condition, var_list)
    call eval_node_compile_genexpr (en1, pn_expr, var_list, result_type)
    result_type = major_result_type (result_type, en1%result_type)
    pn_next => parse_node_get_next_ptr (pn)
    if (associated (pn_next)) then
        call eval_node_compile_elsif &
            (en2, pn_next, pn_elsif_expr, var_list, result_type)
        result_type = major_result_type (result_type, en2%result_type)
    else if (associated (pn_elsif_expr)) then
        call eval_node_compile_genexpr &
            (en2, pn_elsif_expr, var_list, result_type)
        result_type = major_result_type (result_type, en2%result_type)
    else
        call eval_node_compile_default_else (en2, result_type)
    end if
    call eval_node_create_conditional (en, en0, en1, en2, result_type)
end subroutine eval_node_compile_elsif

```

This makes a default 'else' branch in case it was omitted. The default value just depends on the expected type.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_default_else (en, result_type)
    type(eval_node_t), pointer :: en
    integer, intent(in) :: result_type
    type(subvt_t) :: pval_empty
    type(pdg_array_t) :: aval_undefined
    allocate (en)
    select case (result_type)
    case (V_LOG); call eval_node_init_log (en, .false.)
    case (V_INT); call eval_node_init_int (en, 0)

```

```

case (V_REAL); call eval_node_init_real (en, 0._default)
case (V_CMPLX)
    call eval_node_init_cmplx (en, (0._default, 0._default))
case (V_SEV)
    call subevt_init (pval_empty)
    call eval_node_init_subevt (en, pval_empty)
case (V_PDG)
    call eval_node_init_pdg_array (en, aval_undefined)
case (V_STR)
    call eval_node_init_string (en, var_str (""))
case default
    call msg_bug ("Undefined type for 'else' branch in conditional")
end select
end subroutine eval_node_compile_default_else

```

If the logical expression is constant, we can simplify the conditional node by replacing it with the selected branch. Otherwise, we initialize a true branching.

(Eval trees: procedures) +=

```

subroutine eval_node_create_conditional (en, en0, en1, en2, result_type)
type(eval_node_t), pointer :: en, en0, en1, en2
integer, intent(in) :: result_type
if (en0%type == EN_CONSTANT) then
    if (en0%lval) then
        en => en1
        call eval_node_final_rec (en2)
        deallocate (en2)
    else
        en => en2
        call eval_node_final_rec (en1)
        deallocate (en1)
    end if
else
    allocate (en)
    call eval_node_init_conditional (en, result_type, en0, en1, en2)
end if
end subroutine eval_node_create_conditional

```

Return the numerical result type which should be used for the combination of the two result types.

(Eval trees: procedures) +=

```

function major_result_type (t1, t2) result (t)
integer :: t
integer, intent(in) :: t1, t2
select case (t1)
case (V_INT)
    select case (t2)
    case (V_INT, V_REAL, V_CMPLX)
        t = t2
    case default
        call type_mismatch ()
    end select
case (V_REAL)
    select case (t2)

```

```

        case (V_INT)
            t = t1
        case (V_REAL, V_CMPLX)
            t = t2
        case default
            call type_mismatch ()
        end select
    case (V_CMPLX)
        select case (t2)
            case (V_INT, V_REAL, V_CMPLX)
                t = t1
            case default
                call type_mismatch ()
        end select
    case default
        if (t1 == t2) then
            t = t1
        else
            call type_mismatch ()
        end if
    end select
contains
    subroutine type_mismatch ()
        call msg_bug ("Type mismatch in branches of a conditional expression")
    end subroutine type_mismatch
end function major_result_type

```

Recursively insert conversion nodes where necessary.

```

<Eval trees: procedures>+≡
recursive subroutine conditional_insert_conversion_nodes (en, result_type)
    type(eval_node_t), intent(inout), target :: en
    integer, intent(in) :: result_type
    select case (result_type)
        case (V_INT, V_REAL, V_CMPLX)
            call insert_conversion_node (en%arg1, result_type)
            if (en%arg2%type == EN_CONDITIONAL) then
                call conditional_insert_conversion_nodes (en%arg2, result_type)
            else
                call insert_conversion_node (en%arg2, result_type)
            end if
        end select
    end subroutine conditional_insert_conversion_nodes

```

Logical expressions

A logical expression consists of one or more singlet logical expressions concatenated by ;. This is for allowing side-effects, only the last value is used.

```

<Eval trees: procedures>+≡
recursive subroutine eval_node_compile_lexpr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list

```

```

type(parse_node_t), pointer :: pn_term, pn_sequel, pn_arg
type(eval_node_t), pointer :: en1, en2
if (debug_active (D_MODEL_F)) then
    print *, "read lexpr"; call parse_node_write (pn)
end if
pn_term => parse_node_get_sub_ptr (pn, tag="lsinglet")
call eval_node_compile_lsinglet (en, pn_term, var_list)
pn_sequel => parse_node_get_next_ptr (pn_term, tag="lsequel")
do while (associated (pn_sequel))
    pn_arg => parse_node_get_sub_ptr (pn_sequel, 2, tag="lsinglet")
    en1 => en
    call eval_node_compile_lsinglet (en2, pn_arg, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        call eval_node_init_log (en, ignore_first_ll (en1, en2))
        call eval_node_final_rec (en1)
        call eval_node_final_rec (en2)
        deallocate (en1, en2)
    else
        call eval_node_init_branch &
            (en, var_str ("lsequel"), V_LOG, en1, en2)
        call eval_node_set_op2_log (en, ignore_first_ll)
    end if
    pn_sequel => parse_node_get_next_ptr (pn_sequel)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lexpr"
end if
end subroutine eval_node_compile_lexpr

```

A logical singlet expression consists of one or more logical terms concatenated by or.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lsinglet (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_term, pn_alternative, pn_arg
    type(eval_node_t), pointer :: en1, en2
    if (debug_active (D_MODEL_F)) then
        print *, "read lsinglet"; call parse_node_write (pn)
    end if
    pn_term => parse_node_get_sub_ptr (pn, tag="lterm")
    call eval_node_compile_lterm (en, pn_term, var_list)
    pn_alternative => parse_node_get_next_ptr (pn_term, tag="alternative")
    do while (associated (pn_alternative))
        pn_arg => parse_node_get_sub_ptr (pn_alternative, 2, tag="lterm")
        en1 => en
        call eval_node_compile_lterm (en2, pn_arg, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call eval_node_init_log (en, or_ll (en1, en2))
        end if
    end do
end subroutine eval_node_compile_lsinglet

```

```

        call eval_node_final_rec (en1)
        call eval_node_final_rec (en2)
        deallocate (en1, en2)
    else
        call eval_node_init_branch &
            (en, var_str ("alternative"), V_LOG, en1, en2)
        call eval_node_set_op2_log (en, or_ll)
    end if
    pn_alternative => parse_node_get_next_ptr (pn_alternative)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lsinglet"
end if
end subroutine eval_node_compile_lsinglet

```

A logical term consists of one or more logical values concatenated by `and`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lterm (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_term, pn_coincidence, pn_arg
    type(eval_node_t), pointer :: en1, en2
    if (debug_active (D_MODEL_F)) then
        print *, "read lterm"; call parse_node_write (pn)
    end if
    pn_term => parse_node_get_sub_ptr (pn)
    call eval_node_compile_lvalue (en, pn_term, var_list)
    pn_coincidence => parse_node_get_next_ptr (pn_term, tag="coincidence")
    do while (associated (pn_coincidence))
        pn_arg => parse_node_get_sub_ptr (pn_coincidence, 2)
        en1 => en
        call eval_node_compile_lvalue (en2, pn_arg, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call eval_node_init_log (en, and_ll (en1, en2))
            call eval_node_final_rec (en1)
            call eval_node_final_rec (en2)
            deallocate (en1, en2)
        else
            call eval_node_init_branch &
                (en, var_str ("coincidence"), V_LOG, en1, en2)
            call eval_node_set_op2_log (en, and_ll)
        end if
        pn_coincidence => parse_node_get_next_ptr (pn_coincidence)
    end do
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done lterm"
    end if
end subroutine eval_node_compile_lterm

```

Logical variables are disabled, because they are confused with the l.h.s. of compared expressions.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lvalue (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  if (debug_active (D_MODEL_F)) then
    print *, "read lvalue"; call parse_node_write (pn)
  end if
  select case (char (parse_node_get_rule_key (pn)))
  case ("true")
    allocate (en)
    call eval_node_init_log (en, .true.)
  case ("false")
    allocate (en)
    call eval_node_init_log (en, .false.)
  case ("negation")
    call eval_node_compile_negation (en, pn, var_list)
  case ("lvariable")
    call eval_node_compile_variable (en, pn, var_list, V_LOG)
  case ("lexpr")
    call eval_node_compile_lexpr (en, pn, var_list)
  case ("block_lexpr")
    call eval_node_compile_block_expr (en, pn, var_list, V_LOG)
  case ("conditional_lexpr")
    call eval_node_compile_conditional (en, pn, var_list, V_LOG)
  case ("compared_expr")
    call eval_node_compile_compared_expr (en, pn, var_list, V_REAL)
  case ("compared_sexpr")
    call eval_node_compile_compared_expr (en, pn, var_list, V_STR)
  case ("all_fun", "any_fun", "no_fun", "photon_isolation_fun")
    call eval_node_compile_log_function (en, pn, var_list)
  case ("record_cmd")
    call eval_node_compile_record_cmd (en, pn, var_list)
  case default
    call parse_node_mismatch &
      ("true|false|negation|lvariable|" // &
       "lexpr|block_lexpr|conditional_lexpr|" // &
       "compared_expr|compared_sexpr|logical_pexpr", pn)
  end select
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lvalue"
  end if
end subroutine eval_node_compile_lvalue

```

A negation consists of the keyword not and a logical value.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_negation (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list

```



```

type(parse_node_t), pointer :: pn_arg
type(eval_node_t), pointer :: en1
if (debug_active (D_MODEL_F)) then
    print *, "read negation"; call parse_node_write (pn)
end if
pn_arg => parse_node_get_sub_ptr (pn, 2)
call eval_node_compile_lvalue (en1, pn_arg, var_list)
allocate (en)
if (en1%type == EN_CONSTANT) then
    call eval_node_init_log (en, not_1 (en1))
    call eval_node_final_rec (en1)
    deallocate (en1)
else
    call eval_node_init_branch (en, var_str ("not"), V_LOG, en1)
    call eval_node_set_op1_log (en, not_1)
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done negation"
end if
end subroutine eval_node_compile_negation

```

Comparisons

Up to the loop, this is easy. There is always at least one comparison. This is evaluated, and the result is the logical node **en**. If it is constant, we keep its second sub-node as **en2**. (Thus, at the very end **en2** has to be deleted if **en** is (still) constant.)

If there is another comparison, we first check if the first comparison was constant. In that case, there are two possibilities: (i) it was true. Then, its right-hand side is compared with the new right-hand side, and the result replaces the previous one which is deleted. (ii) it was false. In this case, the result of the whole comparison is false, and we can exit the loop without evaluating anything else.

Now assume that the first comparison results in a valid branch, its second sub-node kept as **en2**. We first need a copy of this, which becomes the new left-hand side. If **en2** is constant, we make an identical constant node **en1**. Otherwise, we make **en1** an appropriate pointer node. Next, the first branch is saved as **en0** and we evaluate the comparison between **en1** and the a right-hand side. If this turns out to be constant, there are again two possibilities: (i) true, then we revert to the previous result. (ii) false, then the wh

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_compared_expr (en, pn, var_list, type)
type(eval_node_t), pointer :: en
type(parse_node_t), intent(in) :: pn
type(var_list_t), intent(in), target :: var_list
integer, intent(in) :: type
type(parse_node_t), pointer :: pn_comparison, pn_expr1
type(eval_node_t), pointer :: en0, en1, en2
if (debug_active (D_MODEL_F)) then
    print *, "read comparison"; call parse_node_write (pn)

```

```

end if
select case (type)
case (V_INT, V_REAL)
    pn_expr1 => parse_node_get_sub_ptr (pn, tag="expr")
    call eval_node_compile_expr (en1, pn_expr1, var_list)
    pn_comparison => parse_node_get_next_ptr (pn_expr1, tag="comparison")
case (V_STR)
    pn_expr1 => parse_node_get_sub_ptr (pn, tag="sexpr")
    call eval_node_compile_sexpr (en1, pn_expr1, var_list)
    pn_comparison => parse_node_get_next_ptr (pn_expr1, tag="str_comparison")
end select
call eval_node_compile_comparison &
    (en, en1, en2, pn_comparison, var_list, type)
pn_comparison => parse_node_get_next_ptr (pn_comparison)
SCAN_FURTHER: do while (associated (pn_comparison))
    if (en%type == EN_CONSTANT) then
        if (en%lval) then
            en1 => en2
            call eval_node_final_rec (en); deallocate (en)
            call eval_node_compile_comparison &
                (en, en1, en2, pn_comparison, var_list, type)
        else
            exit SCAN_FURTHER
        end if
    else
        allocate (en1)
        if (en2%type == EN_CONSTANT) then
            select case (en2%result_type)
            case (V_INT); call eval_node_init_int    (en1, en2%ival)
            case (V_REAL); call eval_node_init_real  (en1, en2%rval)
            case (V_STR); call eval_node_init_string (en1, en2%sval)
            end select
        else
            select case (en2%result_type)
            case (V_INT); call eval_node_init_int_ptr &
                (en1, var_str ("(previous)"), en2%ival, en2%value_is_known)
            case (V_REAL); call eval_node_init_real_ptr &
                (en1, var_str ("(previous)"), en2%rval, en2%value_is_known)
            case (V_STR); call eval_node_init_string_ptr &
                (en1, var_str ("(previous)"), en2%sval, en2%value_is_known)
            end select
        end if
        en0 => en
        call eval_node_compile_comparison &
            (en, en1, en2, pn_comparison, var_list, type)
        if (en%type == EN_CONSTANT) then
            if (en%lval) then
                call eval_node_final_rec (en); deallocate (en)
                en => en0
            else
                call eval_node_final_rec (en0); deallocate (en0)
                exit SCAN_FURTHER
            end if
        else
    
```

```

        en1 => en
        allocate (en)
        call eval_node_init_branch (en, var_str ("and"), V_LOG, en0, en1)
        call eval_node_set_op2_log (en, and_ll)
    end if
end if
pn_comparison => parse_node_get_next_ptr (pn_comparison)
end do SCAN_FURTHER
if (en%type == EN_CONSTANT .and. associated (en2)) then
    call eval_node_final_rec (en2); deallocate (en2)
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done compared_expr"
end if
end subroutine eval_node_compile_compared_expr

```

This takes two extra arguments: **en1**, the left-hand-side of the comparison, is already allocated and evaluated. **en2** (the right-hand side) and **en** (the result) are allocated by the routine. **pn** is the parse node which contains the operator and the right-hand side as subnodes.

If the result of the comparison is constant, **en1** is deleted but **en2** is kept, because it may be used in a subsequent comparison. **en** then becomes a constant. If the result is variable, **en** becomes a branch node which refers to **en1** and **en2**.

(*Eval trees: procedures*)+≡

```

recursive subroutine eval_node_compile_comparison &
    (en, en1, en2, pn, var_list, type)
    type(eval_node_t), pointer :: en, en1, en2
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(in) :: type
    type(parse_node_t), pointer :: pn_op, pn_arg
    type(string_t) :: key
    integer :: t1, t2
    real(default), pointer :: tolerance_ptr
    pn_op => parse_node_get_sub_ptr (pn)
    key = parse_node_get_key (pn_op)
    select case (type)
    case (V_INT, V_REAL)
        pn_arg => parse_node_get_next_ptr (pn_op, tag="expr")
        call eval_node_compile_expr (en2, pn_arg, var_list)
    case (V_STR)
        pn_arg => parse_node_get_next_ptr (pn_op, tag="sexpr")
        call eval_node_compile_sexpr (en2, pn_arg, var_list)
    end select
    t1 = en1%result_type
    t2 = en2%result_type
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        call var_list%get_rptr (var_str ("tolerance"), tolerance_ptr)
        en1%tolerance => tolerance_ptr
        select case (char (key))
        case ("<")

```

```

select case (t1)
case (V_INT)
  select case (t2)
    case (V_INT); call eval_node_init_log (en, comp_lt_ii (en1, en2))
    case (V_REAL); call eval_node_init_log (en, comp_ll_ir (en1, en2))
  end select
case (V_REAL)
  select case (t2)
    case (V_INT); call eval_node_init_log (en, comp_ll_ri (en1, en2))
    case (V_REAL); call eval_node_init_log (en, comp_ll_rr (en1, en2))
  end select
end select
case ">")
  select case (t1)
  case (V_INT)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_gt_ii (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_gg_ir (en1, en2))
    end select
  case (V_REAL)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_gg_ri (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_gg_rr (en1, en2))
    end select
  end select
case "<=")
  select case (t1)
  case (V_INT)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_le_ii (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_ls_ir (en1, en2))
    end select
  case (V_REAL)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_ls_ri (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_ls_rr (en1, en2))
    end select
  end select
case ">=")
  select case (t1)
  case (V_INT)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_ge_ii (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_gs_ir (en1, en2))
    end select
  case (V_REAL)
    select case (t2)
      case (V_INT); call eval_node_init_log (en, comp_gs_ri (en1, en2))
      case (V_REAL); call eval_node_init_log (en, comp_gs_rr (en1, en2))
    end select
  end select
case "=="
  select case (t1)
  case (V_INT)

```

```

        select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_eq_ii (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_se_ir (en1, en2))
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_se_ri (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_se_rr (en1, en2))
        end select
    case (V_STR)
        select case (t2)
        case (V_STR); call eval_node_init_log (en, comp_eq_ss (en1, en2))
        end select
    end select
case ("<>")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_ne_ii (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_ns_ir (en1, en2))
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_ns_ri (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_ns_rr (en1, en2))
        end select
    case (V_STR)
        select case (t2)
        case (V_STR); call eval_node_init_log (en, comp_ne_ss (en1, en2))
        end select
    end select
end select
call eval_node_final_rec (en1)
deallocate (en1)
else
call eval_node_init_branch (en, key, V_LOG, en1, en2)
select case (char (key))
case ("<")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_lt_ii)
        case (V_REAL); call eval_node_set_op2_log (en, comp_ll_ir)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_ll_ri)
        case (V_REAL); call eval_node_set_op2_log (en, comp_ll_rr)
        end select
    end select
case (">")
    select case (t1)
    case (V_INT)
        select case (t2)

```

```

        case (V_INT); call eval_node_set_op2_log (en, comp_gt_ii)
        case (V_REAL); call eval_node_set_op2_log (en, comp_gg_ir)
    end select
case (V_REAL)
    select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_gg_ri)
        case (V_REAL); call eval_node_set_op2_log (en, comp_gg_rr)
    end select
end select
case ("<=")
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_le_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ls_ir)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ls_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ls_rr)
            end select
        end select
    end select
case (">=")
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ge_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_gs_ir)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_gs_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_gs_rr)
            end select
        end select
    end select
case ("==")
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_eq_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_se_ir)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_se_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_se_rr)
            end select
        case (V_STR)
            select case (t2)
                case (V_STR); call eval_node_set_op2_log (en, comp_eq_ss)
            end select
        end select
    end select
case ("<>")
    select case (t1)

```

```

        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ne_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ns_ir)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ns_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ns_rr)
            end select
        case (V_STR)
            select case (t2)
                case (V_STR); call eval_node_set_op2_log (en, comp_ne_ss)
            end select
        end select
    end select
    call var_list%get_rptr (var_str ("tolerance"), tolerance_ptr)
    en1%tolerance => tolerance_ptr
end if
end subroutine eval_node_compile_comparison

```

Recording analysis data

The `record` command is actually a logical expression which always evaluates `true`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_record_cmd (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_key, pn_tag, pn_arg
    type(parse_node_t), pointer :: pn_arg1, pn_arg2, pn_arg3, pn_arg4
    type(eval_node_t), pointer :: en0, en1, en2, en3, en4
    real(default), pointer :: event_weight
    if (debug_active (D_MODEL_F)) then
        print *, "read record_cmd"; call parse_node_write (pn)
    end if
    pn_key => parse_node_get_sub_ptr (pn)
    pn_tag => parse_node_get_next_ptr (pn_key)
    pn_arg => parse_node_get_next_ptr (pn_tag)
    select case (char (parse_node_get_key (pn_key)))
        case ("record")
            call var_list%get_rptr (var_str ("event_weight"), event_weight)
        case ("record_unweighted")
            event_weight => null ()
        case ("record_excess")
            call var_list%get_rptr (var_str ("event_excess"), event_weight)
    end select
    select case (char (parse_node_get_rule_key (pn_tag)))
        case ("analysis_id")
            allocate (en0)
            call eval_node_init_string (en0, parse_node_get_string (pn_tag))

```

```

case default
  call eval_node_compile_sexpr (en0, pn_tag, var_list)
end select
allocate (en)
if (associated (pn_arg)) then
  pn_arg1 => parse_node_get_sub_ptr (pn_arg)
  call eval_node_compile_expr (en1, pn_arg1, var_list)
  if (en1%result_type == V_INT) &
    call insert_conversion_node (en1, V_REAL)
  pn_arg2 => parse_node_get_next_ptr (pn_arg1)
  if (associated (pn_arg2)) then
    call eval_node_compile_expr (en2, pn_arg2, var_list)
    if (en2%result_type == V_INT) &
      call insert_conversion_node (en2, V_REAL)
  pn_arg3 => parse_node_get_next_ptr (pn_arg2)
  if (associated (pn_arg3)) then
    call eval_node_compile_expr (en3, pn_arg3, var_list)
    if (en3%result_type == V_INT) &
      call insert_conversion_node (en3, V_REAL)
  pn_arg4 => parse_node_get_next_ptr (pn_arg3)
  if (associated (pn_arg4)) then
    call eval_node_compile_expr (en4, pn_arg4, var_list)
    if (en4%result_type == V_INT) &
      call insert_conversion_node (en4, V_REAL)
    call eval_node_init_record_cmd &
      (en, event_weight, en0, en1, en2, en3, en4)
  else
    call eval_node_init_record_cmd &
      (en, event_weight, en0, en1, en2, en3)
  end if
else
  call eval_node_init_record_cmd (en, event_weight, en0, en1, en2)
end if
else
  call eval_node_init_record_cmd (en, event_weight, en0, en1)
end if
else
  call eval_node_init_record_cmd (en, event_weight, en0)
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done record_cmd"
end if
end subroutine eval_node_compile_record_cmd

```

Particle-list expressions

A particle expression is a subevent or a concatenation of particle-list terms (using join).

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_pexpr (en, pn, var_list)
  type(eval_node_t), pointer :: en

```



```

type(parse_node_t), intent(in) :: pn
type(var_list_t), intent(in), target :: var_list
type(parse_node_t), pointer :: pn_pterm, pn_concatenation, pn_op, pn_arg
type(eval_node_t), pointer :: en1, en2
type(subevt_t) :: subevt
if (debug_active (D_MODEL_F)) then
  print *, "read pexpr"; call parse_node_write (pn)
end if
pn_pterm => parse_node_get_sub_ptr (pn)
call eval_node_compile_pterm (en, pn_pterm, var_list)
pn_concatenation => &
  parse_node_get_next_ptr (pn_pterm, tag="pconcatenation")
do while (associated (pn_concatenation))
  pn_op => parse_node_get_sub_ptr (pn_concatenation)
  pn_arg => parse_node_get_next_ptr (pn_op)
  en1 => en
  call eval_node_compile_pterm (en2, pn_arg, var_list)
  allocate (en)
  if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
    call subevt_join (subevt, en1%pval, en2%pval)
    call eval_node_init_subevt (en, subevt)
    call eval_node_final_rec (en1)
    call eval_node_final_rec (en2)
    deallocate (en1, en2)
  else
    call eval_node_init_branch &
      (en, var_str ("join"), V_SEV, en1, en2)
    call eval_node_set_op2_sev (en, join_pp)
  end if
  pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
end do
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done pexpr"
end if
end subroutine eval_node_compile_pexpr

```

A particle term is a subevent or a combination of particle-list values (using combine).

(Eval trees: procedures) +=

```

recursive subroutine eval_node_compile_pterm (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_pvalue, pn_combination, pn_op, pn_arg
  type(eval_node_t), pointer :: en1, en2
  type(subevt_t) :: subevt
  if (debug_active (D_MODEL_F)) then
    print *, "read pterm"; call parse_node_write (pn)
  end if
  pn_pvalue => parse_node_get_sub_ptr (pn)
  call eval_node_compile_pvalue (en, pn_pvalue, var_list)
  pn_combination => &

```

```

        parse_node_get_next_ptr (pn_pvalue, tag="pcombination")
do while (associated (pn_combination))
    pn_op => parse_node_get_sub_ptr (pn_combination)
    pn_arg => parse_node_get_next_ptr (pn_op)
    en1 => en
    call eval_node_compile_pvalue (en2, pn_arg, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        call subevt_combine (subevt, en1%pval, en2%pval)
        call eval_node_init_subevt (en, subevt)
        call eval_node_final_rec (en1)
        call eval_node_final_rec (en2)
        deallocate (en1, en2)
    else
        call eval_node_init_branch &
            (en, var_str ("combine"), V_SEV, en1, en2)
        call eval_node_set_op2_sev (en, combine_pp)
    end if
    pn_combination => parse_node_get_next_ptr (pn_combination)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done pterm"
end if
end subroutine eval_node_compile_pterm

```

A particle-list value is a PDG-code array, a particle identifier, a variable, a (grouped) pexpr, a block pexpr, a conditional, or a particle-list function.

The `cexpr` node is responsible for transforming a constant PDG-code array into a subevent. It takes the code array as its first argument, the event subevent as its second argument, and the requested particle type (incoming/outgoing) as its zero-th argument. The result is the list of particles in the event that match the code array.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_pvalue (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_prefix_cexpr
    type(eval_node_t), pointer :: en1, en2, en0
    type(string_t) :: key
    type(subevt_t), pointer :: evt_ptr
    logical, pointer :: known
    if (debug_active (D_MODEL_F)) then
        print *, "read pvalue"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("pexpr_src")
        call eval_node_compile_prefix_cexpr (en1, pn, var_list)
        allocate (en2)
        if (var_list%contains (var_str ("@evt"))) then
            call var_list%get_pptr (var_str ("@evt"), evt_ptr, known)
            call eval_node_init_subevt_ptr (en2, var_str ("@evt"), evt_ptr, known)

```

```

allocate (en)
call eval_node_init_branch &
      (en, var_str ("prt_selection"), V_SEV, en1, en2)
call eval_node_set_op2_sev (en, select_pdg_ca)
allocate (en0)
pn_prefix_cexpr => parse_node_get_sub_ptr (pn)
key = parse_node_get_rule_key (pn_prefix_cexpr)
select case (char (key))
case ("beam_prt")
      call eval_node_init_int (en0, PRT_BEAM)
      en%arg0 => en0
case ("incoming_prt")
      call eval_node_init_int (en0, PRT_INCOMING)
      en%arg0 => en0
case ("outgoing_prt")
      call eval_node_init_int (en0, PRT_OUTGOING)
      en%arg0 => en0
case ("unspecified_prt")
      call eval_node_init_int (en0, PRT_OUTGOING)
      en%arg0 => en0
end select
else
      call parse_node_write (pn)
      call msg_bug (" Missing event data while compiling pvalue")
end if
case ("pvariable")
      call eval_node_compile_variable (en, pn, var_list, V_SEV)
case ("pexpr")
      call eval_node_compile_pexpr (en, pn, var_list)
case ("block_pexpr")
      call eval_node_compile_block_expr (en, pn, var_list, V_SEV)
case ("conditional_pexpr")
      call eval_node_compile_conditional (en, pn, var_list, V_SEV)
case ("join_fun", "combine_fun", "collect_fun", "cluster_fun", &
      "select_fun", "extract_fun", "sort_fun", "select_b_jet_fun", &
      "select_non_bjet_fun", "select_c_jet_fun", &
      "select_light_jet_fun", "photon_reco_fun")
      call eval_node_compile_prt_function (en, pn, var_list)
case default
      call parse_node_mismatch &
            ("prefix_cexpr|pvariable|" // &
            "grouped_pexpr|block_pexpr|conditional_pexpr|" // &
            "prt_function", pn)
end select
if (debug_active (D_MODEL_F)) then
      call eval_node_write (en)
      print *, "done pvalue"
end if
end subroutine eval_node_compile_pvalue

```

Particle functions

This combines the treatment of 'join', 'combine', 'collect', 'cluster', 'select', and 'extract', as well as the functions for b , c and light jet selection and photon recombination which all have the same syntax. The one or two argument nodes are allocated. If there is a condition, the condition node is also allocated as a logical expression, for which the variable list is augmented by the appropriate (unary/binary) observables.

(*Eval trees: procedures*) \equiv

```
recursive subroutine eval_node_compile_prt_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_clause, pn_key, pn_cond, pn_args
  type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
  type(eval_node_t), pointer :: en0, en1, en2
  type(string_t) :: key
  if (debug_active (D_MODEL_F)) then
    print *, "read prt_function"; call parse_node_write (pn)
  end if
  pn_clause => parse_node_get_sub_ptr (pn)
  pn_key   => parse_node_get_sub_ptr (pn_clause)
  pn_cond => parse_node_get_next_ptr (pn_key)
  if (associated (pn_cond)) &
    pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
  pn_args => parse_node_get_next_ptr (pn_clause)
  pn_arg1 => parse_node_get_sub_ptr (pn_args)
  pn_arg2 => parse_node_get_next_ptr (pn_arg1)
  key = parse_node_get_key (pn_key)
  call eval_node_compile_pexpr (en1, pn_arg1, var_list)
  allocate (en)
  if (.not. associated (pn_arg2)) then
    select case (char (key))
    case ("collect")
      call eval_node_init_prt_fun_unary (en, en1, key, collect_p)
    case ("cluster")
      if (fastjet_available ()) then
        call fastjet_init ()
      else
        call msg_fatal &
          ("'cluster' function requires FastJet, which is not enabled")
      end if
      en1%var_list => var_list
      call eval_node_init_prt_fun_unary (en, en1, key, cluster_p)
      call var_list%get_iptr (var_str ("jet_algorithm"), en1%jet_algorithm)
      call var_list%get_rptr (var_str ("jet_r"), en1%jet_r)
      call var_list%get_rptr (var_str ("jet_p"), en1%jet_p)
      call var_list%get_rptr (var_str ("jet_ycut"), en1%jet_ycut)
      call var_list%get_rptr (var_str ("jet_dcut"), en1%jet_dcut)
    case ("photon_recombination")
      en1%var_list => var_list
      call eval_node_init_prt_fun_unary &
        (en, en1, key, photon_recombination_p)
      call var_list%get_rptr (var_str ("photon_rec_r0"), en1%photon_rec_r0)
```

```

case ("select")
  call eval_node_init_prt_fun_unary (en, en1, key, select_p)
case ("extract")
  call eval_node_init_prt_fun_unary (en, en1, key, extract_p)
case ("sort")
  call eval_node_init_prt_fun_unary (en, en1, key, sort_p)
case ("select_b_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_b_jet_p)
case ("select_non_b_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_non_b_jet_p)
case ("select_c_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_c_jet_p)
case ("select_light_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_light_jet_p)
case default
  call msg_bug (" Unary particle function '" // char (key) // &
    "' undefined")
end select
else
  call eval_node_compile_pexpr (en2, pn_arg2, var_list)
  select case (char (key))
  case ("join")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, join_pp)
  case ("combine")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, combine_pp)
  case ("collect")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, collect_pp)
  case ("select")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, select_pp)
  case ("sort")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, sort_pp)
  case default
    call msg_bug (" Binary particle function '" // char (key) // &
      "' undefined")
  end select
end if
if (associated (pn_cond)) then
  call eval_node_set_observables (en, var_list)
  select case (char (key))
  case ("extract", "sort")
    call eval_node_compile_expr (en0, pn_arg0, en%var_list)
  case default
    call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
  end select
  en%arg0 => en0
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done prt_function"
end if
end subroutine eval_node_compile_prt_function

```

The `eval` expression is similar, but here the expression `arg0` is mandatory, and the whole thing evaluates to a numeric value. To guarantee initialization of

variables defined on subevents instead of a single (namely the first) particle of a subevent, we make sure that `en` points to the subevent stored in `en1`.

(Eval trees: procedures)+≡

```
recursive subroutine eval_node_compile_eval_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_key, pn_arg0, pn_args, pn_arg1, pn_arg2
  type(eval_node_t), pointer :: en0, en1, en2
  type(string_t) :: key
  if (debug_active (D_MODEL_F)) then
    print *, "read eval_function"; call parse_node_write (pn)
  end if
  pn_key => parse_node_get_sub_ptr (pn)
  pn_arg0 => parse_node_get_next_ptr (pn_key)
  pn_args => parse_node_get_next_ptr (pn_arg0)
  pn_arg1 => parse_node_get_sub_ptr (pn_args)
  pn_arg2 => parse_node_get_next_ptr (pn_arg1)
  key = parse_node_get_key (pn_key)
  call eval_node_compile_pexpr (en1, pn_arg1, var_list)
  allocate (en)
  if (.not. associated (pn_arg2)) then
    call eval_node_init_eval_fun_unary (en, en1, key)
  else
    call eval_node_compile_pexpr (en2, pn_arg2, var_list)
    call eval_node_init_eval_fun_binary (en, en1, en2, key)
  end if
  en%pval => en1%pval
  call eval_node_set_observables (en, var_list)
  call eval_node_compile_expr (en0, pn_arg0, en%var_list)
  if (en0%result_type == V_INT) &
    call insert_conversion_node (en0, V_REAL)
  if (en0%result_type /= V_REAL) &
    call msg_fatal (" 'eval' function does not result in real value")
  call eval_node_set_expr (en, en0)
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done eval_function"
  end if
end subroutine eval_node_compile_eval_function
```

Logical functions of subevents. For `photon_isolation` there is a conditional selection expression instead of a mandatory logical expression, so in the case of the absence of the selection we have to create a logical `eval_node_t` with value `.true..`

(Eval trees: procedures)+≡

```
recursive subroutine eval_node_compile_log_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_clause, pn_key, pn_str, pn_cond
  type(parse_node_t), pointer :: pn_arg0, pn_args, pn_arg1, pn_arg2
  type(eval_node_t), pointer :: en0, en1, en2
```

```

type(string_t) :: key
if (debug_active (D_MODEL_F)) then
    print *, "read log_function"; call parse_node_write (pn)
end if
select case (char (parse_node_get_rule_key (pn)))
case ("all_fun", "any_fun", "no_fun")
    pn_key => parse_node_get_sub_ptr (pn)
    pn_arg0 => parse_node_get_next_ptr (pn_key)
    pn_args => parse_node_get_next_ptr (pn_arg0)
case ("photon_isolation_fun")
    pn_clause => parse_node_get_sub_ptr (pn)
    pn_key => parse_node_get_sub_ptr (pn_clause)
    pn_cond => parse_node_get_next_ptr (pn_key)
    if (associated (pn_cond)) then
        pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
    else
        pn_arg0 => null ()
    end if
    pn_args => parse_node_get_next_ptr (pn_clause)
case default
    call parse_node_mismatch ("all_fun|any_fun|" // &
        "no_fun|photon_isolation_fun", pn)
end select
pn_arg1 => parse_node_get_sub_ptr (pn_args)
pn_arg2 => parse_node_get_next_ptr (pn_arg1)
key = parse_node_get_key (pn_key)
call eval_node_compile_pexpr (en1, pn_arg1, var_list)
allocate (en)
if (.not. associated (pn_arg2)) then
    select case (char (key))
    case ("all")
        call eval_node_init_log_fun_unary (en, en1, key, all_p)
    case ("any")
        call eval_node_init_log_fun_unary (en, en1, key, any_p)
    case ("no")
        call eval_node_init_log_fun_unary (en, en1, key, no_p)
    case default
        call msg_bug ("Unary logical particle function '" // char (key) // &
            "' undefined")
    end select
else
    call eval_node_compile_pexpr (en2, pn_arg2, var_list)
    select case (char (key))
    case ("all")
        call eval_node_init_log_fun_binary (en, en1, en2, key, all_pp)
    case ("any")
        call eval_node_init_log_fun_binary (en, en1, en2, key, any_pp)
    case ("no")
        call eval_node_init_log_fun_binary (en, en1, en2, key, no_pp)
    case ("photon_isolation")
        en1%var_list => var_list
        call var_list%get_rptr (var_str ("photon_iso_eps"), en1%photon_iso_eps)
        call var_list%get_rptr (var_str ("photon_iso_n"), en1%photon_iso_n)
        call var_list%get_rptr (var_str ("photon_iso_r0"), en1%photon_iso_r0)
    end select
end if

```

```

        call eval_node_init_log_fun_binary (en, en1, en2, key, photon_isolation_pp)
    case default
        call msg_bug ("Binary logical particle function '" // char (key) // &
            "' undefined")
    end select
end if
if (associated (pn_arg0)) then
    call eval_node_set_observables (en, var_list)
    select case (char (key))
    case ("all", "any", "no", "photon_isolation")
        call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
    case default
        call msg_bug ("Compiling logical particle function: missing mode")
    end select
    call eval_node_set_expr (en, en0, V_LOG)
else
    select case (char (key))
    case ("photon_isolation")
        allocate (en0)
        call eval_node_init_log (en0, .true.)
        call eval_node_set_expr (en, en0, V_LOG)
    case default
        call msg_bug ("Only photon isolation can be called unconditionally")
    end select
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done log_function"
end if
end subroutine eval_node_compile_log_function

```

Count function of subevents.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_count_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_clause, pn_key, pn_cond, pn_args
    type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
    type(eval_node_t), pointer :: en0, en1, en2
    type(string_t) :: key
    if (debug_active (D_MODEL_F)) then
        print *, "read count_function"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("count_fun")
        pn_clause => parse_node_get_sub_ptr (pn)
        pn_key => parse_node_get_sub_ptr (pn_clause)
        pn_cond => parse_node_get_next_ptr (pn_key)
        if (associated (pn_cond)) then
            pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
        else
            pn_arg0 => null ()
        end if
    end if

```



```

        pn_args => parse_node_get_next_ptr (pn_clause)
    end select
    pn_arg1 => parse_node_get_sub_ptr (pn_args)
    pn_arg2 => parse_node_get_next_ptr (pn_arg1)
    key = parse_node_get_key (pn_key)
    call eval_node_compile_pexpr (en1, pn_arg1, var_list)
    allocate (en)
    if (.not. associated (pn_arg2)) then
        select case (char (key))
            case ("count")
                call eval_node_init_int_fun_unary (en, en1, key, count_a)
            case default
                call msg_bug ("Unary subevent function '" // char (key) // &
                    "' undefined")
        end select
    else
        call eval_node_compile_pexpr (en2, pn_arg2, var_list)
        select case (char (key))
            case ("count")
                call eval_node_init_int_fun_binary (en, en1, en2, key, count_pp)
            case default
                call msg_bug ("Binary subevent function '" // char (key) // &
                    "' undefined")
        end select
    end if
    if (associated (pn_arg0)) then
        call eval_node_set_observables (en, var_list)
        select case (char (key))
            case ("count")
                call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
                call eval_node_set_expr (en, en0, V_INT)
            case default
                call msg_bug ("Subevent function '" // char (key) // &
                    "' undefined")
        end select
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done count_function"
    end if
end subroutine eval_node_compile_count_function

```

Numeric functions of subevents.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_numeric_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_key, pn_args
    type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
    type(eval_node_t), pointer :: en0, en1
    type(string_t) :: key
    if (debug_active (D_MODEL_F)) then
        print *, "read numeric_function"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
        case ("sum_fun", "prod_fun")

```

```

        if (debug_active (D_MODEL_F)) then
            print *, "read sum_fun"; call parse_node_write (pn)
        end if
        pn_key => parse_node_get_sub_ptr (pn)
        pn_arg0 => parse_node_get_next_ptr (pn_key)
        pn_args => parse_node_get_next_ptr (pn_arg0)
    end select
    pn_arg1 => parse_node_get_sub_ptr (pn_args)
    pn_arg2 => parse_node_get_next_ptr (pn_arg1)
    key = parse_node_get_key (pn_key)
    call eval_node_compile_pexpr (en1, pn_arg1, var_list)
    if (associated (pn_arg2)) then
        call msg_fatal ("The " // char (key) // &
            " function can only be used for unary observables.")
    end if
    allocate (en)
    select case (char (key))
    case ("sum")
        call eval_node_init_real_fun_cum (en, en1, key, sum_a)
    case ("prod")
        call eval_node_init_real_fun_cum (en, en1, key, prod_a)
    case default
        call msg_bug ("Unary subevent function '" // char (key) // &
            "' undefined")
    end select
    call eval_node_set_observables (en, var_list)
    call eval_node_compile_expr (en0, pn_arg0, en%var_list)
    if (en0%result_type == V_INT) &
        call insert_conversion_node (en0, V_REAL)
    call eval_node_set_expr (en, en0, V_REAL)
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done numeric_function"
    end if
end subroutine eval_node_compile_numeric_function

```

PDG-code arrays

A PDG-code expression is (optionally) prefixed by `beam`, `incoming`, or `outgoing`, a block, or a conditional. In any case, it evaluates to a constant.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_prefix_cexpr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_avalue, pn_prt
    type(string_t) :: key
    if (debug_active (D_MODEL_F)) then
        print *, "read prefix_cexpr"; call parse_node_write (pn)
    end if
    pn_avalue => parse_node_get_sub_ptr (pn)
    key = parse_node_get_rule_key (pn_avalue)

```

```

select case (char (key))
case ("beam_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
case ("incoming_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
case ("outgoing_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
case ("unspecified_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 1)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
case default
    call parse_node_mismatch &
        ("beam_prt|incoming_prt|outgoing_prt|unspecified_prt", &
         pn_avalue)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done prefix_cexpr"
end if
end subroutine eval_node_compile_prefix_cexpr

```

A PDG array is a string of PDG code definitions (or aliases), concatenated by ','. The code definitions may be variables which are not defined at compile time, so we have to allocate sub-nodes. This analogous to `eval_node_compile_term`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_cexpr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_prt, pn_concatenation
    type(eval_node_t), pointer :: en1, en2
    type(pdg_array_t) :: aval
    if (debug_active (D_MODEL_F)) then
        print *, "read cexpr"; call parse_node_write (pn)
    end if
    pn_prt => parse_node_get_sub_ptr (pn)
    call eval_node_compile_avalue (en, pn_prt, var_list)
    pn_concatenation => parse_node_get_next_ptr (pn_prt)
    do while (associated (pn_concatenation))
        pn_prt => parse_node_get_sub_ptr (pn_concatenation, 2)
        en1 => en
        call eval_node_compile_avalue (en2, pn_prt, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call concat_cc (aval, en1, en2)
            call eval_node_init_pdg_array (en, aval)
            call eval_node_final_rec (en1)
            call eval_node_final_rec (en2)
            deallocate (en1, en2)
        else

```

```

        call eval_node_init_branch (en, var_str (":"), V_PDG, en1, en2)
        call eval_node_set_op2_pdg (en, concat_cc)
    end if
    pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done cexpr"
end if
end subroutine eval_node_compile_cexpr

```

Compile a PDG-code type value. It may be either an integer expression or a variable of type PDG array, optionally quoted.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_avalue (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read avalue"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("pdg_code")
        call eval_node_compile_pdg_code (en, pn, var_list)
    case ("cvariable", "variable", "prt_name")
        call eval_node_compile_cvariable (en, pn, var_list)
    case ("cexpr")
        call eval_node_compile_cexpr (en, pn, var_list)
    case ("block_cexpr")
        call eval_node_compile_block_expr (en, pn, var_list, V_PDG)
    case ("conditional_cexpr")
        call eval_node_compile_conditional (en, pn, var_list, V_PDG)
    case default
        call parse_node_mismatch &
            ("grouped_cexpr|block_cexpr|conditional_cexpr|" // &
             "pdg_code|cvariable|prt_name", pn)
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done avalue"
    end if
end subroutine eval_node_compile_avalue

```

Compile a PDG-code expression, which is the key PDG with an integer expression as argument. The procedure is analogous to `eval_node_compile_unary_function`.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_pdg_code (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_arg
    type(eval_node_t), pointer :: en1
    type(string_t) :: key

```

```

type(pdg_array_t) :: aval
integer :: t
if (debug_active (D_MODEL_F)) then
    print *, "read PDG code"; call parse_node_write (pn)
end if
pn_arg => parse_node_get_sub_ptr (pn, 2)
call eval_node_compile_expr &
    (en1, parse_node_get_sub_ptr (pn_arg, tag="expr"), var_list)
t = en1%result_type
allocate (en)
key = "PDG"
if (en1%type == EN_CONSTANT) then
    select case (t)
    case (V_INT)
        call pdg_i (aval, en1)
        call eval_node_init_pdg_array (en, aval)
    case default; call eval_type_error (pn, char (key), t)
    end select
    call eval_node_final_rec (en1)
    deallocate (en1)
else
    select case (t)
    case (V_INT); call eval_node_set_op1_pdg (en, pdg_i)
    case default; call eval_type_error (pn, char (key), t)
    end select
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done function"
end if
end subroutine eval_node_compile_pdg_code

```

This is entirely analogous to `eval_node_compile_variable`. However, PDG-array variables occur in different contexts.

To avoid name clashes between PDG-array variables and ordinary variables, we prepend a character (*). This is not visible to the user.

<Eval trees: procedures>+≡

```

subroutine eval_node_compile_cvariable (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_name
    type(string_t) :: var_name
    type(pdg_array_t), pointer :: aptr
    type(pdg_array_t), target, save :: no_aval
    logical, pointer :: known
    logical, target, save :: unknown = .false.
    if (debug_active (D_MODEL_F)) then
        print *, "read cvariable"; call parse_node_write (pn)
    end if
    pn_name => pn
    var_name = parse_node_get_string (pn_name)
    allocate (en)

```

```

if (var_list%contains (var_name)) then
  call var_list%get_aptr (var_name, aptr, known)
  call eval_node_init_pdg_array_ptr (en, var_name, aptr, known)
else
  call parse_node_write (pn)
  call msg_error ("This PDG-array variable is undefined at this point")
  call eval_node_init_pdg_array_ptr (en, var_name, no_aval, unknown)
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done cvariable"
end if
end subroutine eval_node_compile_cvariable

```

String expressions

A string expression is either a string value or a concatenation of string values.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_sexpr (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_svalue, pn_concatenation, pn_op, pn_arg
  type(eval_node_t), pointer :: en1, en2
  type(string_t) :: string
  if (debug_active (D_MODEL_F)) then
    print *, "read sexpr"; call parse_node_write (pn)
  end if
  pn_svalue => parse_node_get_sub_ptr (pn)
  call eval_node_compile_svalue (en, pn_svalue, var_list)
  pn_concatenation => &
    parse_node_get_next_ptr (pn_svalue, tag="str_concatenation")
  do while (associated (pn_concatenation))
    pn_op => parse_node_get_sub_ptr (pn_concatenation)
    pn_arg => parse_node_get_next_ptr (pn_op)
    en1 => en
    call eval_node_compile_svalue (en2, pn_arg, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
      call concat_ss (string, en1, en2)
      call eval_node_init_string (en, string)
      call eval_node_final_rec (en1)
      call eval_node_final_rec (en2)
      deallocate (en1, en2)
    else
      call eval_node_init_branch &
        (en, var_str ("concat"), V_STR, en1, en2)
      call eval_node_set_op2_str (en, concat_ss)
    end if
    pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
  end do
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
  end if
end subroutine eval_node_compile_sexpr

```

```

        print *, "done sexpr"
    end if
end subroutine eval_node_compile_sexpr

```

A string value is a string literal, a variable, a (grouped) sexpr, a block sexpr, or a conditional.

```

<Eval trees: procedures>+≡
recursive subroutine eval_node_compile_svalue (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read svalue"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("svariable")
        call eval_node_compile_variable (en, pn, var_list, V_STR)
    case ("sexpr")
        call eval_node_compile_sexpr (en, pn, var_list)
    case ("block_sexpr")
        call eval_node_compile_block_expr (en, pn, var_list, V_STR)
    case ("conditional_sexpr")
        call eval_node_compile_conditional (en, pn, var_list, V_STR)
    case ("sprintf_fun")
        call eval_node_compile_sprintf (en, pn, var_list)
    case ("string_literal")
        allocate (en)
        call eval_node_init_string (en, parse_node_get_string (pn))
    case default
        call parse_node_mismatch &
            ("svariable|" // &
             "grouped_sexpr|block_sexpr|conditional_sexpr|" // &
             "string_function|string_literal", pn)
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done svalue"
    end if
end subroutine eval_node_compile_svalue

```

There is currently one string function, `sprintf`. For `sprintf`, the first argument (no brackets) is the format string, the optional arguments in brackets are the expressions or variables to be formatted.

```

<Eval trees: procedures>+≡
recursive subroutine eval_node_compile_sprintf (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_clause, pn_key, pn_args
    type(parse_node_t), pointer :: pn_arg0
    type(eval_node_t), pointer :: en0, en1
    integer :: n_args
    type(string_t) :: key

```

```

if (debug_active (D_MODEL_F)) then
    print *, "read sprintf_fun"; call parse_node_write (pn)
end if
pn_clause => parse_node_get_sub_ptr (pn)
pn_key   => parse_node_get_sub_ptr (pn_clause)
pn_arg0  => parse_node_get_next_ptr (pn_key)
pn_args  => parse_node_get_next_ptr (pn_clause)
call eval_node_compile_sexpr (en0, pn_arg0, var_list)
if (associated (pn_args)) then
    call eval_node_compile_sprintf_args (en1, pn_args, var_list, n_args)
else
    n_args = 0
    en1 => null ()
end if
allocate (en)
key = parse_node_get_key (pn_key)
call eval_node_init_format_string (en, en0, en1, key, n_args)
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done sprintf_fun"
end if
end subroutine eval_node_compile_sprintf

```

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_sprintf_args (en, pn, var_list, n_args)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(out) :: n_args
    type(parse_node_t), pointer :: pn_arg
    integer :: i
    type(eval_node_t), pointer :: en1, en2
    n_args = parse_node_get_n_sub (pn)
    en => null ()
    do i = n_args, 1, -1
        pn_arg => parse_node_get_sub_ptr (pn, i)
        select case (char (parse_node_get_rule_key (pn_arg)))
            case ("lvariable")
                call eval_node_compile_variable (en1, pn_arg, var_list, V_LOG)
            case ("svariable")
                call eval_node_compile_variable (en1, pn_arg, var_list, V_STR)
            case ("expr")
                call eval_node_compile_expr (en1, pn_arg, var_list)
            case default
                call parse_node_mismatch ("variable|svariable|lvariable|expr", pn_arg)
        end select
        if (associated (en)) then
            en2 => en
            allocate (en)
            call eval_node_init_branch &
                (en, var_str ("sprintf_arg"), V_NONE, en1, en2)
        else
            allocate (en)
            call eval_node_init_branch &

```



```

                (en, var_str ("sprintf_arg"), V_NONE, en1)
            end if
        end do
    end subroutine eval_node_compile_sprintf_args

```

Evaluation. We allocate the argument list and apply the Fortran wrapper for the `sprintf` function.

(Eval trees: procedures)+≡

```

subroutine evaluate_sprintf (string, n_args, en_fmt, en_arg)
    type(string_t), intent(out) :: string
    integer, intent(in) :: n_args
    type(eval_node_t), pointer :: en_fmt
    type(eval_node_t), intent(in), optional, target :: en_arg
    type(eval_node_t), pointer :: en_branch, en_var
    type(sprintf_arg_t), dimension(:), allocatable :: arg
    type(string_t) :: fmt
    logical :: autoformat
    integer :: i, j, sprintf_argc
    autoformat = .not. associated (en_fmt)
    if (autoformat) fmt = ""
    if (present (en_arg)) then
        sprintf_argc = 0
        en_branch => en_arg
        do i = 1, n_args
            select case (en_branch%arg1%result_type)
                case (V_CMPLX); sprintf_argc = sprintf_argc + 2
                case default ; sprintf_argc = sprintf_argc + 1
            end select
            en_branch => en_branch%arg2
        end do
        allocate (arg (sprintf_argc))
        j = 1
        en_branch => en_arg
        do i = 1, n_args
            en_var => en_branch%arg1
            select case (en_var%result_type)
                case (V_LOG)
                    call sprintf_arg_init (arg(j), en_var%lval)
                    if (autoformat) fmt = fmt // "%s "
                case (V_INT);
                    call sprintf_arg_init (arg(j), en_var%ival)
                    if (autoformat) fmt = fmt // "%i "
                case (V_REAL);
                    call sprintf_arg_init (arg(j), en_var%rval)
                    if (autoformat) fmt = fmt // "%g "
                case (V_STR)
                    call sprintf_arg_init (arg(j), en_var%sval)
                    if (autoformat) fmt = fmt // "%s "
                case (V_CMPLX)
                    call sprintf_arg_init (arg(j), real (en_var%cval, default))
                    j = j + 1
                    call sprintf_arg_init (arg(j), aimag (en_var%cval))
                    if (autoformat) fmt = fmt // " (%g + %g * I) "
            end select
        end do
    end if
    string = trim (fmt)
end subroutine evaluate_sprintf

```

```

        case default
            call eval_node_write (en_var)
            call msg_error ("sprintf is implemented " &
                // "for logical, integer, real, and string values only")
        end select
        j = j + 1
        en_branch => en_branch%arg2
    end do
else
    allocate (arg(0))
end if
if (autoformat) then
    string = sprintf (trim (fmt), arg)
else
    string = sprintf (en_fmt%sval, arg)
end if
end subroutine evaluate_sprintf

```

28.3.5 Auxiliary functions for the compiler

Issue an error that the current node could not be compiled because of type mismatch:

(Eval trees: procedures)+≡

```

subroutine eval_type_error (pn, string, t)
    type(parse_node_t), intent(in) :: pn
    character(*), intent(in) :: string
    integer, intent(in) :: t
    type(string_t) :: type
    select case (t)
        case (V_NONE); type = "(none)"
        case (V_LOG); type = "'logical'"
        case (V_INT); type = "'integer'"
        case (V_REAL); type = "'real'"
        case (V_CMPLX); type = "'complex'"
        case default; type = "(unknown)"
    end select
    call parse_node_write (pn)
    call msg_fatal (" The " // string // &
        " operation is not defined for the given argument type " // &
        char (type))
end subroutine eval_type_error

```

If two numerics are combined, the result is integer if both arguments are integer, if one is integer and the other real or both are real, than its argument is real, otherwise complex.

(Eval trees: procedures)+≡

```

function numeric_result_type (t1, t2) result (t)
    integer, intent(in) :: t1, t2
    integer :: t
    if (t1 == V_INT .and. t2 == V_INT) then
        t = V_INT
    else if (t1 == V_INT .and. t2 == V_REAL) then

```

```

        t = V_REAL
    else if (t1 == V_REAL .and. t2 == V_INT) then
        t = V_REAL
    else if (t1 == V_REAL .and. t2 == V_REAL) then
        t = V_REAL
    else
        t = V_CMPLX
    end if
end function numeric_result_type

```

28.3.6 Evaluation

Evaluation is done recursively. For leaf nodes nothing is to be done.

Evaluating particle-list functions: First, we evaluate the particle lists. If a condition is present, we assign the particle pointers of the condition node to the allocated particle entries in the parent node, keeping in mind that the observables in the variable stack used for the evaluation of the condition also contain pointers to these entries. Then, the assigned procedure is evaluated, which sets the subevent in the parent node. If required, the procedure evaluates the condition node once for each (pair of) particles to determine the result.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_evaluate (en)
    type(eval_node_t), intent(inout) :: en
    logical :: exist
    select case (en%type)
    case (EN_UNARY)
        if (associated(en%arg1)) then
            call eval_node_evaluate(en%arg1)
            en%value_is_known = en%arg1%value_is_known
        else
            en%value_is_known = .false.
        end if
        if (en%value_is_known) then
            select case (en%result_type)
            case (V_LOG); en%lval = en%op1_log(en%arg1)
            case (V_INT); en%ival = en%op1_int(en%arg1)
            case (V_REAL); en%rval = en%op1_real(en%arg1)
            case (V_CMPLX); en%cval = en%op1_cmplx(en%arg1)
            case (V_PDG);
                call en%op1_pdg(en%aval, en%arg1)
            case (V_SEV)
                if (associated(en%arg0)) then
                    call en%op1_sev(en%pval, en%arg1, en%arg0)
                else
                    call en%op1_sev(en%pval, en%arg1)
                end if
            case (V_STR)
                call en%op1_str(en%sval, en%arg1)
            end select
        end if
    case (EN_BINARY)
        if (associated(en%arg1) .and. associated(en%arg2)) then

```

```

        call eval_node_evaluate (en%arg1)
        call eval_node_evaluate (en%arg2)
        en%value_is_known = &
            en%arg1%value_is_known .and. en%arg2%value_is_known
    else
        en%value_is_known = .false.
    end if
    if (en%value_is_known) then
        select case (en%result_type)
        case (V_LOG); en%lval = en%op2_log (en%arg1, en%arg2)
        case (V_INT); en%ival = en%op2_int (en%arg1, en%arg2)
        case (V_REAL); en%rval = en%op2_real (en%arg1, en%arg2)
        case (V_CMPLX); en%cval = en%op2_cmplx (en%arg1, en%arg2)
        case (V_PDG)
            call en%op2_pdg (en%aval, en%arg1, en%arg2)
        case (V_SEV)
            if (associated (en%arg0)) then
                call en%op2_sev (en%pval, en%arg1, en%arg2, en%arg0)
            else
                call en%op2_sev (en%pval, en%arg1, en%arg2)
            end if
        case (V_STR)
            call en%op2_str (en%sval, en%arg1, en%arg2)
        end select
    end if
case (EN_BLOCK)
    if (associated (en%arg1) .and. associated (en%arg0)) then
        call eval_node_evaluate (en%arg1)
        call eval_node_evaluate (en%arg0)
        en%value_is_known = en%arg0%value_is_known
    else
        en%value_is_known = .false.
    end if
    if (en%value_is_known) then
        select case (en%result_type)
        case (V_LOG); en%lval = en%arg0%lval
        case (V_INT); en%ival = en%arg0%ival
        case (V_REAL); en%rval = en%arg0%rval
        case (V_CMPLX); en%cval = en%arg0%cval
        case (V_PDG); en%aval = en%arg0%aval
        case (V_SEV); en%pval = en%arg0%pval
        case (V_STR); en%sval = en%arg0%sval
        end select
    end if
case (EN_CONDITIONAL)
    if (associated (en%arg0)) then
        call eval_node_evaluate (en%arg0)
        en%value_is_known = en%arg0%value_is_known
    else
        en%value_is_known = .false.
    end if
    if (en%arg0%value_is_known) then
        if (en%arg0%lval) then
            call eval_node_evaluate (en%arg1)

```

```

en%value_is_known = en%arg1%value_is_known
if (en%value_is_known) then
  select case (en%result_type)
    case (V_LOG); en%lval = en%arg1%lval
    case (V_INT); en%ival = en%arg1%ival
    case (V_REAL); en%rval = en%arg1%rval
    case (V_CMPLX); en%cval = en%arg1%cval
    case (V_PDG); en%aval = en%arg1%aval
    case (V_SEV); en%pval = en%arg1%pval
    case (V_STR); en%sval = en%arg1%sval
  end select
end if
else
  call eval_node_evaluate (en%arg2)
  en%value_is_known = en%arg2%value_is_known
  if (en%value_is_known) then
    select case (en%result_type)
      case (V_LOG); en%lval = en%arg2%lval
      case (V_INT); en%ival = en%arg2%ival
      case (V_REAL); en%rval = en%arg2%rval
      case (V_CMPLX); en%cval = en%arg2%cval
      case (V_PDG); en%aval = en%arg2%aval
      case (V_SEV); en%pval = en%arg2%pval
      case (V_STR); en%sval = en%arg2%sval
    end select
  end if
end if
end if
case (EN_RECORD_CMD)
  exist = .true.
  en%lval = .false.
  call eval_node_evaluate (en%arg0)
  if (en%arg0%value_is_known) then
    if (associated (en%arg1)) then
      call eval_node_evaluate (en%arg1)
      if (en%arg1%value_is_known) then
        if (associated (en%arg2)) then
          call eval_node_evaluate (en%arg2)
          if (en%arg2%value_is_known) then
            if (associated (en%arg3)) then
              call eval_node_evaluate (en%arg3)
              if (en%arg3%value_is_known) then
                if (associated (en%arg4)) then
                  call eval_node_evaluate (en%arg4)
                  if (en%arg4%value_is_known) then
                    if (associated (en%rval)) then
                      call analysis_record_data (en%arg0%sval, &
                        en%arg1%rval, en%arg2%rval, &
                        en%arg3%rval, en%arg4%rval, &
                        weight=en%rval, exist=exist, &
                        success=en%lval)
                    else
                      call analysis_record_data (en%arg0%sval, &
                        en%arg1%rval, en%arg2%rval, &

```

```

                                en%arg3%rval, en%arg4%rval, &
                                exist=exist, success=en%lval)
                                end if
                                end if
                                else
                                if (associated (en%rval)) then
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, en%arg2%rval, &
                                en%arg3%rval, &
                                weight=en%rval, exist=exist, &
                                success=en%lval)
                                else
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, en%arg2%rval, &
                                en%arg3%rval, &
                                exist=exist, success=en%lval)
                                end if
                                end if
                                end if
                                else
                                if (associated (en%rval)) then
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, en%arg2%rval, &
                                weight=en%rval, exist=exist, &
                                success=en%lval)
                                else
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, en%arg2%rval, &
                                exist=exist, success=en%lval)
                                end if
                                end if
                                end if
                                else
                                if (associated (en%rval)) then
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, &
                                weight=en%rval, exist=exist, success=en%lval)
                                else
                                call analysis_record_data (en%arg0%sval, &
                                en%arg1%rval, &
                                exist=exist, success=en%lval)
                                end if
                                end if
                                end if
                                else
                                if (associated (en%rval)) then
                                call analysis_record_data (en%arg0%sval, 1._default, &
                                weight=en%rval, exist=exist, success=en%lval)
                                else
                                call analysis_record_data (en%arg0%sval, 1._default, &
                                exist=exist, success=en%lval)
                                end if
                                end if
                                if (.not. exist) then

```

```

        call msg_error ("Analysis object '" // char (en%arg0% sval) &
            // "' is undefined")
        en%arg0%value_is_known = .false.
    end if
end if
case (EN_OBS1_INT)
    en%ival = en%obs1_int (en%prt1)
    en%value_is_known = .true.
case (EN_OBS2_INT)
    en%ival = en%obs2_int (en%prt1, en%prt2)
    en%value_is_known = .true.
case (EN_OBS1_REAL)
    en%rval = en%obs1_real (en%prt1)
    en%value_is_known = .true.
case (EN_OBS2_REAL)
    en%rval = en%obs2_real (en%prt1, en%prt2)
    en%value_is_known = .true.
case (EN_OBSEV_INT)
    en%ival = en%obsev_int (en%pval)
    en%value_is_known = .true.
case (EN_OBSEV_REAL)
    en%rval = en%obsev_real (en%pval)
    en%value_is_known = .true.
case (EN_PRT_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_sev (en%pval, en%arg1, en%arg0)
        else
            call en%op1_sev (en%pval, en%arg1)
        end if
    end if
case (EN_PRT_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. en%arg2%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_sev (en%pval, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_sev (en%pval, en%arg1, en%arg2)
        end if
    end if
case (EN_EVAL_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%pval%is_nonempty ()
    if (en%value_is_known) then

```

```

        en%arg0%index => en%index
        en%index = 1
        en%arg0%prt1 => en%prt1
        en%prt1 = en%arg1%pval%get_prt (1)
        call eval_node_evaluate (en%arg0)
        en%rval = en%arg0%rval
    end if
case (EN_EVAL_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%pval%is_nonempty () .and. en%arg2%pval%is_nonempty ()
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%arg0%prt2 => en%prt2
        en%index = 1
        call eval_pp (en%arg1, en%arg2, en%arg0, en%rval, en%value_is_known)
    end if
case (EN_LOG_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%lval = en%op1_cut (en%arg1, en%arg0)
    end if
case (EN_LOG_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%arg0%prt2 => en%prt2
        en%lval = en%op2_cut (en%arg1, en%arg2, en%arg0)
    end if
case (EN_INT_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_evi (en%ival, en%arg1, en%arg0)
        else
            call en%op1_evi (en%ival, en%arg1)
        end if
    end if
case (EN_INT_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. &

```



```

        en%arg2%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_evi (en%ival, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_evi (en%ival, en%arg1, en%arg2)
        end if
    end if
case (EN_REAL_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_evr (en%rval, en%arg1, en%arg0)
        else
            call en%op1_evr (en%rval, en%arg1)
        end if
    end if
case (EN_REAL_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. &
        en%arg2%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_evr (en%rval, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_evr (en%rval, en%arg1, en%arg2)
        end if
    end if
case (EN_REAL_FUN_CUM)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%rval = en%opcum_evr (en%arg1, en%arg0)
    end if
case (EN_FORMAT_STR)
    if (associated (en%arg0)) then
        call eval_node_evaluate (en%arg0)
        en%value_is_known = en%arg0%value_is_known
    else
        en%value_is_known = .true.
    end if

```

```

        if (associated (en%arg1)) then
            call eval_node_evaluate (en%arg1)
            en%value_is_known = &
                en%value_is_known .and. en%arg1%value_is_known
            if (en%value_is_known) then
                call evaluate_sprintf (en%sval, en%ival, en%arg0, en%arg1)
            end if
        else
            if (en%value_is_known) then
                call evaluate_sprintf (en%sval, en%ival, en%arg0)
            end if
        end if
    end select
    if (debug2_active (D_MODEL_F)) then
        print *, "eval_node_evaluate"
        call eval_node_write (en)
    end if
end subroutine eval_node_evaluate

```

Test method

This is called from a unit test: initialize a particular observable.

```

<Eval trees: eval node: TBP>+≡
    procedure :: test_obs => eval_node_test_obs

<Eval trees: sub interfaces>+≡
    module subroutine eval_node_test_obs (node, var_list, var_name)
        class(eval_node_t), intent(inout) :: node
        type(var_list_t), intent(in) :: var_list
        type(string_t), intent(in) :: var_name
    end subroutine eval_node_test_obs

<Eval trees: procedures>+≡
    module subroutine eval_node_test_obs (node, var_list, var_name)
        class(eval_node_t), intent(inout) :: node
        type(var_list_t), intent(in) :: var_list
        type(string_t), intent(in) :: var_name
        procedure(obs_unary_int), pointer :: obs1_iptr
        type(prt_t), pointer :: p1
        call var_list%get_obs1_iptr (var_name, obs1_iptr, p1)
        call eval_node_init_obs1_int_ptr (node, var_name, obs1_iptr, p1)
    end subroutine eval_node_test_obs

```

28.3.7 Evaluation syntax

We have two different flavors of the syntax: with and without particles.

```

<Eval trees: public>+≡
    public :: syntax_expr
    public :: syntax_pexpr

```

```

<Eval trees: variables>+=
  type(syntax_t), target, save :: syntax_expr
  type(syntax_t), target, save :: syntax_pexpr

```

These are for testing only and may be removed:

```

<Eval trees: public>+=
  public :: syntax_expr_init
  public :: syntax_pexpr_init

<Eval trees: sub interfaces>+=
  module subroutine syntax_expr_init ()
  end subroutine syntax_expr_init
  module subroutine syntax_pexpr_init ()
  end subroutine syntax_pexpr_init

<Eval trees: procedures>+=
  module subroutine syntax_expr_init ()
    type(ifile_t) :: ifile
    call define_expr_syntax (ifile, particles=.false., analysis=.false.)
    call syntax_init (syntax_expr, ifile)
    call ifile_final (ifile)
  end subroutine syntax_expr_init

  module subroutine syntax_pexpr_init ()
    type(ifile_t) :: ifile
    call define_expr_syntax (ifile, particles=.true., analysis=.false.)
    call syntax_init (syntax_pexpr, ifile)
    call ifile_final (ifile)
  end subroutine syntax_pexpr_init

<Eval trees: public>+=
  public :: syntax_expr_final
  public :: syntax_pexpr_final

<Eval trees: sub interfaces>+=
  module subroutine syntax_expr_final ()
  end subroutine syntax_expr_final
  module subroutine syntax_pexpr_final ()
  end subroutine syntax_pexpr_final

<Eval trees: procedures>+=
  module subroutine syntax_expr_final ()
    call syntax_final (syntax_expr)
  end subroutine syntax_expr_final

  module subroutine syntax_pexpr_final ()
    call syntax_final (syntax_pexpr)
  end subroutine syntax_pexpr_final

<Eval trees: public>+=
  public :: syntax_pexpr_write

<Eval trees: sub interfaces>+=
  module subroutine syntax_pexpr_write (unit)
    integer, intent(in), optional :: unit
  end subroutine syntax_pexpr_write

```

<Eval trees: procedures>+≡

```
module subroutine syntax_pexpr_write (unit)
  integer, intent(in), optional :: unit
  call syntax_write (syntax_pexpr, unit)
end subroutine syntax_pexpr_write
```

<Eval trees: public>+≡

```
public :: define_expr_syntax
```

Numeric expressions.

<Eval trees: sub interfaces>+≡

```
module subroutine define_expr_syntax (ifile, particles, analysis)
  type(ifile_t), intent(inout) :: ifile
  logical, intent(in) :: particles, analysis
end subroutine define_expr_syntax
```

<Eval trees: procedures>+≡

```
module subroutine define_expr_syntax (ifile, particles, analysis)
  type(ifile_t), intent(inout) :: ifile
  logical, intent(in) :: particles, analysis
  type(string_t) :: numeric_pexpr
  type(string_t) :: var_plist, var_alias
  if (particles) then
    numeric_pexpr = " | numeric_pexpr"
    var_plist = " | var_plist"
    var_alias = " | var_alias"
  else
    numeric_pexpr = ""
    var_plist = ""
    var_alias = ""
  end if
  call ifile_append (ifile, "SEQ expr = subexpr addition*")
  call ifile_append (ifile, "ALT subexpr = addition | term")
  call ifile_append (ifile, "SEQ addition = plus_or_minus term")
  call ifile_append (ifile, "SEQ term = factor multiplication*")
  call ifile_append (ifile, "SEQ multiplication = times_or_over factor")
  call ifile_append (ifile, "SEQ factor = value exponentiation?")
  call ifile_append (ifile, "SEQ exponentiation = to_the value")
  call ifile_append (ifile, "ALT plus_or_minus = '+' | '-'")
  call ifile_append (ifile, "ALT times_or_over = '*' | '/'")
  call ifile_append (ifile, "ALT to_the = '^' | '**")
  call ifile_append (ifile, "KEY '+'")
  call ifile_append (ifile, "KEY '-'")
  call ifile_append (ifile, "KEY '*'")
  call ifile_append (ifile, "KEY '/'")
  call ifile_append (ifile, "KEY '^'")
  call ifile_append (ifile, "KEY '**")
  call ifile_append (ifile, "ALT value = signed_value | unsigned_value")
  call ifile_append (ifile, "SEQ signed_value = '-' unsigned_value")
  call ifile_append (ifile, "ALT unsigned_value = " // &
    "numeric_value | constant | variable | " // &
    "result | " // &
    "grouped_expr | block_expr | conditional_expr | " // &
    "unary_function | binary_function" // &
    numeric_pexpr)
```

```

call ifile_append (ifile, "ALT numeric_value = integer_value | " &
// "real_value | complex_value")
call ifile_append (ifile, "SEQ integer_value = integer_literal unit_expr?")
call ifile_append (ifile, "SEQ real_value = real_literal unit_expr?")
call ifile_append (ifile, "SEQ complex_value = complex_literal unit_expr?")
call ifile_append (ifile, "INT integer_literal")
call ifile_append (ifile, "REA real_literal")
call ifile_append (ifile, "COM complex_literal")
call ifile_append (ifile, "SEQ unit_expr = unit unit_power?")
call ifile_append (ifile, "ALT unit = " // &
"TeV | GeV | MeV | keV | eV | meV | " // &
"nbarn | pbarn | fbarn | abarn | " // &
"rad | mrad | degree | '",'")
call ifile_append (ifile, "KEY TeV")
call ifile_append (ifile, "KEY GeV")
call ifile_append (ifile, "KEY MeV")
call ifile_append (ifile, "KEY keV")
call ifile_append (ifile, "KEY eV")
call ifile_append (ifile, "KEY meV")
call ifile_append (ifile, "KEY nbarn")
call ifile_append (ifile, "KEY pbarn")
call ifile_append (ifile, "KEY fbarn")
call ifile_append (ifile, "KEY abarn")
call ifile_append (ifile, "KEY rad")
call ifile_append (ifile, "KEY mrad")
call ifile_append (ifile, "KEY degree")
call ifile_append (ifile, "KEY '",'")
call ifile_append (ifile, "SEQ unit_power = '^' frac_expr")
call ifile_append (ifile, "ALT frac_expr = frac | grouped_frac")
call ifile_append (ifile, "GRO grouped_frac = ( frac_expr )")
call ifile_append (ifile, "SEQ frac = signed_int div?")
call ifile_append (ifile, "ALT signed_int = " &
// "neg_int | pos_int | integer_literal")
call ifile_append (ifile, "SEQ neg_int = '-' integer_literal")
call ifile_append (ifile, "SEQ pos_int = '+' integer_literal")
call ifile_append (ifile, "SEQ div = '/' integer_literal")
call ifile_append (ifile, "ALT constant = pi | I")
call ifile_append (ifile, "KEY pi")
call ifile_append (ifile, "KEY I")
call ifile_append (ifile, "IDE variable")
call ifile_append (ifile, "SEQ result = result_key result_arg")
call ifile_append (ifile, "ALT result_key = " // &
"num_id | integral | error")
call ifile_append (ifile, "KEY num_id")
call ifile_append (ifile, "KEY integral")
call ifile_append (ifile, "KEY error")
call ifile_append (ifile, "GRO result_arg = ( process_id )")
call ifile_append (ifile, "IDE process_id")
call ifile_append (ifile, "SEQ unary_function = fun_unary function_arg1")
call ifile_append (ifile, "SEQ binary_function = fun_binary function_arg2")
call ifile_append (ifile, "ALT fun_unary = " // &
"complex | real | int | nint | floor | ceiling | abs | conjg | sgn | " // &
"sqrt | exp | log | log10 | " // &
"sin | cos | tan | asin | acos | atan | " // &

```

```

    "sinh | cosh | tanh | asinh | acosh | atanh")
call ifile_append (ifile, "KEY complex")
call ifile_append (ifile, "KEY real")
call ifile_append (ifile, "KEY int")
call ifile_append (ifile, "KEY nint")
call ifile_append (ifile, "KEY floor")
call ifile_append (ifile, "KEY ceiling")
call ifile_append (ifile, "KEY abs")
call ifile_append (ifile, "KEY conjg")
call ifile_append (ifile, "KEY sgn")
call ifile_append (ifile, "KEY sqrt")
call ifile_append (ifile, "KEY exp")
call ifile_append (ifile, "KEY log")
call ifile_append (ifile, "KEY log10")
call ifile_append (ifile, "KEY sin")
call ifile_append (ifile, "KEY cos")
call ifile_append (ifile, "KEY tan")
call ifile_append (ifile, "KEY asin")
call ifile_append (ifile, "KEY acos")
call ifile_append (ifile, "KEY atan")
call ifile_append (ifile, "KEY sinh")
call ifile_append (ifile, "KEY cosh")
call ifile_append (ifile, "KEY tanh")
call ifile_append (ifile, "KEY asinh")
call ifile_append (ifile, "KEY acosh")
call ifile_append (ifile, "KEY atanh")
call ifile_append (ifile, "ALT fun_binary = max | min | mod | modulo")
call ifile_append (ifile, "KEY max")
call ifile_append (ifile, "KEY min")
call ifile_append (ifile, "KEY mod")
call ifile_append (ifile, "KEY modulo")
call ifile_append (ifile, "ARG function_arg1 = ( expr )")
call ifile_append (ifile, "ARG function_arg2 = ( expr, expr )")
call ifile_append (ifile, "GRO grouped_expr = ( expr )")
call ifile_append (ifile, "SEQ block_expr = let var_spec in expr")
call ifile_append (ifile, "KEY let")
call ifile_append (ifile, "ALT var_spec = " // &
    "var_num | var_int | var_real | var_complex | " // &
    "var_logical" // var_plist // var_alias // " | var_string")
call ifile_append (ifile, "SEQ var_num = var_name '=' expr")
call ifile_append (ifile, "SEQ var_int = int var_name '=' expr")
call ifile_append (ifile, "SEQ var_real = real var_name '=' expr")
call ifile_append (ifile, "SEQ var_complex = complex var_name '=' complex_expr")
call ifile_append (ifile, "ALT complex_expr = " // &
    "cexpr_real | cexpr_complex")
call ifile_append (ifile, "ARG cexpr_complex = ( expr, expr )")
call ifile_append (ifile, "SEQ cexpr_real = expr")
call ifile_append (ifile, "IDE var_name")
call ifile_append (ifile, "KEY '='")
call ifile_append (ifile, "KEY in")
call ifile_append (ifile, "SEQ conditional_expr = " // &
    "if lexpr then expr maybe_elseif_expr maybe_else_expr endif")
call ifile_append (ifile, "SEQ maybe_elseif_expr = elseif_expr*")
call ifile_append (ifile, "SEQ maybe_else_expr = else_expr?")

```

```

call ifile_append (ifile, "SEQ elsif_expr = elsif lexpr then expr")
call ifile_append (ifile, "SEQ else_expr = else expr")
call ifile_append (ifile, "KEY if")
call ifile_append (ifile, "KEY then")
call ifile_append (ifile, "KEY elsif")
call ifile_append (ifile, "KEY else")
call ifile_append (ifile, "KEY endif")
call define_lexpr_syntax (ifile, particles, analysis)
call define_sexpr_syntax (ifile)
if (particles) then
    call define_pexpr_syntax (ifile)
    call define_cexpr_syntax (ifile)
    call define_var_plist_syntax (ifile)
    call define_var_alias_syntax (ifile)
    call define_numeric_pexpr_syntax (ifile)
    call define_logical_pexpr_syntax (ifile)
end if

end subroutine define_expr_syntax

```

Logical expressions.

(Eval trees: procedures)+≡

```

subroutine define_lexpr_syntax (ifile, particles, analysis)
    type(ifile_t), intent(inout) :: ifile
    logical, intent(in) :: particles, analysis
    type(string_t) :: logical_pexpr, record_cmd
    if (particles) then
        logical_pexpr = " | logical_pexpr"
    else
        logical_pexpr = ""
    end if
    if (analysis) then
        record_cmd = " | record_cmd"
    else
        record_cmd = ""
    end if
    call ifile_append (ifile, "SEQ lexpr = lsinglet lsequel*")
    call ifile_append (ifile, "SEQ lsequel = ';' lsinglet")
    call ifile_append (ifile, "SEQ lsinglet = lterm alternative*")
    call ifile_append (ifile, "SEQ alternative = or lterm")
    call ifile_append (ifile, "SEQ lterm = lvalue coincidence*")
    call ifile_append (ifile, "SEQ coincidence = and lvalue")
    call ifile_append (ifile, "KEY ';'")
    call ifile_append (ifile, "KEY or")
    call ifile_append (ifile, "KEY and")
    call ifile_append (ifile, "ALT lvalue = " // &
        "true | false | lvariable | negation | " // &
        "grouped_lexpr | block_lexpr | conditional_lexpr | " // &
        "compared_expr | compared_sexpr" // &
        logical_pexpr // record_cmd)
    call ifile_append (ifile, "KEY true")
    call ifile_append (ifile, "KEY false")
    call ifile_append (ifile, "SEQ lvariable = '?' alt_lvariable")

```

```

call ifile_append (ifile, "KEY '?'")
call ifile_append (ifile, "ALT alt_lvariable = variable | grouped_lexpr")
call ifile_append (ifile, "SEQ negation = not lvalue")
call ifile_append (ifile, "KEY not")
call ifile_append (ifile, "GRO grouped_lexpr = ( lexpr )")
call ifile_append (ifile, "SEQ block_lexpr = let var_spec in lexpr")
call ifile_append (ifile, "ALT var_logical = " // &
    "var_logical_new | var_logical_spec")
call ifile_append (ifile, "SEQ var_logical_new = logical var_logical_spec")
call ifile_append (ifile, "KEY logical")
call ifile_append (ifile, "SEQ var_logical_spec = '?' var_name = lexpr")
call ifile_append (ifile, "SEQ conditional_lexpr = " // &
    "if lexpr then lexpr maybe_elseif_lexpr maybe_else_lexpr endif")
call ifile_append (ifile, "SEQ maybe_elseif_lexpr = elseif_lexpr*")
call ifile_append (ifile, "SEQ maybe_else_lexpr = else_lexpr?")
call ifile_append (ifile, "SEQ elseif_lexpr = elseif lexpr then lexpr")
call ifile_append (ifile, "SEQ else_lexpr = else lexpr")
call ifile_append (ifile, "SEQ compared_expr = expr comparison+")
call ifile_append (ifile, "SEQ comparison = compare expr")
call ifile_append (ifile, "ALT compare = " // &
    "< | > | <= | >= | == | <>")
call ifile_append (ifile, "KEY '<')
call ifile_append (ifile, "KEY '>')
call ifile_append (ifile, "KEY '<='")
call ifile_append (ifile, "KEY '>='")
call ifile_append (ifile, "KEY '=='")
call ifile_append (ifile, "KEY '<>')
call ifile_append (ifile, "SEQ compared_sexpr = sexpr str_comparison+")
call ifile_append (ifile, "SEQ str_comparison = str_compare sexpr")
call ifile_append (ifile, "ALT str_compare = '== | '<>')
if (analysis) then
    call ifile_append (ifile, "SEQ record_cmd = " // &
        "record_key analysis_tag record_arg?")
    call ifile_append (ifile, "ALT record_key = " // &
        "record | record_unweighted | record_excess")
    call ifile_append (ifile, "KEY record")
    call ifile_append (ifile, "KEY record_unweighted")
    call ifile_append (ifile, "KEY record_excess")
    call ifile_append (ifile, "ALT analysis_tag = analysis_id | sexpr")
    call ifile_append (ifile, "IDE analysis_id")
    call ifile_append (ifile, "ARG record_arg = ( expr+ )")
end if
end subroutine define_lexpr_syntax

```

String expressions.

(Eval trees: procedures)+≡

```

subroutine define_sexpr_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "SEQ sexpr = svalue str_concatenation*")
    call ifile_append (ifile, "SEQ str_concatenation = '&' svalue")
    call ifile_append (ifile, "KEY '&')
    call ifile_append (ifile, "ALT svalue = " // &
        "grouped_sexpr | block_sexpr | conditional_sexpr | " // &
        "svariable | string_function | string_literal")

```



```

call ifile_append (ifile, "GRO grouped_sexpr = ( sexpr )")
call ifile_append (ifile, "SEQ block_sexpr = let var_spec in sexpr")
call ifile_append (ifile, "SEQ conditional_sexpr = " // &
    "if lexpr then sexpr maybe_elseif_sexpr maybe_else_sexpr endif")
call ifile_append (ifile, "SEQ maybe_elseif_sexpr = elseif_sexpr*")
call ifile_append (ifile, "SEQ maybe_else_sexpr = else_sexpr?")
call ifile_append (ifile, "SEQ elseif_sexpr = elseif lexpr then sexpr")
call ifile_append (ifile, "SEQ else_sexpr = else sexpr")
call ifile_append (ifile, "SEQ svariable = '$' alt_svariable")
call ifile_append (ifile, "KEY '$'")
call ifile_append (ifile, "ALT alt_svariable = variable | grouped_sexpr")
call ifile_append (ifile, "ALT var_string = " // &
    "var_string_new | var_string_spec")
call ifile_append (ifile, "SEQ var_string_new = string var_string_spec")
call ifile_append (ifile, "KEY string")
call ifile_append (ifile, "SEQ var_string_spec = '$' var_name = sexpr") ! $
call ifile_append (ifile, "ALT string_function = sprintf_fun")
call ifile_append (ifile, "SEQ sprintf_fun = sprintf_clause sprintf_args?")
call ifile_append (ifile, "SEQ sprintf_clause = sprintf sexpr")
call ifile_append (ifile, "KEY sprintf")
call ifile_append (ifile, "ARG sprintf_args = ( sprintf_arg* )")
call ifile_append (ifile, "ALT sprintf_arg = " &
    // "lvariable | svariable | expr")
call ifile_append (ifile, "QUO string_literal = '...'"')
end subroutine define_sexpr_syntax

```

Eval trees that evaluate to subevents.

(Eval trees: procedures)+≡

```

subroutine define_pexpr_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "SEQ pexpr = pterm pconcatenation*")
    call ifile_append (ifile, "SEQ pconcatenation = '&' pterm")
    ! call ifile_append (ifile, "KEY '&'")    !!! (Key exists already)
    call ifile_append (ifile, "SEQ pterm = pvalue pcombination*")
    call ifile_append (ifile, "SEQ pcombination = '+' pvalue")
    ! call ifile_append (ifile, "KEY '+'")    !!! (Key exists already)
    call ifile_append (ifile, "ALT pvalue = " // &
        "pexpr_src | pvariable | " // &
        "grouped_pexpr | block_pexpr | conditional_pexpr | " // &
        "prt_function")
    call ifile_append (ifile, "SEQ pexpr_src = prefix_cexpr")
    call ifile_append (ifile, "ALT prefix_cexpr = " // &
        "beam_prt | incoming_prt | outgoing_prt | unspecified_prt")
    call ifile_append (ifile, "SEQ beam_prt = beam cexpr")
    call ifile_append (ifile, "KEY beam")
    call ifile_append (ifile, "SEQ incoming_prt = incoming cexpr")
    call ifile_append (ifile, "KEY incoming")
    call ifile_append (ifile, "SEQ outgoing_prt = outgoing cexpr")
    call ifile_append (ifile, "KEY outgoing")
    call ifile_append (ifile, "SEQ unspecified_prt = cexpr")
    call ifile_append (ifile, "SEQ pvariable = '@' alt_pvariable")
    call ifile_append (ifile, "KEY '@'")
    call ifile_append (ifile, "ALT alt_pvariable = variable | grouped_pexpr")
    call ifile_append (ifile, "GRO grouped_pexpr = '[' pexpr ']'")

```

```

call ifile_append (ifile, "SEQ block_pexpr = let var_spec in pexpr")
call ifile_append (ifile, "SEQ conditional_pexpr = " // &
    "if lexpr then pexpr maybe_elseif_pexpr maybe_else_pexpr endif")
call ifile_append (ifile, "SEQ maybe_elseif_pexpr = elseif_pexpr*")
call ifile_append (ifile, "SEQ maybe_else_pexpr = else_pexpr?")
call ifile_append (ifile, "SEQ elseif_pexpr = elseif lexpr then pexpr")
call ifile_append (ifile, "SEQ else_pexpr = else pexpr")
call ifile_append (ifile, "ALT prt_function = " // &
    "join_fun | combine_fun | collect_fun | cluster_fun | " // &
    "photon_reco_fun | " // &
    "select_fun | extract_fun | sort_fun | " // &
    "select_b_jet_fun | select_non_b_jet_fun | " // &
    "select_c_jet_fun | select_light_jet_fun")
call ifile_append (ifile, "SEQ join_fun = join_clause pargs2")
call ifile_append (ifile, "SEQ combine_fun = combine_clause pargs2")
call ifile_append (ifile, "SEQ collect_fun = collect_clause pargs1")
call ifile_append (ifile, "SEQ cluster_fun = cluster_clause pargs1")
call ifile_append (ifile, "SEQ photon_reco_fun = photon_reco_clause pargs1")
call ifile_append (ifile, "SEQ select_fun = select_clause pargs1")
call ifile_append (ifile, "SEQ extract_fun = extract_clause pargs1")
call ifile_append (ifile, "SEQ sort_fun = sort_clause pargs1")
call ifile_append (ifile, "SEQ select_b_jet_fun = " // &
    "select_b_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_non_b_jet_fun = " // &
    "select_non_b_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_c_jet_fun = " // &
    "select_c_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_light_jet_fun = " // &
    "select_light_jet_clause pargs1")
call ifile_append (ifile, "SEQ join_clause = join condition?")
call ifile_append (ifile, "SEQ combine_clause = combine condition?")
call ifile_append (ifile, "SEQ collect_clause = collect condition?")
call ifile_append (ifile, "SEQ cluster_clause = cluster condition?")
call ifile_append (ifile, "SEQ photon_reco_clause = photon_recombination condition?")
call ifile_append (ifile, "SEQ select_clause = select condition?")
call ifile_append (ifile, "SEQ extract_clause = extract position?")
call ifile_append (ifile, "SEQ sort_clause = sort criterion?")
call ifile_append (ifile, "SEQ select_b_jet_clause = " // &
    "select_b_jet condition?")
call ifile_append (ifile, "SEQ select_non_b_jet_clause = " // &
    "select_non_b_jet condition?")
call ifile_append (ifile, "SEQ select_c_jet_clause = " // &
    "select_c_jet condition?")
call ifile_append (ifile, "SEQ select_light_jet_clause = " // &
    "select_light_jet condition?")
call ifile_append (ifile, "KEY join")
call ifile_append (ifile, "KEY combine")
call ifile_append (ifile, "KEY collect")
call ifile_append (ifile, "KEY cluster")
call ifile_append (ifile, "KEY photon_recombination")
call ifile_append (ifile, "KEY select")
call ifile_append (ifile, "SEQ condition = if lexpr")
call ifile_append (ifile, "KEY extract")
call ifile_append (ifile, "SEQ position = index expr")

```

```

call ifile_append (ifile, "KEY sort")
call ifile_append (ifile, "KEY select_b_jet")
call ifile_append (ifile, "KEY select_non_b_jet")
call ifile_append (ifile, "KEY select_c_jet")
call ifile_append (ifile, "KEY select_light_jet")
call ifile_append (ifile, "SEQ criterion = by expr")
call ifile_append (ifile, "KEY index")
call ifile_append (ifile, "KEY by")
call ifile_append (ifile, "ARG pargs2 = '[' pexpr, pexpr ']')")
call ifile_append (ifile, "ARG pargs1 = '[' pexpr, pexpr? ']')")
end subroutine define_pexpr_syntax

```

Eval trees that evaluate to PDG-code arrays.

(Eval trees: procedures)+≡

```

subroutine define_cexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ cexpr = avalue concatenation*")
  call ifile_append (ifile, "SEQ concatenation = ':' avalue")
  call ifile_append (ifile, "KEY ':'")
  call ifile_append (ifile, "ALT avalue = " // &
    "grouped_cexpr | block_cexpr | conditional_cexpr | " // &
    "variable | pdg_code | prt_name")
  call ifile_append (ifile, "GRO grouped_cexpr = ( cexpr )")
  call ifile_append (ifile, "SEQ block_cexpr = let var_spec in cexpr")
  call ifile_append (ifile, "SEQ conditional_cexpr = " // &
    "if lexpr then cexpr maybe_elseif_cexpr maybe_else_cexpr endif")
  call ifile_append (ifile, "SEQ maybe_elseif_cexpr = elseif_cexpr*")
  call ifile_append (ifile, "SEQ maybe_else_cexpr = else_cexpr?")
  call ifile_append (ifile, "SEQ elseif_cexpr = elseif lexpr then cexpr")
  call ifile_append (ifile, "SEQ else_cexpr = else cexpr")
  call ifile_append (ifile, "SEQ pdg_code = pdg pdg_arg")
  call ifile_append (ifile, "KEY pdg")
  call ifile_append (ifile, "ARG pdg_arg = ( expr )")
  call ifile_append (ifile, "QUO prt_name = '""'...'""'")
end subroutine define_cexpr_syntax

```

Extra variable types.

(Eval trees: procedures)+≡

```

subroutine define_var_plist_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "ALT var_plist = var_plist_new | var_plist_spec")
  call ifile_append (ifile, "SEQ var_plist_new = subevt var_plist_spec")
  call ifile_append (ifile, "KEY subevt")
  call ifile_append (ifile, "SEQ var_plist_spec = '@' var_name '=' pexpr")
end subroutine define_var_plist_syntax

subroutine define_var_alias_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ var_alias = alias var_name '=' cexpr")
  call ifile_append (ifile, "KEY alias")
end subroutine define_var_alias_syntax

```

Particle-list expressions that evaluate to numeric values

```

<Eval trees: procedures>+≡
subroutine define_numeric_pexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "ALT numeric_pexpr = " &
    // "eval_fun | count_fun | sum_fun | " &
    // "prod_fun")
  call ifile_append (ifile, "SEQ eval_fun = eval expr pargs1")
  call ifile_append (ifile, "SEQ count_fun = count_clause pargs1")
  call ifile_append (ifile, "SEQ count_clause = count condition?")
  call ifile_append (ifile, "SEQ sum_fun = sum expr pargs1")
  call ifile_append (ifile, "SEQ prod_fun = prod expr pargs1")
  call ifile_append (ifile, "KEY eval")
  call ifile_append (ifile, "KEY count")
  call ifile_append (ifile, "KEY sum")
  call ifile_append (ifile, "KEY prod")
end subroutine define_numeric_pexpr_syntax

```

Particle-list functions that evaluate to logical values.

```

<Eval trees: procedures>+≡
subroutine define_logical_pexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "ALT logical_pexpr = " // &
    "all_fun | any_fun | no_fun | " // &
    "photon_isolation_fun")
  call ifile_append (ifile, "SEQ all_fun = all lexpr pargs1")
  call ifile_append (ifile, "SEQ any_fun = any lexpr pargs1")
  call ifile_append (ifile, "SEQ no_fun = no lexpr pargs1")
  call ifile_append (ifile, "SEQ photon_isolation_fun = " // &
    "photon_isolation_clause pargs2")
  call ifile_append (ifile, "SEQ photon_isolation_clause = " // &
    "photon_isolation condition?")
  call ifile_append (ifile, "KEY all")
  call ifile_append (ifile, "KEY any")
  call ifile_append (ifile, "KEY no")
  call ifile_append (ifile, "KEY photon_isolation")
end subroutine define_logical_pexpr_syntax

```

All characters that can occur in expressions (apart from alphanumeric).

```

<Eval trees: procedures>+≡
subroutine lexer_init_eval_tree (lexer, particles)
  type(lexer_t), intent(out) :: lexer
  logical, intent(in) :: particles
  type(keyword_list_t), pointer :: keyword_list
  if (particles) then
    keyword_list => syntax_get_keyword_list_ptr (syntax_pexpr)
  else
    keyword_list => syntax_get_keyword_list_ptr (syntax_expr)
  end if
  call lexer_init (lexer, &
    comment_chars = "#!", &
    quote_chars = "'", &
    quote_match = "'", &

```

```

        single_chars = "() [] , ; : & % ? $ @ " , &
        special_class = [ "+-*/^", "<>=~ " ] , &
        keyword_list = keyword_list)
    end subroutine lexer_init_eval_tree

```

28.3.8 Set up appropriate parse trees

Parse an input stream as a specific flavor of expression. The appropriate expression syntax has to be available.

(Eval trees: public)+≡

```

    public :: parse_tree_init_expr
    public :: parse_tree_init_lexpr
    public :: parse_tree_init_pexpr
    public :: parse_tree_init_cexpr
    public :: parse_tree_init_sexpr

```

(Eval trees: sub interfaces)+≡

```

    module subroutine parse_tree_init_expr (parse_tree, stream, particles)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
        logical, intent(in) :: particles
    end subroutine parse_tree_init_expr
    module subroutine parse_tree_init_lexpr (parse_tree, stream, particles)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
        logical, intent(in) :: particles
    end subroutine parse_tree_init_lexpr
    module subroutine parse_tree_init_pexpr (parse_tree, stream)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
    end subroutine parse_tree_init_pexpr
    module subroutine parse_tree_init_cexpr (parse_tree, stream)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
    end subroutine parse_tree_init_cexpr
    module subroutine parse_tree_init_sexpr (parse_tree, stream, particles)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
        logical, intent(in) :: particles
    end subroutine parse_tree_init_sexpr

```

(Eval trees: procedures)+≡

```

    module subroutine parse_tree_init_expr (parse_tree, stream, particles)
        type(parse_tree_t), intent(out) :: parse_tree
        type(stream_t), intent(inout), target :: stream
        logical, intent(in) :: particles
        type(lexer_t) :: lexer
        call lexer_init_eval_tree (lexer, particles)
        call lexer_assign_stream (lexer, stream)
        if (particles) then
            call parse_tree_init &
                (parse_tree, syntax_pexpr, lexer, var_str ("expr"))
        else

```

```

        call parse_tree_init &
            (parse_tree, syntax_expr, lexer, var_str ("expr"))
    end if
    call lexer_final (lexer)
end subroutine parse_tree_init_expr

module subroutine parse_tree_init_lexpr (parse_tree, stream, particles)
    type(parse_tree_t), intent(out) :: parse_tree
    type(stream_t), intent(inout), target :: stream
    logical, intent(in) :: particles
    type(lexer_t) :: lexer
    call lexer_init_eval_tree (lexer, particles)
    call lexer_assign_stream (lexer, stream)
    if (particles) then
        call parse_tree_init &
            (parse_tree, syntax_pexpr, lexer, var_str ("lexpr"))
    else
        call parse_tree_init &
            (parse_tree, syntax_expr, lexer, var_str ("lexpr"))
    end if
    call lexer_final (lexer)
end subroutine parse_tree_init_lexpr

module subroutine parse_tree_init_pexpr (parse_tree, stream)
    type(parse_tree_t), intent(out) :: parse_tree
    type(stream_t), intent(inout), target :: stream
    type(lexer_t) :: lexer
    call lexer_init_eval_tree (lexer, .true.)
    call lexer_assign_stream (lexer, stream)
    call parse_tree_init &
        (parse_tree, syntax_pexpr, lexer, var_str ("pexpr"))
    call lexer_final (lexer)
end subroutine parse_tree_init_pexpr

module subroutine parse_tree_init_cexpr (parse_tree, stream)
    type(parse_tree_t), intent(out) :: parse_tree
    type(stream_t), intent(inout), target :: stream
    type(lexer_t) :: lexer
    call lexer_init_eval_tree (lexer, .true.)
    call lexer_assign_stream (lexer, stream)
    call parse_tree_init &
        (parse_tree, syntax_pexpr, lexer, var_str ("cexpr"))
    call lexer_final (lexer)
end subroutine parse_tree_init_cexpr

module subroutine parse_tree_init_sexpr (parse_tree, stream, particles)
    type(parse_tree_t), intent(out) :: parse_tree
    type(stream_t), intent(inout), target :: stream
    logical, intent(in) :: particles
    type(lexer_t) :: lexer
    call lexer_init_eval_tree (lexer, particles)
    call lexer_assign_stream (lexer, stream)
    if (particles) then
        call parse_tree_init &

```

```

        (parse_tree, syntax_pexpr, lexer, var_str ("sexpr"))
    else
        call parse_tree_init &
            (parse_tree, syntax_expr, lexer, var_str ("sexpr"))
    end if
    call lexer_final (lexer)
end subroutine parse_tree_init_sexpr

```

28.3.9 The evaluation tree

The evaluation tree contains the initial variable list and the root node.

```

<Eval trees: public>+≡
    public :: eval_tree_t

<Eval trees: types>+≡
    type, extends (expr_t) :: eval_tree_t
    private
        type(parse_node_t), pointer :: pn => null ()
        type(var_list_t) :: var_list
        type(eval_node_t), pointer :: root => null ()
    contains
        <Eval trees: eval tree: TBP>
    end type eval_tree_t

```

Init from stream, using a temporary parse tree.

```

<Eval trees: eval tree: TBP>≡
    procedure :: init_stream => eval_tree_init_stream

<Eval trees: sub interfaces>+≡
    module subroutine eval_tree_init_stream &
        (eval_tree, stream, var_list, subevt, result_type)
        class(eval_tree_t), intent(out), target :: eval_tree
        type(stream_t), intent(inout), target :: stream
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), target, optional :: subevt
        integer, intent(in), optional :: result_type
    end subroutine eval_tree_init_stream

<Eval trees: procedures>+≡
    module subroutine eval_tree_init_stream &
        (eval_tree, stream, var_list, subevt, result_type)
        class(eval_tree_t), intent(out), target :: eval_tree
        type(stream_t), intent(inout), target :: stream
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), target, optional :: subevt
        integer, intent(in), optional :: result_type
        type(parse_tree_t) :: parse_tree
        type(parse_node_t), pointer :: nd_root
        integer :: type
        type = V_REAL; if (present (result_type)) type = result_type
        select case (type)
        case (V_INT, V_REAL, V_CMPLX)
            call parse_tree_init_expr (parse_tree, stream, present (subevt))

```

```

case (V_LOG)
  call parse_tree_init_lexpr (parse_tree, stream, present (subevt))
case (V_SEV)
  call parse_tree_init_pexpr (parse_tree, stream)
case (V_PDG)
  call parse_tree_init_cexpr (parse_tree, stream)
case (V_STR)
  call parse_tree_init_sexpr (parse_tree, stream, present (subevt))
end select
nd_root => parse_tree%get_root_ptr ()
if (associated (nd_root)) then
  select case (type)
  case (V_INT, V_REAL, V_CMPLX)
    call eval_tree_init_expr (eval_tree, nd_root, var_list, subevt)
  case (V_LOG)
    call eval_tree_init_lexpr (eval_tree, nd_root, var_list, subevt)
  case (V_SEV)
    call eval_tree_init_pexpr (eval_tree, nd_root, var_list, subevt)
  case (V_PDG)
    call eval_tree_init_cexpr (eval_tree, nd_root, var_list, subevt)
  case (V_STR)
    call eval_tree_init_sexpr (eval_tree, nd_root, var_list, subevt)
  end select
end if
call parse_tree_final (parse_tree)
end subroutine eval_tree_init_stream

```

API (to be superseded by the methods below): Init from a given parse-tree node. If we evaluate an expression that contains particle-list references, the original subevent has to be supplied. The initial variable list is optional.

<Eval trees: eval tree: TBP>+≡

```

procedure :: init_expr => eval_tree_init_expr
procedure :: init_lexpr => eval_tree_init_lexpr
procedure :: init_pexpr => eval_tree_init_pexpr
procedure :: init_cexpr => eval_tree_init_cexpr
procedure :: init_sexpr => eval_tree_init_sexpr

```

<Eval trees: sub interfaces>+≡

```

module subroutine eval_tree_init_expr &
  (expr, parse_node, var_list, subevt)
  class(eval_tree_t), intent(out), target :: expr
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subevt_t), intent(in), optional, target :: subevt
end subroutine eval_tree_init_expr
module subroutine eval_tree_init_lexpr &
  (expr, parse_node, var_list, subevt)
  class(eval_tree_t), intent(out), target :: expr
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subevt_t), intent(in), optional, target :: subevt
end subroutine eval_tree_init_lexpr
module subroutine eval_tree_init_pexpr &
  (expr, parse_node, var_list, subevt)

```



```

        class(eval_tree_t), intent(out), target :: expr
        type(parse_node_t), intent(in), target :: parse_node
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), optional, target :: subevt
    end subroutine eval_tree_init_pexpr
module subroutine eval_tree_init_cexpr &
    (expr, parse_node, var_list, subevt)
    class(eval_tree_t), intent(out), target :: expr
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
end subroutine eval_tree_init_cexpr
module subroutine eval_tree_init_sexpr &
    (expr, parse_node, var_list, subevt)
    class(eval_tree_t), intent(out), target :: expr
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
end subroutine eval_tree_init_sexpr

<Eval trees: procedures>+=
module subroutine eval_tree_init_expr &
    (expr, parse_node, var_list, subevt)
    class(eval_tree_t), intent(out), target :: expr
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    call eval_tree_link_var_list (expr, var_list)
    if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
    call eval_node_compile_expr &
        (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_expr

module subroutine eval_tree_init_lexpr &
    (expr, parse_node, var_list, subevt)
    class(eval_tree_t), intent(out), target :: expr
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    call eval_tree_link_var_list (expr, var_list)
    if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
    call eval_node_compile_lexpr &
        (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_lexpr

module subroutine eval_tree_init_pexpr &
    (expr, parse_node, var_list, subevt)
    class(eval_tree_t), intent(out), target :: expr
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    call eval_tree_link_var_list (expr, var_list)
    if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
    call eval_node_compile_pexpr &
        (expr%root, parse_node, expr%var_list)

```

```

end subroutine eval_tree_init_pexpr

module subroutine eval_tree_init_cexpr &
  (expr, parse_node, var_list, subevt)
  class(eval_tree_t), intent(out), target :: expr
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subevt_t), intent(in), optional, target :: subevt
  call eval_tree_link_var_list (expr, var_list)
  if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
  call eval_node_compile_cexpr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_cexpr

module subroutine eval_tree_init_sexpr &
  (expr, parse_node, var_list, subevt)
  class(eval_tree_t), intent(out), target :: expr
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subevt_t), intent(in), optional, target :: subevt
  call eval_tree_link_var_list (expr, var_list)
  if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
  call eval_node_compile_sexpr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_sexpr

```

Alternative: set up the expression using the parse node that has already been stored. We assume that the subevt or any other variable that may be referred to has already been added to the local variable list.

(Eval trees: eval tree: TBP)+≡

```

procedure :: setup_expr  => eval_tree_setup_expr
procedure :: setup_lexpr => eval_tree_setup_lexpr
procedure :: setup_pexpr => eval_tree_setup_pexpr
procedure :: setup_cexpr => eval_tree_setup_cexpr
procedure :: setup_sexpr => eval_tree_setup_sexpr

```

(Eval trees: sub interfaces)+≡

```

module subroutine eval_tree_setup_expr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
end subroutine eval_tree_setup_expr
module subroutine eval_tree_setup_lexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
end subroutine eval_tree_setup_lexpr
module subroutine eval_tree_setup_pexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
end subroutine eval_tree_setup_pexpr
module subroutine eval_tree_setup_cexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
end subroutine eval_tree_setup_cexpr
module subroutine eval_tree_setup_sexpr (expr, vars)

```

```

        class(eval_tree_t), intent(inout), target :: expr
        class(vars_t), intent(in), target :: vars
    end subroutine eval_tree_setup_sexpr
<Eval trees: procedures>+≡
module subroutine eval_tree_setup_expr (expr, vars)
    class(eval_tree_t), intent(inout), target :: expr
    class(vars_t), intent(in), target :: vars
    call eval_tree_link_var_list (expr, vars)
    call eval_node_compile_expr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_expr

module subroutine eval_tree_setup_lexpr (expr, vars)
    class(eval_tree_t), intent(inout), target :: expr
    class(vars_t), intent(in), target :: vars
    call eval_tree_link_var_list (expr, vars)
    call eval_node_compile_lexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_lexpr

module subroutine eval_tree_setup_pexpr (expr, vars)
    class(eval_tree_t), intent(inout), target :: expr
    class(vars_t), intent(in), target :: vars
    call eval_tree_link_var_list (expr, vars)
    call eval_node_compile_pexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_pexpr

module subroutine eval_tree_setup_cexpr (expr, vars)
    class(eval_tree_t), intent(inout), target :: expr
    class(vars_t), intent(in), target :: vars
    call eval_tree_link_var_list (expr, vars)
    call eval_node_compile_cexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_cexpr

module subroutine eval_tree_setup_sexpr (expr, vars)
    class(eval_tree_t), intent(inout), target :: expr
    class(vars_t), intent(in), target :: vars
    call eval_tree_link_var_list (expr, vars)
    call eval_node_compile_sexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_sexpr

```

This extra API function handles numerical constant expressions only. The only nontrivial part is the optional unit.

```

<Eval trees: eval tree: TBP>+≡
    procedure :: init_numeric_value => eval_tree_init_numeric_value
<Eval trees: sub interfaces>+≡
    module subroutine eval_tree_init_numeric_value (eval_tree, parse_node)
        class(eval_tree_t), intent(out), target :: eval_tree
        type(parse_node_t), intent(in), target :: parse_node
    end subroutine eval_tree_init_numeric_value
<Eval trees: procedures>+≡
    module subroutine eval_tree_init_numeric_value (eval_tree, parse_node)
        class(eval_tree_t), intent(out), target :: eval_tree
        type(parse_node_t), intent(in), target :: parse_node

```

```

        call eval_node_compile_numeric_value (eval_tree%root, parse_node)
    end subroutine eval_tree_init_numeric_value

```

Initialize the variable list, linking it to a context variable list.

```

<Eval trees: procedures>+≡
subroutine eval_tree_link_var_list (eval_tree, vars)
    type(eval_tree_t), intent(inout), target :: eval_tree
    class(vars_t), intent(in), target :: vars
    call eval_tree%var_list%link (vars)
end subroutine eval_tree_link_var_list

```

Include a subevent object in the initialization. We add a pointer to this as variable @evt in the local variable list.

```

<Eval trees: procedures>+≡
subroutine eval_tree_set_subevt (eval_tree, subevt)
    type(eval_tree_t), intent(inout), target :: eval_tree
    type(subevt_t), intent(in), target :: subevt
    logical, save, target :: known = .true.
    call eval_tree%var_list%append_subevt_ptr &
        (var_str("@evt"), subevt, known, intrinsic=.true.)
end subroutine eval_tree_set_subevt

```

Finalizer.

```

<Eval trees: eval tree: TBP>+≡
procedure :: final => eval_tree_final

<Eval trees: sub interfaces>+≡
module subroutine eval_tree_final (expr)
    class(eval_tree_t), intent(inout) :: expr
end subroutine eval_tree_final

<Eval trees: procedures>+≡
module subroutine eval_tree_final (expr)
    class(eval_tree_t), intent(inout) :: expr
    call expr%var_list%final ()
    if (associated (expr%root)) then
        call eval_node_final_rec (expr%root)
        deallocate (expr%root)
    end if
end subroutine eval_tree_final

```

```

<Eval trees: eval tree: TBP>+≡
procedure :: evaluate => eval_tree_evaluate

<Eval trees: sub interfaces>+≡
module subroutine eval_tree_evaluate (expr)
    class(eval_tree_t), intent(inout) :: expr
end subroutine eval_tree_evaluate

<Eval trees: procedures>+≡
module subroutine eval_tree_evaluate (expr)
    class(eval_tree_t), intent(inout) :: expr
    if (associated (expr%root)) then
        call eval_node_evaluate (expr%root)
    end if
end subroutine eval_tree_evaluate

```

```

        end if
    end subroutine eval_tree_evaluate

```

Check if the eval tree is allocated.

```

<Eval trees: procedures>+≡
function eval_tree_is_defined (eval_tree) result (flag)
    logical :: flag
    type(eval_tree_t), intent(in) :: eval_tree
    flag = associated (eval_tree%root)
end function eval_tree_is_defined

```

Check if the eval tree result is constant.

```

<Eval trees: procedures>+≡
function eval_tree_is_constant (eval_tree) result (flag)
    logical :: flag
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        flag = eval_tree%root%type == EN_CONSTANT
    else
        flag = .false.
    end if
end function eval_tree_is_constant

```

Insert a conversion node at the root, if necessary (only for real/int conversion)

```

<Eval trees: procedures>+≡
subroutine eval_tree_convert_result (eval_tree, result_type)
    type(eval_tree_t), intent(inout) :: eval_tree
    integer, intent(in) :: result_type
    if (associated (eval_tree%root)) then
        call insert_conversion_node (eval_tree%root, result_type)
    end if
end subroutine eval_tree_convert_result

```

Return the value of the top node, after evaluation. If the tree is empty, return the type of V_NONE. When extracting the value, no check for existence is done. For numeric values, the functions are safe against real/integer mismatch.

```

<Eval trees: eval tree: TBP>+≡
procedure :: is_known => eval_tree_result_is_known
procedure :: get_log => eval_tree_get_log
procedure :: get_int => eval_tree_get_int
procedure :: get_real => eval_tree_get_real
procedure :: get_cmplx => eval_tree_get_cmplx
procedure :: get_pdg_array => eval_tree_get_pdg_array
procedure :: get_subevt => eval_tree_get_subevt
procedure :: get_string => eval_tree_get_string

<Eval trees: sub interfaces>+≡
module function eval_tree_get_result_type (expr) result (type)
    integer :: type
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_result_type
module function eval_tree_result_is_known (expr) result (flag)

```

```

    logical :: flag
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_result_is_known
module function eval_tree_result_is_known_ptr (expr) result (ptr)
    logical, pointer :: ptr
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_result_is_known_ptr
module function eval_tree_get_log (expr) result (lval)
    logical :: lval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_log
module function eval_tree_get_int (expr) result (ival)
    integer :: ival
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_int
module function eval_tree_get_real (expr) result (rval)
    real(default) :: rval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_real
module function eval_tree_get_cmplx (expr) result (cval)
    complex(default) :: cval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_cmplx
module function eval_tree_get_pdg_array (expr) result (aval)
    type(pdg_array_t) :: aval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_pdg_array
module function eval_tree_get_subevt (expr) result (pval)
    type(subevt_t) :: pval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_subevt
module function eval_tree_get_string (expr) result (sval)
    type(string_t) :: sval
    class(eval_tree_t), intent(in) :: expr
end function eval_tree_get_string

```

(Eval trees: procedures)+≡

```

module function eval_tree_get_result_type (expr) result (type)
    integer :: type
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        type = expr%root%result_type
    else
        type = V_NONE
    end if
end function eval_tree_get_result_type

module function eval_tree_result_is_known (expr) result (flag)
    logical :: flag
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
        case (V_LOG, V_INT, V_REAL)
            flag = expr%root%value_is_known
        case default

```

```

        flag = .true.
    end select
else
    flag = .false.
end if
end function eval_tree_result_is_known

module function eval_tree_result_is_known_ptr (expr) result (ptr)
    logical, pointer :: ptr
    class(eval_tree_t), intent(in) :: expr
    logical, target, save :: known = .true.
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_LOG, V_INT, V_REAL)
                ptr => expr%root%value_is_known
            case default
                ptr => known
        end select
    else
        ptr => null ()
    end if
end function eval_tree_result_is_known_ptr

module function eval_tree_get_log (expr) result (lval)
    logical :: lval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) lval = expr%root%lval
end function eval_tree_get_log

module function eval_tree_get_int (expr) result (ival)
    integer :: ival
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_INT); ival = expr%root%ival
            case (V_REAL); ival = expr%root%rval
            case (V_CMPLX); ival = expr%root%cval
        end select
    end if
end function eval_tree_get_int

module function eval_tree_get_real (expr) result (rval)
    real(default) :: rval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_REAL); rval = expr%root%rval
            case (V_INT); rval = expr%root%ival
            case (V_CMPLX); rval = expr%root%cval
        end select
    end if
end function eval_tree_get_real

module function eval_tree_get_cmplx (expr) result (cval)

```

```

complex(default) :: cval
class(eval_tree_t), intent(in) :: expr
if (associated (expr%root)) then
  select case (expr%root%result_type)
    case (V_CMLX); cval = expr%root%cval
    case (V_REAL); cval = expr%root%rval
    case (V_INT);  cval = expr%root%ival
  end select
end if
end function eval_tree_get_cmlx

module function eval_tree_get_pdg_array (expr) result (aval)
  type(pdg_array_t) :: aval
  class(eval_tree_t), intent(in) :: expr
  if (associated (expr%root)) then
    aval = expr%root%aval
  end if
end function eval_tree_get_pdg_array

module function eval_tree_get_subevt (expr) result (pval)
  type(subevt_t) :: pval
  class(eval_tree_t), intent(in) :: expr
  if (associated (expr%root)) then
    pval = expr%root%pval
  end if
end function eval_tree_get_subevt

module function eval_tree_get_string (expr) result (sval)
  type(string_t) :: sval
  class(eval_tree_t), intent(in) :: expr
  if (associated (expr%root)) then
    sval = expr%root%sval
  end if
end function eval_tree_get_string

```

Return a pointer to the value of the top node.

(Eval trees: procedures)+≡

```

function eval_tree_get_log_ptr (eval_tree) result (lval)
  logical, pointer :: lval
  type(eval_tree_t), intent(in) :: eval_tree
  if (associated (eval_tree%root)) then
    lval => eval_tree%root%lval
  else
    lval => null ()
  end if
end function eval_tree_get_log_ptr

function eval_tree_get_int_ptr (eval_tree) result (ival)
  integer, pointer :: ival
  type(eval_tree_t), intent(in) :: eval_tree
  if (associated (eval_tree%root)) then
    ival => eval_tree%root%ival
  else

```



```

        ival => null ()
    end if
end function eval_tree_get_int_ptr

function eval_tree_get_real_ptr (eval_tree) result (rval)
    real(default), pointer :: rval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        rval => eval_tree%root%rval
    else
        rval => null ()
    end if
end function eval_tree_get_real_ptr

function eval_tree_get_cmplx_ptr (eval_tree) result (cval)
    complex(default), pointer :: cval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        cval => eval_tree%root%cval
    else
        cval => null ()
    end if
end function eval_tree_get_cmplx_ptr

function eval_tree_get_subevt_ptr (eval_tree) result (pval)
    type(subevt_t), pointer :: pval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        pval => eval_tree%root%pval
    else
        pval => null ()
    end if
end function eval_tree_get_subevt_ptr

function eval_tree_get_pdg_array_ptr (eval_tree) result (aval)
    type(pdg_array_t), pointer :: aval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        aval => eval_tree%root%aval
    else
        aval => null ()
    end if
end function eval_tree_get_pdg_array_ptr

function eval_tree_get_string_ptr (eval_tree) result (sval)
    type(string_t), pointer :: sval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        sval => eval_tree%root%sval
    else
        sval => null ()
    end if
end function eval_tree_get_string_ptr

```

```

<Eval trees: eval tree: TBP>+≡
    procedure :: write => eval_tree_write

<Eval trees: sub interfaces>+≡
    module subroutine eval_tree_write (expr, unit, write_vars)
        class(eval_tree_t), intent(in) :: expr
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: write_vars
    end subroutine eval_tree_write

<Eval trees: procedures>+≡
    module subroutine eval_tree_write (expr, unit, write_vars)
        class(eval_tree_t), intent(in) :: expr
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: write_vars
        integer :: u
        logical :: vl
        u = given_output_unit (unit); if (u < 0) return
        vl = .false.; if (present (write_vars)) vl = write_vars
        write (u, "(1x,A)") "Evaluation tree:"
        if (associated (expr%root)) then
            call eval_node_write_rec (expr%root, unit)
        else
            write (u, "(3x,A)") "[empty]"
        end if
        if (vl) call expr%var_list%write (unit)
    end subroutine eval_tree_write

```

Use the written representation for generating an MD5 sum:

```

<Eval trees: procedures>+≡
    function eval_tree_get_md5sum (eval_tree) result (md5sum_et)
        character(32) :: md5sum_et
        type(eval_tree_t), intent(in) :: eval_tree
        integer :: u
        u = free_unit ()
        open (unit = u, status = "scratch", action = "readwrite")
        call eval_tree_write (eval_tree, unit=u)
        rewind (u)
        md5sum_et = md5sum (u)
        close (u)
    end function eval_tree_get_md5sum

```

28.3.10 Direct evaluation

These procedures create an eval tree and evaluate it on-the-fly, returning only the final value. The evaluation must yield a well-defined value, unless the `is_known` flag is present, which will be set accordingly.

```

<Eval trees: public>+≡
    public :: eval_log
    public :: eval_int
    public :: eval_real
    public :: eval_cmplx
    public :: eval_subevt

```

```

public :: eval_pdg_array
public :: eval_string

(Eval trees: sub interfaces) +=
  module function eval_log &
    (parse_node, var_list, subevt, is_known) result (lval)
    logical :: lval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_log
  module function eval_int &
    (parse_node, var_list, subevt, is_known) result (ival)
    integer :: ival
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_int
  module function eval_real &
    (parse_node, var_list, subevt, is_known) result (rval)
    real(default) :: rval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_real
  module function eval_cmplx &
    (parse_node, var_list, subevt, is_known) result (cval)
    complex(default) :: cval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_cmplx
  module function eval_subevt &
    (parse_node, var_list, subevt, is_known) result (pval)
    type(subevt_t) :: pval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_subevt
  module function eval_pdg_array &
    (parse_node, var_list, subevt, is_known) result (aval)
    type(pdg_array_t) :: aval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
  end function eval_pdg_array
  module function eval_string &
    (parse_node, var_list, subevt, is_known) result (sval)
    type(string_t) :: sval

```

```

    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
end function eval_string

```

<Eval trees: procedures>+≡

```

module function eval_log &
    (parse_node, var_list, subevt, is_known) result (lval)
    logical :: lval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_lexpr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        lval = eval_tree_get_log (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
        lval = .false.
    end if
    call eval_tree_final (eval_tree)
end function eval_log

```

```

module function eval_int &
    (parse_node, var_list, subevt, is_known) result (ival)
    integer :: ival
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_expr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        ival = eval_tree_get_int (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
        ival = 0
    end if
    call eval_tree_final (eval_tree)
end function eval_int

```

```

module function eval_real &
    (parse_node, var_list, subevt, is_known) result (rval)

```

```

real(default) :: rval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subvt_t), intent(in), optional, target :: subvt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_expr &
    (eval_tree, parse_node, var_list, subvt)
call eval_tree_evaluate (eval_tree)
if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    rval = eval_tree_get_real (eval_tree)
else if (present (is_known)) then
    is_known = .false.
else
    call eval_tree_unknown (eval_tree, parse_node)
    rval = 0
end if
call eval_tree_final (eval_tree)
end function eval_real

module function eval_cmplx &
    (parse_node, var_list, subvt, is_known) result (cval)
complex(default) :: cval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subvt_t), intent(in), optional, target :: subvt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_expr &
    (eval_tree, parse_node, var_list, subvt)
call eval_tree_evaluate (eval_tree)
if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    cval = eval_tree_get_cmplx (eval_tree)
else if (present (is_known)) then
    is_known = .false.
else
    call eval_tree_unknown (eval_tree, parse_node)
    cval = 0
end if
call eval_tree_final (eval_tree)
end function eval_cmplx

module function eval_subvt &
    (parse_node, var_list, subvt, is_known) result (pval)
type(subvt_t) :: pval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subvt_t), intent(in), optional, target :: subvt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_pexpr &
    (eval_tree, parse_node, var_list, subvt)

```

```

call eval_tree_evaluate (eval_tree)
if (eval_tree_result_is_known (eval_tree)) then
  if (present (is_known)) is_known = .true.
  pval = eval_tree_get_subvt (eval_tree)
else if (present (is_known)) then
  is_known = .false.
else
  call eval_tree_unknown (eval_tree, parse_node)
end if
call eval_tree_final (eval_tree)
end function eval_subvt

module function eval_pdg_array &
  (parse_node, var_list, subvt, is_known) result (aval)
  type(pdg_array_t) :: aval
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subvt_t), intent(in), optional, target :: subvt
  logical, intent(out), optional :: is_known
  type(eval_tree_t), target :: eval_tree
  call eval_tree_init_cexpr &
    (eval_tree, parse_node, var_list, subvt)
  call eval_tree_evaluate (eval_tree)
  if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    aval = eval_tree_get_pdg_array (eval_tree)
  else if (present (is_known)) then
    is_known = .false.
  else
    call eval_tree_unknown (eval_tree, parse_node)
  end if
  call eval_tree_final (eval_tree)
end function eval_pdg_array

module function eval_string &
  (parse_node, var_list, subvt, is_known) result (sval)
  type(string_t) :: sval
  type(parse_node_t), intent(in), target :: parse_node
  type(var_list_t), intent(in), target :: var_list
  type(subvt_t), intent(in), optional, target :: subvt
  logical, intent(out), optional :: is_known
  type(eval_tree_t), target :: eval_tree
  call eval_tree_init_sexpr &
    (eval_tree, parse_node, var_list, subvt)
  call eval_tree_evaluate (eval_tree)
  if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    sval = eval_tree_get_string (eval_tree)
  else if (present (is_known)) then
    is_known = .false.
  else
    call eval_tree_unknown (eval_tree, parse_node)
    sval = ""
  end if
end if

```

```

        call eval_tree_final (eval_tree)
    end function eval_string

```

Here is a variant that returns numeric values of all possible kinds, the appropriate kind to be selected later:

```

<Eval trees: public>+≡
    public :: eval_numeric

<Eval trees: sub interfaces>+≡
    module subroutine eval_numeric &
        (parse_node, var_list, subevt, ival, rval, cval, &
         is_known, result_type)
        type(parse_node_t), intent(in), target :: parse_node
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), optional, target :: subevt
        integer, intent(out), optional :: ival
        real(default), intent(out), optional :: rval
        complex(default), intent(out), optional :: cval
        logical, intent(out), optional :: is_known
        integer, intent(out), optional :: result_type
    end subroutine eval_numeric

<Eval trees: procedures>+≡
    module subroutine eval_numeric &
        (parse_node, var_list, subevt, ival, rval, cval, &
         is_known, result_type)
        type(parse_node_t), intent(in), target :: parse_node
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), optional, target :: subevt
        integer, intent(out), optional :: ival
        real(default), intent(out), optional :: rval
        complex(default), intent(out), optional :: cval
        logical, intent(out), optional :: is_known
        integer, intent(out), optional :: result_type
        type(eval_tree_t), target :: eval_tree
        call eval_tree_init_expr &
            (eval_tree, parse_node, var_list, subevt)
        call eval_tree_evaluate (eval_tree)
        if (eval_tree_result_is_known (eval_tree)) then
            if (present (ival)) ival = eval_tree_get_int (eval_tree)
            if (present (rval)) rval = eval_tree_get_real (eval_tree)
            if (present (cval)) cval = eval_tree_get_cmplx (eval_tree)
            if (present (is_known)) is_known = .true.
        else
            call eval_tree_unknown (eval_tree, parse_node)
            if (present (ival)) ival = 0
            if (present (rval)) rval = 0
            if (present (cval)) cval = 0
            if (present (is_known)) is_known = .false.
        end if
        if (present (result_type)) &
            result_type = eval_tree_get_result_type (eval_tree)
        call eval_tree_final (eval_tree)
    end subroutine eval_numeric

```

Error message with debugging info:

```

<Eval trees: procedures>+≡
  subroutine eval_tree_unknown (eval_tree, parse_node)
    type(eval_tree_t), intent(in) :: eval_tree
    type(parse_node_t), intent(in) :: parse_node
    call parse_node_write_rec (parse_node)
    call eval_tree_write (eval_tree)
    call msg_error ("Evaluation yields an undefined result, inserting default")
  end subroutine eval_tree_unknown

```

28.3.11 Factory Type

Since `eval_tree_t` is an implementation of `expr_t`, we also need a matching factory type and build method.

```

<Eval trees: public>+≡
  public :: eval_tree_factory_t

<Eval trees: types>+≡
  type, extends (expr_factory_t) :: eval_tree_factory_t
  private
    type(parse_node_t), pointer :: pn => null ()
  contains
    <Eval trees: eval tree factory: TBP>
  end type eval_tree_factory_t

```

Output: delegate to the output of the embedded parse node.

```

<Eval trees: eval tree factory: TBP>≡
  procedure :: write => eval_tree_factory_write

<Eval trees: sub interfaces>+≡
  module subroutine eval_tree_factory_write (expr_factory, unit)
    class(eval_tree_factory_t), intent(in) :: expr_factory
    integer, intent(in), optional :: unit
  end subroutine eval_tree_factory_write

<Eval trees: procedures>+≡
  module subroutine eval_tree_factory_write (expr_factory, unit)
    class(eval_tree_factory_t), intent(in) :: expr_factory
    integer, intent(in), optional :: unit
    if (associated (expr_factory%pn)) then
      call parse_node_write_rec (expr_factory%pn, unit)
    end if
  end subroutine eval_tree_factory_write

```

Initializer: take a parse node and hide it thus from the environment.

```

<Eval trees: eval tree factory: TBP>+≡
  procedure :: init => eval_tree_factory_init

<Eval trees: sub interfaces>+≡
  module subroutine eval_tree_factory_init (expr_factory, pn)
    class(eval_tree_factory_t), intent(out) :: expr_factory
    type(parse_node_t), intent(in), pointer :: pn
  end subroutine eval_tree_factory_init

```



```

<Eval trees: procedures>+≡
  module subroutine eval_tree_factory_init (expr_factory, pn)
    class(eval_tree_factory_t), intent(out) :: expr_factory
    type(parse_node_t), intent(in), pointer :: pn
    expr_factory%pn => pn
  end subroutine eval_tree_factory_init

```

Factory method: allocate expression with correct eval tree type. If the stored parse node is not associate, don't allocate. Gfortran 7/8/9 bug, has to remain in the module.

```

<Eval trees: eval tree factory: TBP>+≡
  procedure :: build => eval_tree_factory_build

<Eval trees: main procedures>≡
  subroutine eval_tree_factory_build (expr_factory, expr)
    class(eval_tree_factory_t), intent(in) :: expr_factory
    class(expr_t), intent(out), allocatable :: expr
    if (associated (expr_factory%pn)) then
      allocate (eval_tree_t :: expr)
      select type (expr)
        type is (eval_tree_t)
          expr%pn => expr_factory%pn
        end select
      end if
    end subroutine eval_tree_factory_build

```

28.3.12 Unit tests

Test module, followed by the corresponding implementation module.

```

<eval_trees_ut.f90>≡
  <File header>

  module eval_trees_ut
    use unit_tests
    use eval_trees_uti

    <Standard module head>

    <Eval trees: public test>

    contains

    <Eval trees: test driver>

  end module eval_trees_ut

<eval_trees_uti.f90>≡
  <File header>

  module eval_trees_uti

    <Use kinds>

```

⟨Use strings⟩

```
use ifiles
use lexers
use lorentz
use syntax_rules, only: syntax_write
use pdg_arrays
use subevents
use variables
use observables
```

```
use eval_trees
```

⟨Standard module head⟩

⟨Eval trees: test declarations⟩

```
contains
```

⟨Eval trees: tests⟩

```
end module eval_trees_util
```

API: driver for the unit tests below.

⟨Eval trees: public test⟩≡

```
public :: expressions_test
```

⟨Eval trees: test driver⟩≡

```
subroutine expressions_test (u, results)
  integer, intent(in) :: u
  type (test_results_t), intent(inout) :: results
```

⟨Eval trees: execute tests⟩

```
end subroutine expressions_test
```

Testing the routines of the expressions module. First a simple unary observable and the node evaluation.

⟨Eval trees: execute tests⟩≡

```
call test (expressions_1, "expressions_1", &
  "check simple observable", &
  u, results)
```

⟨Eval trees: test declarations⟩≡

```
public :: expressions_1
```

⟨Eval trees: tests⟩≡

```
subroutine expressions_1 (u)
  integer, intent(in) :: u
  type(var_list_t), pointer :: var_list => null ()
  type(eval_node_t), pointer :: node => null ()
  type(prt_t), pointer :: prt => null ()
  type(string_t) :: var_name
```

```
write (u, "(A)")  "* Test output: Expressions"
```

```
write (u, "(A)")  "* Purpose: test simple observable and node evaluation"
```

```
write (u, "(A)")
```

```

write (u, "(A)")  "* Setting a unary observable:"
write (u, "(A)")

allocate (var_list)
allocate (prt)
call var_list_set_observables_unary (var_list, prt)
call var_list%write (u)

write (u, "(A)")  "* Evaluating the observable node:"
write (u, "(A)")

var_name = "PDG"

allocate (node)
call node%test_obs (var_list, var_name)
call node%write (u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call node%final_rec ()
deallocate (node)
!!! Workaround for NAGFOR 6.2
! call var_list%final ()
deallocate (var_list)
deallocate (prt)

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_1"

end subroutine expressions_1

```

Parse a complicated expression, transfer it to a parse tree and evaluate.

```

<Eval trees: execute tests>+≡
  call test (expressions_2, "expressions_2", &
    "check expression transfer to parse tree", &
    u, results)

<Eval trees: test declarations>+≡
  public :: expressions_2

<Eval trees: tests>+≡
  subroutine expressions_2 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(eval_tree_t) :: eval_tree
    type(string_t) :: expr_text
    type(var_list_t), pointer :: var_list => null ()

    write (u, "(A)")  "* Test output: Expressions"
    write (u, "(A)")  "* Purpose: test parse routines"
    write (u, "(A)")

```

```

call syntax_expr_init ()
call syntax_write (syntax_expr, u)
allocate (var_list)
call var_list%append_real (var_str ("tolerance"), 0._default)
call var_list%append_real (var_str ("x"), -5._default)
call var_list%append_int (var_str ("foo"), -27)
call var_list%append_real (var_str ("mb"), 4._default)
expr_text = &
    "let real twopi = 2 * pi in" // &
    "  twopi * sqrt (25.d0 - mb^2)" // &
    " / (let int mb_or_0 = max (mb, 0) in" // &
    "    1 + (if -1 TeV <= x < mb_or_0 then abs(x) else x endif))"
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call var_list%write (u)
call eval_tree%init_stream (stream, var_list=var_list)
call eval_tree%evaluate ()
call eval_tree%write (u)

write (u, "(A)")  "* Input string:"
write (u, "(A,A)")  "    ", char (expr_text)
write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stream_final (stream)
call ifile_final (ifile)
call eval_tree%final ()
call var_list%final ()
deallocate (var_list)
call syntax_expr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_2"

end subroutine expressions_2

```

Test a subevent expression.

<Eval trees: execute tests>+≡

```

call test (expressions_3, "expressions_3", &
    "check subevent expressions", &
    u, results)

```

<Eval trees: test declarations>+≡

```

public :: expressions_3

```

<Eval trees: tests>+≡

```

subroutine expressions_3 (u)
    integer, intent(in) :: u
    type(subvt_t) :: subvt

    write (u, "(A)")  "* Test output: Expressions"
    write (u, "(A)")  "* Purpose: test subevent expressions"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize subevent:"

```

```

write (u, "(A)")

call subevt_init (subevt)
call subevt%reset (1)
call subevt%set_incoming (1, 22, &
    vector4_moving (1.e3_default, 1.e3_default, 1), 0._default, [2])
call subevt%write (u)
call subevt%reset (4)
call subevt%reset (3)
call subevt%set_incoming (1, 21, &
    vector4_moving (1.e3_default, 1.e3_default, 3), 0._default, [1])
call subevt_polarize (subevt, 1, -1)
call subevt%set_outgoing (2, 1, &
    vector4_moving (0._default, 1.e3_default, 3), &
    -1.e6_default, [7])
call subevt%set_composite (3, &
    vector4_moving (-1.e3_default, 0._default, 3), [2, 7])
call subevt%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_3"

end subroutine expressions_3

```

Test expressions from a PDG array.

```

<Eval trees: execute tests>+≡
    call test (expressions_4, "expressions_4", &
        "check pdg array expressions", &
        u, results)

<Eval trees: test declarations>+≡
    public :: expressions_4

<Eval trees: tests>+≡
    subroutine expressions_4 (u)
        integer, intent(in) :: u
        type(subevt_t), target :: subevt
        type(string_t) :: expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(eval_tree_t) :: eval_tree
        type(var_list_t), pointer :: var_list => null ()
        type(pdg_array_t) :: aval

        write (u, "(A)")  "* Test output: Expressions"
        write (u, "(A)")  "* Purpose: test pdg array expressions"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization:"
        write (u, "(A)")

        call syntax_pexpr_init ()
        call syntax_write (syntax_pexpr, u)
        allocate (var_list)
        call var_list%append_real (var_str ("tolerance"), 0._default)

```

```

aval = 0
call var_list%append_pdg_array (var_str ("particle"), aval)
aval = [11,-11]
call var_list%append_pdg_array (var_str ("lepton"), aval)
aval = 22
call var_list%append_pdg_array (var_str ("photon"), aval)
aval = 1
call var_list%append_pdg_array (var_str ("u"), aval)
call subevt_init (subevt)
call subevt%reset (6)
call subevt%set_incoming (1, 1, &
    vector4_moving (1._default, 1._default, 1), 0._default)
call subevt%set_incoming (2, -1, &
    vector4_moving (2._default, 2._default, 1), 0._default)
call subevt%set_outgoing (3, 22, &
    vector4_moving (3._default, 3._default, 1), 0._default)
call subevt%set_outgoing (4, 22, &
    vector4_moving (4._default, 4._default, 1), 0._default)
call subevt%set_outgoing (5, 11, &
    vector4_moving (5._default, 5._default, 1), 0._default)
call subevt%set_outgoing (6, -11, &
    vector4_moving (6._default, 6._default, 1), 0._default)
write (u, "(A)")
write (u, "(A)")  "* Expression:"
expr_text = &
    "let alias quark = pdg(1):pdg(2):pdg(3) in" // &
    "  any E > 3 GeV " // &
    "    [sort by - Pt " // &
    "      [select if Index < 6 " // &
    "        [photon:pdg(-11):pdg(3):quark " // &
    "          & incoming particle]]]" // &
    "  and" // &
    "  eval Theta [extract index -1 [photon]] > 45 degree" // &
    "  and" // &
    "  count [incoming photon] * 3 > 0"
write (u, "(A,A)")  "  ", char (expr_text)
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Extract the evaluation tree:"
write (u, "(A)")

call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call eval_tree%init_stream (stream, var_list, subevt, V_LOG)
call eval_tree%write (u)
call eval_tree%evaluate ()

write (u, "(A)")
write (u, "(A)")  "* Evaluate the tree:"
write (u, "(A)")

call eval_tree%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call stream_final (stream)
call ifile_final (ifile)
call eval_tree%final ()
call var_list%final ()
deallocate (var_list)
call syntax_pexpr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_4"

end subroutine expressions_4

```

28.4 Physics Models

A model object represents a physics model. It contains a table of particle data, a list of parameters, and a vertex table. The list of parameters is a variable list which includes the real parameters (which are pointers to the particle data table) and PDG array variables for the particles themselves. The vertex list is used for phase-space generation, not for calculating the matrix element.

The actual numeric model data are in the base type `model_data_t`, as part of the `qft` section. We implement the `model_t` as an extension of this, for convenient direct access to the base-type methods via inheritance. (Alternatively, we could delegate these calls explicitly.) The extension contains administrative additions, such as the methods for recalculating derived data and keeping the parameter set consistent. It thus acts as a proxy of the actual model-data object towards the WHIZARD package. There are further proxy objects, such as the `parameter_t` array which provides the interface to the actual numeric parameters.

Model definitions are read from model files. Therefore, this module contains a parser for model files. The parameter definitions (derived parameters) are Sindarin expressions.

The models, as read from file, are stored in a model library which is a simple list of model definitions. For setting up a process object we should make a copy (an instance) of a model, which gets the current parameter values from the global variable list.

28.4.1 Module

```
<models.f90>≡  
<File header>  
  
module models  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use kinds>  
    use kinds, only: c_default_float  
    <Use strings>  
    use os_interface  
    use model_data  
  
    use syntax_rules  
    use parser  
    use variables  
    use expr_base  
    use eval_trees  
  
    <Standard module head>  
  
    <Models: public>  
  
    <Models: parameters>  
  
    <Models: types>
```



```

    <Models: interfaces>

    <Models: variables>

    interface
    <Models: sub interfaces>
    end interface

contains

    <Models: main procedures>

end module models

<models_sub.f90>≡
    <File header>

submodule (models) models_s

    use io_units
    use diagnostics
    use md5
    use physics_defs, only: UNDEFINED

    use ifiles
    use lexers
    use pdg_arrays
    use ttv_formfactors, only: init_parameters

    implicit none

contains

    <Models: procedures>

end submodule models_s

```

28.4.2 Physics Parameters

A parameter has a name, a value. Derived parameters also have a definition in terms of other parameters, which is stored as an `eval_tree`. External parameters are set by an external program.

This parameter object should be considered as a proxy object. The parameter name and value are stored in a corresponding `modelpar_data_t` object which is located in a `model_data_t` object. The latter is a component of the `model_t` handler. Methods of `parameter_t` can be delegated to the `par_data_t` component.

The `block_name` and `block_index` values, if nonempty, indicate the possibility of reading this parameter from a SLHA-type input file. (Within the `parameter_t` object, this info is just used for I/O, the actual block register is located in the parent `model_t` object.)

The `pn` component is a pointer to the parameter definition inside the model parse tree. It allows us to recreate the `eval_tree` when making copies (instances) of the parameter object.

```

<Models: parameters>≡
  integer, parameter :: PAR_NONE = 0, PAR_UNUSED = -1
  integer, parameter :: PAR_INDEPENDENT = 1, PAR_DERIVED = 2
  integer, parameter :: PAR_EXTERNAL = 3

<Models: types>≡
  type :: parameter_t
    private
    integer :: type = PAR_NONE
    class(modelpar_data_t), pointer :: data => null ()
    type(string_t) :: block_name
    integer, dimension(:), allocatable :: block_index
    type(parse_node_t), pointer :: pn => null ()
    class(expr_t), allocatable :: expr
  contains
    <Models: parameter: TBP>
  end type parameter_t

```

Initialization depends on parameter type. Independent parameters are initialized by a constant value or a constant numerical expression (which may contain a unit). Derived parameters are initialized by an arbitrary numerical expression, which makes use of the current variable list. The expression is evaluated by the function `parameter_reset`.

This implementation supports only real parameters and real values.

```

<Models: parameter: TBP>≡
  procedure :: init_independent_value => parameter_init_independent_value
  procedure :: init_independent => parameter_init_independent
  procedure :: init_derived => parameter_init_derived
  procedure :: init_external => parameter_init_external
  procedure :: init_unused => parameter_init_unused

<Models: sub interfaces>≡
  module subroutine parameter_init_independent_value &
    (par, par_data, name, value)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
  end subroutine parameter_init_independent_value
  module subroutine parameter_init_external (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
  end subroutine parameter_init_external
  module subroutine parameter_init_unused (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
  end subroutine parameter_init_unused

```

<Models: procedures>≡

```

module subroutine parameter_init_independent_value &
    (par, par_data, name, value)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    par%type = PAR_INDEPENDENT
    par%data => par_data
    call par%data%init (name, value)
end subroutine parameter_init_independent_value

module subroutine parameter_init_external (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    par%type = PAR_EXTERNAL
    par%data => par_data
    call par%data%init (name, 0._default)
end subroutine parameter_init_external

module subroutine parameter_init_unused (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    par%type = PAR_UNUSED
    par%data => par_data
    call par%data%init (name, 0._default)
end subroutine parameter_init_unused

```

Gfortran 7/8/9 bug: these have to remain in the main module.

<Models: main procedures>≡

```

subroutine parameter_init_independent (par, par_data, name, pn)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn
    par%type = PAR_INDEPENDENT
    par%pn => pn
    allocate (eval_tree_t :: par%expr)
    select type (expr => par%expr)
    type is (eval_tree_t)
        call expr%init_numeric_value (pn)
    end select
    par%data => par_data
    call par%data%init (name, par%expr%get_real ())
end subroutine parameter_init_independent

subroutine parameter_init_derived (par, par_data, name, pn, var_list)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn

```

```

    type(var_list_t), intent(in), target :: var_list
    par%type = PAR_DERIVED
    par%pn => pn
    allocate (eval_tree_t :: par%expr)
    select type (expr => par%expr)
    type is (eval_tree_t)
        call expr%init_expr (pn, var_list=var_list)
    end select
    par%data => par_data
!    call par%expr%evaluate ()
    call par%data%init (name, 0._default)
end subroutine parameter_init_derived

```

The finalizer is needed for the evaluation tree in the definition.

```

<Models: parameter: TBP>+≡
    procedure :: final => parameter_final

<Models: sub interfaces>+≡
    module subroutine parameter_final (par)
        class(parameter_t), intent(inout) :: par
    end subroutine parameter_final

<Models: procedures>+≡
    module subroutine parameter_final (par)
        class(parameter_t), intent(inout) :: par
        if (allocated (par%expr)) then
            call par%expr%final ()
        end if
    end subroutine parameter_final

```

All derived parameters should be recalculated if some independent parameters have changed:

```

<Models: parameter: TBP>+≡
    procedure :: reset_derived => parameter_reset_derived

<Models: sub interfaces>+≡
    module subroutine parameter_reset_derived (par)
        class(parameter_t), intent(inout) :: par
    end subroutine parameter_reset_derived

<Models: procedures>+≡
    module subroutine parameter_reset_derived (par)
        class(parameter_t), intent(inout) :: par
        select case (par%type)
        case (PAR_DERIVED)
            call par%expr%evaluate ()
            par%data = par%expr%get_real ()
        end select
    end subroutine parameter_reset_derived

```

Output. [We should have a formula format for the eval tree, suitable for input and output!]

```

<Models: parameter: TBP>+≡
    procedure :: write => parameter_write

```

```

<Models: sub interfaces>+≡
    module subroutine parameter_write (par, unit, write_defs)
        class(parameter_t), intent(in) :: par
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: write_defs
    end subroutine parameter_write

<Models: procedures>+≡
    module subroutine parameter_write (par, unit, write_defs)
        class(parameter_t), intent(in) :: par
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: write_defs
        logical :: defs
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        defs = .false.; if (present (write_defs)) defs = write_defs
        select case (par%type)
        case (PAR_INDEPENDENT)
            write (u, "(3x,A)", advance="no") "parameter"
            call par%data%write (u)
        case (PAR_DERIVED)
            write (u, "(3x,A)", advance="no") "derived"
            call par%data%write (u)
        case (PAR_EXTERNAL)
            write (u, "(3x,A)", advance="no") "external"
            call par%data%write (u)
        case (PAR_UNUSED)
            write (u, "(3x,A)", advance="no") "unused"
            write (u, "(1x,A)", advance="no") char (par%data%get_name ())
        end select
        select case (par%type)
        case (PAR_INDEPENDENT)
            if (allocated (par%block_index)) then
                write (u, "(1x,A,1x,A,*(1x,IO))" &
                    "slha_entry", char (par%block_name), par%block_index)
            else
                write (u, "(A)")
            end if
        case (PAR_DERIVED)
            if (defs) then
                call par%expr%write (unit)
            else
                write (u, "(A)")
            end if
        case default
            write (u, "(A)")
        end select
    end subroutine parameter_write

```

Screen output variant. Restrict output to the given parameter type.

```

<Models: parameter: TBP>+≡
    procedure :: show => parameter_show

<Models: sub interfaces>+≡
    module subroutine parameter_show (par, l, u, party)

```

```

        class(parameter_t), intent(in) :: par
        integer, intent(in) :: l, u
        integer, intent(in) :: partype
    end subroutine parameter_show
<Models: procedures>+=
module subroutine parameter_show (par, l, u, partype)
    class(parameter_t), intent(in) :: par
    integer, intent(in) :: l, u
    integer, intent(in) :: partype
    if (par%type == partype) then
        call par%data%show (l, u)
    end if
end subroutine parameter_show

```

28.4.3 SLHA block register

For the optional SLHA interface, the model record contains a register of SLHA-type block names together with index values, which point to a particular parameter. These are private types:

```

<Models: types>+=
    type :: slha_entry_t
        integer, dimension(:), allocatable :: block_index
        integer :: i_par = 0
    end type slha_entry_t

<Models: types>+=
    type :: slha_block_t
        type(string_t) :: name
        integer :: n_entry = 0
        type(slha_entry_t), dimension(:), allocatable :: entry
    end type slha_block_t

```

28.4.4 Model Object

A model object holds all information about parameters, particles, and vertices. For models that require an external program for parameter calculation, there is the pointer to a function that does this calculation, given the set of independent and derived parameters.

As explained above, the type inherits from `model_data_t`, which is the actual storage for the model data.

When reading a model, we create a parse tree. Parameter definitions are available via parse nodes. Since we may need those later when making model instances, we keep the whole parse tree in the model definition (but not in the instances).

```

<Models: public>=
    public :: model_t

```

```

<Models: types>+=
  type, extends (model_data_t) :: model_t
    private
      character(32) :: md5sum = ""
      logical :: ufo_model = .false.
      type(string_t) :: ufo_path
      type(string_t), dimension(:), allocatable :: schemes
      type(string_t), allocatable :: selected_scheme
      type(parameter_t), dimension(:), allocatable :: par
      integer :: n_slha_block = 0
      type(slha_block_t), dimension(:), allocatable :: slha_block
      integer :: max_par_name_length = 0
      integer :: max_field_name_length = 0
      type(var_list_t) :: var_list
      type(string_t) :: dlname
      procedure(model_init_external_parameters), nopass, pointer :: &
        init_external_parameters => null ()
      type(dlaccess_t) :: dlaccess
      type(parse_tree_t) :: parse_tree
    contains
      <Models: model: TBP>
    end type model_t

```

This is the interface for a procedure that initializes the calculation of external parameters, given the array of all parameters.

```

<Models: interfaces>=
  abstract interface
    subroutine model_init_external_parameters (par) bind (C)
      import
      real(c_default_float), dimension(*), intent(inout) :: par
    end subroutine model_init_external_parameters
  end interface

```

Initialization: Specify the number of parameters, particles, vertices and allocate memory. If an associated DL library is specified, load this library.

The model may already carry scheme information, so we have to save and restore the scheme number when actually initializing the `model_data_t` base.

```

<Models: model: TBP>=
  generic :: init => model_init
  procedure, private :: model_init

<Models: sub interfaces>+=
  module subroutine model_init &
    (model, name, libname, os_data, n_par, n_prt, n_vtx, ufo)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name, libname
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: n_par, n_prt, n_vtx
    logical, intent(in), optional :: ufo
  end subroutine model_init

<Models: procedures>+=
  module subroutine model_init &
    (model, name, libname, os_data, n_par, n_prt, n_vtx, ufo)

```

```

class(model_t), intent(inout) :: model
type(string_t), intent(in) :: name, libname
type(os_data_t), intent(in) :: os_data
integer, intent(in) :: n_par, n_prt, n_vtx
logical, intent(in), optional :: ufo
type(c_funptr) :: c_fptr
type(string_t) :: libpath
integer :: scheme_num
scheme_num = model%get_scheme_num ()
call model%basic_init (name, n_par, n_prt, n_vtx)
if (present (ufo)) model%ufo_model = ufo
call model%set_scheme_num (scheme_num)
if (libname /= "") then
  if (.not. os_data%use_testfiles) then
    libpath = os_data%whizard_models_libpath_local
    model%dlname = os_get_dlname ( &
      libpath // "/" // libname, os_data, ignore=.true.)
  end if
  if (model%dlname == "") then
    libpath = os_data%whizard_models_libpath
    model%dlname = os_get_dlname (libpath // "/" // libname, os_data)
  end if
else
  model%dlname = ""
end if
if (model%dlname /= "") then
  if (.not. dlaccess_is_open (model%dlaccess)) then
    if (logging) &
      call msg_message ("Loading model auxiliary library '" &
        // char (libpath) // "/" // char (model%dlname) // "'")
    call dlaccess_init (model%dlaccess, os_data%whizard_models_libpath, &
      model%dlname, os_data)
    if (dlaccess_has_error (model%dlaccess)) then
      call msg_message (char (dlaccess_get_error (model%dlaccess)))
      call msg_fatal ("Loading model auxiliary library '" &
        // char (model%dlname) // "' failed")
      return
    end if
    c_fptr = dlaccess_get_c_funptr (model%dlaccess, &
      var_str ("init_external_parameters"))
    if (dlaccess_has_error (model%dlaccess)) then
      call msg_message (char (dlaccess_get_error (model%dlaccess)))
      call msg_fatal ("Loading function from auxiliary library '" &
        // char (model%dlname) // "' failed")
      return
    end if
    call c_f_procpointer (c_fptr, model% init_external_parameters)
  end if
end if
end subroutine model_init

```

For a model instance, we do not attempt to load a DL library. This is the core of the full initializer above.


```

<Models: model: TBP>+≡
  procedure, private :: basic_init => model_basic_init

<Models: sub interfaces>+≡
  module subroutine model_basic_init (model, name, n_par, n_prt, n_vtx)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    integer, intent(in) :: n_par, n_prt, n_vtx
  end subroutine model_basic_init

<Models: procedures>+≡
  module subroutine model_basic_init (model, name, n_par, n_prt, n_vtx)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    integer, intent(in) :: n_par, n_prt, n_vtx
    allocate (model%par (n_par))
    call model%model_data_t%init (name, n_par, 0, n_prt, n_vtx)
  end subroutine model_basic_init

```

Finalization: The variable list contains allocated pointers, also the parse tree. We also close the DL access object, if any, that enables external parameter calculation.

```

<Models: model: TBP>+≡
  procedure :: final => model_final

<Models: sub interfaces>+≡
  module subroutine model_final (model)
    class(model_t), intent(inout) :: model
  end subroutine model_final

<Models: procedures>+≡
  module subroutine model_final (model)
    class(model_t), intent(inout) :: model
    integer :: i
    if (allocated (model%par)) then
      do i = 1, size (model%par)
        call model%par(i)%final ()
      end do
    end if
    call model%var_list%final (follow_link=.false.)
    if (model%dlname /= "") call dlaccess_final (model%dlaccess)
    call parse_tree_final (model%parse_tree)
    call model%model_data_t%final ()
  end subroutine model_final

```

Output. By default, the output is in the form of an input file. If `verbose` is true, for each derived parameter the definition (eval tree) is displayed, and the vertex hash table is shown.

```

<Models: model: TBP>+≡
  procedure :: write => model_write

<Models: sub interfaces>+≡
  module subroutine model_write (model, unit, verbose, &
    show_md5sum, show_variables, show_parameters, &
    show_particles, show_vertices, show_scheme)

```

```

class(model_t), intent(in) :: model
integer, intent(in), optional :: unit
logical, intent(in), optional :: verbose
logical, intent(in), optional :: show_md5sum
logical, intent(in), optional :: show_variables
logical, intent(in), optional :: show_parameters
logical, intent(in), optional :: show_particles
logical, intent(in), optional :: show_vertices
logical, intent(in), optional :: show_scheme
end subroutine model_write

```

(Models: procedures)+≡

```

module subroutine model_write (model, unit, verbose, &
    show_md5sum, show_variables, show_parameters, &
    show_particles, show_vertices, show_scheme)
class(model_t), intent(in) :: model
integer, intent(in), optional :: unit
logical, intent(in), optional :: verbose
logical, intent(in), optional :: show_md5sum
logical, intent(in), optional :: show_variables
logical, intent(in), optional :: show_parameters
logical, intent(in), optional :: show_particles
logical, intent(in), optional :: show_vertices
logical, intent(in), optional :: show_scheme
logical :: verb, show_md5, show_par, show_var
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
verb = .false.; if (present (verbose)) verb = verbose
show_md5 = .true.; if (present (show_md5sum)) &
    show_md5 = show_md5sum
show_par = .true.; if (present (show_parameters)) &
    show_par = show_parameters
show_var = verb; if (present (show_variables)) &
    show_var = show_variables
write (u, "(A,A,A)") 'model ', char (model%get_name ()), ' '
if (show_md5 .and. model%md5sum /= "") &
    write (u, "(1x,A,A,A)") "! md5sum = '", model%md5sum, "' "
if (model%is_ufo_model ()) then
    write (u, "(1x,A)") "! model derived from UFO source"
else if (model%has_schemes ()) then
    write (u, "(1x,A)", advance="no") "! schemes ="
    do i = 1, size (model%schemes)
        if (i > 1) write (u, "(",',')", advance="no")
        write (u, "(1x,A,A,A)", advance="no") &
            "'", char (model%schemes(i)), "' "
    end do
    write (u, *)
    if (allocated (model%selected_scheme)) then
        write (u, "(1x,A,A,A,I0,A)") &
            "! selected scheme = '", char (model%get_scheme ()), &
            "' (" , model%get_scheme_num (), ")"
    end if
end if
if (show_par) then
    write (u, "(A)")

```

```

        do i = 1, size (model%par)
            call model%par(i)%write (u, write_defs=verbose)
        end do
    end if
    call model%model_data_t%write (unit, verbose, &
        show_md5sum, show_variables, &
        show_parameters=.false., &
        show_particles=show_particles, &
        show_vertices=show_vertices, &
        show_scheme=show_scheme)
    if (show_var) then
        write (u, "(A)")
        call model%var_list%write (unit, follow_link=.false.)
    end if
end subroutine model_write

```

Screen output, condensed form.

```

<Models: model: TBP>+≡
    procedure :: show => model_show

<Models: sub interfaces>+≡
    module subroutine model_show (model, unit)
        class(model_t), intent(in) :: model
        integer, intent(in), optional :: unit
    end subroutine model_show

<Models: procedures>+≡
    module subroutine model_show (model, unit)
        class(model_t), intent(in) :: model
        integer, intent(in), optional :: unit
        integer :: i, u, l
        u = given_output_unit (unit)
        write (u, "(A,1x,A)") "Model:", char (model%get_name ())
        if (model%has_schemes ()) then
            write (u, "(2x,A,A,A,I0,A)") "Scheme: '", &
                char (model%get_scheme ()), "' (" , model%get_scheme_num (), ")"
        end if
        l = model%max_field_name_length
        call model%show_fields (l, u)
        l = model%max_par_name_length
        if (any (model%par%type == PAR_INDEPENDENT)) then
            write (u, "(2x,A)") "Independent parameters:"
            do i = 1, size (model%par)
                call model%par(i)%show (l, u, PAR_INDEPENDENT)
            end do
        end if
        if (any (model%par%type == PAR_DERIVED)) then
            write (u, "(2x,A)") "Derived parameters:"
            do i = 1, size (model%par)
                call model%par(i)%show (l, u, PAR_DERIVED)
            end do
        end if
        if (any (model%par%type == PAR_EXTERNAL)) then
            write (u, "(2x,A)") "External parameters:"
            do i = 1, size (model%par)

```

```

        call model%par(i)%show (1, u, PAR_EXTERNAL)
    end do
end if
if (any (model%par%type == PAR_UNUSED)) then
    write (u, "(2x,A)") "Unused parameters:"
    do i = 1, size (model%par)
        call model%par(i)%show (1, u, PAR_UNUSED)
    end do
end if
end if
end subroutine model_show

```

Show all fields/particles.

<Models: model: TBP>+≡

```

    procedure :: show_fields => model_show_fields

```

<Models: sub interfaces>+≡

```

    module subroutine model_show_fields (model, l, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in) :: l
        integer, intent(in), optional :: unit
    end subroutine model_show_fields

```

<Models: procedures>+≡

```

    module subroutine model_show_fields (model, l, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in) :: l
        integer, intent(in), optional :: unit
        type(field_data_t), pointer :: field
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(2x,A)") "Particles:"
        do i = 1, model%get_n_field ()
            field => model%get_field_ptr_by_index (i)
            call field%show (1, u)
        end do
    end subroutine model_show_fields

```

Show the list of stable, unstable, polarized, or unpolarized particles, respectively.

<Models: model: TBP>+≡

```

    procedure :: show_stable => model_show_stable
    procedure :: show_unstable => model_show_unstable
    procedure :: show_polarized => model_show_polarized
    procedure :: show_unpolarized => model_show_unpolarized

```

<Models: sub interfaces>+≡

```

    module subroutine model_show_stable (model, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in), optional :: unit
    end subroutine model_show_stable
    module subroutine model_show_unstable (model, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in), optional :: unit
    end subroutine model_show_unstable
    module subroutine model_show_polarized (model, unit)

```

```

        class(model_t), intent(in), target :: model
        integer, intent(in), optional :: unit
    end subroutine model_show_polarized
module subroutine model_show_unpolarized (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
end subroutine model_show_unpolarized

<Models: procedures>+≡
module subroutine model_show_stable (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: field
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(A,1x)", advance="no") "Stable particles:"
    do i = 1, model%get_n_field ()
        field => model%get_field_ptr_by_index (i)
        if (field%is_stable (.false.)) then
            write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
        end if
        if (field%has_antiparticle ()) then
            if (field%is_stable (.true.)) then
                write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
            end if
        end if
    end do
    write (u, *)
end subroutine model_show_stable

module subroutine model_show_unstable (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: field
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(A,1x)", advance="no") "Unstable particles:"
    do i = 1, model%get_n_field ()
        field => model%get_field_ptr_by_index (i)
        if (.not. field%is_stable (.false.)) then
            write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
        end if
        if (field%has_antiparticle ()) then
            if (.not. field%is_stable (.true.)) then
                write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
            end if
        end if
    end do
    write (u, *)
end subroutine model_show_unstable

module subroutine model_show_polarized (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: field

```

```

integer :: u, i
u = given_output_unit (unit)
write (u, "(A,1x)", advance="no") "Polarized particles:"
do i = 1, model%get_n_field ()
  field => model%get_field_ptr_by_index (i)
  if (field%is_polarized (.false.)) then
    write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
  end if
  if (field%has_antiparticle ()) then
    if (field%is_polarized (.true.)) then
      write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
    end if
  end if
end do
write (u, *)
end subroutine model_show_polarized

module subroutine model_show_unpolarized (model, unit)
  class(model_t), intent(in), target :: model
  integer, intent(in), optional :: unit
  type(field_data_t), pointer :: field
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(A,1x)", advance="no") "Unpolarized particles:"
  do i = 1, model%get_n_field ()
    field => model%get_field_ptr_by_index (i)
    if (.not. field%is_polarized (.false.)) then
      write (u, "(1x,A)", advance="no") &
        char (field%get_name (.false.))
    end if
    if (field%has_antiparticle ()) then
      if (.not. field%is_polarized (.true.)) then
        write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
      end if
    end if
  end do
  write (u, *)
end subroutine model_show_unpolarized

```

Retrieve the MD5 sum of a model (actually, of the model file).

<Models: model: TBP>+≡

```
procedure :: get_md5sum => model_get_md5sum
```

<Models: sub interfaces>+≡

```

module function model_get_md5sum (model) result (md5sum)
  character(32) :: md5sum
  class(model_t), intent(in) :: model
end function model_get_md5sum

```

<Models: procedures>+≡

```

module function model_get_md5sum (model) result (md5sum)
  character(32) :: md5sum
  class(model_t), intent(in) :: model
  md5sum = model%md5sum
end function model_get_md5sum

```

Parameters are defined by an expression which may be constant or arbitrary.

(Models: model: TBP)+≡

```

procedure :: &
    set_parameter_constant => model_set_parameter_constant
procedure, private :: &
    set_parameter_parse_node => model_set_parameter_parse_node
procedure :: &
    set_parameter_external => model_set_parameter_external
procedure :: &
    set_parameter_unused => model_set_parameter_unused

```

(Models: sub interfaces)+≡

```

module subroutine model_set_parameter_constant (model, i, name, value)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
end subroutine model_set_parameter_constant
module subroutine model_set_parameter_parse_node &
    (model, i, name, pn, constant)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn
    logical, intent(in) :: constant
end subroutine model_set_parameter_parse_node
module subroutine model_set_parameter_external (model, i, name)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
end subroutine model_set_parameter_external
module subroutine model_set_parameter_unused (model, i, name)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
end subroutine model_set_parameter_unused

```

(Models: procedures)+≡

```

module subroutine model_set_parameter_constant (model, i, name, value)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    logical, save, target :: known = .true.
    class(modelpar_data_t), pointer :: par_data
    real(default), pointer :: value_ptr
    par_data => model%get_par_real_ptr (i)
    call model%par(i)%init_independent_value (par_data, name, value)
    value_ptr => par_data%get_real_ptr ()
    call model%var_list%append_real_ptr (name, value_ptr, &
        is_known=known, intrinsic=.true.)
    model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_constant

```

```

module subroutine model_set_parameter_parse_node &
  (model, i, name, pn, constant)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(string_t), intent(in) :: name
  type(parse_node_t), intent(in), target :: pn
  logical, intent(in) :: constant
  logical, save, target :: known = .true.
  class(modelpar_data_t), pointer :: par_data
  real(default), pointer :: value_ptr
  par_data => model%get_par_real_ptr (i)
  if (constant) then
    call model%par(i)%init_independent (par_data, name, pn)
  else
    call model%par(i)%init_derived (par_data, name, pn, model%var_list)
  end if
  value_ptr => par_data%get_real_ptr ()
  call model%var_list%append_real_ptr (name, value_ptr, &
    is_known=known, locked=.not.constant, intrinsic=.true.)
  model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_parse_node

module subroutine model_set_parameter_external (model, i, name)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(string_t), intent(in) :: name
  logical, save, target :: known = .true.
  class(modelpar_data_t), pointer :: par_data
  real(default), pointer :: value_ptr
  par_data => model%get_par_real_ptr (i)
  call model%par(i)%init_external (par_data, name)
  value_ptr => par_data%get_real_ptr ()
  call model%var_list%append_real_ptr (name, value_ptr, &
    is_known=known, locked=.true., intrinsic=.true.)
  model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_external

module subroutine model_set_parameter_unused (model, i, name)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(string_t), intent(in) :: name
  class(modelpar_data_t), pointer :: par_data
  par_data => model%get_par_real_ptr (i)
  call model%par(i)%init_unused (par_data, name)
  call model%var_list%append_real (name, locked=.true., intrinsic=.true.)
  model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_unused

```

Make a copy of a parameter. We assume that the `model_data_t` parameter arrays have already been copied, so names and values are available in the current model, and can be used as targets. The eval tree should not be copied, since it should refer to the new variable list. The safe solution is to make use of the above initializers, which also take care of the building a new variable list.


```

<Models: model: TBP>+≡
  procedure, private :: copy_parameter => model_copy_parameter

<Models: sub interfaces>+≡
  module subroutine model_copy_parameter (model, i, par)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(parameter_t), intent(in) :: par
  end subroutine model_copy_parameter

<Models: procedures>+≡
  module subroutine model_copy_parameter (model, i, par)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(parameter_t), intent(in) :: par
    type(string_t) :: name
    real(default) :: value
    name = par%data%get_name ()
    select case (par%type)
    case (PAR_INDEPENDENT)
      if (associated (par%pn)) then
        call model%set_parameter_parse_node (i, name, par%pn, &
          constant = .true.)
      else
        value = par%data%get_real ()
        call model%set_parameter_constant (i, name, value)
      end if
      if (allocated (par%block_index)) then
        model%par(i)%block_name = par%block_name
        model%par(i)%block_index = par%block_index
      end if
    case (PAR_DERIVED)
      call model%set_parameter_parse_node (i, name, par%pn, &
        constant = .false.)
    case (PAR_EXTERNAL)
      call model%set_parameter_external (i, name)
    case (PAR_UNUSED)
      call model%set_parameter_unused (i, name)
    end select
  end subroutine model_copy_parameter

```

Recalculate all derived parameters.

```

<Models: model: TBP>+≡
  procedure :: update_parameters => model_parameters_update

<Models: sub interfaces>+≡
  module subroutine model_parameters_update (model)
    class(model_t), intent(inout) :: model
  end subroutine model_parameters_update

<Models: procedures>+≡
  module subroutine model_parameters_update (model)
    class(model_t), intent(inout) :: model
    integer :: i
    real(default), dimension(:), allocatable :: par
    do i = 1, size (model%par)

```

```

        call model%par(i)%reset_derived ()
    end do
    if (associated (model%init_external_parameters)) then
        allocate (par (model%get_n_real ()))
        call model%real_parameters_to_c_array (par)
        call model%init_external_parameters (par)
        call model%real_parameters_from_c_array (par)
        if (model%get_name() == var_str ("SM_tt_threshold")) &
            call set_threshold_parameters ()
    end if
contains
    subroutine set_threshold_parameters ()
        real(default) :: mpole, wtop
        !!! !!! !!! Workaround for OS-X and BSD which do not load
        !!! !!! !!! the global values created previously. Therefore
        !!! !!! !!! a second initialization for the threshold model,
        !!! !!! !!! where M1S is required to compute the top mass.
        call init_parameters (mpole, wtop, &
            par(20), par(21), par(22), &
            par(19), par(39), par(4), par(1), &
            par(2), par(10), par(24), par(25), &
            par(23), par(26), par(27), par(29), &
            par(30), par(31), par(32), par(33), &
            par(36) > 0._default, par(28))
    end subroutine set_threshold_parameters
end subroutine model_parameters_update

```

Initialize field data with PDG long name and PDG code.

```

<Models: model: TBP>+≡
    procedure, private :: init_field => model_init_field

<Models: sub interfaces>+≡
    module subroutine model_init_field (model, i, longname, pdg)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: longname
        integer, intent(in) :: pdg
    end subroutine model_init_field

<Models: procedures>+≡
    module subroutine model_init_field (model, i, longname, pdg)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: longname
        integer, intent(in) :: pdg
        type(field_data_t), pointer :: field
        field => model%get_field_ptr_by_index (i)
        call field%init (longname, pdg)
    end subroutine model_init_field

```

Copy field data for index i from another particle which serves as a template.
The name should be the unique long name.

```

<Models: model: TBP>+≡
    procedure, private :: copy_field => model_copy_field

```

```

<Models: sub interfaces>+≡
    module subroutine model_copy_field (model, i, name_src)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: name_src
    end subroutine model_copy_field

```

```

<Models: procedures>+≡
    module subroutine model_copy_field (model, i, name_src)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: name_src
        type(field_data_t), pointer :: field_src, field
        field_src => model%get_field_ptr (name_src)
        field => model%get_field_ptr_by_index (i)
        call field%copy_from (field_src)
    end subroutine model_copy_field

```

28.4.5 Model Access via Variables

Write the model variable list.

```

<Models: model: TBP>+≡
    procedure :: write_var_list => model_write_var_list

<Models: sub interfaces>+≡
    module subroutine model_write_var_list (model, unit, follow_link)
        class(model_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: follow_link
    end subroutine model_write_var_list

<Models: procedures>+≡
    module subroutine model_write_var_list (model, unit, follow_link)
        class(model_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: follow_link
        call model%var_list%write (unit, follow_link)
    end subroutine model_write_var_list

```

Link a variable list to the model variables.

```

<Models: model: TBP>+≡
    procedure :: link_var_list => model_link_var_list

<Models: sub interfaces>+≡
    module subroutine model_link_var_list (model, var_list)
        class(model_t), intent(inout) :: model
        type(var_list_t), intent(in), target :: var_list
    end subroutine model_link_var_list

<Models: procedures>+≡
    module subroutine model_link_var_list (model, var_list)
        class(model_t), intent(inout) :: model
        type(var_list_t), intent(in), target :: var_list
        call model%var_list%link (var_list)
    end subroutine model_link_var_list

```

```
end subroutine model_link_var_list
```

Check if the model contains a named variable.

```
<Models: model: TBP>+≡
  procedure :: var_exists => model_var_exists

<Models: sub interfaces>+≡
  module function model_var_exists (model, name) result (flag)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    logical :: flag
  end function model_var_exists

<Models: procedures>+≡
  module function model_var_exists (model, name) result (flag)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    logical :: flag
    flag = model%var_list%contains (name, follow_link=.false.)
  end function model_var_exists
```

Check if the model variable is a derived parameter, i.e., locked.

```
<Models: model: TBP>+≡
  procedure :: var_is_locked => model_var_is_locked

<Models: sub interfaces>+≡
  module function model_var_is_locked (model, name) result (flag)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    logical :: flag
  end function model_var_is_locked

<Models: procedures>+≡
  module function model_var_is_locked (model, name) result (flag)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    logical :: flag
    flag = model%var_list%is_locked (name, follow_link=.false.)
  end function model_var_is_locked
```

Set a model parameter via the named variable. We assume that the variable exists and is writable, i.e., non-locked. We update the model and variable list, so independent and derived parameters are always synchronized.

```
<Models: model: TBP>+≡
  procedure :: set_real => model_var_set_real

<Models: sub interfaces>+≡
  module subroutine model_var_set_real (model, name, rval, verbose, pacified)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    real(default), intent(in) :: rval
    logical, intent(in), optional :: verbose, pacified
  end subroutine model_var_set_real
```

```

<Models: procedures>+≡
  module subroutine model_var_set_real (model, name, rval, verbose, pacified)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    real(default), intent(in) :: rval
    logical, intent(in), optional :: verbose, pacified
    call model%var_list%set_real (name, rval, &
      is_known=.true., ignore=.false., &
      verbose=verbose, model_name=model%get_name (), pacified=pacified)
    call model%update_parameters ()
  end subroutine model_var_set_real

```

Retrieve a model parameter value.

```

<Models: model: TBP>+≡
  procedure :: get_rval => model_var_get_rval

<Models: sub interfaces>+≡
  module function model_var_get_rval (model, name) result (rval)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    real(default) :: rval
  end function model_var_get_rval

<Models: procedures>+≡
  module function model_var_get_rval (model, name) result (rval)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    real(default) :: rval
    rval = model%var_list%get_rval (name, follow_link=.false.)
  end function model_var_get_rval

```

[To be deleted] Return a pointer to the variable list.

```

<Models: model: TBP>+≡
  procedure :: get_var_list_ptr => model_get_var_list_ptr

<Models: sub interfaces>+≡
  module function model_get_var_list_ptr (model) result (var_list)
    type(var_list_t), pointer :: var_list
    class(model_t), intent(in), target :: model
  end function model_get_var_list_ptr

<Models: procedures>+≡
  module function model_get_var_list_ptr (model) result (var_list)
    type(var_list_t), pointer :: var_list
    class(model_t), intent(in), target :: model
    var_list => model%var_list
  end function model_get_var_list_ptr

```

28.4.6 UFO models

A single flag identifies a model as a UFO model. There is no other distinction, but the flag allows us to handle built-in and UFO models with the same name in parallel.

```

<Models: model: TBP>+≡

```

```

        procedure :: is_ufo_model => model_is_ufo_model
<Models: sub interfaces>+≡
        module function model_is_ufo_model (model) result (flag)
            class(model_t), intent(in) :: model
            logical :: flag
            end function model_is_ufo_model
<Models: procedures>+≡
        module function model_is_ufo_model (model) result (flag)
            class(model_t), intent(in) :: model
            logical :: flag
            flag = model%ufo_model
            end function model_is_ufo_model

```

Return the UFO path used for fetching the UFO source.

```

<Models: model: TBP>+≡
        procedure :: get_ufo_path => model_get_ufo_path
<Models: sub interfaces>+≡
        module function model_get_ufo_path (model) result (path)
            class(model_t), intent(in) :: model
            type(string_t) :: path
            end function model_get_ufo_path
<Models: procedures>+≡
        module function model_get_ufo_path (model) result (path)
            class(model_t), intent(in) :: model
            type(string_t) :: path
            if (model%ufo_model) then
                path = model%ufo_path
            else
                path = ""
            end if
            end function model_get_ufo_path

```

Call OMega and generate a model file from an UFO source file. We start with a file name; the model name is expected to be the base name, stripping extensions.

The path search either takes `ufo_path_requested`, or searches first in the working directory, then in a hard-coded UFO model directory.

```

<Models: procedures>+≡
        subroutine model_generate_ufo (filename, os_data, ufo_path, &
            ufo_path_requested)
            type(string_t), intent(in) :: filename
            type(os_data_t), intent(in) :: os_data
            type(string_t), intent(out) :: ufo_path
            type(string_t), intent(in), optional :: ufo_path_requested
            type(string_t) :: model_name, omega_path, ufo_dir, ufo_init
            logical :: exist
            call get_model_name (filename, model_name)
            call msg_message ("Model: Generating model '" // char (model_name) &
                // "' from UFO sources")
            if (present (ufo_path_requested)) then
                call msg_message ("Model: Searching for UFO sources in '" &
                    // char (ufo_path_requested) // "'")
            end if
        end subroutine model_generate_ufo

```

```

    ufo_path = ufo_path_requested
    ufo_dir = ufo_path_requested // "/" // model_name
    ufo_init = ufo_dir // "/" // "__init__.py"
    inquire (file = char (ufo_init), exist = exist)
else
    call msg_message ("Model: Searching for UFO sources in &
        &working directory")
    ufo_path = "."
    ufo_dir = ufo_path // "/" // model_name
    ufo_init = ufo_dir // "/" // "__init__.py"
    inquire (file = char (ufo_init), exist = exist)
    if (.not. exist) then
        ufo_path = char (os_data%whizard_modelpath_ufo)
        ufo_dir = ufo_path // "/" // model_name
        ufo_init = ufo_dir // "/" // "__init__.py"
        call msg_message ("Model: Searching for UFO sources in '" &
            // char (os_data%whizard_modelpath_ufo) // "'")
        inquire (file = char (ufo_init), exist = exist)
    end if
end if
if (exist) then
    call msg_message ("Model: Found UFO sources for model '" &
        // char (model_name) // "'")
else
    call msg_fatal ("Model: UFO sources for model '" &
        // char (model_name) // "' not found")
end if
omega_path = os_data%whizard_omega_binpath // "/omega_UFO.opt"
call os_system_call (omega_path &
    // " -model:UFO_dir " // ufo_dir &
    // " -model:exec" &
    // " -model:write_WHIZARD" &
    // " > " // filename)
inquire (file = char (filename), exist = exist)
if (exist) then
    call msg_message ("Model: Model file '" // char (filename) //&
        "' generated")
else
    call msg_fatal ("Model: Model file '" // char (filename) &
        // "' could not be generated")
end if
contains
subroutine get_model_name (filename, model_name)
    type(string_t), intent(in) :: filename
    type(string_t), intent(out) :: model_name
    type(string_t) :: string
    string = filename
    call split (string, model_name, ".")
end subroutine get_model_name
end subroutine model_generate_ufo

```

28.4.7 Scheme handling

A model can specify a set of allowed schemes that steer the setup of model variables. The model file can contain scheme-specific declarations that are selected by a `select scheme` clause. Scheme support is optional.

If enabled, the model object contains a list of allowed schemes, and the model reader takes the active scheme as an argument. After the model has been read, the scheme is fixed and can no longer be modified.

The model supports schemes if the scheme array is allocated.

```
<Models: model: TBP>+≡
    procedure :: has_schemes => model_has_schemes

<Models: sub interfaces>+≡
    module function model_has_schemes (model) result (flag)
        logical :: flag
        class(model_t), intent(in) :: model
    end function model_has_schemes

<Models: procedures>+≡
    module function model_has_schemes (model) result (flag)
        logical :: flag
        class(model_t), intent(in) :: model
        flag = allocated (model%schemes)
    end function model_has_schemes
```

Enable schemes: fix the list of allowed schemes.

```
<Models: model: TBP>+≡
    procedure :: enable_schemes => model_enable_schemes

<Models: sub interfaces>+≡
    module subroutine model_enable_schemes (model, scheme)
        class(model_t), intent(inout) :: model
        type(string_t), dimension(:), intent(in) :: scheme
    end subroutine model_enable_schemes

<Models: procedures>+≡
    module subroutine model_enable_schemes (model, scheme)
        class(model_t), intent(inout) :: model
        type(string_t), dimension(:), intent(in) :: scheme
        allocate (model%schemes (size (scheme)), source = scheme)
    end subroutine model_enable_schemes
```

Find the scheme. Check if the scheme is allowed. The numeric index of the selected scheme is stored in the `model_data_t` base object.

If no argument is given, select the first scheme. The numeric scheme ID will then be 1, while a model without schemes retains 0.

```
<Models: model: TBP>+≡
    procedure :: set_scheme => model_set_scheme

<Models: sub interfaces>+≡
    module subroutine model_set_scheme (model, scheme)
        class(model_t), intent(inout) :: model
        type(string_t), intent(in), optional :: scheme
    end subroutine model_set_scheme
```


<Models: procedures>+≡

```

module subroutine model_set_scheme (model, scheme)
  class(model_t), intent(inout) :: model
  type(string_t), intent(in), optional :: scheme
  logical :: ok
  integer :: i
  if (model%has_schemes ()) then
    if (present (scheme)) then
      ok = .false.
      CHECK_SCHEME: do i = 1, size (model%schemes)
        if (scheme == model%schemes(i)) then
          allocate (model%selected_scheme, source = scheme)
          call model%set_scheme_num (i)
          ok = .true.
          exit CHECK_SCHEME
        end if
      end do CHECK_SCHEME
      if (.not. ok) then
        call msg_fatal &
          ("Model '" // char (model%get_name ()) &
           // "': scheme '" // char (scheme) // "' not supported")
      end if
    else
      allocate (model%selected_scheme, source = model%schemes(1))
      call model%set_scheme_num (1)
    end if
  else
    if (present (scheme)) then
      call msg_error &
        ("Model '" // char (model%get_name ()) &
         // "' does not support schemes")
    end if
  end if
end subroutine model_set_scheme

```

Get the scheme. Note that the base `model_data_t` provides a `get_scheme_num` getter function.

<Models: model: TBP>+≡

```

procedure :: get_scheme => model_get_scheme

```

<Models: sub interfaces>+≡

```

module function model_get_scheme (model) result (scheme)
  class(model_t), intent(in) :: model
  type(string_t) :: scheme
end function model_get_scheme

```

<Models: procedures>+≡

```

module function model_get_scheme (model) result (scheme)
  class(model_t), intent(in) :: model
  type(string_t) :: scheme
  if (allocated (model%selected_scheme)) then
    scheme = model%selected_scheme
  else
    scheme = ""
  end if
end function

```

```
end function model_get_scheme
```

Check if a model has been set up with a specific name and (if applicable) scheme. This helps in determining whether we need a new model object.

A UFO model is considered to be distinct from a non-UFO model. We assume that if `ufo` is asked for, there is no scheme argument. Furthermore, if there is an `ufo_path` requested, it must coincide with the `ufo_path` of the model. If not, the model `ufo_path` is not checked.

```
<Models: model: TBP>+≡
```

```
procedure :: matches => model_matches
```

```
<Models: sub interfaces>+≡
```

```
module function model_matches &
  (model, name, scheme, ufo, ufo_path) result (flag)
  logical :: flag
  class(model_t), intent(in) :: model
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: scheme
  logical, intent(in), optional :: ufo
  type(string_t), intent(in), optional :: ufo_path
end function model_matches
```

```
<Models: procedures>+≡
```

```
module function model_matches &
  (model, name, scheme, ufo, ufo_path) result (flag)
  logical :: flag
  class(model_t), intent(in) :: model
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: scheme
  logical, intent(in), optional :: ufo
  type(string_t), intent(in), optional :: ufo_path
  logical :: ufo_model
  ufo_model = .false.; if (present (ufo)) ufo_model = ufo
  if (name /= model%get_name ()) then
    flag = .false.
  else if (ufo_model .neqv. model%is_ufo_model ()) then
    flag = .false.
  else if (ufo_model) then
    if (present (ufo_path)) then
      flag = model%get_ufo_path () == ufo_path
    else
      flag = .true.
    end if
  else if (model%has_schemes ()) then
    if (present (scheme)) then
      flag = model%get_scheme () == scheme
    else
      flag = model%get_scheme_num () == 1
    end if
  else if (present (scheme)) then
    flag = .false.
  else
    flag = .true.
  end if
```

```
end function model_matches
```

28.4.8 SLHA-type interface

Abusing the original strict SUSY Les Houches Accord (SLHA), we support reading parameter data from some custom SLHA-type input file. To this end, the `model` object stores a list of model-specific block names together with information how to find a parameter in the model record, given a block name and index vector.

Check if the model supports custom SLHA block info. This is the case if `n_slha_block` is nonzero, i.e., after SLHA block names have been parsed and registered.

```
<Models: model: TBP>+≡
  procedure :: supports_custom_slha => model_supports_custom_slha

<Models: sub interfaces>+≡
  module function model_supports_custom_slha (model) result (flag)
    class(model_t), intent(in) :: model
    logical :: flag
  end function model_supports_custom_slha

<Models: procedures>+≡
  module function model_supports_custom_slha (model) result (flag)
    class(model_t), intent(in) :: model
    logical :: flag

    flag = model%n_slha_block > 0

  end function model_supports_custom_slha
```

Return the block names for all SLHA block references.

```
<Models: model: TBP>+≡
  procedure :: get_custom_slha_blocks => model_get_custom_slha_blocks

<Models: sub interfaces>+≡
  module subroutine model_get_custom_slha_blocks (model, block_name)
    class(model_t), intent(in) :: model
    type(string_t), dimension(:), allocatable :: block_name
  end subroutine model_get_custom_slha_blocks

<Models: procedures>+≡
  module subroutine model_get_custom_slha_blocks (model, block_name)
    class(model_t), intent(in) :: model
    type(string_t), dimension(:), allocatable :: block_name

    integer :: i

    allocate (block_name (model%n_slha_block))
    do i = 1, size (block_name)
      block_name(i) = model%slha_block(i)%name
    end do

  end subroutine model_get_custom_slha_blocks
```

This routine registers a SLHA block reference. We have the index of a (new) parameter entry and a parse node from the model file which specifies a block name and an index array.

(Models: procedures)+≡

```

subroutine model_record_slha_block_entry (model, i_par, node)
  class(model_t), intent(inout) :: model
  integer, intent(in) :: i_par
  type(parse_node_t), intent(in), target :: node

  type(parse_node_t), pointer :: node_block_name, node_index
  type(string_t) :: block_name
  integer :: n_index, i, i_block
  integer, dimension(:), allocatable :: block_index

  node_block_name => node%get_sub_ptr (2)
  select case (char (node_block_name%get_rule_key ()))
  case ("block_name")
    block_name = node_block_name%get_string ()
  case ("QNUMBERS")
    block_name = "QNUMBERS"
  case default
    block_name = node_block_name%get_string ()
  end select
  n_index = node%get_n_sub () - 2
  allocate (block_index (n_index))
  node_index => node_block_name%get_next_ptr ()
  do i = 1, n_index
    block_index(i) = node_index%get_integer ()
    node_index => node_index%get_next_ptr ()
  end do
  i_block = 0
  FIND_BLOCK: do i = 1, model%n_slha_block
    if (model%slha_block(i)%name == block_name) then
      i_block = i
      exit FIND_BLOCK
    end if
  end do FIND_BLOCK
  if (i_block == 0) then
    call model_add_slha_block (model, block_name)
    i_block = model%n_slha_block
  end if
  associate (b => model%slha_block(i_block))
    call add_slha_block_entry (b, block_index, i_par)
  end associate
  model%par(i_par)%block_name = block_name
  model%par(i_par)%block_index = block_index
end subroutine model_record_slha_block_entry

```

Add a new entry to the SLHA block register, increasing the array size if necessary

(Models: procedures)+≡

```

subroutine model_add_slha_block (model, block_name)
  class(model_t), intent(inout) :: model
  type(string_t), intent(in) :: block_name

```

```

if (.not. allocated (model%slha_block)) allocate (model%slha_block (1))
if (model%n_slha_block == size (model%slha_block)) call grow
model%n_slha_block = model%n_slha_block + 1
associate (b => model%slha_block(model%n_slha_block))
    b%name = block_name
    allocate (b%entry (1))
end associate

contains

subroutine grow
    type(slha_block_t), dimension(:), allocatable :: b_tmp
    call move_alloc (model%slha_block, b_tmp)
    allocate (model%slha_block (2 * size (b_tmp)))
    model%slha_block(:size (b_tmp)) = b_tmp(:)
end subroutine grow

end subroutine model_add_slha_block

```

Add a new entry to a block-register record. The entry establishes a pointer-target relation between an index array within the SLHA block and a parameter-data record. We increase the entry array as needed.

(Models: procedures)+≡

```

subroutine add_slha_block_entry (b, block_index, i_par)
    type(slha_block_t), intent(inout) :: b
    integer, dimension(:), intent(in) :: block_index
    integer, intent(in) :: i_par

    if (b%n_entry == size (b%entry)) call grow
    b%n_entry = b%n_entry + 1
    associate (entry => b%entry(b%n_entry))
        entry%block_index = block_index
        entry%i_par = i_par
    end associate

contains

subroutine grow
    type(slha_entry_t), dimension(:), allocatable :: entry_tmp
    call move_alloc (b%entry, entry_tmp)
    allocate (b%entry (2 * size (entry_tmp)))
    b%entry(:size (entry_tmp)) = entry_tmp(:)
end subroutine grow

end subroutine add_slha_block_entry

```

The lookup routine returns a pointer to the appropriate `par_data` record, if `block_name` and `block_index` are valid. The latter point to the `slha_block_t` register within the `model_t` object, if it is allocated.

This should only be needed during I/O (i.e., while reading the SLHA file), so a simple linear search for each parameter should not be a performance problem.

(Models: model: TBP)+≡

```

    procedure :: slha_lookup => model_slha_lookup
<Models: sub interfaces>+≡
    module subroutine model_slha_lookup &
        (model, block_name, block_index, par_data)
        class(model_t), intent(in) :: model
        type(string_t), intent(in) :: block_name
        integer, dimension(:), intent(in) :: block_index
        class(modelpar_data_t), pointer, intent(out) :: par_data
    end subroutine model_slha_lookup

<Models: procedures>+≡
    module subroutine model_slha_lookup &
        (model, block_name, block_index, par_data)
        class(model_t), intent(in) :: model
        type(string_t), intent(in) :: block_name
        integer, dimension(:), intent(in) :: block_index
        class(modelpar_data_t), pointer, intent(out) :: par_data

    integer :: i, j

    par_data => null ()
    if (allocated (model%slha_block)) then
        do i = 1, model%n_slha_block
            associate (block => model%slha_block(i))
                if (block%name == block_name) then
                    do j = 1, block%n_entry
                        associate (entry => block%entry(j))
                            if (size (entry%block_index) == size (block_index)) then
                                if (all (entry%block_index == block_index)) then
                                    par_data => model%par(entry%i_par)%data
                                    return
                                end if
                            end if
                        end associate
                    end do
                end if
            end associate
        end do
    end if

    end subroutine model_slha_lookup

```

Modify the value of a parameter, identified by block name and index array.

```

<Models: model: TBP>+≡
    procedure :: slha_set_par => model_slha_set_par

<Models: sub interfaces>+≡
    module subroutine model_slha_set_par (model, block_name, block_index, value)
        class(model_t), intent(inout) :: model
        type(string_t), intent(in) :: block_name
        integer, dimension(:), intent(in) :: block_index
        real(default), intent(in) :: value
    end subroutine model_slha_set_par

```

```

<Models: procedures>+≡
module subroutine model_slha_set_par (model, block_name, block_index, value)
  class(model_t), intent(inout) :: model
  type(string_t), intent(in) :: block_name
  integer, dimension(:), intent(in) :: block_index
  real(default), intent(in) :: value

  class(modelpar_data_t), pointer :: par_data

  call model%slha_lookup (block_name, block_index, par_data)
  if (associated (par_data)) then
    par_data = value
  end if

end subroutine model_slha_set_par

```

28.4.9 Reading models from file

This procedure defines the model-file syntax for the parser, returning an internal file (ifile).

Note that arithmetic operators are defined as keywords in the expression syntax, so we exclude them here.

```

<Models: procedures>+≡
subroutine define_model_file_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ model_def = model_name_def " // &
    "scheme_header parameters external_pars particles vertices")
  call ifile_append (ifile, "SEQ model_name_def = model model_name")
  call ifile_append (ifile, "KEY model")
  call ifile_append (ifile, "QUO model_name = '...'"")
  call ifile_append (ifile, "SEQ scheme_header = scheme_decl?")
  call ifile_append (ifile, "SEQ scheme_decl = schemes '=' scheme_list")
  call ifile_append (ifile, "KEY schemes")
  call ifile_append (ifile, "LIS scheme_list = scheme_name+")
  call ifile_append (ifile, "QUO scheme_name = '...'"")
  call ifile_append (ifile, "SEQ parameters = generic_par_def*")
  call ifile_append (ifile, "ALT generic_par_def = &
    &parameter_def | derived_def | unused_def | scheme_block")
  call ifile_append (ifile, "SEQ parameter_def = parameter par_name " // &
    "'=' any_real_value slha_annotation?")
  call ifile_append (ifile, "ALT any_real_value = " &
    // "neg_real_value | pos_real_value | real_value")
  call ifile_append (ifile, "SEQ neg_real_value = '-' real_value")
  call ifile_append (ifile, "SEQ pos_real_value = '+' real_value")
  call ifile_append (ifile, "KEY parameter")
  call ifile_append (ifile, "IDE par_name")
  ! call ifile_append (ifile, "KEY '='")          !!! Key already exists
  call ifile_append (ifile, "SEQ slha_annotation = " // &
    "slha_entry slha_block_name slha_entry_index*")
  call ifile_append (ifile, "KEY slha_entry")
  call ifile_append (ifile, "IDE slha_block_name")
  call ifile_append (ifile, "INT slha_entry_index")

```

```

call ifile_append (ifile, "SEQ derived_def = derived par_name " // &
"=' expr")
call ifile_append (ifile, "KEY derived")
call ifile_append (ifile, "SEQ unused_def = unused par_name")
call ifile_append (ifile, "KEY unused")
call ifile_append (ifile, "SEQ external_pars = external_def*")
call ifile_append (ifile, "SEQ external_def = external par_name")
call ifile_append (ifile, "KEY external")
call ifile_append (ifile, "SEQ scheme_block = &
&scheme_block_beg scheme_block_body scheme_block_end")
call ifile_append (ifile, "SEQ scheme_block_beg = select scheme")
call ifile_append (ifile, "SEQ scheme_block_body = scheme_block_case*")
call ifile_append (ifile, "SEQ scheme_block_case = &
&scheme scheme_id parameters")
call ifile_append (ifile, "ALT scheme_id = scheme_list | other")
call ifile_append (ifile, "SEQ scheme_block_end = end select")
call ifile_append (ifile, "KEY select")
call ifile_append (ifile, "KEY scheme")
call ifile_append (ifile, "KEY other")
call ifile_append (ifile, "KEY end")
call ifile_append (ifile, "SEQ particles = particle_def*")
call ifile_append (ifile, "SEQ particle_def = particle name_def " // &
"prt_pdg prt_details")
call ifile_append (ifile, "KEY particle")
call ifile_append (ifile, "SEQ prt_pdg = signed_int")
call ifile_append (ifile, "ALT prt_details = prt_src | prt_properties")
call ifile_append (ifile, "SEQ prt_src = like name_def prt_properties")
call ifile_append (ifile, "KEY like")
call ifile_append (ifile, "SEQ prt_properties = prt_property*")
call ifile_append (ifile, "ALT prt_property = " // &
"parton | invisible | gauge | left | right | " // &
"prt_name | prt_anti | prt_tex_name | prt_tex_anti | " // &
"prt_spin | prt_isospin | prt_charge | " // &
"prt_color | prt_mass | prt_width")
call ifile_append (ifile, "KEY parton")
call ifile_append (ifile, "KEY invisible")
call ifile_append (ifile, "KEY gauge")
call ifile_append (ifile, "KEY left")
call ifile_append (ifile, "KEY right")
call ifile_append (ifile, "SEQ prt_name = name name_def+")
call ifile_append (ifile, "SEQ prt_anti = anti name_def+")
call ifile_append (ifile, "SEQ prt_tex_name = tex_name name_def")
call ifile_append (ifile, "SEQ prt_tex_anti = tex_anti name_def")
call ifile_append (ifile, "KEY name")
call ifile_append (ifile, "KEY anti")
call ifile_append (ifile, "KEY tex_name")
call ifile_append (ifile, "KEY tex_anti")
call ifile_append (ifile, "ALT name_def = name_string | name_id")
call ifile_append (ifile, "QUO name_string = '...'"")
call ifile_append (ifile, "IDE name_id")
call ifile_append (ifile, "SEQ prt_spin = spin frac")
call ifile_append (ifile, "KEY spin")
call ifile_append (ifile, "SEQ prt_isospin = isospin frac")
call ifile_append (ifile, "KEY isospin")

```



```

call ifile_append (ifile, "SEQ prt_charge = charge frac")
call ifile_append (ifile, "KEY charge")
call ifile_append (ifile, "SEQ prt_color = color integer_literal")
call ifile_append (ifile, "KEY color")
call ifile_append (ifile, "SEQ prt_mass = mass par_name")
call ifile_append (ifile, "KEY mass")
call ifile_append (ifile, "SEQ prt_width = width par_name")
call ifile_append (ifile, "KEY width")
call ifile_append (ifile, "SEQ vertices = vertex_def*")
call ifile_append (ifile, "SEQ vertex_def = vertex name_def+")
call ifile_append (ifile, "KEY vertex")
call define_expr_syntax (ifile, particles=.false., analysis=.false.)
end subroutine define_model_file_syntax

```

The model-file syntax and lexer are fixed, therefore stored as module variables:

```

<Models: variables>≡
  type(syntax_t), target, save :: syntax_model_file

<Models: public>+≡
  public :: syntax_model_file_init

<Models: sub interfaces>+≡
  module subroutine syntax_model_file_init ()
  end subroutine syntax_model_file_init

<Models: procedures>+≡
  module subroutine syntax_model_file_init ()
    type(ifile_t) :: ifile
    call define_model_file_syntax (ifile)
    call syntax_init (syntax_model_file, ifile)
    call ifile_final (ifile)
  end subroutine syntax_model_file_init

<Models: procedures>+≡
  subroutine lexer_init_model_file (lexer)
    type(lexer_t), intent(out) :: lexer
    call lexer_init (lexer, &
      comment_chars = "#!", &
      quote_chars = '"{', &
      quote_match = '"}', &
      single_chars = ":(,)", &
      special_class = [ "+-*/^", "<=> " ], &
      keyword_list = syntax_get_keyword_list_ptr (syntax_model_file))
  end subroutine lexer_init_model_file

<Models: public>+≡
  public :: syntax_model_file_final

<Models: sub interfaces>+≡
  module subroutine syntax_model_file_final ()
  end subroutine syntax_model_file_final

<Models: procedures>+≡
  module subroutine syntax_model_file_final ()
    call syntax_final (syntax_model_file)
  end subroutine syntax_model_file_final

```

```

end subroutine syntax_model_file_final

<Models: public>+≡
public :: syntax_model_file_write

<Models: sub interfaces>+≡
module subroutine syntax_model_file_write (unit)
integer, intent(in), optional :: unit
end subroutine syntax_model_file_write

<Models: procedures>+≡
module subroutine syntax_model_file_write (unit)
integer, intent(in), optional :: unit
call syntax_write (syntax_model_file, unit)
end subroutine syntax_model_file_write

```

Read a model from file. Handle all syntax and respect the provided scheme.

The `ufo` flag just says that the model object should be tagged as being derived from an UFO model. The UFO model path may be requested by the caller. If not, we use a standard path search for UFO models. There is no difference in the contents of the file or the generated model object.

```

<Models: model: TBP>+≡
procedure :: read => model_read

<Models: sub interfaces>+≡
module subroutine model_read (model, filename, os_data, exist, &
scheme, ufo, ufo_path_requested, rebuild_mdl)
class(model_t), intent(out), target :: model
type(string_t), intent(in) :: filename
type(os_data_t), intent(in) :: os_data
logical, intent(out), optional :: exist
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path_requested
logical, intent(in), optional :: rebuild_mdl
end subroutine model_read

<Models: procedures>+≡
module subroutine model_read (model, filename, os_data, exist, &
scheme, ufo, ufo_path_requested, rebuild_mdl)
class(model_t), intent(out), target :: model
type(string_t), intent(in) :: filename
type(os_data_t), intent(in) :: os_data
logical, intent(out), optional :: exist
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path_requested
logical, intent(in), optional :: rebuild_mdl
type(string_t) :: file
type(stream_t), target :: stream
type(lexer_t) :: lexer
integer :: unit
character(32) :: model_md5sum
type(parse_node_t), pointer :: nd_model_def, nd_model_name_def
type(parse_node_t), pointer :: nd_schemes, nd_scheme_decl

```

```

type(parse_node_t), pointer :: nd_parameters
type(parse_node_t), pointer :: nd_external_pars
type(parse_node_t), pointer :: nd_particles, nd_vertices
type(string_t) :: model_name, lib_name
integer :: n_parblock, n_par, i_par, n_ext, n_prt, n_vtx
type(parse_node_t), pointer :: nd_par_def
type(parse_node_t), pointer :: nd_ext_def
type(parse_node_t), pointer :: nd_prt
type(parse_node_t), pointer :: nd_vtx
logical :: ufo_model, model_exist, rebuild
ufo_model = .false.; if (present (ufo)) ufo_model = ufo
rebuild = .true.; if (present (rebuild_mdl)) rebuild = rebuild_mdl
file = filename
inquire (file=char(file), exist=model_exist)
if ((.not. model_exist) .and. (.not. os_data%use_testfiles)) then
    file = os_data%whizard_modelpath_local // "/" // filename
    inquire (file = char (file), exist = model_exist)
end if
if (.not. model_exist) then
    file = os_data%whizard_modelpath // "/" // filename
    inquire (file = char (file), exist = model_exist)
end if
if (ufo_model .and. rebuild) then
    file = filename
    call model_generate_ufo (filename, os_data, model%ufo_path, &
        ufo_path_requested=ufo_path_requested)
    inquire (file = char (file), exist = model_exist)
end if
if (.not. model_exist) then
    call msg_fatal ("Model file '" // char (filename) // "' not found")
    if (present (exist)) exist = .false.
    return
end if
if (present (exist)) exist = .true.

if (logging) call msg_message ("Reading model file '" // char (file) // "'")

unit = free_unit ()
open (file=char(file), unit=unit, action="read", status="old")
model_md5sum = md5sum (unit)
close (unit)

call lexer_init_model_file (lexer)
call stream_init (stream, char (file))
call lexer_assign_stream (lexer, stream)
call parse_tree_init (model%parse_tree, syntax_model_file, lexer)
call stream_final (stream)
call lexer_final (lexer)

nd_model_def => model%parse_tree%get_root_ptr ()
nd_model_name_def => parse_node_get_sub_ptr (nd_model_def)
model_name = parse_node_get_string &
    (parse_node_get_sub_ptr (nd_model_name_def, 2))
nd_schemes => nd_model_name_def%get_next_ptr ()

```

```

call find_block &
    ("scheme_header", nd_schemes, nd_scheme_decl, nd_next=nd_parameters)
call find_block &
    ("parameters", nd_parameters, nd_par_def, n_parblock, nd_external_pars)
call find_block &
    ("external_pars", nd_external_pars, nd_ext_def, n_ext, nd_particles)
call find_block &
    ("particles", nd_particles, nd_prt, n_prt, nd_vertices)
call find_block &
    ("vertices", nd_vertices, nd_vtx, n_vtx)

if (associated (nd_external_pars)) then
    lib_name = "external." // model_name
else
    lib_name = ""
end if

if (associated (nd_scheme_decl)) then
    call handle_schemes (nd_scheme_decl, scheme)
end if

n_par = 0
call count_parameters (nd_par_def, n_parblock, n_par)

call model%init &
    (model_name, lib_name, os_data, n_par + n_ext, n_prt, n_vtx, ufo)
model%md5sum = model_md5sum

if (associated (nd_par_def)) then
    i_par = 0
    call handle_parameters (nd_par_def, n_parblock, i_par)
end if
if (associated (nd_ext_def)) then
    call handle_external (nd_ext_def, n_par, n_ext)
end if
call model%update_parameters ()
if (associated (nd_prt)) then
    call handle_fields (nd_prt, n_prt)
end if
if (associated (nd_vtx)) then
    call handle_vertices (nd_vtx, n_vtx)
end if

call model%freeze_vertices ()
call model%append_field_vars ()

contains

subroutine find_block (key, nd, nd_item, n_item, nd_next)
    character(*), intent(in) :: key
    type(parse_node_t), pointer, intent(inout) :: nd
    type(parse_node_t), pointer, intent(out) :: nd_item
    integer, intent(out), optional :: n_item

```

```

type(parse_node_t), pointer, intent(out), optional :: nd_next
if (associated (nd)) then
    if (nd%get_rule_key () == key) then
        nd_item => nd%get_sub_ptr ()
        if (present (n_item)) n_item = nd%get_n_sub ()
        if (present (nd_next)) nd_next => nd%get_next_ptr ()
    else
        nd_item => null ()
        if (present (n_item)) n_item = 0
        if (present (nd_next)) nd_next => nd
        nd => null ()
    end if
else
    nd_item => null ()
    if (present (n_item)) n_item = 0
    if (present (nd_next)) nd_next => null ()
end if
end subroutine find_block

subroutine handle_schemes (nd_scheme_decl, scheme)
type(parse_node_t), pointer, intent(in) :: nd_scheme_decl
type(string_t), intent(in), optional :: scheme
type(parse_node_t), pointer :: nd_list, nd_entry
type(string_t), dimension(:), allocatable :: schemes
integer :: i, n_schemes
nd_list => nd_scheme_decl%get_sub_ptr (3)
nd_entry => nd_list%get_sub_ptr ()
n_schemes = nd_list%get_n_sub ()
allocate (schemes (n_schemes))
do i = 1, n_schemes
    schemes(i) = nd_entry%get_string ()
    nd_entry => nd_entry%get_next_ptr ()
end do
if (present (scheme)) then
    do i = 1, n_schemes
        if (schemes(i) == scheme) goto 10    ! block exit
    end do
    call msg_fatal ("Scheme '" // char (scheme) &
        // "' is not supported by model '" // char (model_name) // "'")
end if
10 continue
call model%enable_schemes (schemes)
call model%set_scheme (scheme)
end subroutine handle_schemes

subroutine select_scheme (nd_scheme_block, n_parblock_sub, nd_par_def)
type(parse_node_t), pointer, intent(in) :: nd_scheme_block
integer, intent(out) :: n_parblock_sub
type(parse_node_t), pointer, intent(out) :: nd_par_def
type(parse_node_t), pointer :: nd_scheme_body
type(parse_node_t), pointer :: nd_scheme_case, nd_scheme_id, nd_scheme
type(string_t) :: scheme
integer :: n_cases, i
scheme = model%get_scheme ()

```

```

nd_scheme_body => nd_scheme_block%get_sub_ptr (2)
nd_parameters => null ()
select case (char (nd_scheme_body%get_rule_key ()))
case ("scheme_block_body")
    n_cases = nd_scheme_body%get_n_sub ()
    FIND_SCHEME: do i = 1, n_cases
        nd_scheme_case => nd_scheme_body%get_sub_ptr (i)
        nd_scheme_id => nd_scheme_case%get_sub_ptr (2)
        select case (char (nd_scheme_id%get_rule_key ()))
        case ("scheme_list")
            nd_scheme => nd_scheme_id%get_sub_ptr ()
            do while (associated (nd_scheme))
                if (scheme == nd_scheme%get_string ()) then
                    nd_parameters => nd_scheme_id%get_next_ptr ()
                    exit FIND_SCHEME
                end if
                nd_scheme => nd_scheme%get_next_ptr ()
            end do
        case ("other")
            nd_parameters => nd_scheme_id%get_next_ptr ()
            exit FIND_SCHEME
        case default
            print *, "'", char (nd_scheme_id%get_rule_key ()), "'"
            call msg_bug ("Model read: impossible scheme rule")
        end select
    end do FIND_SCHEME
end select
if (associated (nd_parameters)) then
    select case (char (nd_parameters%get_rule_key ()))
    case ("parameters")
        n_parblock_sub = nd_parameters%get_n_sub ()
        if (n_parblock_sub > 0) then
            nd_par_def => nd_parameters%get_sub_ptr ()
        else
            nd_par_def => null ()
        end if
    case default
        n_parblock_sub = 0
        nd_par_def => null ()
    end select
else
    n_parblock_sub = 0
    nd_par_def => null ()
end if
end subroutine select_scheme

recursive subroutine count_parameters (nd_par_def_in, n_parblock, n_par)
    type(parse_node_t), pointer, intent(in) :: nd_par_def_in
    integer, intent(in) :: n_parblock
    integer, intent(inout) :: n_par
    type(parse_node_t), pointer :: nd_par_def, nd_par_key
    type(parse_node_t), pointer :: nd_par_def_sub
    integer :: n_parblock_sub
    integer :: i

```

```

nd_par_def => nd_par_def_in
do i = 1, n_parblock
  nd_par_key => nd_par_def%get_sub_ptr ()
  select case (char (nd_par_key%get_rule_key ()))
  case ("parameter", "derived", "unused")
    n_par = n_par + 1
  case ("scheme_block_beg")
    call select_scheme (nd_par_def, n_parblock_sub, nd_par_def_sub)
    if (n_parblock_sub > 0) then
      call count_parameters (nd_par_def_sub, n_parblock_sub, n_par)
    end if
  case default
    print *, "'", char (nd_par_key%get_rule_key ()), "'"
    call msg_bug ("Model read: impossible parameter rule")
  end select
  nd_par_def => parse_node_get_next_ptr (nd_par_def)
end do
end subroutine count_parameters

recursive subroutine handle_parameters (nd_par_def_in, n_parblock, i_par)
  type(parse_node_t), pointer, intent(in) :: nd_par_def_in
  integer, intent(in) :: n_parblock
  integer, intent(inout) :: i_par
  type(parse_node_t), pointer :: nd_par_def, nd_par_key
  type(parse_node_t), pointer :: nd_par_def_sub
  integer :: n_parblock_sub
  integer :: i
  nd_par_def => nd_par_def_in
  do i = 1, n_parblock
    nd_par_key => nd_par_def%get_sub_ptr ()
    select case (char (nd_par_key%get_rule_key ()))
    case ("parameter")
      i_par = i_par + 1
      call model%read_parameter (i_par, nd_par_def)
    case ("derived")
      i_par = i_par + 1
      call model%read_derived (i_par, nd_par_def)
    case ("unused")
      i_par = i_par + 1
      call model%read_unused (i_par, nd_par_def)
    case ("scheme_block_beg")
      call select_scheme (nd_par_def, n_parblock_sub, nd_par_def_sub)
      if (n_parblock_sub > 0) then
        call handle_parameters (nd_par_def_sub, n_parblock_sub, i_par)
      end if
    end select
    nd_par_def => parse_node_get_next_ptr (nd_par_def)
  end do
end subroutine handle_parameters

subroutine handle_external (nd_ext_def, n_par, n_ext)
  type(parse_node_t), pointer, intent(inout) :: nd_ext_def
  integer, intent(in) :: n_par, n_ext
  integer :: i

```

```

do i = n_par + 1, n_par + n_ext
  call model%read_external (i, nd_ext_def)
  nd_ext_def => parse_node_get_next_ptr (nd_ext_def)
end do
!   real(c_default_float), dimension(:), allocatable :: par
!   if (associated (model%init_external_parameters)) then
!     allocate (par (model%get_n_real ()))
!     call model%real_parameters_to_c_array (par)
!     call model%init_external_parameters (par)
!     call model%real_parameters_from_c_array (par)
!   end if
end subroutine handle_external

subroutine handle_fields (nd_prt, n_prt)
  type(parse_node_t), pointer, intent(inout) :: nd_prt
  integer, intent(in) :: n_prt
  integer :: i
  do i = 1, n_prt
    call model%read_field (i, nd_prt)
    nd_prt => parse_node_get_next_ptr (nd_prt)
  end do
end subroutine handle_fields

subroutine handle_vertices (nd_vtx, n_vtx)
  type(parse_node_t), pointer, intent(inout) :: nd_vtx
  integer, intent(in) :: n_vtx
  integer :: i
  do i = 1, n_vtx
    call model%read_vertex (i, nd_vtx)
    nd_vtx => parse_node_get_next_ptr (nd_vtx)
  end do
end subroutine handle_vertices

end subroutine model_read

```

Parameters are real values (literal) with an optional unit.

(Models: model: TBP)+≡

```
procedure, private :: read_parameter => model_read_parameter
```

(Models: sub interfaces)+≡

```

module subroutine model_read_parameter (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in), target :: node
end subroutine model_read_parameter

```

(Models: procedures)+≡

```

module subroutine model_read_parameter (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in), target :: node
  type(parse_node_t), pointer :: node_name, node_val, node_slha_entry
  type(string_t) :: name
  node_name => parse_node_get_sub_ptr (node, 2)
  name = parse_node_get_string (node_name)

```



```

node_val => parse_node_get_next_ptr (node_name, 2)
call model%set_parameter_parse_node (i, name, node_val, constant=.true.)
node_slha_entry => parse_node_get_next_ptr (node_val)
if (associated (node_slha_entry)) then
    call model_record_slha_block_entry (model, i, node_slha_entry)
end if
end subroutine model_read_parameter

```

Derived parameters have any numeric expression as their definition. Don't evaluate the expression, yet.

```

<Models: model: TBP>+≡
    procedure, private :: read_derived => model_read_derived

<Models: sub interfaces>+≡
    module subroutine model_read_derived (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
    end subroutine model_read_derived

<Models: procedures>+≡
    module subroutine model_read_derived (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
        type(string_t) :: name
        type(parse_node_t), pointer :: pn_expr
        name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
        pn_expr => parse_node_get_sub_ptr (node, 4)
        call model%set_parameter_parse_node (i, name, pn_expr, constant=.false.)
    end subroutine model_read_derived

```

External parameters have no definition; they are handled by an external library.

```

<Models: model: TBP>+≡
    procedure, private :: read_external => model_read_external

<Models: sub interfaces>+≡
    module subroutine model_read_external (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
    end subroutine model_read_external

<Models: procedures>+≡
    module subroutine model_read_external (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
        type(string_t) :: name
        name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
        call model%set_parameter_external (i, name)
    end subroutine model_read_external

```

Ditto for unused parameters, they are there just for reserving the name.

<Models: model: TBP>+≡

```
procedure, private :: read_unused => model_read_unused
```

<Models: sub interfaces>+≡

```
module subroutine model_read_unused (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in), target :: node
end subroutine model_read_unused
```

<Models: procedures>+≡

```
module subroutine model_read_unused (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in), target :: node
  type(string_t) :: name
  name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
  call model%set_parameter_unused (i, name)
end subroutine model_read_unused
```

<Models: model: TBP>+≡

```
procedure, private :: read_field => model_read_field
```

<Models: sub interfaces>+≡

```
module subroutine model_read_field (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in) :: node
end subroutine model_read_field
```

<Models: procedures>+≡

```
module subroutine model_read_field (model, i, node)
  class(model_t), intent(inout), target :: model
  integer, intent(in) :: i
  type(parse_node_t), intent(in) :: node
  type(parse_node_t), pointer :: nd_src, nd_props, nd_prop
  type(string_t) :: longname
  integer :: pdg
  type(string_t) :: name_src
  type(string_t), dimension(:), allocatable :: name
  type(field_data_t), pointer :: field, field_src
  longname = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
  pdg = read_frac (parse_node_get_sub_ptr (node, 3))
  field => model%get_field_ptr_by_index (i)
  call field%init (longname, pdg)
  nd_src => parse_node_get_sub_ptr (node, 4)
  if (associated (nd_src)) then
    if (parse_node_get_rule_key (nd_src) == "prt_src") then
      name_src = parse_node_get_string (parse_node_get_sub_ptr (nd_src, 2))
      field_src => model%get_field_ptr (name_src, check=.true.)
      call field%copy_from (field_src)
      nd_props => parse_node_get_sub_ptr (nd_src, 3)
    else
      nd_props => nd_src
    end if
  end if
```

```

nd_prop => parse_node_get_sub_ptr (nd_props)
do while (associated (nd_prop))
  select case (char (parse_node_get_rule_key (nd_prop)))
  case ("invisible")
    call field%set (is_visible=.false.)
  case ("parton")
    call field%set (is_parton=.true.)
  case ("gauge")
    call field%set (is_gauge=.true.)
  case ("left")
    call field%set (is_left_handed=.true.)
  case ("right")
    call field%set (is_right_handed=.true.)
  case ("prt_name")
    call read_names (nd_prop, name)
    call field%set (name=name)
  case ("prt_anti")
    call read_names (nd_prop, name)
    call field%set (anti=name)
  case ("prt_tex_name")
    call field%set ( &
      tex_name = parse_node_get_string &
      (parse_node_get_sub_ptr (nd_prop, 2)))
  case ("prt_tex_anti")
    call field%set ( &
      tex_anti = parse_node_get_string &
      (parse_node_get_sub_ptr (nd_prop, 2)))
  case ("prt_spin")
    call field%set ( &
      spin_type = read_frac &
      (parse_node_get_sub_ptr (nd_prop, 2), 2))
  case ("prt_isospin")
    call field%set ( &
      isospin_type = read_frac &
      (parse_node_get_sub_ptr (nd_prop, 2), 2))
  case ("prt_charge")
    call field%set ( &
      charge_type = read_frac &
      (parse_node_get_sub_ptr (nd_prop, 2), 3))
  case ("prt_color")
    call field%set ( &
      color_type = parse_node_get_integer &
      (parse_node_get_sub_ptr (nd_prop, 2)))
  case ("prt_mass")
    call field%set ( &
      mass_data = model%get_par_data_ptr &
      (parse_node_get_string &
      (parse_node_get_sub_ptr (nd_prop, 2))))
  case ("prt_width")
    call field%set ( &
      width_data = model%get_par_data_ptr &
      (parse_node_get_string &
      (parse_node_get_sub_ptr (nd_prop, 2))))
  case default

```

```

        call msg_bug (" Unknown particle property '" &
            // char (parse_node_get_rule_key (nd_prop)) // "'")
    end select
    if (allocated (name)) deallocate (name)
    nd_prop => parse_node_get_next_ptr (nd_prop)
end do
end if
call field%freeze ()
end subroutine model_read_field

```

<Models: model: TBP>+≡

```

procedure, private :: read_vertex => model_read_vertex

```

<Models: sub interfaces>+≡

```

module subroutine model_read_vertex (model, i, node)
    class(model_t), intent(inout) :: model
    integer, intent(in) :: i
    type(parse_node_t), intent(in) :: node
end subroutine model_read_vertex

```

<Models: procedures>+≡

```

module subroutine model_read_vertex (model, i, node)
    class(model_t), intent(inout) :: model
    integer, intent(in) :: i
    type(parse_node_t), intent(in) :: node
    type(string_t), dimension(:), allocatable :: name
    call read_names (node, name)
    call model%set_vertex (i, name)
end subroutine model_read_vertex

```

<Models: procedures>+≡

```

subroutine read_names (node, name)
    type(parse_node_t), intent(in) :: node
    type(string_t), dimension(:), allocatable, intent(inout) :: name
    type(parse_node_t), pointer :: nd_name
    integer :: n_names, i
    n_names = parse_node_get_n_sub (node) - 1
    allocate (name (n_names))
    nd_name => parse_node_get_sub_ptr (node, 2)
    do i = 1, n_names
        name(i) = parse_node_get_string (nd_name)
        nd_name => parse_node_get_next_ptr (nd_name)
    end do
end subroutine read_names

```

There is an optional argument for the base.

<Models: procedures>+≡

```

function read_frac (nd_frac, base) result (qn_type)
    integer :: qn_type
    type(parse_node_t), intent(in) :: nd_frac
    integer, intent(in), optional :: base
    type(parse_node_t), pointer :: nd_num, nd_den
    integer :: num, den
    nd_num => parse_node_get_sub_ptr (nd_frac)

```

```

nd_den => parse_node_get_next_ptr (nd_num)
select case (char (parse_node_get_rule_key (nd_num)))
case ("integer_literal")
    num = parse_node_get_integer (nd_num)
case ("neg_int")
    num = - parse_node_get_integer (parse_node_get_sub_ptr (nd_num, 2))
case ("pos_int")
    num = parse_node_get_integer (parse_node_get_sub_ptr (nd_num, 2))
case default
    call parse_tree_bug (nd_num, "int|neg_int|pos_int")
end select
if (associated (nd_den)) then
    den = parse_node_get_integer (parse_node_get_sub_ptr (nd_den, 2))
else
    den = 1
end if
if (present (base)) then
    if (den == 1) then
        qn_type = sign (1 + abs (num) * base, num)
    else if (den == base) then
        qn_type = sign (abs (num) + 1, num)
    else
        call parse_node_write_rec (nd_frac)
        call msg_fatal (" Fractional quantum number: wrong denominator")
    end if
else
    if (den == 1) then
        qn_type = num
    else
        call parse_node_write_rec (nd_frac)
        call msg_fatal (" Wrong type: no fraction expected")
    end if
end if
end function read_frac

```

Append field (PDG-array) variables to the variable list, based on the field content.

<Models: model: TBP>+≡

```

procedure, private :: append_field_vars => model_append_field_vars

```

<Models: sub interfaces>+≡

```

module subroutine model_append_field_vars (model)
    class(model_t), intent(inout) :: model
end subroutine model_append_field_vars

```

<Models: procedures>+≡

```

module subroutine model_append_field_vars (model)
    class(model_t), intent(inout) :: model
    type(pdg_array_t) :: aval
    type(field_data_t), dimension(:), pointer :: field_array
    type(field_data_t), pointer :: field
    type(string_t) :: name
    type(string_t), dimension(:), allocatable :: name_array
    integer, dimension(:), allocatable :: pdg
    logical, dimension(:), allocatable :: mask

```

```

integer :: i, j
field_array => model%get_field_array_ptr ()
aval = UNDEFINED
call model%var_list%append_pdg_array (var_str ("particle"), &
    aval, locked = .true., intrinsic=.true.)
do i = 1, size (field_array)
    aval = field_array(i)%get_pdg ()
    name = field_array(i)%get_longname ()
    call model%var_list%append_pdg_array &
        (name, aval, locked=.true., intrinsic=.true.)
    call field_array(i)%get_name_array (.false., name_array)
    do j = 1, size (name_array)
        call model%var_list%append_pdg_array (name_array(j), &
            aval, locked=.true., intrinsic=.true.)
    end do
    model%max_field_name_length = &
        max (model%max_field_name_length, len (name_array(1)))
    aval = - field_array(i)%get_pdg ()
    call field_array(i)%get_name_array (.true., name_array)
    do j = 1, size (name_array)
        call model%var_list%append_pdg_array (name_array(j), &
            aval, locked=.true., intrinsic=.true.)
    end do
    if (size (name_array) > 0) then
        model%max_field_name_length = &
            max (model%max_field_name_length, len (name_array(1)))
    end if
end do
call model%get_all_pdg (pdg)
allocate (mask (size (pdg)))
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_charge_type () /= 1
end do
aval = pack (pdg, mask)
call model%var_list%append_pdg_array (var_str ("charged"), &
    aval, locked = .true., intrinsic=.true.)
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_charge_type () == 1
end do
aval = pack (pdg, mask)
call model%var_list%append_pdg_array (var_str ("neutral"), &
    aval, locked = .true., intrinsic=.true.)
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_color_type () /= 1
end do
aval = pack (pdg, mask)
call model%var_list%append_pdg_array (var_str ("colored"), &
    aval, locked = .true., intrinsic=.true.)
end subroutine model_append_field_vars

```

28.4.10 Test models

```
<Models: public>+≡
    public :: create_test_model

<Models: sub interfaces>+≡
    module subroutine create_test_model (model_name, test_model)
        type(string_t), intent(in) :: model_name
        type(model_t), intent(out), pointer :: test_model
    end subroutine create_test_model

<Models: procedures>+≡
    module subroutine create_test_model (model_name, test_model)
        type(string_t), intent(in) :: model_name
        type(model_t), intent(out), pointer :: test_model
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (model_name, model_name // var_str (".mdl"), os_data, test_model)
    end subroutine create_test_model
```

28.4.11 Model list

List of currently active models

```
<Models: types>+≡
    type, extends (model_t) :: model_entry_t
        type(model_entry_t), pointer :: next => null ()
    end type model_entry_t

<Models: public>+≡
    public :: model_list_t

<Models: types>+≡
    type :: model_list_t
        type(model_entry_t), pointer :: first => null ()
        type(model_entry_t), pointer :: last => null ()
        type(model_list_t), pointer :: context => null ()
    contains
        <Models: model list: TBP>
    end type model_list_t
```

Write an account of the model list. We write linked lists first, starting from the global context.

```
<Models: model list: TBP>≡
    procedure :: write => model_list_write

<Models: sub interfaces>+≡
    recursive module subroutine model_list_write &
        (object, unit, verbose, follow_link)
        class(model_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
```

```

        logical, intent(in), optional :: follow_link
    end subroutine model_list_write

<Models: procedures>+≡
    recursive module subroutine model_list_write &
        (object, unit, verbose, follow_link)
        class(model_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: follow_link
        type(model_entry_t), pointer :: current
        logical :: rec
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        rec = .true.; if (present (follow_link)) rec = follow_link
        if (rec .and. associated (object%context)) then
            call object%context%write (unit, verbose, follow_link)
        end if
        current => object%first
        if (associated (current)) then
            do while (associated (current))
                call current%write (unit, verbose)
                current => current%next
                if (associated (current)) write (u, *)
            end do
        end if
    end subroutine model_list_write

```

Link this list to another one.

```

<Models: model list: TBP>+≡
    procedure :: link => model_list_link

<Models: sub interfaces>+≡
    module subroutine model_list_link (model_list, context)
        class(model_list_t), intent(inout) :: model_list
        type(model_list_t), intent(in), target :: context
    end subroutine model_list_link

<Models: procedures>+≡
    module subroutine model_list_link (model_list, context)
        class(model_list_t), intent(inout) :: model_list
        type(model_list_t), intent(in), target :: context
        model_list%context => context
    end subroutine model_list_link

```

(Private, used below:) Append an existing model, for which we have allocated a pointer entry, to the model list. The original pointer becomes disassociated, and the model should now be considered as part of the list. We assume that this model is not yet part of the list.

If we provide a model argument, this returns a pointer to the new entry.

```

<Models: model list: TBP>+≡
    procedure, private :: import => model_list_import

```



```

<Models: sub interfaces>+≡
  module subroutine model_list_import (model_list, current, model)
    class(model_list_t), intent(inout) :: model_list
    type(model_entry_t), pointer, intent(inout) :: current
    type(model_t), optional, pointer, intent(out) :: model
  end subroutine model_list_import

```

```

<Models: procedures>+≡
  module subroutine model_list_import (model_list, current, model)
    class(model_list_t), intent(inout) :: model_list
    type(model_entry_t), pointer, intent(inout) :: current
    type(model_t), optional, pointer, intent(out) :: model
    if (associated (current)) then
      if (associated (model_list%first)) then
        model_list%last%next => current
      else
        model_list%first => current
      end if
      model_list%last => current
      if (present (model)) model => current%model_t
      current => null ()
    end if
  end subroutine model_list_import

```

Currently test only:

Add a new model with given name to the list, if it does not yet exist. If successful, return a pointer to the new model.

```

<Models: model list: TBP>+≡
  procedure :: add => model_list_add

```

```

<Models: sub interfaces>+≡
  module subroutine model_list_add (model_list, &
    name, os_data, n_par, n_prt, n_vtx, model)
    class(model_list_t), intent(inout) :: model_list
    type(string_t), intent(in) :: name
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: n_par, n_prt, n_vtx
    type(model_t), pointer :: model
  end subroutine model_list_add

```

```

<Models: procedures>+≡
  module subroutine model_list_add (model_list, &
    name, os_data, n_par, n_prt, n_vtx, model)
    class(model_list_t), intent(inout) :: model_list
    type(string_t), intent(in) :: name
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: n_par, n_prt, n_vtx
    type(model_t), pointer :: model
    type(model_entry_t), pointer :: current
    if (model_list%model_exists (name, follow_link=.false.)) then
      model => null ()
    else
      allocate (current)
      call current%init (name, var_str (""), os_data, &
        n_par, n_prt, n_vtx)
    end if
  end subroutine model_list_add

```

```

        call model_list%import (current, model)
    end if
end subroutine model_list_add

```

Read a new model from file and add to the list, if it does not yet exist. Finalize the model by allocating the vertex table. Return a pointer to the new model. If unsuccessful, return the original pointer.

The model is always inserted in the last link of a chain of model lists. This way, we avoid loading models twice from different contexts. When a model is modified, we should first allocate a local copy.

(Models: model list: TBP)+≡

```

    procedure :: read_model => model_list_read_model

```

(Models: sub interfaces)+≡

```

    module subroutine model_list_read_model &
        (model_list, name, filename, os_data, model, &
         scheme, ufo, ufo_path, rebuild_mdl)
    class(model_list_t), intent(inout), target :: model_list
    type(string_t), intent(in) :: name, filename
    type(os_data_t), intent(in) :: os_data
    type(model_t), pointer, intent(inout) :: model
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    logical, intent(in), optional :: rebuild_mdl
    end subroutine model_list_read_model

```

(Models: procedures)+≡

```

    module subroutine model_list_read_model &
        (model_list, name, filename, os_data, model, &
         scheme, ufo, ufo_path, rebuild_mdl)
    class(model_list_t), intent(inout), target :: model_list
    type(string_t), intent(in) :: name, filename
    type(os_data_t), intent(in) :: os_data
    type(model_t), pointer, intent(inout) :: model
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    logical, intent(in), optional :: rebuild_mdl
    class(model_list_t), pointer :: global_model_list
    type(model_entry_t), pointer :: current
    logical :: exist
    if (.not. model_list%model_exists (name, &
        scheme, ufo, ufo_path, follow_link=.true.)) then
        allocate (current)
        call current%read (filename, os_data, exist, &
            scheme=scheme, ufo=ufo, ufo_path_requested=ufo_path, &
            rebuild_mdl=rebuild_mdl)
        if (.not. exist) return
        if (current%get_name () /= name) then
            call msg_fatal ("Model file '" // char (filename) // &
                "' contains model '" // char (current%get_name ()) // &
                "' instead of '" // char (name) // "'")
            call current%final (); deallocate (current)

```

```

        return
    end if
    global_model_list => model_list
    do while (associated (global_model_list%context))
        global_model_list => global_model_list%context
    end do
    call global_model_list%import (current, model)
else
    model => model_list%get_model_ptr (name, scheme, ufo, ufo_path)
end if
end subroutine model_list_read_model

```

Append a copy of an existing model to a model list. Optionally, return pointer to the new entry.

<Models: model list: TBP>+≡

```

    procedure :: append_copy => model_list_append_copy

```

<Models: sub interfaces>+≡

```

    module subroutine model_list_append_copy (model_list, orig, model)
        class(model_list_t), intent(inout) :: model_list
        type(model_t), intent(in), target :: orig
        type(model_t), intent(out), pointer, optional :: model
    end subroutine model_list_append_copy

```

<Models: procedures>+≡

```

    module subroutine model_list_append_copy (model_list, orig, model)
        class(model_list_t), intent(inout) :: model_list
        type(model_t), intent(in), target :: orig
        type(model_t), intent(out), pointer, optional :: model
        type(model_entry_t), pointer :: copy
        allocate (copy)
        call copy%init_instance (orig)
        call model_list%import (copy, model)
    end subroutine model_list_append_copy

```

Check if a model exists by examining the list. Check recursively unless told otherwise.

<Models: model list: TBP>+≡

```

    procedure :: model_exists => model_list_model_exists

```

<Models: sub interfaces>+≡

```

    recursive module function model_list_model_exists &
        (model_list, name, scheme, ufo, ufo_path, follow_link) result (exists)
        class(model_list_t), intent(in) :: model_list
        logical :: exists
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: scheme
        logical, intent(in), optional :: ufo
        type(string_t), intent(in), optional :: ufo_path
        logical, intent(in), optional :: follow_link
    end function model_list_model_exists

```

<Models: procedures>+≡

```

    recursive module function model_list_model_exists &
        (model_list, name, scheme, ufo, ufo_path, follow_link) result (exists)

```

```

class(model_list_t), intent(in) :: model_list
logical :: exists
type(string_t), intent(in) :: name
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path
logical, intent(in), optional :: follow_link
type(model_entry_t), pointer :: current
logical :: rec
rec = .true.; if (present (follow_link)) rec = follow_link
current => model_list%first
do while (associated (current))
    if (current%matches (name, scheme, ufo, ufo_path)) then
        exists = .true.
        return
    end if
    current => current%next
end do
if (rec .and. associated (model_list%context)) then
    exists = model_list%context%model_exists (name, &
        scheme, ufo, ufo_path, follow_link)
else
    exists = .false.
end if
end function model_list_model_exists

```

Return a pointer to a named model. Search recursively unless told otherwise.

(Models: model list: TBP)+≡

```

procedure :: get_model_ptr => model_list_get_model_ptr

```

(Models: sub interfaces)+≡

```

recursive module function model_list_get_model_ptr &
    (model_list, name, scheme, ufo, ufo_path, follow_link) result (model)
class(model_list_t), intent(in) :: model_list
type(model_t), pointer :: model
type(string_t), intent(in) :: name
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path
logical, intent(in), optional :: follow_link
end function model_list_get_model_ptr

```

(Models: procedures)+≡

```

recursive module function model_list_get_model_ptr &
    (model_list, name, scheme, ufo, ufo_path, follow_link) result (model)
class(model_list_t), intent(in) :: model_list
type(model_t), pointer :: model
type(string_t), intent(in) :: name
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path
logical, intent(in), optional :: follow_link
type(model_entry_t), pointer :: current
logical :: rec
rec = .true.; if (present (follow_link)) rec = follow_link

```

```

current => model_list%first
do while (associated (current))
  if (current%matches (name, scheme, ufo, ufo_path)) then
    model => current%model_t
    return
  end if
  current => current%next
end do
if (rec .and. associated (model_list%context)) then
  model => model_list%context%get_model_ptr (name, &
    scheme, ufo, ufo_path, follow_link)
else
  model => null ()
end if
end function model_list_get_model_ptr

```

Delete the list of models. No recursion.

```

<Models: model list: TBP>+≡
  procedure :: final => model_list_final

<Models: sub interfaces>+≡
  module subroutine model_list_final (model_list)
    class(model_list_t), intent(inout) :: model_list
  end subroutine model_list_final

<Models: procedures>+≡
  module subroutine model_list_final (model_list)
    class(model_list_t), intent(inout) :: model_list
    type(model_entry_t), pointer :: current
    model_list%last => null ()
    do while (associated (model_list%first))
      current => model_list%first
      model_list%first => model_list%first%next
      call current%final ()
      deallocate (current)
    end do
  end subroutine model_list_final

```

28.4.12 Model instances

A model instance is a copy of a model object. The parameters are true copies. The particle data and the variable list pointers should point to the copy, so modifying the parameters has only a local effect. Hence, we build them up explicitly. The vertex array is also rebuilt, it contains particle pointers. Finally, the vertex hash table can be copied directly since it contains no pointers.

The `multiplicity` entry depends on the association of the `mass_data` entry and therefore has to be set at the end.

The instance must carry the `target` attribute.

Parameters: the `copy_parameter` method essentially copies the parameter decorations (parse node, expression etc.). The current parameter values are part of the `model_data_t` base type and are copied afterwards via its `copy_from` method.

Note: the parameter set is initialized for real parameters only.

In order for the local model to be able to use the correct UFO model setup, UFO model information has to be transferred.

```

<Models: model: TBP>+≡
    procedure :: init_instance => model_copy

<Models: sub interfaces>+≡
    module subroutine model_copy (model, orig)
        class(model_t), intent(out), target :: model
        type(model_t), intent(in) :: orig
    end subroutine model_copy

<Models: procedures>+≡
    module subroutine model_copy (model, orig)
        class(model_t), intent(out), target :: model
        type(model_t), intent(in) :: orig
        integer :: n_par, n_prt, n_vtx
        integer :: i
        n_par = orig%get_n_real ()
        n_prt = orig%get_n_field ()
        n_vtx = orig%get_n_vtx ()
        call model%basic_init (orig%get_name (), n_par, n_prt, n_vtx)
        if (allocated (orig%schemes)) then
            model%schemes = orig%schemes
            if (allocated (orig%selected_scheme)) then
                model%selected_scheme = orig%selected_scheme
                call model%set_scheme_num (orig%get_scheme_num ())
            end if
        end if
        if (allocated (orig%slha_block)) then
            model%slha_block = orig%slha_block
        end if
        model%md5sum = orig%md5sum
        model%ufo_model = orig%ufo_model
        model%ufo_path = orig%ufo_path
        if (allocated (orig%par)) then
            do i = 1, n_par
                call model%copy_parameter (i, orig%par(i))
            end do
        end if
        model%init_external_parameters => orig%init_external_parameters
        call model%model_data_t%copy_from (orig)
        model%max_par_name_length = orig%max_par_name_length
        call model%append_field_vars ()
    end subroutine model_copy

```

28.4.13 Unit tests

Test module, followed by the corresponding implementation module.

```

<models_ut.f90>≡
    <File header>

    module models_ut

```

```

    use unit_tests
    use models_uti

    <Standard module head>

    <Models: public test>

contains

    <Models: test driver>

end module models_ut
<models_uti.f90>≡
    <File header>

module models_uti

    <Use kinds>
    <Use strings>
    use file_utils, only: delete_file
    use physics_defs, only: SCALAR, SPINOR
    use os_interface
    use model_data
    use variables

    use models

    <Standard module head>

    <Models: test declarations>

contains

    <Models: tests>

end module models_uti
API: driver for the unit tests below.
<Models: public test>≡
    public :: models_test
<Models: test driver>≡
    subroutine models_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Models: execute tests>
    end subroutine models_test

```

Construct a Model

Here, we construct a toy model explicitly without referring to a file.

```

<Models: execute tests>≡
    call test (models_1, "models_1", &

```

```

        "construct model", &
        u, results)

<Models: test declarations>≡
    public :: models_1

<Models: tests>≡
    subroutine models_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(string_t) :: model_name
        type(string_t) :: x_longname
        type(string_t), dimension(2) :: parname
        type(string_t), dimension(2) :: x_name
        type(string_t), dimension(1) :: x_anti
        type(string_t) :: x_tex_name, x_tex_anti
        type(string_t) :: y_longname
        type(string_t), dimension(2) :: y_name
        type(string_t) :: y_tex_name
        type(field_data_t), pointer :: field

        write (u, "(A)")  "* Test output: models_1"
        write (u, "(A)")  "* Purpose: create a model"
        write (u, *)

        model_name = "Test model"
        call model_list%add (model_name, os_data, 2, 2, 3, model)
        parname(1) = "mx"
        parname(2) = "coup"
        call model%set_parameter_constant (1, parname(1), 10._default)
        call model%set_parameter_constant (2, parname(2), 1.3_default)
        x_longname = "X_LEPTON"
        x_name(1) = "X"
        x_name(2) = "x"
        x_anti(1) = "Xbar"
        x_tex_name = "X~+"
        x_tex_anti = "X~- "
        field => model%get_field_ptr_by_index (1)
        call field%init (x_longname, 99)
        call field%set ( &
            .true., .false., .false., .false., .false., &
            name=x_name, anti=x_anti, tex_name=x_tex_name, tex_anti=x_tex_anti, &
            spin_type=SPINOR, isospin_type=-3, charge_type=2, &
            mass_data=model%get_par_data_ptr (parname(1)))
        y_longname = "Y_COLORON"
        y_name(1) = "Y"
        y_name(2) = "yc"
        y_tex_name = "Y~0"
        field => model%get_field_ptr_by_index (2)
        call field%init (y_longname, 97)
        call field%set ( &
            .false., .false., .true., .false., .false., &
            name=y_name, tex_name=y_tex_name, &

```



```

        spin_type=SCALAR, isospin_type=2, charge_type=1, color_type=8)
    call model%set_vertex (1, [99, 99, 99])
    call model%set_vertex (2, [99, 99, 99, 99])
    call model%set_vertex (3, [99, 97, 99])
    call model_list%write (u)

    call model_list%final ()

    write (u, *)
    write (u, "(A)")  "* Test output end: models_1"

end subroutine models_1

```

Read a Model

Read a predefined model from file.

```

<Models: execute tests>+≡
    call test (models_2, "models_2", &
        "read model", &
        u, results)

<Models: test declarations>+≡
    public :: models_2

<Models: tests>+≡
    subroutine models_2 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(var_list_t), pointer :: var_list
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_2"
        write (u, "(A)")  "* Purpose: read a model from file"
        write (u, *)

        call syntax_model_file_init ()
        call os_data%init ()

        call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
            os_data, model)
        call model_list%write (u)

        write (u, *)
        write (u, "(A)")  "* Variable list"
        write (u, *)

        var_list => model%get_var_list_ptr ()
        call var_list%write (u)

        write (u, *)
        write (u, "(A)")  "* Cleanup"

        call model_list%final ()

```

```

call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_2"

end subroutine models_2

```

Model Instance

Read a predefined model from file and create an instance.

```

<Models: execute tests>+≡
call test (models_3, "models_3", &
    "model instance", &
    u, results)

<Models: test declarations>+≡
public :: models_3

<Models: tests>+≡
subroutine models_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(var_list_t), pointer :: var_list
    type(model_t), pointer :: instance

    write (u, "(A)")  "* Test output: models_3"
    write (u, "(A)")  "* Purpose: create a model instance"
    write (u, *)

    call syntax_model_file_init ()
    call os_data%init ()

    call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
        os_data, model)
    allocate (instance)
    call instance%init_instance (model)

    call model%write (u)

    write (u, *)
    write (u, "(A)")  "* Variable list"
    write (u, *)

    var_list => instance%get_var_list_ptr ()
    call var_list%write (u)

    write (u, *)
    write (u, "(A)")  "* Cleanup"

    call instance%final ()
    deallocate (instance)

```

```

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_3"

end subroutine models_3

```

Unstable and Polarized Particles

Read a predefined model from file and define decays and polarization.

```

<Models: execute tests>+≡
  call test (models_4, "models_4", &
    "handle decays and polarization", &
    u, results)

<Models: test declarations>+≡
  public :: models_4

<Models: tests>+≡
  subroutine models_4 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model, model_instance
    character(32) :: md5sum

    write (u, "(A)")  "* Test output: models_4"
    write (u, "(A)")  "* Purpose: set and unset decays and polarization"
    write (u, *)

    call syntax_model_file_init ()
    call os_data%init ()

    write (u, "(A)")  "* Read model from file"

    call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
      os_data, model)

    md5sum = model%get_parameters_md5sum ()
    write (u, *)
    write (u, "(1x,3A)")  "MD5 sum (parameters) = '", md5sum, "'"

    write (u, *)
    write (u, "(A)")  "* Set particle decays and polarization"
    write (u, *)

    call model%set_unstable (25, [var_str ("dec1"), var_str ("dec2")])
    call model%set_polarized (6)
    call model%set_unstable (-6, [var_str ("fdec")])

    call model%write (u)

    md5sum = model%get_parameters_md5sum ()

```

```

write (u, *)
write (u, "(1x,3A)") "MD5 sum (parameters) = '", md5sum, "'"

write (u, *)
write (u, "(A)")  "* Create a model instance"

allocate (model_instance)
call model_instance%init_instance (model)

write (u, *)
write (u, "(A)")  "* Revert particle decays and polarization"
write (u, *)

call model%set_stable (25)
call model%set_unpolarized (6)
call model%set_stable (-6)

call model%write (u)

md5sum = model%get_parameters_md5sum ()
write (u, *)
write (u, "(1x,3A)") "MD5 sum (parameters) = '", md5sum, "'"

write (u, *)
write (u, "(A)")  "* Show the model instance"
write (u, *)

call model_instance%write (u)

md5sum = model_instance%get_parameters_md5sum ()
write (u, *)
write (u, "(1x,3A)") "MD5 sum (parameters) = '", md5sum, "'"

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_instance%final ()
deallocate (model_instance)
call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_4"

end subroutine models_4

```

Model Variables

Read a predefined model from file and modify some parameters.

Note that the MD5 sum is not modified by this.

```

(Models: execute tests)+≡
call test (models_5, "models_5", &

```

```

        "handle parameters", &
        u, results)
<Models: test declarations>+≡
    public :: models_5
<Models: tests>+≡
    subroutine models_5 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(model_t), pointer :: model, model_instance
        character(32) :: md5sum

        write (u, "(A)")  "* Test output: models_5"
        write (u, "(A)")  "* Purpose: access and modify model variables"
        write (u, *)

        call syntax_model_file_init ()
        call os_data%init ()

        write (u, "(A)")  "* Read model from file"

        call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
            os_data, model)

        write (u, *)

        call model%write (u, &
            show_md5sum = .true., &
            show_variables = .true., &
            show_parameters = .true., &
            show_particles = .false., &
            show_vertices = .false.)

        write (u, *)
        write (u, "(A)")  "* Check parameter status"
        write (u, *)

        write (u, "(1x,A,L1)") "xy exists = ", model%var_exists (var_str ("xx"))
        write (u, "(1x,A,L1)") "ff exists = ", model%var_exists (var_str ("ff"))
        write (u, "(1x,A,L1)") "mf exists = ", model%var_exists (var_str ("mf"))
        write (u, "(1x,A,L1)") "ff locked = ", model%var_is_locked (var_str ("ff"))
        write (u, "(1x,A,L1)") "mf locked = ", model%var_is_locked (var_str ("mf"))

        write (u, *)
        write (u, "(1x,A,F6.2)") "ff = ", model%get_rval (var_str ("ff"))
        write (u, "(1x,A,F6.2)") "mf = ", model%get_rval (var_str ("mf"))

        write (u, *)
        write (u, "(A)")  "* Modify parameter"
        write (u, *)

        call model%set_real (var_str ("ff"), 1._default)

```

```

call model%write (u, &
    show_md5sum = .true., &
    show_variables = .true., &
    show_parameters = .true., &
    show_particles = .false., &
    show_vertices = .false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_5"

end subroutine models_5

```

Read model with disordered parameters

Read a model from file where the ordering of independent and derived parameters is non-canonical.

```

<Models: execute tests>+≡
    call test (models_6, "models_6", &
        "read model parameters", &
        u, results)

<Models: test declarations>+≡
    public :: models_6

<Models: tests>+≡
    subroutine models_6 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(var_list_t), pointer :: var_list
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_6"
        write (u, "(A)")  "* Purpose: read a model from file &
            &with non-canonical parameter ordering"
        write (u, *)

        open (newunit=um, file="Test6.mdl", status="replace", action="readwrite")
        write (um, "(A)")  'model "Test6"'
        write (um, "(A)")  ' parameter a = 1.000000000000E+00'
        write (um, "(A)")  ' derived b = 2 * a'
        write (um, "(A)")  ' parameter c = 3.000000000000E+00'
        write (um, "(A)")  ' unused d'

        rewind (um)

```

```

do
    read (um, "(A)", end=1) buffer
    write (u, "(A)") trim (buffer)
end do
1 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

call model_list%read_model (var_str ("Test6"), var_str ("Test6.mdl"), &
    os_data, model)

write (u, *)
write (u, "(A)")  "* Variable list"
write (u, *)

var_list => model%get_var_list_ptr ()
call var_list%write (u)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_6"

end subroutine models_6

```

Read model with schemes

Read a model from file which supports scheme selection in the parameter list.

```

<Models: execute tests>+≡
    call test (models_7, "models_7", &
        "handle schemes", &
        u, results)

<Models: test declarations>+≡
    public :: models_7

<Models: tests>+≡
    subroutine models_7 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(var_list_t), pointer :: var_list
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_7"
        write (u, "(A)")  "* Purpose: read a model from file &

```

```

        &with scheme selection"
write (u, *)

open (newunit=um, file="Test7.mdl", status="replace", action="readwrite")
write (um, "(A)") 'model "Test7"'
write (um, "(A)") ' schemes = "foo", "bar", "gee"'
write (um, "(A)") ''
write (um, "(A)") ' select scheme'
write (um, "(A)") ' scheme "foo"'
write (um, "(A)") ' parameter a = 1'
write (um, "(A)") ' derived b = 2 * a'
write (um, "(A)") ' scheme other'
write (um, "(A)") ' parameter b = 4'
write (um, "(A)") ' derived a = b / 2'
write (um, "(A)") ' end select'
write (um, "(A)") ''
write (um, "(A)") ' parameter c = 3'
write (um, "(A)") ''
write (um, "(A)") ' select scheme'
write (um, "(A)") ' scheme "foo", "gee"'
write (um, "(A)") ' derived d = b + c'
write (um, "(A)") ' scheme other'
write (um, "(A)") ' unused d'
write (um, "(A)") ' end select'

rewind (um)
do
    read (um, "(A)", end=1) buffer
    write (u, "(A)") trim (buffer)
end do
1 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

write (u, *)
write (u, "(A)")  "** Model output, default scheme (= foo)"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model)
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

write (u, *)
write (u, "(A)")  "** Model output, scheme foo"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model, scheme = var_str ("foo"))

```



```

call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

write (u, *)
write (u, "(A)")  "* Model output, scheme bar"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model, scheme = var_str ("bar"))
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

write (u, *)
write (u, "(A)")  "* Model output, scheme gee"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model, scheme = var_str ("gee"))
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_7"

contains

subroutine show_var_list ()
    write (u, *)
    write (u, "(A)")  "* Variable list"
    write (u, *)
    var_list => model%get_var_list_ptr ()
    call var_list%write (u)
end subroutine show_var_list

subroutine show_par_array ()
    real(default), dimension(:), allocatable :: par
    integer :: n
    write (u, *)
    write (u, "(A)")  "* Parameter array"
    write (u, *)
    n = model%get_n_real ()

```

```

        allocate (par (n))
        call model%real_parameters_to_array (par)
        write (u, 1) par
1       format (1X,F6.3)
        end subroutine show_par_array

end subroutine models_7

```

Read and handle UFO model

Read a model from file which is considered as an UFO model. In fact, it is a mock model file which just follows our naming convention for UFO models. Compare this to an equivalent non-UFO model.

```

<Models: execute tests>+≡
    call test (models_8, "models_8", &
               "handle UFO-derived models", &
               u, results)

<Models: test declarations>+≡
    public :: models_8

<Models: tests>+≡
    subroutine models_8 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(string_t) :: model_name
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_8"
        write (u, "(A)")  "* Purpose: distinguish models marked as UFO-derived"
        write (u, *)

        call os_data%init ()

        call show_model_list_status ()
        model_name = "models_8_M"

        write (u, *)
        write (u, "(A)")  "* Write WHIZARD model"
        write (u, *)

        open (newunit=um, file=char (model_name // ".mdl"), &
              status="replace", action="readwrite")
        write (um, "(A)")  'model "models_8_M"'
        write (um, "(A)")  ' parameter a = 1'

        rewind (um)
        do
            read (um, "(A)", end=1) buffer
            write (u, "(A)") trim (buffer)

```

```

end do
1  continue
   close (um)

   write (u, *)
   write (u, "(A)")  "** Write UFO model"
   write (u, *)

   open (newunit=um, file=char (model_name // ".ufo.mdl"), &
        status="replace", action="readwrite")
   write (um, "(A)")  'model "models_8_M"'
   write (um, "(A)")  ' parameter a = 2'

   rewind (um)
   do
       read (um, "(A)", end=2)  buffer
       write (u, "(A)")  trim (buffer)
   end do
2  continue
   close (um)

   call syntax_model_file_init ()
   call os_data%init ()

   write (u, *)
   write (u, "(A)")  "** Read WHIZARD model"
   write (u, *)

   call model_list%read_model (model_name, model_name // ".mdl", &
        os_data, model)
   call model%write (u, show_md5sum=.false.)

   call show_model_list_status ()

   write (u, *)
   write (u, "(A)")  "** Read UFO model"
   write (u, *)

   call model_list%read_model (model_name, model_name // ".ufo.mdl", &
        os_data, model, ufo=.true., rebuild_mdl = .false.)
   call model%write (u, show_md5sum=.false.)

   call show_model_list_status ()

   write (u, *)
   write (u, "(A)")  "** Reload WHIZARD model"
   write (u, *)

   call model_list%read_model (model_name, model_name // ".mdl", &
        os_data, model)
   call model%write (u, show_md5sum=.false.)

   call show_model_list_status ()

```

```

write (u, *)
write (u, "(A)")  "* Reload UFO model"
write (u, *)

call model_list%read_model (model_name, model_name // ".ufo.mdl", &
    os_data, model, ufo=.true., rebuild_md1 = .false.)
call model%write (u, show_md5sum=.false.)

call show_model_list_status ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_8"

contains

subroutine show_model_list_status ()
    write (u, "(A)")  "* Model list status"
    write (u, *)
    write (u, "(A,1x,L1)")  "WHIZARD model exists =", &
        model_list%model_exists (model_name)
    write (u, "(A,1x,L1)")  "UFO model exists =", &
        model_list%model_exists (model_name, ufo=.true.)
end subroutine show_model_list_status

end subroutine models_8

```

Generate UFO model file

Generate the necessary .ufo.mdl file from source, calling OMega, and load the model.

Note: There must not be another unit test which works with the same UFO model. The model file is deleted explicitly at the end of this test.

```

<Models: execute tests>+≡
    call test (models_9, "models_9", &
        "generate UFO-derived model file", &
        u, results)

<Models: test declarations>+≡
    public :: models_9

<Models: tests>+≡
    subroutine models_9 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list

```

```

type(string_t) :: model_name, model_file_name
type(model_t), pointer :: model

write (u, "(A)")  "* Test output: models_9"
write (u, "(A)")  "* Purpose: enable the UFO Standard Model (test version)"
write (u, *)

call os_data%init ()
call syntax_model_file_init ()

os_data%whizard_modelpath_ufo = "../models/UFO"

model_name = "SM"
model_file_name = model_name // ".models_9" // ".ufo.mdl"

write (u, "(A)")  "* Generate and read UFO model"
write (u, *)

call delete_file (char (model_file_name))

call model_list%read_model (model_name, model_file_name, os_data, model, ufo=.true.)
call model%write (u, show_md5sum=.false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_9"

end subroutine models_9

```

Read model with schemes

Read a model from file which contains `slha_entry` qualifiers for parameters.

```

<Models: execute tests>+≡
  call test (models_10, "models_10", &
    "handle slha_entry option", &
    u, results)

<Models: test declarations>+≡
  public :: models_10

<Models: tests>+≡
  subroutine models_10 (u)
    integer, intent(in) :: u
    integer :: um
    character(80) :: buffer
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(var_list_t), pointer :: var_list
    type(model_t), pointer :: model

```

```

type(string_t), dimension(:), allocatable :: slha_block_name
integer :: i

write (u, "(A)")  "*" Test output: models_10"
write (u, "(A)")  "*" Purpose: read a model from file &
                  &with slha_entry options"
write (u, *)

open (newunit=um, file="Test10.mdl", status="replace", action="readwrite")
write (um, "(A)") 'model "Test10"'
write (um, "(A)") ' parameter a = 1    slha_entry F00 1'
write (um, "(A)") ' parameter b = 4    slha_entry BAR 2 1'

rewind (um)
do
    read (um, "(A)", end=1) buffer
    write (u, "(A)") trim (buffer)
end do
1 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

write (u, *)
write (u, "(A)")  "*" Model output, default scheme (= foo)"
write (u, *)

call model_list%read_model (var_str ("Test10"), var_str ("Test10.mdl"), &
                           os_data, model)
call model%write (u, show_md5sum=.false.)

write (u, *)
write (u, "(A)")  "*" Check that model contains slha_entry options"
write (u, *)

write (u, "(A,1x,L1)") &
    "supports_custom_slha =", model%supports_custom_slha ()

write (u, *)
write (u, "(A)")  "custom_slha_blocks ="
call model%get_custom_slha_blocks (slha_block_name)
do i = 1, size (slha_block_name)
    write (u, "(1x,A)", advance="no") char (slha_block_name(i))
end do
write (u, *)

write (u, *)
write (u, "(A)")  "*" Parameter lookup"
write (u, *)

call show_slha ("F00", [1])
call show_slha ("F00", [2])
call show_slha ("BAR", [2, 1])

```

```

call show_slha ("GEE", [3])

write (u, *)
write (u, "(A)")  "** Modify parameter via SLHA block interface"
write (u, *)

call model%slha_set_par (var_str ("FOO"), [1], 7._default)
call show_slha ("FOO", [1])

write (u, *)
write (u, "(A)")  "** Show var list with modified parameter"
write (u, *)

call show_var_list ()

write (u, *)
write (u, "(A)")  "** Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "** Test output end: models_10"

contains

subroutine show_slha (block_name, block_index)
  character(*), intent(in) :: block_name
  integer, dimension(:), intent(in) :: block_index
  class(modelpar_data_t), pointer :: par_data
  write (u, "(A,(1x,I0))", advance="no") block_name, block_index
  write (u, "(' => ')", advance="no")
  call model%slha_lookup (var_str (block_name), block_index, par_data)
  if (associated (par_data)) then
    call par_data%write (u)
    write (u, *)
  else
    write (u, "(' - ')")
  end if
end subroutine show_slha

subroutine show_var_list ()
  var_list => model%get_var_list_ptr ()
  call var_list%write (u)
end subroutine show_var_list

end subroutine models_10

```

28.5 The SUSY Les Houches Accord

The SUSY Les Houches Accord defines a standard interfaces for storing the physics data of SUSY models. Here, we provide the means for reading, storing, and writing such data.

```
<slha_interface.f90>≡  
  <File header>  
  
  module slha_interface  
  
    <Use kinds>  
    <Use strings>  
    use os_interface  
    use lexers  
    use parser  
    use variables  
    use models  
  
    <Standard module head>  
  
    <SLHA: public>  
  
    <SLHA: types>  
  
    interface  
    <SLHA: sub interfaces>  
    end interface  
  
    save  
  
  end module slha_interface  
<slha_interface_sub.f90>≡  
  <File header>  
  
  submodule (slha_interface) slha_interface_s  
  
    use io_units  
    use constants  
    use string_utils, only: upper_case  
    use system_defs, only: VERSION_STRING  
    use system_defs, only: EOF  
    use diagnostics  
    use ifiles  
    use syntax_rules  
  
    implicit none  
  
    <SLHA: parameters>  
  
    <SLHA: variables>  
  
  contains
```



```
⟨SLHA: procedures⟩
```

```
end submodule slha_interface_s
```

28.5.1 Preprocessor

SLHA is a mixed-format standard. It should be read in assuming free format (but line-oriented), but it has some fixed-format elements.

To overcome this difficulty, we implement a preprocessing step which transforms the SLHA into a format that can be swallowed by our generic free-format lexer and parser. Each line with a blank first character is assumed to be a data line. We prepend a 'DATA' keyword to these lines. Furthermore, to enforce line-orientation, each line is appended a '\$' key which is recognized by the parser. To do this properly, we first remove trailing comments, and skip lines consisting only of comments.

The preprocessor reads from a stream and puts out an `ifile`. Blocks that are not recognized are skipped. For some blocks, data items are quoted, so they can be read as strings if necessary.

A name clash occurs if the block name is identical to a keyword. This can happen for custom SLHA models and files. In that case, we prepend an underscore, which will be silently suppressed where needed.

```
⟨SLHA: parameters⟩≡
```

```
integer, parameter :: MODE_SKIP = 0, MODE_DATA = 1, MODE_INFO = 2
```

```
⟨SLHA: procedures⟩≡
```

```
subroutine slha_preprocess (stream, custom_block_name, ifile)
  type(stream_t), intent(inout), target :: stream
  type(string_t), dimension(:), intent(in) :: custom_block_name
  type(ifile_t), intent(out) :: ifile
  type(string_t) :: buffer, line, item
  integer :: iostat
  integer :: mode
  mode = MODE
  SCAN_FILE: do
    call stream_get_record (stream, buffer, iostat)
    select case (iostat)
    case (0)
      call split (buffer, line, "#")
      if (len_trim (line) == 0) cycle SCAN_FILE
      select case (char (extract (line, 1, 1)))
      case ("B", "b")
        call check_block_handling (line, custom_block_name, mode)
        call ifile_append (ifile, line // "$")
      case ("D", "d")
        mode = MODE_DATA
        call ifile_append (ifile, line // "$")
      case (" ")
        select case (mode)
        case (MODE_DATA)
          call ifile_append (ifile, "DATA" // line // "$")
        case (MODE_INFO)
```

```

        line = adjustl (line)
        call split (line, item, " ")
        call ifile_append (ifile, "INFO" // " " // item // " " &
            // ' "' // trim (adjustl (line)) // ' " $')
    end select
case default
    call msg_message (char (line))
    call msg_fatal ("SLHA: Incomprehensible line")
end select
case (EOF)
    exit SCAN_FILE
case default
    call msg_fatal ("SLHA: I/O error occurred while reading SLHA input")
end select
end do SCAN_FILE
end subroutine slha_preprocess

```

Return the mode that we should treat this block with. We add the `custom_block_name` array to the set of supported blocks, which otherwise includes only hard-coded block names. Those custom blocks are data blocks.

Unknown blocks will be skipped altogether. The standard does not specify their internal format at all, so we must not parse their content.

If the name of a (custom) block clashes with a keyword of the SLHA syntax, we append an underscore to the block name, modifying the current line string. This should be silently suppressed when actually parsing block names.

```

<SLHA: procedures> +=
subroutine check_block_handling (line, custom_block_name, mode)
    type(string_t), intent(inout) :: line
    type(string_t), dimension(:), intent(in) :: custom_block_name
    integer, intent(out) :: mode
    type(string_t) :: buffer, key, block_name
    integer :: i
    buffer = trim (line)
    call split (buffer, key, " ")
    buffer = adjustl (buffer)
    call split (buffer, block_name, " ")
    buffer = adjustl (buffer)
    block_name = trim (adjustl (upper_case (block_name)))
    select case (char (block_name))
    case ("MODSEL", "MINPAR", "SMINPUTS")
        mode = MODE_DATA
    case ("MASS")
        mode = MODE_DATA
    case ("NMIX", "UMIX", "VMIX", "STOPMIX", "SBOTMIX", "STAUMIX")
        mode = MODE_DATA
    case ("NMHMIX", "NMAMIX", "NMNMIX", "NMSSMRUN")
        mode = MODE_DATA
    case ("ALPHA", "HMIX")
        mode = MODE_DATA
    case ("AU", "AD", "AE")
        mode = MODE_DATA
    case ("SPINFO", "DCINFO")
        mode = MODE_INFO
    end select
end subroutine

```

```

case default
  mode = MODE_SKIP
  CHECK_CUSTOM_NAMES: do i = 1, size (custom_block_name)
    if (block_name == custom_block_name(i)) then
      mode = MODE_DATA
      call mangle_keywords (block_name)
      line = key // " " // block_name // " " // trim (buffer)
      exit CHECK_CUSTOM_NAMES
    end if
  end do CHECK_CUSTOM_NAMES
end select
end subroutine check_block_handling

```

Append an underscore to specific block names:

```

<SLHA: procedures>+=
subroutine mangle_keywords (name)
  type(string_t), intent(inout) :: name
  select case (char (name))
  case ("BLOCK", "DATA", "INFO", "DECAY")
    name = name // "_"
  end select
end subroutine mangle_keywords

```

Remove the underscore again:

```

<SLHA: procedures>+=
subroutine demangle_keywords (name)
  type(string_t), intent(inout) :: name
  select case (char (name))
  case ("BLOCK_", "DATA_", "INFO_", "DECAY_")
    name = extract (name, 1, len(name)-1)
  end select
end subroutine demangle_keywords

```

28.5.2 Lexer and syntax

```

<SLHA: variables>=
  type(syntax_t), target :: syntax_slha

<SLHA: public>=
  public :: syntax_slha_init

<SLHA: sub interfaces>=
  module subroutine syntax_slha_init ()
    end subroutine syntax_slha_init

<SLHA: procedures>+=
  module subroutine syntax_slha_init ()
    type(ifile_t) :: ifile
    call define_slha_syntax (ifile)
    call syntax_init (syntax_slha, ifile)
    call ifile_final (ifile)
  end subroutine syntax_slha_init

```

```

<SLHA: public>+=
    public :: syntax_slha_final

<SLHA: sub interfaces>+=
    module subroutine syntax_slha_final ()
    end subroutine syntax_slha_final

<SLHA: procedures>+=
    module subroutine syntax_slha_final ()
    call syntax_final (syntax_slha)
    end subroutine syntax_slha_final

<SLHA: public>+=
    public :: syntax_slha_write

<SLHA: sub interfaces>+=
    module subroutine syntax_slha_write (unit)
    integer, intent(in), optional :: unit
    end subroutine syntax_slha_write

<SLHA: procedures>+=
    module subroutine syntax_slha_write (unit)
    integer, intent(in), optional :: unit
    call syntax_write (syntax_slha, unit)
    end subroutine syntax_slha_write

<SLHA: procedures>+=
    subroutine define_slha_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "SEQ slha = chunk*")
    call ifile_append (ifile, "ALT chunk = block_def | decay_def")
    call ifile_append (ifile, "SEQ block_def = " &
        // "BLOCK blockgen '$' block_line*")
    call ifile_append (ifile, "ALT blockgen = block_spec | q_spec")
    call ifile_append (ifile, "KEY BLOCK")
    call ifile_append (ifile, "SEQ q_spec = QNUMBERS pdg_code")
    call ifile_append (ifile, "KEY QNUMBERS")
    call ifile_append (ifile, "SEQ block_spec = block_name qvalue?")
    call ifile_append (ifile, "IDE block_name")
    call ifile_append (ifile, "SEQ qvalue = qname '=' qitem")
    call ifile_append (ifile, "IDE qname")
    call ifile_append (ifile, "ALT qitem = signed_real | real")
    call ifile_append (ifile, "SEQ signed_real = sign real")
    call ifile_append (ifile, "KEY '='")
    call ifile_append (ifile, "REA real")
    call ifile_append (ifile, "KEY '$'")
    call ifile_append (ifile, "ALT block_line = block_data | block_info")
    call ifile_append (ifile, "SEQ block_data = DATA data_line '$'")
    call ifile_append (ifile, "KEY DATA")
    call ifile_append (ifile, "SEQ data_line = data_item+")
    call ifile_append (ifile, "ALT data_item = signed_number | number")
    call ifile_append (ifile, "SEQ signed_number = sign number")
    call ifile_append (ifile, "ALT sign = '+' | '-'")
    call ifile_append (ifile, "ALT number = integer | real")
    call ifile_append (ifile, "INT integer")
    call ifile_append (ifile, "KEY '-'")

```

```

call ifile_append (ifile, "KEY '+'")
call ifile_append (ifile, "SEQ block_info = INFO info_line '$'")
call ifile_append (ifile, "KEY INFO")
call ifile_append (ifile, "SEQ info_line = integer string_literal")
call ifile_append (ifile, "QUO string_literal = '...'"")
call ifile_append (ifile, "SEQ decay_def = " &
    // "DECAY decay_spec '$' decay_data*")
call ifile_append (ifile, "KEY DECAY")
call ifile_append (ifile, "SEQ decay_spec = pdg_code data_item")
call ifile_append (ifile, "ALT pdg_code = signed_integer | integer")
call ifile_append (ifile, "SEQ signed_integer = sign integer")
call ifile_append (ifile, "SEQ decay_data = DATA decay_line '$'")
call ifile_append (ifile, "SEQ decay_line = data_item integer pdg_code+")
end subroutine define_slha_syntax

```

The SLHA specification allows for string data items in certain places. Currently, we do not interpret them, but the strings, which are not quoted, must be parsed somehow. The hack for this problem is to allow essentially all characters as special characters, so the string can be read before it is discarded.

<SLHA: public>+≡

```
public :: lexer_init_slha
```

<SLHA: sub interfaces>+≡

```

module subroutine lexer_init_slha (lexer)
    type(lexer_t), intent(out) :: lexer
end subroutine lexer_init_slha

```

<SLHA: procedures>+≡

```

module subroutine lexer_init_slha (lexer)
    type(lexer_t), intent(out) :: lexer
    call lexer_init (lexer, &
        comment_chars = "#", &
        quote_chars = "'", &
        quote_match = "'", &
        single_chars = "+-=$", &
        special_class = [ " " ], &
        keyword_list = syntax_get_keyword_list_ptr (syntax_slha), &
        upper_case_keywords = .true.) ! $
end subroutine lexer_init_slha

```

28.5.3 Interpreter

Find blocks

From the parse tree, find the node that represents a particular block. If **required** is true, issue an error if not found. Since **block_name** is always invoked with capital letters, we have to capitalize **pn_block_name**.

<SLHA: procedures>+≡

```

function slha_get_block_ptr &
    (parse_tree, block_name, required) result (pn_block)
    type(parse_node_t), pointer :: pn_block
    type(parse_tree_t), intent(in) :: parse_tree

```

```

type(string_t), intent(in) :: block_name
type(string_t) :: block_def
logical, intent(in) :: required
type(parse_node_t), pointer :: pn_root, pn_block_spec, pn_block_name
pn_root => parse_tree%get_root_ptr ()
pn_block => parse_node_get_sub_ptr (pn_root)
do while (associated (pn_block))
  select case (char (parse_node_get_rule_key (pn_block)))
    case ("block_def")
      pn_block_spec => parse_node_get_sub_ptr (pn_block, 2)
      pn_block_name => parse_node_get_sub_ptr (pn_block_spec)
      select case (char (pn_block_name%get_rule_key ()))
        case ("block_name")
          block_def = trim (adjustl (upper_case &
            (pn_block_name%get_string ())))
        case ("QNUMBERS")
          block_def = "QNUMBERS"
      end select
      if (block_def == block_name) then
        return
      end if
    end select
    pn_block => parse_node_get_next_ptr (pn_block)
  end do
  if (required) then
    call msg_fatal ("SLHA: block '" // char (block_name) // "' not found")
  end if
end function slha_get_block_ptr

```

Scan the file for the first/next DECAY block.

(SLHA: procedures)+≡

```

function slha_get_first_decay_ptr (parse_tree) result (pn_decay)
  type(parse_node_t), pointer :: pn_decay
  type(parse_tree_t), intent(in) :: parse_tree
  type(parse_node_t), pointer :: pn_root
  pn_root => parse_tree%get_root_ptr ()
  pn_decay => parse_node_get_sub_ptr (pn_root)
  do while (associated (pn_decay))
    select case (char (parse_node_get_rule_key (pn_decay)))
      case ("decay_def")
        return
    end select
    pn_decay => parse_node_get_next_ptr (pn_decay)
  end do
end function slha_get_first_decay_ptr

function slha_get_next_decay_ptr (pn_block) result (pn_decay)
  type(parse_node_t), pointer :: pn_decay
  type(parse_node_t), intent(in), target :: pn_block
  pn_decay => parse_node_get_next_ptr (pn_block)
  do while (associated (pn_decay))
    select case (char (parse_node_get_rule_key (pn_decay)))
      case ("decay_def")
        return
    end select
  end do
end function slha_get_next_decay_ptr

```

```

        end select
        pn_decay => parse_node_get_next_ptr (pn_decay)
    end do
end function slha_get_next_decay_ptr

```

Extract and transfer data from blocks

Given the parse node of a block, find the parse node of a particular switch or data line. Return this node and the node of the data item following the integer code.

(SLHA: procedures)+≡

```

subroutine slha_find_index_ptr (pn_block, pn_data, pn_item, code)
    type(parse_node_t), intent(in), target :: pn_block
    type(parse_node_t), intent(out), pointer :: pn_data
    type(parse_node_t), intent(out), pointer :: pn_item
    integer, intent(in) :: code
    pn_data => parse_node_get_sub_ptr (pn_block, 4)
    call slha_next_index_ptr (pn_data, pn_item, code)
end subroutine slha_find_index_ptr

subroutine slha_find_index_pair_ptr (pn_block, pn_data, pn_item, code1, code2)
    type(parse_node_t), intent(in), target :: pn_block
    type(parse_node_t), intent(out), pointer :: pn_data
    type(parse_node_t), intent(out), pointer :: pn_item
    integer, intent(in) :: code1, code2
    pn_data => parse_node_get_sub_ptr (pn_block, 4)
    call slha_next_index_pair_ptr (pn_data, pn_item, code1, code2)
end subroutine slha_find_index_pair_ptr

```

Starting from the pointer to a data line, find a data line with the given integer code.

(SLHA: procedures)+≡

```

subroutine slha_next_index_ptr (pn_data, pn_item, code)
    type(parse_node_t), intent(inout), pointer :: pn_data
    integer, intent(in) :: code
    type(parse_node_t), intent(out), pointer :: pn_item
    type(parse_node_t), pointer :: pn_line, pn_code
    do while (associated (pn_data))
        pn_line => parse_node_get_sub_ptr (pn_data, 2)
        pn_code => parse_node_get_sub_ptr (pn_line)
        select case (char (parse_node_get_rule_key (pn_code)))
            case ("integer")
                if (parse_node_get_integer (pn_code) == code) then
                    pn_item => parse_node_get_next_ptr (pn_code)
                    return
                end if
            end select
        pn_data => parse_node_get_next_ptr (pn_data)
    end do
    pn_item => null ()
end subroutine slha_next_index_ptr

```

Starting from the pointer to a data line, find a data line with the given integer code pair.

<SLHA: procedures>+≡

```

subroutine slha_next_index_pair_ptr (pn_data, pn_item, code1, code2)
  type(parse_node_t), intent(inout), pointer :: pn_data
  integer, intent(in) :: code1, code2
  type(parse_node_t), intent(out), pointer :: pn_item
  type(parse_node_t), pointer :: pn_line, pn_code1, pn_code2
  do while (associated (pn_data))
    pn_line => parse_node_get_sub_ptr (pn_data, 2)
    pn_code1 => parse_node_get_sub_ptr (pn_line)
    select case (char (parse_node_get_rule_key (pn_code1)))
    case ("integer")
      if (parse_node_get_integer (pn_code1) == code1) then
        pn_code2 => parse_node_get_next_ptr (pn_code1)
        if (associated (pn_code2)) then
          select case (char (parse_node_get_rule_key (pn_code2)))
          case ("integer")
            if (parse_node_get_integer (pn_code2) == code2) then
              pn_item => parse_node_get_next_ptr (pn_code2)
              return
            end if
          end select
        end if
      end if
    end select
    pn_data => parse_node_get_next_ptr (pn_data)
  end do
  pn_item => null ()
end subroutine slha_next_index_pair_ptr

```

Handle info data

Return all strings with index i. The result is an allocated string array. Since we do not know the number of matching entries in advance, we build an intermediate list which is transferred to the final array and deleted before exiting.

<SLHA: types>≡

```

type :: str_entry_t
  type(string_t) :: str
  type(str_entry_t), pointer :: next => null ()
end type str_entry_t

```

<SLHA: procedures>+≡

```

subroutine retrieve_strings_in_block (pn_block, code, str_array)
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code
  type(string_t), dimension(:), allocatable, intent(out) :: str_array
  type(parse_node_t), pointer :: pn_data, pn_item
  type(str_entry_t), pointer :: first => null ()
  type(str_entry_t), pointer :: current => null ()
  integer :: n
  n = 0

```



```

call slha_find_index_ptr (pn_block, pn_data, pn_item, code)
if (associated (pn_item)) then
  n = n + 1
  allocate (first)
  first%str = parse_node_get_string (pn_item)
  current => first
  do while (associated (pn_data))
    pn_data => parse_node_get_next_ptr (pn_data)
    call slha_next_index_ptr (pn_data, pn_item, code)
    if (associated (pn_item)) then
      n = n + 1
      allocate (current%next)
      current => current%next
      current%str = parse_node_get_string (pn_item)
    end if
  end do
  allocate (str_array (n))
  n = 0
  do while (associated (first))
    n = n + 1
    current => first
    str_array(n) = current%str
    first => first%next
    deallocate (current)
  end do
else
  allocate (str_array (0))
end if
end subroutine retrieve_strings_in_block

```

Transfer data from SLHA to variables

Extract real parameter with index *i*. If it does not exist, retrieve it from the variable list, using the given name.

(SLHA: procedures) +=

```

function get_parameter_in_block (pn_block, code, name, var_list) result (var)
  real(default) :: var
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_data, pn_item
  call slha_find_index_ptr (pn_block, pn_data, pn_item, code)
  if (associated (pn_item)) then
    var = get_real_parameter (pn_item)
  else
    var = var_list%get_rval (name)
  end if
end function get_parameter_in_block

```

Extract a real data item with index *i*. If it does exist, set it in the variable list, using the given name. If the variable is not present in the variable list, ignore

it.

```
(SLHA: procedures)+≡  
subroutine set_data_item (pn_block, code, name, var_list)  
  type(parse_node_t), intent(in), target :: pn_block  
  integer, intent(in) :: code  
  type(string_t), intent(in) :: name  
  type(var_list_t), intent(inout), target :: var_list  
  type(parse_node_t), pointer :: pn_data, pn_item  
  call slha_find_index_ptr (pn_block, pn_data, pn_item, code)  
  if (associated (pn_item)) then  
    call var_list%set_real (name, get_real_parameter (pn_item), &  
      is_known=.true., ignore=.true.)  
  end if  
end subroutine set_data_item
```

Extract a real matrix element with index i,j. If it does exists, set it in the variable list, using the given name. If the variable is not present in the variable list, ignore it.

```
(SLHA: procedures)+≡  
subroutine set_matrix_element (pn_block, code1, code2, name, var_list)  
  type(parse_node_t), intent(in), target :: pn_block  
  integer, intent(in) :: code1, code2  
  type(string_t), intent(in) :: name  
  type(var_list_t), intent(inout), target :: var_list  
  type(parse_node_t), pointer :: pn_data, pn_item  
  call slha_find_index_pair_ptr (pn_block, pn_data, pn_item, code1, code2)  
  if (associated (pn_item)) then  
    call var_list%set_real (name, get_real_parameter (pn_item), &  
      is_known=.true., ignore=.true.)  
  end if  
end subroutine set_matrix_element
```

Transfer data from variables to SLHA

Get a real/integer parameter with index i from the variable list and write it to the current output file. In the integer case, we account for the fact that the variable is type real. If it does not exist, do nothing.

```
(SLHA: procedures)+≡  
subroutine write_integer_data_item (u, code, name, var_list, comment)  
  integer, intent(in) :: u  
  integer, intent(in) :: code  
  type(string_t), intent(in) :: name  
  type(var_list_t), intent(in) :: var_list  
  character(*), intent(in) :: comment  
  integer :: item  
  if (var_list%contains (name)) then  
    item = nint (var_list%get_rval (name))  
    call write_integer_parameter (u, code, item, comment)  
  end if  
end subroutine write_integer_data_item
```

```

subroutine write_real_data_item (u, code, name, var_list, comment)
  integer, intent(in) :: u
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in) :: var_list
  character(*), intent(in) :: comment
  real(default) :: item
  if (var_list%contains (name)) then
    item = var_list%get_rval (name)
    call write_real_parameter (u, code, item, comment)
  end if
end subroutine write_real_data_item

```

Get a real data item with two integer indices from the variable list and write it to the current output file. If it does not exist, do nothing.

(SLHA: procedures)+≡

```

subroutine write_matrix_element (u, code1, code2, name, var_list, comment)
  integer, intent(in) :: u
  integer, intent(in) :: code1, code2
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in) :: var_list
  character(*), intent(in) :: comment
  real(default) :: item
  if (var_list%contains (name)) then
    item = var_list%get_rval (name)
    call write_real_matrix_element (u, code1, code2, item, comment)
  end if
end subroutine write_matrix_element

```

28.5.4 Auxiliary function

Write a block header.

(SLHA: procedures)+≡

```

subroutine write_block_header (u, name, comment)
  integer, intent(in) :: u
  character(*), intent(in) :: name, comment
  write (u, "(A,1x,A,3x,'#',1x,A)") "BLOCK", name, comment
end subroutine write_block_header

```

Extract a real parameter that may be defined real or integer, signed or unsigned.

(SLHA: procedures)+≡

```

function get_real_parameter (pn_item) result (var)
  real(default) :: var
  type(parse_node_t), intent(in), target :: pn_item
  type(parse_node_t), pointer :: pn_sign, pn_var
  integer :: sign
  select case (char (parse_node_get_rule_key (pn_item)))
  case ("signed_number")
    pn_sign => parse_node_get_sub_ptr (pn_item)
    pn_var => parse_node_get_next_ptr (pn_sign)
    select case (char (parse_node_get_key (pn_sign)))

```

```

        case ("+"); sign = +1
        case ("-"); sign = -1
    end select
    case default
        sign = +1
        pn_var => pn_item
    end select
    select case (char (parse_node_get_rule_key (pn_var)))
    case ("integer"); var = sign * parse_node_get_integer (pn_var)
    case ("real");    var = sign * parse_node_get_real (pn_var)
    end select
end function get_real_parameter

```

Auxiliary: Extract an integer parameter that may be defined signed or unsigned.
A real value is an error.

(SLHA: procedures)+≡

```

function get_integer_parameter (pn_item) result (var)
    integer :: var
    type(parse_node_t), intent(in), target :: pn_item
    type(parse_node_t), pointer :: pn_sign, pn_var
    integer :: sign
    select case (char (parse_node_get_rule_key (pn_item)))
    case ("signed_integer")
        pn_sign => parse_node_get_sub_ptr (pn_item)
        pn_var => parse_node_get_next_ptr (pn_sign)
        select case (char (parse_node_get_key (pn_sign)))
        case ("+"); sign = +1
        case ("-"); sign = -1
        end select
    case ("integer")
        sign = +1
        pn_var => pn_item
    case default
        call parse_node_write (pn_var)
        call msg_error ("SLHA: Integer parameter expected")
        var = 0
        return
    end select
    var = sign * parse_node_get_integer (pn_var)
end function get_integer_parameter

```

Write an integer parameter with a single index directly to file, using the required output format.

(SLHA: procedures)+≡

```

subroutine write_integer_parameter (u, code, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code
    integer, intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I9, 3x, 3x, I9, 4x, 3x, '#', 1x, A)
    write (u, 1) code, item, comment
end subroutine write_integer_parameter

```

Write a real parameter with two indices directly to file, using the required output format.

```
<SLHA: procedures>+=
  subroutine write_real_parameter (u, code, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code
    real(default), intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I9, 3x, 1P, E16.8, 0P, 3x, '#', 1x, A)
    write (u, 1) code, item, comment
  end subroutine write_real_parameter
```

Write a real parameter with a single index directly to file, using the required output format.

```
<SLHA: procedures>+=
  subroutine write_real_matrix_element (u, code1, code2, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code1, code2
    real(default), intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I2, 1x, I2, 3x, 1P, E16.8, 0P, 3x, '#', 1x, A)
    write (u, 1) code1, code2, item, comment
  end subroutine write_real_matrix_element
```

The concrete SLHA interpreter

SLHA codes for particular physics models

```
<SLHA: parameters>+=
  integer, parameter :: MDL_MSSM = 0
  integer, parameter :: MDL_NMSSM = 1
```

Take the parse tree and extract relevant data. Select the correct model and store all data that is present in the appropriate variable list. Finally, update the variable record.

We assume that if the model contains custom SLHA block names, we just have to scan those to get complete information. Block names could coincide with the SLHA standard block names, but we do not have to assume this. This will be the situation for an UFO-generated file. In particular, an UFO file should contain all expressions necessary for computing dependent parameters, so we can forget about the strict SLHA standard and its hard-coded conventions.

If there are no custom SLHA block names, we should assume that the model is a standard SUSY model, and the parameters and hard-coded blocks can be read as specified by the original SLHA standard. There are hard-coded block names and parameter calculations.

Public for use in unit test.

```
<SLHA: public>+=
  public :: slha_interpret_parse_tree

<SLHA: sub interfaces>+=
  module subroutine slha_interpret_parse_tree &
    (parse_tree, model, input, spectrum, decays)
```

```

        type(parse_tree_t), intent(in) :: parse_tree
        type(model_t), intent(inout), target :: model
        logical, intent(in) :: input, spectrum, decays
    end subroutine slha_interpret_parse_tree
<SLHA: procedures>+≡
module subroutine slha_interpret_parse_tree &
    (parse_tree, model, input, spectrum, decays)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    logical, intent(in) :: input, spectrum, decays
    logical :: errors
    integer :: mssm_type
    if (model%supports_custom_slha ()) then
        call slha_handle_custom_file (parse_tree, model)
    else
        call slha_handle_MODSEL (parse_tree, model, mssm_type)
        if (input) then
            call slha_handle_SMINPUTS (parse_tree, model)
            call slha_handle_MINPAR (parse_tree, model, mssm_type)
        end if
        if (spectrum) then
            call slha_handle_info_block (parse_tree, "SPINFO", errors)
            if (errors) return
            call slha_handle_MASS (parse_tree, model)
            call slha_handle_matrix_block (parse_tree, "NMIX", "mn_", 4, 4, model)
            call slha_handle_matrix_block (parse_tree, "NMNMIX", "mixn_", 5, 5, model)
            call slha_handle_matrix_block (parse_tree, "UMIX", "mu_", 2, 2, model)
            call slha_handle_matrix_block (parse_tree, "VMIX", "mv_", 2, 2, model)
            call slha_handle_matrix_block (parse_tree, "STOPMIX", "mt_", 2, 2, model)
            call slha_handle_matrix_block (parse_tree, "SBOTMIX", "mb_", 2, 2, model)
            call slha_handle_matrix_block (parse_tree, "STAUMIX", "ml_", 2, 2, model)
            call slha_handle_matrix_block (parse_tree, "NMHMX", "mixh0_", 3, 3, model)
            call slha_handle_matrix_block (parse_tree, "NMAMIX", "mixa0_", 2, 3, model)
            call slha_handle_ALPHA (parse_tree, model)
            call slha_handle_HMIX (parse_tree, model)
            call slha_handle_NMSSMRUN (parse_tree, model)
            call slha_handle_matrix_block (parse_tree, "AU", "Au_", 3, 3, model)
            call slha_handle_matrix_block (parse_tree, "AD", "Ad_", 3, 3, model)
            call slha_handle_matrix_block (parse_tree, "AE", "Ae_", 3, 3, model)
        end if
    end if
    if (decays) then
        call slha_handle_info_block (parse_tree, "DCINFO", errors)
        if (errors) return
        call slha_handle_decays (parse_tree, model)
    end if
end subroutine slha_interpret_parse_tree

```

Info blocks

Handle the informational blocks SPINFO and DCINFO. The first two items are program name and version. Items with index 3 are warnings. Items with index

4 are errors. We reproduce these as WHIZARD warnings and errors.

<SLHA: procedures>+≡

```

subroutine slha_handle_info_block (parse_tree, block_name, errors)
  type(parse_tree_t), intent(in) :: parse_tree
  character(*), intent(in) :: block_name
  logical, intent(out) :: errors
  type(parse_node_t), pointer :: pn_block
  type(string_t), dimension(:), allocatable :: msg
  integer :: i
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str (block_name), required=.true.)
  if (.not. associated (pn_block)) then
    call msg_error ("SLHA: Missing info block '" &
      // trim (block_name) // "'; ignored.")
    errors = .true.
    return
  end if
  select case (block_name)
  case ("SPINFO")
    call msg_message ("SLHA: SUSY spectrum program info:")
  case ("DCINFO")
    call msg_message ("SLHA: SUSY decay program info:")
  end select
  call retrieve_strings_in_block (pn_block, 1, msg)
  do i = 1, size (msg)
    call msg_message ("SLHA: " // char (msg(i)))
  end do
  call retrieve_strings_in_block (pn_block, 2, msg)
  do i = 1, size (msg)
    call msg_message ("SLHA: " // char (msg(i)))
  end do
  call retrieve_strings_in_block (pn_block, 3, msg)
  do i = 1, size (msg)
    call msg_warning ("SLHA: " // char (msg(i)))
  end do
  call retrieve_strings_in_block (pn_block, 4, msg)
  do i = 1, size (msg)
    call msg_error ("SLHA: " // char (msg(i)))
  end do
  errors = size (msg) > 0
end subroutine slha_handle_info_block

```

MODSEL

Handle the overall model definition. Only certain models are recognized. The soft-breaking model templates that determine the set of input parameters.

This block used to be required, but for generic UFO model support we should allow for its absence. In that case, `mssm_type` will be set to a negative value. If the block is present, the model must be one of the following, or parsing ends with an error.

<SLHA: parameters>+≡

```

integer, parameter :: MSSM_GENERIC = 0

```

```

integer, parameter :: MSSM_SUGRA = 1
integer, parameter :: MSSM_GMSB = 2
integer, parameter :: MSSM_AMSB = 3

```

(SLHA: procedures) +=

```

subroutine slha_handle_MODSEL (parse_tree, model, mssm_type)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(in), target :: model
  integer, intent(out) :: mssm_type
  type(parse_node_t), pointer :: pn_block, pn_data, pn_item
  type(string_t) :: model_name
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("MODSEL"), required=.false.)
  if (.not. associated (pn_block)) then
    mssm_type = -1
    return
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 1)
  if (associated (pn_item)) then
    mssm_type = get_integer_parameter (pn_item)
  else
    mssm_type = MSSM_GENERIC
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 3)
  if (associated (pn_item)) then
    select case (parse_node_get_integer (pn_item))
    case (MDL_MSSM); model_name = "MSSM"
    case (MDL_NMSSM); model_name = "NMSSM"
    case default
      call msg_fatal ("SLHA: unknown model code in MODSEL")
      return
    end select
  else
    model_name = "MSSM"
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 4)
  if (associated (pn_item)) then
    call msg_fatal (" R-parity violation is currently not supported by WHIZARD.")
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 5)
  if (associated (pn_item)) then
    call msg_fatal (" CP violation is currently not supported by WHIZARD.")
  end if
  select case (char (model_name))
  case ("MSSM")
    select case (char (model%get_name ()))
    case ("MSSM", "MSSM_CKM", "MSSM_Grav", "MSSM_Hgg")
      model_name = model%get_name ()
    case default
      call msg_fatal ("Selected model '" &
        // char (model%get_name ()) // "' does not match model '" &
        // char (model_name) // "' in SLHA input file.")
      return
    end select
  end select

```



```

case ("NMSSM")
  select case (char (model%get_name ()))
  case ("NMSSM", "NMSSM_CKM", "NMSSM_Hgg")
    model_name = model%get_name ()
  case default
    call msg_fatal ("Selected model '" &
      // char (model%get_name ()) // "' does not match model '" &
      // char (model_name) // "' in SLHA input file.")
    return
  end select
case default
  call msg_bug ("SLHA model name '" &
    // char (model_name) // "' not recognized.")
  return
end select
call msg_message ("SLHA: Initializing model '" // char (model_name) // "'")
end subroutine slha_handle_MODSEL

```

Write a MODSEL block, based on the contents of the current model.

```

<SLHA: procedures>+≡
subroutine slha_write_MODSEL (u, model, mssm_type)
  integer, intent(in) :: u
  type(model_t), intent(in), target :: model
  integer, intent(out) :: mssm_type
  type(var_list_t), pointer :: var_list
  integer :: model_id
  type(string_t) :: mtype_string
  var_list => model%get_var_list_ptr ()
  if (var_list%contains (var_str ("mtype"))) then
    mssm_type = nint (var_list%get_rval (var_str ("mtype")))
  else
    call msg_error ("SLHA: parameter 'mtype' (SUSY breaking scheme) " &
      // "is unknown in current model, no SLHA output possible")
    mssm_type = -1
    return
  end if
  call write_block_header (u, "MODSEL", "SUSY model selection")
  select case (mssm_type)
  case (0); mtype_string = "Generic MSSM"
  case (1); mtype_string = "SUGRA"
  case (2); mtype_string = "GMSB"
  case (3); mtype_string = "AMSB"
  case default
    mtype_string = "unknown"
  end select
  call write_integer_parameter (u, 1, mssm_type, &
    "SUSY-breaking scheme: " // char (mtype_string))
  select case (char (model%get_name ()))
  case ("MSSM"); model_id = MDL_MSSM
  case ("NMSSM"); model_id = MDL_NMSSM
  case default
    model_id = 0
  end select

```

```

    call write_integer_parameter (u, 3, model_id, &
        "SUSY model type: " // char (model%get_name ()))
end subroutine slha_write_MODSEL

```

SMINPUTS

Read SM parameters and update the variable list accordingly. If a parameter is not defined in the block, we use the previous value from the model variable list. For the basic parameters we have to do a small recalculation, since SLHA uses the G_F - α - m_Z scheme, while WHIZARD derives them from G_F , m_W , and m_Z .

(*SLHA: procedures*)+≡

```

subroutine slha_handle_SMINPUTS (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block
    real(default) :: alpha_em_i, GF, alphas, mZ
    real(default) :: ee, vv, cw_sw, cw2, mW
    real(default) :: mb, mtop, mtau
    type(var_list_t), pointer :: var_list
    var_list => model%get_var_list_ptr ()
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str ("SMINPUTS"), required=.true.)
    if (.not. (associated (pn_block))) return
    alpha_em_i = &
        get_parameter_in_block (pn_block, 1, var_str ("alpha_em_i"), var_list)
    GF = get_parameter_in_block (pn_block, 2, var_str ("GF"), var_list)
    alphas = &
        get_parameter_in_block (pn_block, 3, var_str ("alphas"), var_list)
    mZ = get_parameter_in_block (pn_block, 4, var_str ("mZ"), var_list)
    mb = get_parameter_in_block (pn_block, 5, var_str ("mb"), var_list)
    mtop = get_parameter_in_block (pn_block, 6, var_str ("mtop"), var_list)
    mtau = get_parameter_in_block (pn_block, 7, var_str ("mtau"), var_list)
    ee = sqrt (4 * pi / alpha_em_i)
    vv = 1 / sqrt (sqrt (2._default) * GF)
    cw_sw = ee * vv / (2 * mZ)
    if (2*cw_sw <= 1) then
        cw2 = (1 + sqrt (1 - 4 * cw_sw**2)) / 2
        mW = mZ * sqrt (cw2)
        call var_list%set_real (var_str ("GF"), GF, .true.)
        call var_list%set_real (var_str ("mZ"), mZ, .true.)
        call var_list%set_real (var_str ("mW"), mW, .true.)
        call var_list%set_real (var_str ("mtau"), mtau, .true.)
        call var_list%set_real (var_str ("mb"), mb, .true.)
        call var_list%set_real (var_str ("mtop"), mtop, .true.)
        call var_list%set_real (var_str ("alphas"), alphas, .true.)
    else
        call msg_fatal ("SLHA: Unphysical SM parameter values")
        return
    end if
end subroutine slha_handle_SMINPUTS

```

Write a SMINPUTS block.

(SLHA: procedures)+≡

```

subroutine slha_write_SMINPUTS (u, model)
  integer, intent(in) :: u
  type(model_t), intent(in), target :: model
  type(var_list_t), pointer :: var_list
  var_list => model%get_var_list_ptr ()
  call write_block_header (u, "SMINPUTS", "SM input parameters")
  call write_real_data_item (u, 1, var_str ("alpha_em_i"), var_list, &
    "Inverse electromagnetic coupling alpha (Z pole)")
  call write_real_data_item (u, 2, var_str ("GF"), var_list, &
    "Fermi constant")
  call write_real_data_item (u, 3, var_str ("alphas"), var_list, &
    "Strong coupling alpha_s (Z pole)")
  call write_real_data_item (u, 4, var_str ("mZ"), var_list, &
    "Z mass")
  call write_real_data_item (u, 5, var_str ("mb"), var_list, &
    "b running mass (at mb)")
  call write_real_data_item (u, 6, var_str ("mtop"), var_list, &
    "top mass")
  call write_real_data_item (u, 7, var_str ("mtau"), var_list, &
    "tau mass")
end subroutine slha_write_SMINPUTS

```

MINPAR

The block of SUSY input parameters. They are accessible to WHIZARD, but they only get used when an external spectrum generator is invoked. The precise set of parameters depends on the type of SUSY breaking, which by itself is one of the parameters.

(SLHA: procedures)+≡

```

subroutine slha_handle_MINPAR (parse_tree, model, mssm_type)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  integer, intent(in) :: mssm_type
  type(var_list_t), pointer :: var_list
  type(parse_node_t), pointer :: pn_block
  var_list => model%get_var_list_ptr ()
  call var_list%set_real &
    (var_str ("mtype"), real(mssm_type, default), is_known=.true.)
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("MINPAR"), required=.true.)
  select case (mssm_type)
  case (MSSM_SUGRA)
    call set_data_item (pn_block, 1, var_str ("m_zero"), var_list)
    call set_data_item (pn_block, 2, var_str ("m_half"), var_list)
    call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
    call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
    call set_data_item (pn_block, 5, var_str ("A0"), var_list)
  case (MSSM_GMSB)
    call set_data_item (pn_block, 1, var_str ("Lambda"), var_list)
    call set_data_item (pn_block, 2, var_str ("M_mes"), var_list)
  end select
end subroutine slha_handle_MINPAR

```

```

        call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
        call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
        call set_data_item (pn_block, 5, var_str ("N_5"), var_list)
        call set_data_item (pn_block, 6, var_str ("c_grav"), var_list)
    case (MSSM_AMSB)
        call set_data_item (pn_block, 1, var_str ("m_zero"), var_list)
        call set_data_item (pn_block, 2, var_str ("m_grav"), var_list)
        call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
        call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
    case default
        call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
    end select
end subroutine slha_handle_MINPAR

```

Write a MINPAR block as appropriate for the current model type.

(SLHA: procedures) +=

```

subroutine slha_write_MINPAR (u, model, mssm_type)
    integer, intent(in) :: u
    type(model_t), intent(in), target :: model
    integer, intent(in) :: mssm_type
    type(var_list_t), pointer :: var_list
    var_list => model%get_var_list_ptr ()
    call write_block_header (u, "MINPAR", "Basic SUSY input parameters")
    select case (mssm_type)
    case (MSSM_SUGRA)
        call write_real_data_item (u, 1, var_str ("m_zero"), var_list, &
            "Common scalar mass")
        call write_real_data_item (u, 2, var_str ("m_half"), var_list, &
            "Common gaugino mass")
        call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
            "tan(beta)")
        call write_integer_data_item (u, 4, &
            var_str ("sgn_mu"), var_list, &
            "Sign of mu")
        call write_real_data_item (u, 5, var_str ("A0"), var_list, &
            "Common trilinear coupling")
    case (MSSM_GMSB)
        call write_real_data_item (u, 1, var_str ("Lambda"), var_list, &
            "Soft-breaking scale")
        call write_real_data_item (u, 2, var_str ("M_mes"), var_list, &
            "Messenger scale")
        call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
            "tan(beta)")
        call write_integer_data_item (u, 4, &
            var_str ("sgn_mu"), var_list, &
            "Sign of mu")
        call write_integer_data_item (u, 5, var_str ("N_5"), var_list, &
            "Messenger index")
        call write_real_data_item (u, 6, var_str ("c_grav"), var_list, &
            "Gravitino mass factor")
    case (MSSM_AMSB)
        call write_real_data_item (u, 1, var_str ("m_zero"), var_list, &
            "Common scalar mass")
        call write_real_data_item (u, 2, var_str ("m_grav"), var_list, &

```

```

        "Gravitino mass")
    call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
        "tan(beta)")
    call write_integer_data_item (u, 4, &
        var_str ("sgn_mu"), var_list, &
        "Sign of mu")
case default
    call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
        "tan(beta)")
end select
end subroutine slha_write_MINPAR

```

Mass spectrum

Set masses. Since the particles are identified by PDG code, read the line and try to set the appropriate particle mass in the current model. At the end, update parameters, just in case the W or Z mass was included.

```

<SLHA: procedures>+=
subroutine slha_handle_MASS (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block, pn_data, pn_line, pn_code
    type(parse_node_t), pointer :: pn_mass
    integer :: pdg
    real(default) :: mass
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str ("MASS"), required=.true.)
    if (.not. (associated (pn_block))) return
    pn_data => parse_node_get_sub_ptr (pn_block, 4)
    do while (associated (pn_data))
        pn_line => parse_node_get_sub_ptr (pn_data, 2)
        pn_code => parse_node_get_sub_ptr (pn_line)
        if (associated (pn_code)) then
            pdg = get_integer_parameter (pn_code)
            pn_mass => parse_node_get_next_ptr (pn_code)
            if (associated (pn_mass)) then
                mass = get_real_parameter (pn_mass)
                call model%set_field_mass (pdg, mass)
            else
                call msg_error ("SLHA: Block MASS: Missing mass value")
            end if
        else
            call msg_error ("SLHA: Block MASS: Missing PDG code")
        end if
        pn_data => parse_node_get_next_ptr (pn_data)
    end do
end subroutine slha_handle_MASS

```

Widths

Set widths. For each DECAY block, extract the header, read the PDG code and width, and try to set the appropriate particle width in the current model.

(*SLHA: procedures*) +=

```
subroutine slha_handle_decays (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_decay, pn_decay_spec, pn_code, pn_width
  integer :: pdg
  real(default) :: width
  pn_decay => slha_get_first_decay_ptr (parse_tree)
  do while (associated (pn_decay))
    pn_decay_spec => parse_node_get_sub_ptr (pn_decay, 2)
    pn_code => parse_node_get_sub_ptr (pn_decay_spec)
    pdg = get_integer_parameter (pn_code)
    pn_width => parse_node_get_next_ptr (pn_code)
    width = get_real_parameter (pn_width)
    call model%set_field_width (pdg, width)
    pn_decay => slha_get_next_decay_ptr (pn_decay)
  end do
end subroutine slha_handle_decays
```

Mixing matrices

Read mixing matrices. We can treat all matrices by a single procedure if we just know the block name, variable prefix, and matrix dimension. The matrix dimension must be less than 10. For the pseudoscalar Higgses in NMSSM-type models we need off-diagonal matrices, so we generalize the definition.

(*SLHA: procedures*) +=

```
subroutine slha_handle_matrix_block &
  (parse_tree, block_name, var_prefix, dim1, dim2, model)
  type(parse_tree_t), intent(in) :: parse_tree
  character(*), intent(in) :: block_name, var_prefix
  integer, intent(in) :: dim1, dim2
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_block
  type(var_list_t), pointer :: var_list
  integer :: i, j
  character(len=len(var_prefix)+2) :: var_name
  var_list => model%get_var_list_ptr ()
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str (block_name), required=.false.)
  if (.not. (associated (pn_block))) return
  do i = 1, dim1
    do j = 1, dim2
      write (var_name, "(A,I1,I1)") var_prefix, i, j
      call set_matrix_element (pn_block, i, j, var_str (var_name), var_list)
    end do
  end do
end subroutine slha_handle_matrix_block
```

Higgs data

Read the block ALPHA which holds just the Higgs mixing angle.

```
(SLHA: procedures)+≡
subroutine slha_handle_ALPHA (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_block, pn_line, pn_data, pn_item
  type(var_list_t), pointer :: var_list
  real(default) :: al_h
  var_list => model%get_var_list_ptr ()
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("ALPHA"), required=.false.)
  if (.not. (associated (pn_block))) return
  pn_data => parse_node_get_sub_ptr (pn_block, 4)
  pn_line => parse_node_get_sub_ptr (pn_data, 2)
  pn_item => parse_node_get_sub_ptr (pn_line)
  if (associated (pn_item)) then
    al_h = get_real_parameter (pn_item)
    call var_list%set_real (var_str ("al_h"), al_h, &
      is_known=.true., ignore=.true.)
  end if
end subroutine slha_handle_ALPHA
```

Read the block HMX for the Higgs mixing parameters

```
(SLHA: procedures)+≡
subroutine slha_handle_HMX (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_block
  type(var_list_t), pointer :: var_list
  var_list => model%get_var_list_ptr ()
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("HMX"), required=.false.)
  if (.not. (associated (pn_block))) return
  call set_data_item (pn_block, 1, var_str ("mu_h"), var_list)
  call set_data_item (pn_block, 2, var_str ("tanb_h"), var_list)
end subroutine slha_handle_HMX
```

Read the block NMSSMRUN for the specific NMSSM parameters

```
(SLHA: procedures)+≡
subroutine slha_handle_NMSSMRUN (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_block
  type(var_list_t), pointer :: var_list
  var_list => model%get_var_list_ptr ()
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("NMSSMRUN"), required=.false.)
  if (.not. (associated (pn_block))) return
  call set_data_item (pn_block, 1, var_str ("ls"), var_list)
  call set_data_item (pn_block, 2, var_str ("ks"), var_list)
  call set_data_item (pn_block, 3, var_str ("a_ls"), var_list)
```

```

call set_data_item (pn_block, 4, var_str ("a_ks"), var_list)
call set_data_item (pn_block, 5, var_str ("nmu"), var_list)
end subroutine slha_handle_NMSSMRUN

```

28.5.5 Parsing custom SLHA files

With the introduction of UFO models, we support custom files in generic SLHA format that reset model parameters. In contrast to strict SLHA files, the order and naming of blocks is arbitrary.

We scan the complete file (i.e., preprocessed parse tree), parsing all blocks that contain data lines. For each data line, we identify index array and associated value. Then we set the model parameter that is associated with that block name and index array, if it exists.

```

<SLHA: procedures>+=
subroutine slha_handle_custom_file (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model

  type(parse_node_t), pointer :: pn_root, pn_block
  type(parse_node_t), pointer :: pn_block_spec, pn_block_name
  type(parse_node_t), pointer :: pn_data, pn_line, pn_code, pn_item
  type(string_t) :: block_name
  integer, dimension(:), allocatable :: block_index
  integer :: n_index, i
  real(default) :: value

  pn_root => parse_tree%get_root_ptr ()
  pn_block => pn_root%get_sub_ptr ()
  HANDLE_BLOCKS: do while (associated (pn_block))
    select case (char (pn_block%get_rule_key ()))
      case ("block_def")
        call slha_handle_custom_block (pn_block, model)
      end select
    pn_block => pn_block%get_next_ptr ()
  end do HANDLE_BLOCKS

end subroutine slha_handle_custom_file

<SLHA: procedures>+=
subroutine slha_handle_custom_block (pn_block, model)
  type(parse_node_t), intent(in), target :: pn_block
  type(model_t), intent(inout), target :: model

  type(parse_node_t), pointer :: pn_block_spec, pn_block_name
  type(parse_node_t), pointer :: pn_data, pn_line, pn_code, pn_item
  type(string_t) :: block_name
  integer, dimension(:), allocatable :: block_index
  integer :: n_index, i
  real(default) :: value

  pn_block_spec => parse_node_get_sub_ptr (pn_block, 2)

```



```

pn_block_name => parse_node_get_sub_ptr (pn_block_spec)
select case (char (parse_node_get_rule_key (pn_block_name)))
case ("block_name")
    block_name = trim (adjustl (upper_case (pn_block_name%get_string ())))
case ("QNUMBERS")
    block_name = "QNUMBERS"
end select
call demangle_keywords (block_name)
pn_data => pn_block%get_sub_ptr (4)
HANDLE_LINES: do while (associated (pn_data))
    select case (char (pn_data%get_rule_key ()))
    case ("block_data")
        pn_line => pn_data%get_sub_ptr (2)
        n_index = pn_line%get_n_sub () - 1
        allocate (block_index (n_index))
        pn_code => pn_line%get_sub_ptr ()
        READ_LINE: do i = 1, n_index
            select case (char (pn_code%get_rule_key ()))
            case ("integer"); block_index(i) = pn_code%get_integer ()
            case default
                pn_code => null ()
                exit READ_LINE
            end select
            pn_code => pn_code%get_next_ptr ()
        end do READ_LINE
        if (associated (pn_code)) then
            value = get_real_parameter (pn_code)
            call model%slha_set_par (block_name, block_index, value)
        end if
        deallocate (block_index)
    end select
    pn_data => pn_data%get_next_ptr ()
end do HANDLE_LINES

end subroutine slha_handle_custom_block

```

28.5.6 Parser

Read a SLHA file from stream, including preprocessing, and make up a parse tree.

```

<SLHA: procedures>+≡
subroutine slha_parse_stream (stream, custom_block_name, parse_tree)
    type(stream_t), intent(inout), target :: stream
    type(string_t), dimension(:), intent(in) :: custom_block_name
    type(parse_tree_t), intent(out) :: parse_tree
    type(ifile_t) :: ifile
    type(lexer_t) :: lexer
    type(stream_t), target :: stream_tmp
    call slha_preprocess (stream, custom_block_name, ifile)
    call stream_init (stream_tmp, ifile)
    call lexer_init_slha (lexer)
    call lexer_assign_stream (lexer, stream_tmp)

```

```

    call parse_tree_init (parse_tree, syntax_slha, lexer)
    call lexer_final (lexer)
    call stream_final (stream_tmp)
    call ifile_final (ifile)
end subroutine slha_parse_stream

```

Read a SLHA file chosen by name. Check first the current directory, then the directory where SUSY input files should be located.

The `default_mode` applies to unknown blocks in the SLHA file: this is either `MODE_SKIP` or `MODE_DATA`, corresponding to genuine SUSY and custom file content, respectively.

(SLHA: public)+≡

```
public :: slha_parse_file
```

(SLHA: sub interfaces)+≡

```

module subroutine slha_parse_file &
    (file, custom_block_name, os_data, parse_tree)
    type(string_t), intent(in) :: file
    type(string_t), dimension(:), intent(in) :: custom_block_name
    type(os_data_t), intent(in) :: os_data
    type(parse_tree_t), intent(out) :: parse_tree
end subroutine slha_parse_file

```

(SLHA: procedures)+≡

```

module subroutine slha_parse_file &
    (file, custom_block_name, os_data, parse_tree)
    type(string_t), intent(in) :: file
    type(string_t), dimension(:), intent(in) :: custom_block_name
    type(os_data_t), intent(in) :: os_data
    type(parse_tree_t), intent(out) :: parse_tree
    logical :: exist
    type(string_t) :: filename
    type(stream_t), target :: stream
    call msg_message ("Reading SLHA input file '" // char (file) // "'")
    filename = file
    inquire (file=char(filename), exist=exist)
    if (.not. exist) then
        filename = os_data%whizard_susypath // "/" // file
        inquire (file=char(filename), exist=exist)
        if (.not. exist) then
            call msg_fatal ("SLHA input file '" // char (file) // "' not found")
            return
        end if
    end if
    call stream_init (stream, char (filename))
    call slha_parse_stream (stream, custom_block_name, parse_tree)
    call stream_final (stream)
end subroutine slha_parse_file

```

28.5.7 API

Read the SLHA file, parse it, and interpret the parse tree. The model parameters retrieved from the file will be inserted into the appropriate model, which is

loaded and modified in the background. The pointer to this model is returned as the last argument.

```

<SLHA: public>+≡
    public :: slha_read_file

<SLHA: sub interfaces>+≡
    module subroutine slha_read_file &
        (file, os_data, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        type(model_t), intent(inout), target :: model
        logical, intent(in) :: input, spectrum, decays
    end subroutine slha_read_file

<SLHA: procedures>+≡
    module subroutine slha_read_file &
        (file, os_data, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        type(model_t), intent(inout), target :: model
        logical, intent(in) :: input, spectrum, decays
        type(string_t), dimension(:), allocatable :: custom_block_name
        type(parse_tree_t) :: parse_tree
        call model%get_custom_slha_blocks (custom_block_name)
        call slha_parse_file (file, custom_block_name, os_data, parse_tree)
        if (associated (parse_tree%get_root_ptr ())) then
            call slha_interpret_parse_tree &
                (parse_tree, model, input, spectrum, decays)
            call parse_tree_final (parse_tree)
            call model%update_parameters ()
        end if
    end subroutine slha_read_file

```

Write the SLHA contents, as far as possible, to external file.

```

<SLHA: public>+≡
    public :: slha_write_file

<SLHA: sub interfaces>+≡
    module subroutine slha_write_file (file, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(model_t), target, intent(in) :: model
        logical, intent(in) :: input, spectrum, decays
    end subroutine slha_write_file

<SLHA: procedures>+≡
    module subroutine slha_write_file (file, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(model_t), target, intent(in) :: model
        logical, intent(in) :: input, spectrum, decays
        integer :: mssm_type
        integer :: u
        u = free_unit ()
        call msg_message ("Writing SLHA output file '" // char (file) // "'")
        open (unit=u, file=char(file), action="write", status="replace")
        write (u, "(A)")  "# SUSY Les Houches Accord"
    end subroutine slha_write_file

```

```

write (u, "(A)")  "# Output generated by " // trim (VERSION_STRING)
call slha_write_MODSEL (u, model, mssm_type)
if (input) then
  call slha_write_SMINPUTS (u, model)
  call slha_write_MINPAR (u, model, mssm_type)
end if
if (spectrum) then
  call msg_bug ("SLHA: spectrum output not supported yet")
end if
if (decays) then
  call msg_bug ("SLHA: decays output not supported yet")
end if
close (u)
end subroutine slha_write_file

```

28.5.8 Dispatch

```

⟨SLHA: public⟩+≡
  public :: dispatch_slha

⟨SLHA: sub interfaces⟩+≡
  module subroutine dispatch_slha (var_list, input, spectrum, decays)
    type(var_list_t), intent(inout), target :: var_list
    logical, intent(out) :: input, spectrum, decays
  end subroutine dispatch_slha

⟨SLHA: procedures⟩+≡
  module subroutine dispatch_slha (var_list, input, spectrum, decays)
    type(var_list_t), intent(inout), target :: var_list
    logical, intent(out) :: input, spectrum, decays
    input = var_list%get_lval (var_str ("?slha_read_input"))
    spectrum = var_list%get_lval (var_str ("?slha_read_spectrum"))
    decays = var_list%get_lval (var_str ("?slha_read_decays"))
  end subroutine dispatch_slha

```

28.5.9 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨slha_interface_ut.f90⟩≡
  ⟨File header⟩

  module slha_interface_ut
    use unit_tests
    use slha_interface_util

    ⟨Standard module head⟩

    ⟨SLHA: public test⟩

    contains

    ⟨SLHA: test driver⟩

```

```

end module slha_interface_ut

<slha_interface_util.f90>≡
<File header>

```

```

module slha_interface_util

  <Use strings>
  use io_units
  use os_interface
  use parser
  use model_data
  use variables
  use models

  use slha_interface

  <Standard module head>

  <SLHA: test declarations>

  contains

  <SLHA: tests>

end module slha_interface_util

```

API: driver for the unit tests below.

```

<SLHA: public test>≡
  public :: slha_test

<SLHA: test driver>≡
  subroutine slha_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SLHA: execute tests>
  end subroutine slha_test

```

Checking the basics of the SLHA interface.

```

<SLHA: execute tests>≡
  call test (slha_1, "slha_1", &
    "check SLHA interface", &
    u, results)

<SLHA: test declarations>≡
  public :: slha_1

<SLHA: tests>≡
  subroutine slha_1 (u)
    integer, intent(in) :: u
    type(os_data_t), pointer :: os_data => null ()
    type(parse_tree_t), pointer :: parse_tree => null ()
    integer :: u_file, iostat
    character(80) :: buffer
    character(*), parameter :: file_slha = "slha_test.dat"

```

```

type(model_list_t) :: model_list
type(model_t), pointer :: model => null ()
type(var_list_t), pointer :: var_list
type(string_t), dimension(0) :: empty_string_array

write (u, "(A)")  "* Test output: SLHA Interface"
write (u, "(A)")  "* Purpose: test SLHA file reading and writing"
write (u, "(A)")

write (u, "(A)")  "* Initializing"
write (u, "(A)")

allocate (os_data)
allocate (parse_tree)
call os_data%init ()
call syntax_model_file_init ()
call model_list%read_model &
    (var_str("MSSM"), var_str("MSSM.mdl"), os_data, model)
call syntax_slha_init ()

write (u, "(A)")  "* Reading SLHA file spslap_decays.slha"
write (u, "(A)")

call slha_parse_file (var_str ("spslap_decays.slha"), &
    empty_string_array, os_data, parse_tree)

write (u, "(A)")  "* Writing the parse tree:"
write (u, "(A)")

call parse_tree_write (parse_tree, u)

write (u, "(A)")  "* Interpreting the parse tree"
write (u, "(A)")

call slha_interpret_parse_tree (parse_tree, model, &
    input=.true., spectrum=.true., decays=.true.)
call parse_tree_final (parse_tree)

write (u, "(A)")  "* Writing out the list of variables (reals only):"
write (u, "(A)")

var_list => model%get_var_list_ptr ()
call var_list%write (only_type = V_REAL, unit = u)

write (u, "(A)")
write (u, "(A)")  "* Writing SLHA output to '" // file_slha // "'"
write (u, "(A)")

call slha_write_file (var_str (file_slha), model, input=.true., &
    spectrum=.false., decays=.false.)
u_file = free_unit ()
open (u_file, file = file_slha, action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat)  buffer

```

```

        if (buffer(1:37) == "# Output generated by WHIZARD version") then
            buffer = "[...]"
        end if
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
    write (u, "(A)")

    call parse_tree_final (parse_tree)
    deallocate (parse_tree)
    deallocate (os_data)

    write (u, "(A)")  "* Test output end: slha_1"
    write (u, "(A)")

end subroutine slha_1

```

SLHA interface

This rather trivial sets all input values for the SLHA interface to **false**.

```

<SLHA: execute tests>+=
    call test (slha_2, "slha_2", &
        "SLHA interface", &
        u, results)

<SLHA: test declarations>+=
    public :: slha_2

<SLHA: tests>+=
    subroutine slha_2 (u)
        integer, intent(in) :: u
        type(var_list_t) :: var_list
        logical :: input, spectrum, decays

        write (u, "(A)")  "* Test output: slha_2"
        write (u, "(A)")  "* Purpose: SLHA interface settings"
        write (u, "(A)")

        write (u, "(A)")  "* Default settings"
        write (u, "(A)")

        call var_list%init_defaults (0)
        call dispatch_slha (var_list, &
            input = input, spectrum = spectrum, decays = decays)

        write (u, "(A,1x,L1)") " slha_read_input      =", input
        write (u, "(A,1x,L1)") " slha_read_spectrum =", spectrum
        write (u, "(A,1x,L1)") " slha_read_decays  =", decays

        call var_list%final ()
    end subroutine slha_2

```

```

call var_list%init_defaults (0)

write (u, "(A)")
write (u, "(A)")  "* Set all entries to [false]"
write (u, "(A)")

call var_list%set_log (var_str ("?slha_read_input"), &
    .false., is_known = .true.)
call var_list%set_log (var_str ("?slha_read_spectrum"), &
    .false., is_known = .true.)
call var_list%set_log (var_str ("?slha_read_decays"), &
    .false., is_known = .true.)

call dispatch_slha (var_list, &
    input = input, spectrum = spectrum, decays = decays)

write (u, "(A,1x,L1)")  " slha_read_input      =", input
write (u, "(A,1x,L1)")  " slha_read_spectrum   =", spectrum
write (u, "(A,1x,L1)")  " slha_read_decays     =", decays

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: slha_2"

end subroutine slha_2

```


Chapter 29

Infrastructure for threshold processes

```
<interpolation.f90>≡  
  <File header>  
  
  module interpolation  
    <Use kinds>  
  
    <Standard module head>  
    save  
  
    <Interpolation: public>  
    public :: interpolate_linear, strictly_monotonous  
  
    <Interpolation: interfaces>  
  
    interface  
    <Interpolation: sub interfaces>  
    end interface  
  
  end module interpolation  
<interpolation_sub.f90>≡  
  <File header>  
  
  submodule (interpolation) interpolation_s  
  
    implicit none  
  
    <Interpolation: parameters>  
  
    contains  
  
    <Interpolation: procedures>  
  
  end submodule interpolation_s
```

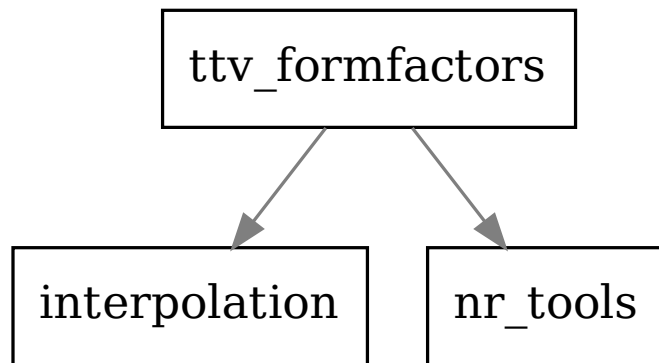


Figure 29.1: Module dependencies in `src/threshold`.

```

<Interpolation: interfaces>≡
  interface interpolate_linear
    module procedure interpolate_linear_1D_complex_array, &
      interpolate_linear_1D_complex_scalar, &
      interpolate_linear_1D_real_array, &
      interpolate_linear_1D_real_scalar, &
      interpolate_linear_2D_complex_array, &
      interpolate_linear_2D_complex_scalar, &
      interpolate_linear_2D_real_array, &
      interpolate_linear_2D_real_scalar, &
      interpolate_linear_3D_complex_array, &
      interpolate_linear_3D_complex_scalar, &
      interpolate_linear_3D_real_array, &
      interpolate_linear_3D_real_scalar
  end interface

  interface strictly_monotonous
    module procedure monotonous
  end interface strictly_monotonous

  interface find_nearest_left
    !!! recursive bisection is slower
    module procedure find_nearest_left_loop
  end interface find_nearest_left

<Interpolation: sub interfaces>≡
  pure module subroutine interpolate_linear_1D_complex_scalar (xa, ya, x, y)
    real(default), dimension(:), intent(in) :: xa
    complex(default), dimension(:), intent(in) :: ya
  
```

```

        real(default), intent(in) :: x
        complex(default), intent(out) :: y
    end subroutine interpolate_linear_1D_complex_scalar

<Interpolation: procedures>≡
    pure module subroutine interpolate_linear_1D_complex_scalar (xa, ya, x, y)
        real(default), dimension(:), intent(in) :: xa
        complex(default), dimension(:), intent(in) :: ya
        real(default), intent(in) :: x
        complex(default), intent(out) :: y
        integer :: ixl
        real(default) :: t
        y = 0.0_default
        !!! don't check this at runtime:
        ! if ( .not.monotonous(xa) ) return
        if ( out_of_range(xa, x) ) return
        ixl = 0
        call find_nearest_left (xa, x, ixl)
        t = ( x - xa(ixl) ) / ( xa(ixl+1) - xa(ixl) )
        y = (1.-t)*ya(ixl) + t*ya(ixl+1)
    end subroutine interpolate_linear_1D_complex_scalar

<Interpolation: sub interfaces>+≡
    pure module subroutine interpolate_linear_2D_complex_scalar (x1a, x2a, ya, x1, x2, y)
        real(default), dimension(:), intent(in) :: x1a
        real(default), dimension(:), intent(in) :: x2a
        complex(default), dimension(:,:), intent(in) :: ya
        real(default), intent(in) :: x1
        real(default), intent(in) :: x2
        complex(default), intent(out) :: y
    end subroutine interpolate_linear_2D_complex_scalar

<Interpolation: procedures>+≡
    pure module subroutine interpolate_linear_2D_complex_scalar (x1a, x2a, ya, x1, x2, y)
        real(default), dimension(:), intent(in) :: x1a
        real(default), dimension(:), intent(in) :: x2a
        complex(default), dimension(:,:), intent(in) :: ya
        real(default), intent(in) :: x1
        real(default), intent(in) :: x2
        complex(default), intent(out) :: y
        integer :: ix1l, ix2l
        real(default) :: t, u
        y = 0.0_default
        !!! don't check this at runtime:
        ! if ( (.not.monotonous(x1a)) .or. (.not.monotonous(x2a)) ) return
        if ( out_of_range(x1a, x1) .or. out_of_range(x2a, x2) ) return
        ix1l = 0
        call find_nearest_left (x1a, x1, ix1l)
        ix2l = 0
        call find_nearest_left (x2a, x2, ix2l)
        t = ( x1 - x1a(ix1l) ) / ( x1a(ix1l+1) - x1a(ix1l) )
        u = ( x2 - x2a(ix2l) ) / ( x2a(ix2l+1) - x2a(ix2l) )
        y = (1.-t)*(1.-u)*ya(ix1l, ix2l) &
            + t*(1.-u)*ya(ix1l+1, ix2l) &
            + t * u * ya(ix1l+1, ix2l+1) &

```

```

      +(1.-t)*      u *ya(ix1l ,ix2l+1)
end subroutine interpolate_linear_2D_complex_scalar

```

(Interpolation: sub interfaces)+≡

```

pure module subroutine interpolate_linear_3D_complex_scalar &
  (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:), intent(in) :: x3a
  complex(default), dimension(:,:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(in) :: x3
  complex(default), intent(out) :: y
end subroutine interpolate_linear_3D_complex_scalar

```

(Interpolation: procedures)+≡

```

pure module subroutine interpolate_linear_3D_complex_scalar &
  (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:), intent(in) :: x3a
  complex(default), dimension(:,:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(in) :: x3
  complex(default), intent(out) :: y
  integer :: ix1l, ix2l, ix3l
  real(default) :: t, u, v
  y = 0.0_default
  !!! don't check this at runtime:
  ! if ( (.not.monotonous(x1a)) .or. (.not.monotonous(x2a)) ) return
  if ( out_of_range(x1a, x1) .or. out_of_range(x2a, x2) .or. out_of_range(x3a, x3) ) return
  ix1l = 0
  call find_nearest_left (x1a, x1, ix1l)
  ix2l = 0
  call find_nearest_left (x2a, x2, ix2l)
  ix3l = 0
  call find_nearest_left (x3a, x3, ix3l)
  t = ( x1 - x1a(ix1l) ) / ( x1a(ix1l+1) - x1a(ix1l) )
  u = ( x2 - x2a(ix2l) ) / ( x2a(ix2l+1) - x2a(ix2l) )
  v = ( x3 - x3a(ix3l) ) / ( x3a(ix3l+1) - x3a(ix3l) )
  y = (1.-t)*(1.-u)*(1.-v)*ya(ix1l ,ix2l ,ix3l ) &
    +(1.-t)*(1.-u)*      v *ya(ix1l ,ix2l ,ix3l+1) &
    +(1.-t)*      u *(1.-v)*ya(ix1l ,ix2l+1,ix3l ) &
    +(1.-t)*      u *      v *ya(ix1l ,ix2l+1,ix3l+1) &
    +      t *(1.-u)*(1.-v)*ya(ix1l+1,ix2l ,ix3l ) &
    +      t *(1.-u)*      v *ya(ix1l+1,ix2l ,ix3l+1) &
    +      t *      u *(1.-v)*ya(ix1l+1,ix2l+1,ix3l ) &
    +      t *      u *      v *ya(ix1l+1,ix2l+1,ix3l+1)
end subroutine interpolate_linear_3D_complex_scalar

```

(Interpolation: sub interfaces)+≡

```

pure module subroutine find_nearest_left_loop (xa, x, ixl)
  real(default), dimension(:), intent(in) :: xa
  real(default), intent(in) :: x
  integer, intent(out) :: ixl
end subroutine find_nearest_left_loop

```

(Interpolation: procedures)+≡

```

pure module subroutine find_nearest_left_loop (xa, x, ixl)
  real(default), dimension(:), intent(in) :: xa
  real(default), intent(in) :: x
  integer, intent(out) :: ixl
  integer :: ixm, ixr
  ixl = 1
  ixr = size(xa)
  do
    if ( ixr-ixl <= 1 ) return
    ixm = (ixr+ixl) / 2
    if ( x < xa(ixm) ) then
      ixr = ixm
    else
      ixl = ixm
    end if
  end do
end subroutine find_nearest_left_loop

```

(Interpolation: procedures)+≡

```

pure recursive subroutine find_nearest_left_rec (xa, x, ixl)
  real(default), dimension(:), intent(in) :: xa
  real(default), intent(in) :: x
  integer, intent(inout) :: ixl
  integer :: nx, bs
  real(default), dimension(:), allocatable :: xa_new
  nx = size(xa)
  bs = nx/2 + 1
  if ( nx < 3 ) then
    ixl = ixl + bs - 1
    return
  else
    if ( x < xa(bs) ) then
      allocate( xa_new(1:bs) )
      xa_new = xa(1:bs)
    else
      ixl = ixl + bs - 1
      allocate( xa_new(bs:nx) )
      xa_new = xa(bs:nx)
    end if
    call find_nearest_left_rec (xa_new, x, ixl)
    deallocate( xa_new )
  end if
end subroutine find_nearest_left_rec

```

(Interpolation: sub interfaces)+≡

```

pure module function monotonous (xa) result (flag)
  real(default), dimension(:), intent(in) :: xa

```

```

        logical :: flag
    end function monotonous

<Interpolation: procedures>+≡
    pure module function monotonous (xa) result (flag)
        real(default), dimension(:), intent(in) :: xa
        integer :: ix
        logical :: flag
        flag = .false.
        do ix = 1, size(xa)-1
            flag = ( xa(ix) < xa(ix+1) )
            if ( .not. flag ) return
        end do
    end function monotonous

<Interpolation: procedures>+≡
    pure function out_of_range (xa, x) result (flag)
        real(default), dimension(:), intent(in) :: xa
        real(default), intent(in) :: x
        logical :: flag
        flag = ( x < xa(1) .or. x > xa(size(xa)) )
    end function out_of_range

<Interpolation: sub interfaces>+≡
    pure module subroutine interpolate_linear_1D_complex_array (xa, ya, x, y)
        real(default), dimension(:), intent(in) :: xa
        complex(default), dimension(:,:), intent(in) :: ya
        real(default), intent(in) :: x
        complex(default), dimension(size(ya(1,:))), intent(out) :: y
    end subroutine interpolate_linear_1D_complex_array

<Interpolation: procedures>+≡
    pure module subroutine interpolate_linear_1D_complex_array (xa, ya, x, y)
        real(default), dimension(:), intent(in) :: xa
        complex(default), dimension(:,:), intent(in) :: ya
        real(default), intent(in) :: x
        complex(default), dimension(size(ya(1,:))), intent(out) :: y
        integer :: iy
        do iy=1, size(y)
            call interpolate_linear_1D_complex_scalar (xa, ya(:,iy), x, y(iy))
        end do
    end subroutine interpolate_linear_1D_complex_array

<Interpolation: sub interfaces>+≡
    pure module subroutine interpolate_linear_1D_real_array (xa, ya, x, y)
        real(default), dimension(:), intent(in) :: xa
        real(default), dimension(:,:), intent(in) :: ya
        real(default), intent(in) :: x
        real(default), dimension(:), intent(out) :: y
    end subroutine interpolate_linear_1D_real_array

<Interpolation: procedures>+≡
    pure module subroutine interpolate_linear_1D_real_array (xa, ya, x, y)
        real(default), dimension(:), intent(in) :: xa

```

```

real(default), dimension(:,:), intent(in) :: ya
real(default), intent(in) :: x
real(default), dimension(:), intent(out) :: y
complex(default), dimension(size(ya(1,:))) :: y_c
call interpolate_linear_1D_complex_array (xa, cmplx(ya,kind=default), x, y_c)
y = real(y_c,kind=default)
end subroutine interpolate_linear_1D_real_array

```

(Interpolation: sub interfaces)+≡

```

pure module subroutine interpolate_linear_1D_real_scalar (xa, ya, x, y)
  real(default), dimension(:), intent(in) :: xa
  real(default), dimension(:), intent(in) :: ya
  real(default), intent(in) :: x
  real(default), intent(out) :: y
  complex(default), dimension(size(ya)) :: ya_c
end subroutine interpolate_linear_1D_real_scalar

```

(Interpolation: procedures)+≡

```

pure module subroutine interpolate_linear_1D_real_scalar (xa, ya, x, y)
  real(default), dimension(:), intent(in) :: xa
  real(default), dimension(:), intent(in) :: ya
  real(default), intent(in) :: x
  real(default), intent(out) :: y
  complex(default), dimension(size(ya)) :: ya_c
  complex(default) :: y_c
  ya_c = cmplx(ya,kind=default)
  call interpolate_linear_1D_complex_scalar (xa, ya_c, x, y_c)
  y = real(y_c,kind=default)
end subroutine interpolate_linear_1D_real_scalar

```

(Interpolation: sub interfaces)+≡

```

pure module subroutine interpolate_linear_2D_complex_array (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  complex(default), dimension(:,:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  complex(default), dimension(size(ya(1,1,:))), intent(out) :: y
end subroutine interpolate_linear_2D_complex_array

```

(Interpolation: procedures)+≡

```

pure module subroutine interpolate_linear_2D_complex_array (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  complex(default), dimension(:,:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  complex(default), dimension(size(ya(1,1,:))), intent(out) :: y
  integer :: iy
  do iy=1, size(y)
    call interpolate_linear_2D_complex_scalar (x1a, x2a, ya(:, :, iy), x1, x2, y(iy))
  end do
end subroutine interpolate_linear_2D_complex_array

```

<Interpolation: sub interfaces>+≡

```
pure module subroutine interpolate_linear_2D_real_array (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), dimension(:), intent(out) :: y
end subroutine interpolate_linear_2D_real_array
```

<Interpolation: procedures>+≡

```
pure module subroutine interpolate_linear_2D_real_array (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), dimension(:), intent(out) :: y
  complex(default), dimension(size(ya(1,1,:))) :: y_c
  call interpolate_linear_2D_complex_array (x1a, x2a, cmplx(ya,kind=default), x1, x2, y_c)
  y = real(y_c,kind=default)
end subroutine interpolate_linear_2D_real_array
```

<Interpolation: sub interfaces>+≡

```
pure module subroutine interpolate_linear_2D_real_scalar (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(out) :: y
end subroutine interpolate_linear_2D_real_scalar
```

<Interpolation: procedures>+≡

```
pure module subroutine interpolate_linear_2D_real_scalar (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(out) :: y
  complex(default), dimension(size(ya(:,1)),size(ya(1,:))) :: ya_c
  complex(default) :: y_c
  ya_c = reshape (ya_c, shape(ya))
  ya_c = cmplx(ya,kind=default)
  call interpolate_linear_2D_complex_scalar (x1a, x2a, ya_c, x1, x2, y_c)
  y = real(y_c,kind=default)
end subroutine interpolate_linear_2D_real_scalar
```

<Interpolation: sub interfaces>+≡

```
pure module subroutine interpolate_linear_3D_complex_array &
  (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
```



```

    real(default), dimension(:), intent(in) :: x3a
    complex(default), dimension(:,:,:), intent(in) :: ya
    real(default), intent(in) :: x1
    real(default), intent(in) :: x2
    real(default), intent(in) :: x3
    complex(default), dimension(size(ya(1,1,1,:))), intent(out) :: y
end subroutine interpolate_linear_3D_complex_array

```

<Interpolation: procedures>+≡

```

pure module subroutine interpolate_linear_3D_complex_array &
    (x1a, x2a, x3a, ya, x1, x2, x3, y)
    real(default), dimension(:), intent(in) :: x1a
    real(default), dimension(:), intent(in) :: x2a
    real(default), dimension(:), intent(in) :: x3a
    complex(default), dimension(:,:,:), intent(in) :: ya
    real(default), intent(in) :: x1
    real(default), intent(in) :: x2
    real(default), intent(in) :: x3
    complex(default), dimension(size(ya(1,1,1,:))), intent(out) :: y
    integer :: iy
    do iy=1, size(y)
        call interpolate_linear_3D_complex_scalar &
            (x1a, x2a, x3a, ya(:, :, :, iy), x1, x2, x3, y(iy))
    end do
end subroutine interpolate_linear_3D_complex_array

```

<Interpolation: sub interfaces>+≡

```

pure module subroutine interpolate_linear_3D_real_array (x1a, x2a, x3a, ya, x1, x2, x3, y)
    real(default), dimension(:), intent(in) :: x1a
    real(default), dimension(:), intent(in) :: x2a
    real(default), dimension(:), intent(in) :: x3a
    real(default), dimension(:,:,:), intent(in) :: ya
    real(default), intent(in) :: x1
    real(default), intent(in) :: x2
    real(default), intent(in) :: x3
    real(default), dimension(:), intent(out) :: y
end subroutine interpolate_linear_3D_real_array

```

<Interpolation: procedures>+≡

```

pure module subroutine interpolate_linear_3D_real_array (x1a, x2a, x3a, ya, x1, x2, x3, y)
    real(default), dimension(:), intent(in) :: x1a
    real(default), dimension(:), intent(in) :: x2a
    real(default), dimension(:), intent(in) :: x3a
    real(default), dimension(:,:,:), intent(in) :: ya
    real(default), intent(in) :: x1
    real(default), intent(in) :: x2
    real(default), intent(in) :: x3
    real(default), dimension(:), intent(out) :: y
    complex(default), dimension(size(ya(1,1,1,:))) :: y_c
    call interpolate_linear_3D_complex_array &
        (x1a, x2a, x3a, cmplx(ya,kind=default), x1, x2, x3, y_c)
    y = real(y_c,kind=default)
end subroutine interpolate_linear_3D_real_array

```

<Interpolation: sub interfaces>+≡

```

pure module subroutine interpolate_linear_3D_real_scalar (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:), intent(in) :: x3a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(in) :: x3
  real(default), intent(out) :: y
end subroutine interpolate_linear_3D_real_scalar

```

<Interpolation: procedures>+≡

```

pure module subroutine interpolate_linear_3D_real_scalar (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:), intent(in) :: x3a
  real(default), dimension(:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(in) :: x3
  real(default), intent(out) :: y
  complex(default), dimension(size(ya(:,1,1)),size(ya(1,:,1)),size(ya(1,1,:))) :: ya_c
  complex(default) :: y_c
  ya_c = cmplx(ya,kind=default)
  call interpolate_linear_3D_complex_scalar (x1a, x2a, x3a, ya_c, x1, x2, x3, y_c)
  y = real(y_c,kind=default)
end subroutine interpolate_linear_3D_real_scalar

```

<nr_tools.f90>≡

```

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! WHIZARD <Version> <Date>

! routine hypgeo and other useful procedures from:
!
! Numerical Recipes in Fortran 77 and 90 (Second Edition)
!
! Book and code Copyright (c) 1986-2001,
! William H. Press, Saul A. Teukolsky,
! William T. Vetterling, Brian P. Flannery.
!
! Information at http://www.nr.com
!
!
! FB: -replaced tabs by 2 whitespaces
!      -reduced hardcoded default stepsize for subroutine 'odeint'
!        called by hypgeo, cf. line 4751
!      -added explicit interface for function 'qgaus' to main module 'nr'
!      -renamed function 'locate' to 'locatenr' to avoid segfault (???)
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

```

```

MODULE nrtype
  INTEGER, PARAMETER :: I4B = SELECTED_INT_KIND(9)
  INTEGER, PARAMETER :: I2B = SELECTED_INT_KIND(4)
  INTEGER, PARAMETER :: I1B = SELECTED_INT_KIND(2)
  INTEGER, PARAMETER :: SP = KIND(1.0)
  INTEGER, PARAMETER :: DP = KIND(1.0D0)
  INTEGER, PARAMETER :: SPC = KIND((1.0,1.0))
  INTEGER, PARAMETER :: DPC = KIND((1.0D0,1.0D0))
  INTEGER, PARAMETER :: LGT = KIND(.true.)
  REAL(SP), PARAMETER :: PI=3.141592653589793238462643383279502884197_sp
  REAL(SP), PARAMETER :: PI02=1.57079632679489661923132169163975144209858_sp
  REAL(SP), PARAMETER :: TWOPI=6.283185307179586476925286766559005768394_sp
  REAL(SP), PARAMETER :: SQRT2=1.41421356237309504880168872420969807856967_sp
  REAL(SP), PARAMETER :: EULER=0.5772156649015328606065120900824024310422_sp
  REAL(DP), PARAMETER :: PI_D=3.141592653589793238462643383279502884197_dp
  REAL(DP), PARAMETER :: PI02_D=1.57079632679489661923132169163975144209858_dp
  REAL(DP), PARAMETER :: TWOPI_D=6.283185307179586476925286766559005768394_dp
  TYPE sprs2_sp
    INTEGER(I4B) :: n,len
    REAL(SP), DIMENSION(:), POINTER :: val
    INTEGER(I4B), DIMENSION(:), POINTER :: irow
    INTEGER(I4B), DIMENSION(:), POINTER :: jcol
  END TYPE sprs2_sp
  TYPE sprs2_dp
    INTEGER(I4B) :: n,len
    REAL(DP), DIMENSION(:), POINTER :: val
    INTEGER(I4B), DIMENSION(:), POINTER :: irow
    INTEGER(I4B), DIMENSION(:), POINTER :: jcol
  END TYPE sprs2_dp
END MODULE nrtype

MODULE nrutil
  USE nrtype
  IMPLICIT NONE
  INTEGER(I4B), PARAMETER :: NPAR_ARTH=16,NPAR2_ARTH=8
  INTEGER(I4B), PARAMETER :: NPAR_GEOP=4,NPAR2_GEOP=2
  INTEGER(I4B), PARAMETER :: NPAR_CUMSUM=16
  INTEGER(I4B), PARAMETER :: NPAR_CUMPROD=8
  INTEGER(I4B), PARAMETER :: NPAR_POLY=8
  INTEGER(I4B), PARAMETER :: NPAR_POLYTERM=8
  INTERFACE array_copy
    MODULE PROCEDURE array_copy_r, array_copy_d, array_copy_i
  END INTERFACE
  INTERFACE swap
    MODULE PROCEDURE swap_i,swap_r,swap_rv,swap_c, &
      swap_cv,swap_cm,swap_z,swap_zv,swap_zm, &
      masked_swap_rs,masked_swap_rv,masked_swap_rm
  END INTERFACE
  INTERFACE reallocate
    MODULE PROCEDURE reallocate_rv,reallocate_rm,&
      reallocate_iv,reallocate_im,reallocate_hv
  END INTERFACE
  INTERFACE imaxloc

```

```

MODULE PROCEDURE imaxloc_r,imaxloc_i
END INTERFACE
INTERFACE assert
MODULE PROCEDURE assert1,assert2,assert3,assert4,assert_v
END INTERFACE
INTERFACE assert_eq
MODULE PROCEDURE assert_eq2,assert_eq3,assert_eq4,assert_eqn
END INTERFACE
INTERFACE arth
MODULE PROCEDURE arth_r, arth_d, arth_i
END INTERFACE
INTERFACE geop
MODULE PROCEDURE geop_r, geop_d, geop_i, geop_c, geop_dv
END INTERFACE
INTERFACE cumsum
MODULE PROCEDURE cumsum_r,cumsum_i
END INTERFACE
INTERFACE poly
MODULE PROCEDURE poly_rr,poly_rrv,poly_dd,poly_ddv,&
poly_rc,poly_cc,poly_msk_rrv,poly_msk_ddv
END INTERFACE
INTERFACE poly_term
MODULE PROCEDURE poly_term_rr,poly_term_cc
END INTERFACE
INTERFACE outerprod
MODULE PROCEDURE outerprod_r,outerprod_d
END INTERFACE
INTERFACE outerdiff
MODULE PROCEDURE outerdiff_r,outerdiff_d,outerdiff_i
END INTERFACE
INTERFACE scatter_add
MODULE PROCEDURE scatter_add_r,scatter_add_d
END INTERFACE
INTERFACE scatter_max
MODULE PROCEDURE scatter_max_r,scatter_max_d
END INTERFACE
INTERFACE diagadd
MODULE PROCEDURE diagadd_rv,diagadd_r
END INTERFACE
INTERFACE diagmult
MODULE PROCEDURE diagmult_rv,diagmult_r
END INTERFACE
INTERFACE get_diag
MODULE PROCEDURE get_diag_rv, get_diag_dv
END INTERFACE
INTERFACE put_diag
MODULE PROCEDURE put_diag_rv, put_diag_r
END INTERFACE
CONTAINS
!BL
SUBROUTINE array_copy_r(src,dest,n_copied,n_not_copied)
REAL(SP), DIMENSION(:), INTENT(IN) :: src
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied

```

```

n_copied=min(size(src),size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_r
!BL
SUBROUTINE array_copy_d(src,dest,n_copied,n_not_copied)
REAL(DP), DIMENSION(:), INTENT(IN) :: src
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src),size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_d
!BL
SUBROUTINE array_copy_i(src,dest,n_copied,n_not_copied)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: src
INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src),size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_i
!BL
!BL
SUBROUTINE swap_i(a,b)
INTEGER(I4B), INTENT(INOUT) :: a,b
INTEGER(I4B) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_i
!BL
SUBROUTINE swap_r(a,b)
REAL(SP), INTENT(INOUT) :: a,b
REAL(SP) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_r
!BL
SUBROUTINE swap_rv(a,b)
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
REAL(SP), DIMENSION(SIZE(a)) :: dum
dum=a
a=b
b=dum
END SUBROUTINE swap_rv
!BL
SUBROUTINE swap_c(a,b)
COMPLEX(SPC), INTENT(INOUT) :: a,b
COMPLEX(SPC) :: dum
dum=a
a=b
b=dum

```

```

        END SUBROUTINE swap_c
!BL
        SUBROUTINE swap_cv(a,b)
        COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: a,b
        COMPLEX(SPC), DIMENSION(SIZE(a)) :: dum
        dum=a
        a=b
        b=dum
        END SUBROUTINE swap_cv
!BL
        SUBROUTINE swap_cm(a,b)
        COMPLEX(SPC), DIMENSION(:, :), INTENT(INOUT) :: a,b
        COMPLEX(SPC), DIMENSION(size(a,1),size(a,2)) :: dum
        dum=a
        a=b
        b=dum
        END SUBROUTINE swap_cm
!BL
        SUBROUTINE swap_z(a,b)
        COMPLEX(DPC), INTENT(INOUT) :: a,b
        COMPLEX(DPC) :: dum
        dum=a
        a=b
        b=dum
        END SUBROUTINE swap_z
!BL
        SUBROUTINE swap_zv(a,b)
        COMPLEX(DPC), DIMENSION(:), INTENT(INOUT) :: a,b
        COMPLEX(DPC), DIMENSION(SIZE(a)) :: dum
        dum=a
        a=b
        b=dum
        END SUBROUTINE swap_zv
!BL
        SUBROUTINE swap_zm(a,b)
        COMPLEX(DPC), DIMENSION(:, :), INTENT(INOUT) :: a,b
        COMPLEX(DPC), DIMENSION(size(a,1),size(a,2)) :: dum
        dum=a
        a=b
        b=dum
        END SUBROUTINE swap_zm
!BL
        SUBROUTINE masked_swap_rs(a,b,mask)
        REAL(SP), INTENT(INOUT) :: a,b
        LOGICAL(LGT), INTENT(IN) :: mask
        REAL(SP) :: swp
        if (mask) then
            swp=a
            a=b
            b=swp
        end if
        END SUBROUTINE masked_swap_rs
!BL
        SUBROUTINE masked_swap_rv(a,b,mask)

```

```

REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(a)) :: swp
where (mask)
    swp=a
    a=b
    b=swp
end where
END SUBROUTINE masked_swap_rv
!BL
SUBROUTINE masked_swap_rm(a,b,mask)
REAL(SP), DIMENSION(:, :), INTENT(INOUT) :: a,b
LOGICAL(LGT), DIMENSION(:, :), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(a,1),size(a,2)) :: swp
where (mask)
    swp=a
    a=b
    b=swp
end where
END SUBROUTINE masked_swap_rm
!BL
!BL
FUNCTION reallocate_rv(p,n)
REAL(SP), DIMENSION(:), POINTER :: p, reallocate_rv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_rv(n),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_rv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_rv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_rv
!BL
FUNCTION reallocate_iv(p,n)
INTEGER(I4B), DIMENSION(:), POINTER :: p, reallocate_iv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_iv(n),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_iv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_iv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_iv
!BL
FUNCTION reallocate_hv(p,n)
CHARACTER(1), DIMENSION(:), POINTER :: p, reallocate_hv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_hv(n),stat=ierr)
if (ierr /= 0) call &

```

```

        nrerror('reallocate_hv: problem in attempt to allocate memory')
    if (.not. associated(p)) RETURN
    nold=size(p)
    reallocate_hv(1:min(nold,n))=p(1:min(nold,n))
    deallocate(p)
END FUNCTION reallocate_hv
!BL
FUNCTION reallocate_rm(p,n,m)
REAL(SP), DIMENSION(:,:), POINTER :: p, reallocate_rm
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_rm(n,m),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_rm: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p,1)
mold=size(p,2)
reallocate_rm(1:min(nold,n),1:min(mold,m))=&
    p(1:min(nold,n),1:min(mold,m))
deallocate(p)
END FUNCTION reallocate_rm
!BL
FUNCTION reallocate_im(p,n,m)
INTEGER(I4B), DIMENSION(:,:), POINTER :: p, reallocate_im
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_im(n,m),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_im: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p,1)
mold=size(p,2)
reallocate_im(1:min(nold,n),1:min(mold,m))=&
    p(1:min(nold,n),1:min(mold,m))
deallocate(p)
END FUNCTION reallocate_im
!BL
FUNCTION ifirstloc(mask)
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
INTEGER(I4B) :: ifirstloc
INTEGER(I4B), DIMENSION(1) :: loc
loc=maxloc(merge(1,0,mask))
ifirstloc=loc(1)
if (.not. mask(ifirstloc)) ifirstloc=size(mask)+1
END FUNCTION ifirstloc
!BL
FUNCTION imaxloc_r(arr)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B) :: imaxloc_r
INTEGER(I4B), DIMENSION(1) :: imax
imax=maxloc(arr(:))
imaxloc_r=imax(1)
END FUNCTION imaxloc_r
!BL

```



```

FUNCTION imaxloc_i(iarr)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: iarr
INTEGER(I4B), DIMENSION(1) :: imax
INTEGER(I4B) :: imaxloc_i
imax=maxloc(iarr(:))
imaxloc_i=imax(1)
END FUNCTION imaxloc_i
!BL
FUNCTION iminloc(arr)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), DIMENSION(1) :: imin
INTEGER(I4B) :: iminloc
imin=minloc(arr(:))
iminloc=imin(1)
END FUNCTION iminloc
!BL
SUBROUTINE assert1(n1,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1
if (.not. n1) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert1'
end if
END SUBROUTINE assert1
!BL
SUBROUTINE assert2(n1,n2,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2
if (.not. (n1 .and. n2)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert2'
end if
END SUBROUTINE assert2
!BL
SUBROUTINE assert3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3
if (.not. (n1 .and. n2 .and. n3)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert3'
end if
END SUBROUTINE assert3
!BL
SUBROUTINE assert4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3,n4
if (.not. (n1 .and. n2 .and. n3 .and. n4)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert4'
end if

```

```

END SUBROUTINE assert4
!BL
SUBROUTINE assert_v(n,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, DIMENSION(:), INTENT(IN) :: n
if (.not. all(n)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert_v'
end if
END SUBROUTINE assert_v
!BL
FUNCTION assert_eq2(n1,n2,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2
INTEGER :: assert_eq2
if (n1 == n2) then
    assert_eq2=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq2'
end if
END FUNCTION assert_eq2
!BL
FUNCTION assert_eq3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3
INTEGER :: assert_eq3
if (n1 == n2 .and. n2 == n3) then
    assert_eq3=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq3'
end if
END FUNCTION assert_eq3
!BL
FUNCTION assert_eq4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3,n4
INTEGER :: assert_eq4
if (n1 == n2 .and. n2 == n3 .and. n3 == n4) then
    assert_eq4=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq4'
end if
END FUNCTION assert_eq4
!BL
FUNCTION assert_eqn(nn,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, DIMENSION(:), INTENT(IN) :: nn

```

```

INTEGER :: assert_eqn
if (all(nn(2:) == nn(1))) then
    assert_eqn=nn(1)
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eqn'
end if
END FUNCTION assert_eqn
!BL
SUBROUTINE nrerror(string)
CHARACTER(LEN=*), INTENT(IN) :: string
write (*,*) 'nrerror: ',string
STOP 'program terminated by nrerror'
END SUBROUTINE nrerror
!BL
FUNCTION arth_r(first,increment,n)
REAL(SP), INTENT(IN) :: first,increment
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: arth_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) arth_r(1)=first
if (n <= NPAR_ARTH) then
    do k=2,n
        arth_r(k)=arth_r(k-1)+increment
    end do
else
    do k=2,NPAR2_ARTH
        arth_r(k)=arth_r(k-1)+increment
    end do
    temp=increment*NPAR2_ARTH
    k=NPAR2_ARTH
    do
        if (k >= n) exit
        k2=k+k
        arth_r(k+1:min(k2,n))=temp+arth_r(1:min(k,n-k))
        temp=temp+temp
        k=k2
    end do
end if
END FUNCTION arth_r
!BL
FUNCTION arth_d(first,increment,n)
REAL(DP), INTENT(IN) :: first,increment
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: arth_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) arth_d(1)=first
if (n <= NPAR_ARTH) then
    do k=2,n
        arth_d(k)=arth_d(k-1)+increment
    end do

```

```

else
  do k=2,NPAR2_ARTH
    arth_d(k)=arth_d(k-1)+increment
  end do
  temp=increment*NPAR2_ARTH
  k=NPAR2_ARTH
  do
    if (k >= n) exit
    k2=k+k
    arth_d(k+1:min(k2,n))=temp+arth_d(1:min(k,n-k))
    temp=temp+temp
    k=k2
  end do
end if
END FUNCTION arth_d
!BL
FUNCTION arth_i(first,increment,n)
INTEGER(I4B), INTENT(IN) :: first,increment,n
INTEGER(I4B), DIMENSION(n) :: arth_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) arth_i(1)=first
if (n <= NPAR_ARTH) then
  do k=2,n
    arth_i(k)=arth_i(k-1)+increment
  end do
else
  do k=2,NPAR2_ARTH
    arth_i(k)=arth_i(k-1)+increment
  end do
  temp=increment*NPAR2_ARTH
  k=NPAR2_ARTH
  do
    if (k >= n) exit
    k2=k+k
    arth_i(k+1:min(k2,n))=temp+arth_i(1:min(k,n-k))
    temp=temp+temp
    k=k2
  end do
end if
END FUNCTION arth_i
!BL
!BL
FUNCTION geop_r(first,factor,n)
REAL(SP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: geop_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) geop_r(1)=first
if (n <= NPAR_GEOP) then
  do k=2,n
    geop_r(k)=geop_r(k-1)*factor
  end do
else

```

```

do k=2,NPAR2_GEOP
    geop_r(k)=geop_r(k-1)*factor
end do
temp=factor**NPAR2_GEOP
k=NPAR2_GEOP
do
    if (k >= n) exit
    k2=k+k
    geop_r(k+1:min(k2,n))=temp*geop_r(1:min(k,n-k))
    temp=temp*temp
    k=k2
end do
end if
END FUNCTION geop_r
!BL
FUNCTION geop_d(first,factor,n)
REAL(DP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: geop_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) geop_d(1)=first
if (n <= NPAR_GEOP) then
    do k=2,n
        geop_d(k)=geop_d(k-1)*factor
    end do
else
    do k=2,NPAR2_GEOP
        geop_d(k)=geop_d(k-1)*factor
    end do
    temp=factor**NPAR2_GEOP
    k=NPAR2_GEOP
    do
        if (k >= n) exit
        k2=k+k
        geop_d(k+1:min(k2,n))=temp*geop_d(1:min(k,n-k))
        temp=temp*temp
        k=k2
    end do
end if
END FUNCTION geop_d
!BL
FUNCTION geop_i(first,factor,n)
INTEGER(I4B), INTENT(IN) :: first,factor,n
INTEGER(I4B), DIMENSION(n) :: geop_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) geop_i(1)=first
if (n <= NPAR_GEOP) then
    do k=2,n
        geop_i(k)=geop_i(k-1)*factor
    end do
else
    do k=2,NPAR2_GEOP
        geop_i(k)=geop_i(k-1)*factor

```

```

end do
temp=factor**NPAR2_GEOP
k=NPAR2_GEOP
do
  if (k >= n) exit
  k2=k+k
  geop_i(k+1:min(k2,n))=temp*geop_i(1:min(k,n-k))
  temp=temp*temp
  k=k2
end do
end if
END FUNCTION geop_i
!BL
FUNCTION geop_c(first,factor,n)
COMPLEX(SP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
COMPLEX(SP), DIMENSION(n) :: geop_c
INTEGER(I4B) :: k,k2
COMPLEX(SP) :: temp
if (n > 0) geop_c(1)=first
if (n <= NPAR_GEOP) then
  do k=2,n
    geop_c(k)=geop_c(k-1)*factor
  end do
else
  do k=2,NPAR2_GEOP
    geop_c(k)=geop_c(k-1)*factor
  end do
  temp=factor**NPAR2_GEOP
  k=NPAR2_GEOP
  do
    if (k >= n) exit
    k2=k+k
    geop_c(k+1:min(k2,n))=temp*geop_c(1:min(k,n-k))
    temp=temp*temp
    k=k2
  end do
end if
END FUNCTION geop_c
!BL
FUNCTION geop_dv(first,factor,n)
REAL(DP), DIMENSION(:), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(size(first),n) :: geop_dv
INTEGER(I4B) :: k,k2
REAL(DP), DIMENSION(size(first)) :: temp
if (n > 0) geop_dv(:,1)=first(:)
if (n <= NPAR_GEOP) then
  do k=2,n
    geop_dv(:,k)=geop_dv(:,k-1)*factor(:)
  end do
else
  do k=2,NPAR2_GEOP
    geop_dv(:,k)=geop_dv(:,k-1)*factor(:)

```

```

end do
temp=factor**NPAR2_GEOP
k=NPAR2_GEOP
do
  if (k >= n) exit
  k2=k+k
  geop_dv(:,k+1:min(k2,n))=geop_dv(:,1:min(k,n-k))*&
    spread(temp,2,size(geop_dv(:,1:min(k,n-k)),2))
  temp=temp*temp
  k=k2
end do
end if
END FUNCTION geop_dv
!BL
!BL
RECURSIVE FUNCTION cumsum_r(arr,seed) RESULT(ans)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
REAL(SP), OPTIONAL, INTENT(IN) :: seed
REAL(SP), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j
REAL(SP) :: sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0.0_sp
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
  do j=2,n
    ans(j)=ans(j-1)+arr(j)
  end do
else
  ans(2:n:2)=cumsum_r(arr(2:n:2)+arr(1:n-1:2),sd)
  ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
END FUNCTION cumsum_r
!BL
RECURSIVE FUNCTION cumsum_i(arr,seed) RESULT(ans)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), OPTIONAL, INTENT(IN) :: seed
INTEGER(I4B), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j,sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0_i4b
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
  do j=2,n
    ans(j)=ans(j-1)+arr(j)
  end do
else
  ans(2:n:2)=cumsum_i(arr(2:n:2)+arr(1:n-1:2),sd)
  ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
end if

```

```

      END FUNCTION cumsum_i
!BL
!BL
      RECURSIVE FUNCTION cumprod(arr,seed) RESULT(ans)
      REAL(SP), DIMENSION(:), INTENT(IN) :: arr
      REAL(SP), OPTIONAL, INTENT(IN) :: seed
      REAL(SP), DIMENSION(size(arr)) :: ans
      INTEGER(I4B) :: n,j
      REAL(SP) :: sd
      n=size(arr)
      if (n == 0_i4b) RETURN
      sd=1.0_sp
      if (present(seed)) sd=seed
      ans(1)=arr(1)*sd
      if (n < NPAR_CUMPROD) then
         do j=2,n
            ans(j)=ans(j-1)*arr(j)
         end do
      else
         ans(2:n:2)=cumprod(arr(2:n:2)*arr(1:n-1:2),sd)
         ans(3:n:2)=ans(2:n-1:2)*arr(3:n:2)
      end if
      END FUNCTION cumprod
!BL
!BL
      FUNCTION poly_rr(x,coeffs)
      REAL(SP), INTENT(IN) :: x
      REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
      REAL(SP) :: poly_rr
      REAL(SP) :: pow
      REAL(SP), DIMENSION(:), ALLOCATABLE :: vec
      INTEGER(I4B) :: i,n,nn
      n=size(coeffs)
      if (n <= 0) then
         poly_rr=0.0_sp
      else if (n < NPAR_POLY) then
         poly_rr=coeffs(n)
         do i=n-1,1,-1
            poly_rr=x*poly_rr+coeffs(i)
         end do
      else
         allocate(vec(n+1))
         pow=x
         vec(1:n)=coeffs
         do
            vec(n+1)=0.0_sp
            nn=ishft(n+1,-1)
            vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
            if (nn == 1) exit
            pow=pow*pow
            n=nn
         end do
         poly_rr=vec(1)
         deallocate(vec)

```



```

        end if
    END FUNCTION poly_rr
!BL
    FUNCTION poly_dd(x,coeffs)
    REAL(DP), INTENT(IN) :: x
    REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs
    REAL(DP) :: poly_dd
    REAL(DP) :: pow
    REAL(DP), DIMENSION(:), ALLOCATABLE :: vec
    INTEGER(I4B) :: i,n,nn
    n=size(coeffs)
    if (n <= 0) then
        poly_dd=0.0_dp
    else if (n < NPAR_POLY) then
        poly_dd=coeffs(n)
        do i=n-1,1,-1
            poly_dd=x*poly_dd+coeffs(i)
        end do
    else
        allocate(vec(n+1))
        pow=x
        vec(1:n)=coeffs
        do
            vec(n+1)=0.0_dp
            nn=ishft(n+1,-1)
            vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
            if (nn == 1) exit
            pow=pow*pow
            n=nn
        end do
        poly_dd=vec(1)
        deallocate(vec)
    end if
    END FUNCTION poly_dd
!BL
    FUNCTION poly_rc(x,coeffs)
    COMPLEX(SPC), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
    COMPLEX(SPC) :: poly_rc
    COMPLEX(SPC) :: pow
    COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
    INTEGER(I4B) :: i,n,nn
    n=size(coeffs)
    if (n <= 0) then
        poly_rc=0.0_sp
    else if (n < NPAR_POLY) then
        poly_rc=coeffs(n)
        do i=n-1,1,-1
            poly_rc=x*poly_rc+coeffs(i)
        end do
    else
        allocate(vec(n+1))
        pow=x
        vec(1:n)=coeffs

```

```

do
  vec(n+1)=0.0_sp
  nn=ishft(n+1,-1)
  vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
  if (nn == 1) exit
  pow=pow*pow
  n=nn
end do
poly_rc=vec(1)
deallocate(vec)
end if
END FUNCTION poly_rc
!BL
FUNCTION poly_cc(x,coeffs)
COMPLEX(SPC), INTENT(IN) :: x
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: coeffs
COMPLEX(SPC) :: poly_cc
COMPLEX(SPC) :: pow
COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n <= 0) then
  poly_cc=0.0_sp
else if (n < NPAR_POLY) then
  poly_cc=coeffs(n)
  do i=n-1,1,-1
    poly_cc=x*poly_cc+coeffs(i)
  end do
else
  allocate(vec(n+1))
  pow=x
  vec(1:n)=coeffs
  do
    vec(n+1)=0.0_sp
    nn=ishft(n+1,-1)
    vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
    if (nn == 1) exit
    pow=pow*pow
    n=nn
  end do
  poly_cc=vec(1)
  deallocate(vec)
end if
END FUNCTION poly_cc
!BL
FUNCTION poly_rrv(x,coeffs)
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(SP), DIMENSION(size(x)) :: poly_rrv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m <= 0) then
  poly_rrv=0.0_sp
else if (m < n .or. m < NPAR_POLY) then

```

```

        poly_rrv=coeffs(m)
        do i=m-1,1,-1
            poly_rrv=x*poly_rrv+coeffs(i)
        end do
    else
        do i=1,n
            poly_rrv(i)=poly_rr(x(i),coeffs)
        end do
    end if
END FUNCTION poly_rrv
!BL
FUNCTION poly_ddv(x,coeffs)
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(DP), DIMENSION(size(x)) :: poly_ddv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m <= 0) then
    poly_ddv=0.0_dp
else if (m < n .or. m < NPAR_POLY) then
    poly_ddv=coeffs(m)
    do i=m-1,1,-1
        poly_ddv=x*poly_ddv+coeffs(i)
    end do
else
    do i=1,n
        poly_ddv(i)=poly_dd(x(i),coeffs)
    end do
end if
END FUNCTION poly_ddv
!BL
FUNCTION poly_msk_rrv(x,coeffs,mask)
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(x)) :: poly_msk_rrv
poly_msk_rrv=unpack(poly_rrv(pack(x,mask),coeffs),mask,0.0_sp)
END FUNCTION poly_msk_rrv
!BL
FUNCTION poly_msk_ddv(x,coeffs,mask)
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(DP), DIMENSION(size(x)) :: poly_msk_ddv
poly_msk_ddv=unpack(poly_ddv(pack(x,mask),coeffs),mask,0.0_dp)
END FUNCTION poly_msk_ddv
!BL
!BL
RECURSIVE FUNCTION poly_term_rr(a,b) RESULT(u)
REAL(SP), DIMENSION(:), INTENT(IN) :: a
REAL(SP), INTENT(IN) :: b
REAL(SP), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)

```

```

    if (n < NPAR_POLYTERM) then
        do j=2,n
            u(j)=a(j)+b*u(j-1)
        end do
    else
        u(2:n:2)=poly_term_rr(a(2:n:2)+a(1:n-1:2)*b,b*b)
        u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
    end if
END FUNCTION poly_term_rr
!BL
RECURSIVE FUNCTION poly_term_cc(a,b) RESULT(u)
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
COMPLEX(SPC), INTENT(IN) :: b
COMPLEX(SPC), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)
if (n < NPAR_POLYTERM) then
    do j=2,n
        u(j)=a(j)+b*u(j-1)
    end do
else
    u(2:n:2)=poly_term_cc(a(2:n:2)+a(1:n-1:2)*b,b*b)
    u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
end if
END FUNCTION poly_term_cc
!BL
!BL
FUNCTION zroots_unity(n,nn)
INTEGER(I4B), INTENT(IN) :: n,nn
COMPLEX(SPC), DIMENSION(nn) :: zroots_unity
INTEGER(I4B) :: k
REAL(SP) :: theta
zroots_unity(1)=1.0
theta=TWOPI/n
k=1
do
    if (k >= nn) exit
    zroots_unity(k+1)=cmplx(cos(k*theta),sin(k*theta),SPC)
    zroots_unity(k+2:min(2*k,nn))=zroots_unity(k+1)*&
        zroots_unity(2:min(k,nn-k))
    k=2*k
end do
END FUNCTION zroots_unity
!BL
FUNCTION outerprod_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerprod_r
outerprod_r = spread(a,dim=2,ncopies=size(b)) * &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_r
!BL
FUNCTION outerprod_d(a,b)

```

```

REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerprod_d
outerprod_d = spread(a,dim=2,ncopies=size(b)) * &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_d
!BL
FUNCTION outerdiv(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiv
outerdiv = spread(a,dim=2,ncopies=size(b)) / &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiv
!BL
FUNCTION outersum(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outersum
outersum = spread(a,dim=2,ncopies=size(b)) + &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outersum
!BL
FUNCTION outerdiff_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiff_r
outerdiff_r = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_r
!BL
FUNCTION outerdiff_d(a,b)
REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerdiff_d
outerdiff_d = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_d
!BL
FUNCTION outerdiff_i(a,b)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: a,b
INTEGER(I4B), DIMENSION(size(a),size(b)) :: outerdiff_i
outerdiff_i = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_i
!BL
FUNCTION outerand(a,b)
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: a,b
LOGICAL(LGT), DIMENSION(size(a),size(b)) :: outerand
outerand = spread(a,dim=2,ncopies=size(b)) .and. &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerand
!BL
SUBROUTINE scatter_add_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_add_r')
```

```

m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=dest(i)+source(j)
end do
END SUBROUTINE scatter_add_r
SUBROUTINE scatter_add_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_add_d')
m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=dest(i)+source(j)
end do
END SUBROUTINE scatter_add_d
SUBROUTINE scatter_max_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_max_r')
m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=max(dest(i),source(j))
end do
END SUBROUTINE scatter_max_r
SUBROUTINE scatter_max_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_max_d')
m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=max(dest(i),source(j))
end do
END SUBROUTINE scatter_max_d
!BL
SUBROUTINE diagadd_rv(mat,diag)
REAL(SP), DIMENSION(:, :), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagadd_rv')
do j=1,n
  mat(j,j)=mat(j,j)+diag(j)
end do
END SUBROUTINE diagadd_rv
!BL
SUBROUTINE diagadd_r(mat,diag)

```

```

REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
    mat(j,j)=mat(j,j)+diag
end do
END SUBROUTINE diagadd_r
!BL
SUBROUTINE diagmult_rv(mat,diag)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagmult_rv')
do j=1,n
    mat(j,j)=mat(j,j)*diag(j)
end do
END SUBROUTINE diagmult_rv
!BL
SUBROUTINE diagmult_r(mat,diag)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
    mat(j,j)=mat(j,j)*diag
end do
END SUBROUTINE diagmult_r
!BL
FUNCTION get_diag_rv(mat)
REAL(SP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(SP), DIMENSION(size(mat,1)) :: get_diag_rv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_rv')
do j=1,size(mat,1)
    get_diag_rv(j)=mat(j,j)
end do
END FUNCTION get_diag_rv
!BL
FUNCTION get_diag_dv(mat)
REAL(DP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(DP), DIMENSION(size(mat,1)) :: get_diag_dv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_dv')
do j=1,size(mat,1)
    get_diag_dv(j)=mat(j,j)
end do
END FUNCTION get_diag_dv
!BL
SUBROUTINE put_diag_rv(diagv,mat)
REAL(SP), DIMENSION(:), INTENT(IN) :: diagv
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n=assert_eq2(size(diagv),min(size(mat,1),size(mat,2)),'put_diag_rv')

```

```

do j=1,n
  mat(j,j)=diagv(j)
end do
END SUBROUTINE put_diag_rv
!BL
SUBROUTINE put_diag_r(scal,mat)
REAL(SP), INTENT(IN) :: scal
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
  mat(j,j)=scal
end do
END SUBROUTINE put_diag_r
!BL
SUBROUTINE unit_matrix(mat)
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: mat
INTEGER(I4B) :: i,n
n=min(size(mat,1),size(mat,2))
mat(:,:)=0.0_sp
do i=1,n
  mat(i,i)=1.0_sp
end do
END SUBROUTINE unit_matrix
!BL
FUNCTION upper_triangle(j,k,extra)
INTEGER(I4B), INTENT(IN) :: j,k
INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
LOGICAL(LGT), DIMENSION(j,k) :: upper_triangle
INTEGER(I4B) :: n
n=0
if (present(extra)) n=extra
upper_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) < n)
END FUNCTION upper_triangle
!BL
FUNCTION lower_triangle(j,k,extra)
INTEGER(I4B), INTENT(IN) :: j,k
INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
LOGICAL(LGT), DIMENSION(j,k) :: lower_triangle
INTEGER(I4B) :: n
n=0
if (present(extra)) n=extra
lower_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) > -n)
END FUNCTION lower_triangle
!BL
FUNCTION vabs(v)
REAL(SP), DIMENSION(:), INTENT(IN) :: v
REAL(SP) :: vabs
vabs=sqrt(dot_product(v,v))
END FUNCTION vabs
!BL
END MODULE nrutil

MODULE ode_path

```



```

USE nrtype
INTEGER(I4B) :: nok,nbad,kount
LOGICAL(LGT), SAVE :: save_steps=.false.
REAL(SP) :: dxsav
REAL(SP), DIMENSION(:), POINTER :: xp
REAL(SP), DIMENSION(:,,:), POINTER :: yp
END MODULE ode_path

MODULE hypgeo_info
USE nrtype
COMPLEX(SPC) :: hypgeo_aa,hypgeo_bb,hypgeo_cc,hypgeo_dz,hypgeo_z0
END MODULE hypgeo_info

MODULE nr
INTERFACE
SUBROUTINE airy(x,ai,bi,aip,bip)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP), INTENT(OUT) :: ai,bi,aip,bip
END SUBROUTINE airy
END INTERFACE
INTERFACE
SUBROUTINE amebsa(p,y,pb,yb,ftol,func,iter,temptr)
USE nrtype
INTEGER(I4B), INTENT(INOUT) :: iter
REAL(SP), INTENT(INOUT) :: yb
REAL(SP), INTENT(IN) :: ftol,temptr
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y,pb
REAL(SP), DIMENSION(:,,:), INTENT(INOUT) :: p
INTERFACE
FUNCTION func(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP) :: func
END FUNCTION func
END INTERFACE
END SUBROUTINE amebsa
END INTERFACE
INTERFACE
SUBROUTINE amoeba(p,y,ftol,func,iter)
USE nrtype
INTEGER(I4B), INTENT(OUT) :: iter
REAL(SP), INTENT(IN) :: ftol
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
REAL(SP), DIMENSION(:,,:), INTENT(INOUT) :: p
INTERFACE
FUNCTION func(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP) :: func
END FUNCTION func
END INTERFACE
END SUBROUTINE amoeba
END INTERFACE

```

```

INTERFACE
  SUBROUTINE anneal(x,y,iorder)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: iorder
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
  END SUBROUTINE anneal
END INTERFACE
INTERFACE
  SUBROUTINE asolve(b,x,itrnsp)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: b
    REAL(DP), DIMENSION(:), INTENT(OUT) :: x
    INTEGER(I4B), INTENT(IN) :: itrnsp
  END SUBROUTINE asolve
END INTERFACE
INTERFACE
  SUBROUTINE atimes(x,r,itrnsp)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: x
    REAL(DP), DIMENSION(:), INTENT(OUT) :: r
    INTEGER(I4B), INTENT(IN) :: itrnsp
  END SUBROUTINE atimes
END INTERFACE
INTERFACE
  SUBROUTINE avevar(data,ave,var)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
    REAL(SP), INTENT(OUT) :: ave,var
  END SUBROUTINE avevar
END INTERFACE
INTERFACE
  SUBROUTINE balanc(a)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
  END SUBROUTINE balanc
END INTERFACE
INTERFACE
  SUBROUTINE banbks(a,m1,m2,al,indx,b)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a,al
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
  END SUBROUTINE banbks
END INTERFACE
INTERFACE
  SUBROUTINE bandec(a,m1,m2,al,indx,d)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: indx
    REAL(SP), INTENT(OUT) :: d
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: al
  END SUBROUTINE bandec

```

```

END INTERFACE
INTERFACE
  SUBROUTINE banmul(a,m1,m2,x,b)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: b
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
  END SUBROUTINE banmul
END INTERFACE
INTERFACE
  SUBROUTINE bcucof(y,y1,y2,y12,d1,d2,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: d1,d2
    REAL(SP), DIMENSION(4), INTENT(IN) :: y,y1,y2,y12
    REAL(SP), DIMENSION(4,4), INTENT(OUT) :: c
  END SUBROUTINE bcucof
END INTERFACE
INTERFACE
  SUBROUTINE bcuint(y,y1,y2,y12,x1l,x1u,x2l,x2u,x1,x2,ansy,&
    ansy1,ansy2)
    USE nrtype
    REAL(SP), DIMENSION(4), INTENT(IN) :: y,y1,y2,y12
    REAL(SP), INTENT(IN) :: x1l,x1u,x2l,x2u,x1,x2
    REAL(SP), INTENT(OUT) :: ansy,ansy1,ansy2
  END SUBROUTINE bcuint
END INTERFACE
INTERFACE beschb
  SUBROUTINE beschb_s(x,gam1,gam2,gampl,gammi)
    USE nrtype
    REAL(DP), INTENT(IN) :: x
    REAL(DP), INTENT(OUT) :: gam1,gam2,gampl,gammi
  END SUBROUTINE beschb_s
!BL
  SUBROUTINE beschb_v(x,gam1,gam2,gampl,gammi)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: x
    REAL(DP), DIMENSION(:), INTENT(OUT) :: gam1,gam2,gampl,gammi
  END SUBROUTINE beschb_v
END INTERFACE
INTERFACE bessi
  FUNCTION bessi_s(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessi_s
  END FUNCTION bessi_s
!BL
  FUNCTION bessi_v(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessi_v
  END FUNCTION bessi_v

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```

END INTERFACE
INTERFACE bessio
  FUNCTION bessio_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessio_s
  END FUNCTION bessio_s
!BL
  FUNCTION bessio_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessio_v
  END FUNCTION bessio_v
END INTERFACE
INTERFACE bess1
  FUNCTION bess1_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bess1_s
  END FUNCTION bess1_s
!BL
  FUNCTION bess1_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bess1_v
  END FUNCTION bess1_v
END INTERFACE
INTERFACE
  SUBROUTINE bessik(x,xnu,ri,rk,rip,rkp)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,xnu
    REAL(SP), INTENT(OUT) :: ri,rk,rip,rkp
  END SUBROUTINE bessik
END INTERFACE
INTERFACE bessj
  FUNCTION bessj_s(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessj_s
  END FUNCTION bessj_s
!BL
  FUNCTION bessj_v(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessj_v
  END FUNCTION bessj_v
END INTERFACE
INTERFACE bessj0
  FUNCTION bessj0_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessj0_s

```

```

        END FUNCTION bessj0_s
!BL
        FUNCTION bessj0_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: bessj0_v
        END FUNCTION bessj0_v
    END INTERFACE
    INTERFACE bessj1
        FUNCTION bessj1_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: bessj1_s
        END FUNCTION bessj1_s
!BL
        FUNCTION bessj1_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: bessj1_v
        END FUNCTION bessj1_v
    END INTERFACE
    INTERFACE bessjy
        SUBROUTINE bessjy_s(x,xnu,rj,ry,rjp,ryp)
        USE nrtype
        REAL(SP), INTENT(IN) :: x,xnu
        REAL(SP), INTENT(OUT) :: rj,ry,rjp,ryp
        END SUBROUTINE bessjy_s
!BL
        SUBROUTINE bessjy_v(x,xnu,rj,ry,rjp,ryp)
        USE nrtype
        REAL(SP), INTENT(IN) :: xnu
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(OUT) :: rj,rjp,ry,ryp
        END SUBROUTINE bessjy_v
    END INTERFACE
    INTERFACE bessk
        FUNCTION bessk_s(n,x)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: bessk_s
        END FUNCTION bessk_s
!BL
        FUNCTION bessk_v(n,x)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: bessk_v
        END FUNCTION bessk_v
    END INTERFACE
    INTERFACE bessk0
        FUNCTION bessk0_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x

```

```

REAL(SP) :: bessk0_s
END FUNCTION bessk0_s
!BL
FUNCTION bessk0_v(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: bessk0_v
END FUNCTION bessk0_v
END INTERFACE
INTERFACE bessk1
FUNCTION bessk1_s(x)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP) :: bessk1_s
END FUNCTION bessk1_s
!BL
FUNCTION bessk1_v(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: bessk1_v
END FUNCTION bessk1_v
END INTERFACE
INTERFACE bessy
FUNCTION bessy_s(n,x)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), INTENT(IN) :: x
REAL(SP) :: bessy_s
END FUNCTION bessy_s
!BL
FUNCTION bessy_v(n,x)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: bessy_v
END FUNCTION bessy_v
END INTERFACE
INTERFACE bessy0
FUNCTION bessy0_s(x)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP) :: bessy0_s
END FUNCTION bessy0_s
!BL
FUNCTION bessy0_v(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: bessy0_v
END FUNCTION bessy0_v
END INTERFACE
INTERFACE bessy1
FUNCTION bessy1_s(x)
USE nrtype
REAL(SP), INTENT(IN) :: x

```

```

      REAL(SP) :: bessy1_s
    END FUNCTION bessy1_s
!BL
    FUNCTION bessy1_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessy1_v
    END FUNCTION bessy1_v
  END INTERFACE
  INTERFACE beta
    FUNCTION beta_s(z,w)
    USE nrtype
    REAL(SP), INTENT(IN) :: z,w
    REAL(SP) :: beta_s
    END FUNCTION beta_s
!BL
    FUNCTION beta_v(z,w)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: z,w
    REAL(SP), DIMENSION(size(z)) :: beta_v
    END FUNCTION beta_v
  END INTERFACE
  INTERFACE betacf
    FUNCTION betacf_s(a,b,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,x
    REAL(SP) :: betacf_s
    END FUNCTION betacf_s
!BL
    FUNCTION betacf_v(a,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,x
    REAL(SP), DIMENSION(size(x)) :: betacf_v
    END FUNCTION betacf_v
  END INTERFACE
  INTERFACE betai
    FUNCTION betai_s(a,b,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,x
    REAL(SP) :: betai_s
    END FUNCTION betai_s
!BL
    FUNCTION betai_v(a,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,x
    REAL(SP), DIMENSION(size(a)) :: betai_v
    END FUNCTION betai_v
  END INTERFACE
  INTERFACE bico
    FUNCTION bico_s(n,k)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n,k
    REAL(SP) :: bico_s
    END FUNCTION bico_s

```

```

!BL
      FUNCTION bico_v(n,k)
      USE nrtype
      INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n,k
      REAL(SP), DIMENSION(size(n)) :: bico_v
      END FUNCTION bico_v
END INTERFACE
INTERFACE
      FUNCTION bnldev(pp,n)
      USE nrtype
      REAL(SP), INTENT(IN) :: pp
      INTEGER(I4B), INTENT(IN) :: n
      REAL(SP) :: bnldev
      END FUNCTION bnldev
END INTERFACE
INTERFACE
      FUNCTION brent(ax,bx,cx,func,tol,xmin)
      USE nrtype
      REAL(SP), INTENT(IN) :: ax,bx,cx,tol
      REAL(SP), INTENT(OUT) :: xmin
      REAL(SP) :: brent
      INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
      END INTERFACE
      END FUNCTION brent
END INTERFACE
INTERFACE
      SUBROUTINE broydn(x,check)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
      LOGICAL(LGT), INTENT(OUT) :: check
      END SUBROUTINE broydn
END INTERFACE
INTERFACE
      SUBROUTINE bsstep(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
      REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
      REAL(SP), INTENT(INOUT) :: x
      REAL(SP), INTENT(IN) :: htry,eps
      REAL(SP), INTENT(OUT) :: hdid,hnext
      INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
      END INTERFACE
      END SUBROUTINE bsstep

```



```

END INTERFACE
INTERFACE
  SUBROUTINE caldat(julian,mm,id,iyyy)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: julian
    INTEGER(I4B), INTENT(OUT) :: mm,id,iyyy
  END SUBROUTINE caldat
END INTERFACE
INTERFACE
  FUNCTION chder(a,b,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP), DIMENSION(size(c)) :: chder
  END FUNCTION chder
END INTERFACE
INTERFACE chebev
  FUNCTION chebev_s(a,b,c,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,x
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP) :: chebev_s
  END FUNCTION chebev_s
!BL
  FUNCTION chebev_v(a,b,c,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: c,x
    REAL(SP), DIMENSION(size(x)) :: chebev_v
  END FUNCTION chebev_v
END INTERFACE
INTERFACE
  FUNCTION chebft(a,b,n,func)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: chebft
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END FUNCTION chebft
END INTERFACE
INTERFACE
  FUNCTION chebpc(c)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP), DIMENSION(size(c)) :: chebpc
  END FUNCTION chebpc
END INTERFACE
INTERFACE

```

```

FUNCTION chint(a,b,c)
  USE nrtype
  REAL(SP), INTENT(IN) :: a,b
  REAL(SP), DIMENSION(:), INTENT(IN) :: c
  REAL(SP), DIMENSION(size(c)) :: chint
END FUNCTION chint
END INTERFACE
INTERFACE
  SUBROUTINE choldc(a,p)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: p
  END SUBROUTINE choldc
END INTERFACE
INTERFACE
  SUBROUTINE cholsl(a,p,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: p,b
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
  END SUBROUTINE cholsl
END INTERFACE
INTERFACE
  SUBROUTINE chsone(bins,ebins,knstrn,df,chsqa,prob)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: knstrn
    REAL(SP), INTENT(OUT) :: df,chsqa,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: bins,ebins
  END SUBROUTINE chsone
END INTERFACE
INTERFACE
  SUBROUTINE chstwo(bins1,bins2,knstrn,df,chsqa,prob)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: knstrn
    REAL(SP), INTENT(OUT) :: df,chsqa,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: bins1,bins2
  END SUBROUTINE chstwo
END INTERFACE
INTERFACE
  SUBROUTINE cisi(x,ci,si)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: ci,si
  END SUBROUTINE cisi
END INTERFACE
INTERFACE
  SUBROUTINE cntab1(nn,chsqa,df,prob,cramrv,ccc)
    USE nrtype
    INTEGER(I4B), DIMENSION(:,:), INTENT(IN) :: nn
    REAL(SP), INTENT(OUT) :: chsqa,df,prob,cramrv,ccc
  END SUBROUTINE cntab1
END INTERFACE
INTERFACE
  SUBROUTINE cntab2(nn,h,hx,hy,hygx,hxgy,uygx,uxgy,uxy)

```

```

        USE nrtype
        INTEGER(I4B), DIMENSION(:,:), INTENT(IN) :: nn
        REAL(SP), INTENT(OUT) :: h,hx,hy,hygx,hxgy,uygx,uxgy,uxy
        END SUBROUTINE cntab2
    END INTERFACE
INTERFACE
    FUNCTION convlv(data,respns,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: data
        REAL(SP), DIMENSION(:), INTENT(IN) :: respns
        INTEGER(I4B), INTENT(IN) :: isign
        REAL(SP), DIMENSION(size(data)) :: convlv
    END FUNCTION convlv
END INTERFACE
INTERFACE
    FUNCTION correl(data1,data2)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
        REAL(SP), DIMENSION(size(data1)) :: correl
    END FUNCTION correl
END INTERFACE
INTERFACE
    SUBROUTINE cosft1(y)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    END SUBROUTINE cosft1
END INTERFACE
INTERFACE
    SUBROUTINE cosft2(y,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE cosft2
END INTERFACE
INTERFACE
    SUBROUTINE covsrt(covar,maska)
        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: covar
        LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
    END SUBROUTINE covsrt
END INTERFACE
INTERFACE
    SUBROUTINE cyclic(a,b,c,alpha,beta,r,x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN):: a,b,c,r
        REAL(SP), INTENT(IN) :: alpha,beta
        REAL(SP), DIMENSION(:), INTENT(OUT):: x
    END SUBROUTINE cyclic
END INTERFACE
INTERFACE
    SUBROUTINE daub4(a,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
        INTEGER(I4B), INTENT(IN) :: isign

```

```

        END SUBROUTINE daub4
    END INTERFACE
    INTERFACE dawson
        FUNCTION dawson_s(x)
            USE nrtype
            REAL(SP), INTENT(IN) :: x
            REAL(SP) :: dawson_s
        END FUNCTION dawson_s
!BL
        FUNCTION dawson_v(x)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(IN) :: x
            REAL(SP), DIMENSION(size(x)) :: dawson_v
        END FUNCTION dawson_v
    END INTERFACE
    INTERFACE
        FUNCTION dbrent(ax,bx,cx,func,dbrent_dfunc,tol,xmin)
            USE nrtype
            REAL(SP), INTENT(IN) :: ax,bx,cx,tol
            REAL(SP), INTENT(OUT) :: xmin
            REAL(SP) :: dbrent
        INTERFACE
            FUNCTION func(x)
                USE nrtype
                REAL(SP), INTENT(IN) :: x
                REAL(SP) :: func
            END FUNCTION func
!BL
            FUNCTION dbrent_dfunc(x)
                USE nrtype
                REAL(SP), INTENT(IN) :: x
                REAL(SP) :: dbrent_dfunc
            END FUNCTION dbrent_dfunc
        END INTERFACE
    END FUNCTION dbrent
    END INTERFACE
    INTERFACE
        SUBROUTINE ddpoly(c,x,pd)
            USE nrtype
            REAL(SP), INTENT(IN) :: x
            REAL(SP), DIMENSION(:), INTENT(IN) :: c
            REAL(SP), DIMENSION(:), INTENT(OUT) :: pd
        END SUBROUTINE ddpoly
    END INTERFACE
    INTERFACE
        FUNCTION decchk(string,ch)
            USE nrtype
            CHARACTER(1), DIMENSION(:), INTENT(IN) :: string
            CHARACTER(1), INTENT(OUT) :: ch
            LOGICAL(LGT) :: decchk
        END FUNCTION decchk
    END INTERFACE
    INTERFACE
        SUBROUTINE dfpmin(p,gtol,iter,fret,func,dfunc)

```

```

USE nrtype
INTEGER(I4B), INTENT(OUT) :: iter
REAL(SP), INTENT(IN) :: gtol
REAL(SP), INTENT(OUT) :: fret
REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
INTERFACE
    FUNCTION func(p)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: p
    REAL(SP) :: func
    END FUNCTION func
!BL
    FUNCTION dfunc(p)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: p
    REAL(SP), DIMENSION(size(p)) :: dfunc
    END FUNCTION dfunc
END INTERFACE
END SUBROUTINE dfpmin
END INTERFACE
INTERFACE
    FUNCTION dfidr(func,x,h,err)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,h
    REAL(SP), INTENT(OUT) :: err
    REAL(SP) :: dfidr
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION dfidr
END INTERFACE
INTERFACE
    SUBROUTINE dftcor(w,delta,a,b,endpts,corre,corim,corfac)
    USE nrtype
    REAL(SP), INTENT(IN) :: w,delta,a,b
    REAL(SP), INTENT(OUT) :: corre,corim,corfac
    REAL(SP), DIMENSION(:), INTENT(IN) :: endpts
    END SUBROUTINE dftcor
END INTERFACE
INTERFACE
    SUBROUTINE dftint(func,a,b,w,cosint,sinint)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,w
    REAL(SP), INTENT(OUT) :: cosint,sinint
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func

```

```

END INTERFACE
END SUBROUTINE dftint
END INTERFACE
INTERFACE
  SUBROUTINE difeq(k,k1,k2,jsf,is1,isf,indexv,s,y)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: is1,isf,jsf,k,k1,k2
  INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indexv
  REAL(SP), DIMENSION(:,:), INTENT(OUT) :: s
  REAL(SP), DIMENSION(:,:), INTENT(IN) :: y
  END SUBROUTINE difeq
END INTERFACE
INTERFACE
  FUNCTION eclass(lista,listb,n)
  USE nrtype
  INTEGER(I4B), DIMENSION(:), INTENT(IN) :: lista,listb
  INTEGER(I4B), INTENT(IN) :: n
  INTEGER(I4B), DIMENSION(n) :: eclass
  END FUNCTION eclass
END INTERFACE
INTERFACE
  FUNCTION eclazz(equiv,n)
  USE nrtype
  INTERFACE
    FUNCTION equiv(i,j)
    USE nrtype
    LOGICAL(LGT) :: equiv
    INTEGER(I4B), INTENT(IN) :: i,j
    END FUNCTION equiv
  END INTERFACE
  INTEGER(I4B), INTENT(IN) :: n
  INTEGER(I4B), DIMENSION(n) :: eclazz
  END FUNCTION eclazz
END INTERFACE
INTERFACE
  FUNCTION ei(x)
  USE nrtype
  REAL(SP), INTENT(IN) :: x
  REAL(SP) :: ei
  END FUNCTION ei
END INTERFACE
INTERFACE
  SUBROUTINE eigsrt(d,v)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
  REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: v
  END SUBROUTINE eigsrt
END INTERFACE
INTERFACE elle
  FUNCTION elle_s(phi,ak)
  USE nrtype
  REAL(SP), INTENT(IN) :: phi,ak
  REAL(SP) :: elle_s
  END FUNCTION elle_s

```

```

!BL
    FUNCTION elle_v(phi,ak)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: phi,ak
    REAL(SP), DIMENSION(size(phi)) :: elle_v
    END FUNCTION elle_v
END INTERFACE
INTERFACE ellf
    FUNCTION ellf_s(phi,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: phi,ak
    REAL(SP) :: ellf_s
    END FUNCTION ellf_s
!BL
    FUNCTION ellf_v(phi,ak)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: phi,ak
    REAL(SP), DIMENSION(size(phi)) :: ellf_v
    END FUNCTION ellf_v
END INTERFACE
INTERFACE ellpi
    FUNCTION ellpi_s(phi,en,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: phi,en,ak
    REAL(SP) :: ellpi_s
    END FUNCTION ellpi_s
!BL
    FUNCTION ellpi_v(phi,en,ak)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: phi,en,ak
    REAL(SP), DIMENSION(size(phi)) :: ellpi_v
    END FUNCTION ellpi_v
END INTERFACE
INTERFACE
    SUBROUTINE elmhes(a)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    END SUBROUTINE elmhes
END INTERFACE
INTERFACE erf
    FUNCTION erf_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: erf_s
    END FUNCTION erf_s
!BL
    FUNCTION erf_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: erf_v
    END FUNCTION erf_v
END INTERFACE
INTERFACE erfc
    FUNCTION erfc_s(x)

```

```

        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: erfc_s
        END FUNCTION erfc_s
!BL
        FUNCTION erfc_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: erfc_v
        END FUNCTION erfc_v
    END INTERFACE
    INTERFACE erfcc
        FUNCTION erfcc_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: erfcc_s
        END FUNCTION erfcc_s
!BL
        FUNCTION erfcc_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: erfcc_v
        END FUNCTION erfcc_v
    END INTERFACE
    INTERFACE
        SUBROUTINE eulsum(sum,term,jterm)
        USE nrtype
        REAL(SP), INTENT(INOUT) :: sum
        REAL(SP), INTENT(IN) :: term
        INTEGER(I4B), INTENT(IN) :: jterm
        END SUBROUTINE eulsum
    END INTERFACE
    INTERFACE
        FUNCTION evlmem(fdt,d,xms)
        USE nrtype
        REAL(SP), INTENT(IN) :: fdt,xms
        REAL(SP), DIMENSION(:), INTENT(IN) :: d
        REAL(SP) :: evlmem
        END FUNCTION evlmem
    END INTERFACE
    INTERFACE expdev
        SUBROUTINE expdev_s(harvest)
        USE nrtype
        REAL(SP), INTENT(OUT) :: harvest
        END SUBROUTINE expdev_s
!BL
        SUBROUTINE expdev_v(harvest)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
        END SUBROUTINE expdev_v
    END INTERFACE
    INTERFACE
        FUNCTION expint(n,x)
        USE nrtype

```



```

    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: expint
    END FUNCTION expint
END INTERFACE
INTERFACE factln
    FUNCTION factln_s(n)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP) :: factln_s
    END FUNCTION factln_s
!BL
    FUNCTION factln_v(n)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n
    REAL(SP), DIMENSION(size(n)) :: factln_v
    END FUNCTION factln_v
END INTERFACE
INTERFACE factrl
    FUNCTION factrl_s(n)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP) :: factrl_s
    END FUNCTION factrl_s
!BL
    FUNCTION factrl_v(n)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n
    REAL(SP), DIMENSION(size(n)) :: factrl_v
    END FUNCTION factrl_v
END INTERFACE
INTERFACE
    SUBROUTINE fasper(x,y,ofac,hifac,px,py,jmax,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), INTENT(IN) :: ofac,hifac
    INTEGER(I4B), INTENT(OUT) :: jmax
    REAL(SP), INTENT(OUT) :: prob
    REAL(SP), DIMENSION(:), POINTER :: px,py
    END SUBROUTINE fasper
END INTERFACE
INTERFACE
    SUBROUTINE fdjac(x,fvec,df)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: fvec
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: df
    END SUBROUTINE fdjac
END INTERFACE
INTERFACE
    SUBROUTINE fgauss(x,a,y,dyda)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: y

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```

        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
    END SUBROUTINE fgauss
END INTERFACE
INTERFACE
    SUBROUTINE fit(x,y,a,b,siga,sigb,chi2,q,sig)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), INTENT(OUT) :: a,b,siga,sigb,chi2,q
    REAL(SP), DIMENSION(:), OPTIONAL, INTENT(IN) :: sig
    END SUBROUTINE fit
END INTERFACE
INTERFACE
    SUBROUTINE fitexy(x,y,sigx,sigy,a,b,siga,sigb,chi2,q)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sigx,sigy
    REAL(SP), INTENT(OUT) :: a,b,siga,sigb,chi2,q
    END SUBROUTINE fitexy
END INTERFACE
INTERFACE
    SUBROUTINE fixrts(d)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
    END SUBROUTINE fixrts
END INTERFACE
INTERFACE
    FUNCTION fleg(x,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: fleg
    END FUNCTION fleg
END INTERFACE
INTERFACE
    SUBROUTINE flmoon(n,nph,jd,frac)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n,nph
    INTEGER(I4B), INTENT(OUT) :: jd
    REAL(SP), INTENT(OUT) :: frac
    END SUBROUTINE flmoon
END INTERFACE
INTERFACE four1
    SUBROUTINE four1_dp(data,isign)
    USE nrtype
    COMPLEX(DPC), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE four1_dp
!BL
    SUBROUTINE four1_sp(data,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE four1_sp
END INTERFACE
INTERFACE

```

```

SUBROUTINE four1_alt(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_alt
END INTERFACE
INTERFACE
SUBROUTINE four1_gather(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_gather
END INTERFACE
INTERFACE
SUBROUTINE four2(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,,:), INTENT(INOUT) :: data
INTEGER(I4B),INTENT(IN) :: isign
END SUBROUTINE four2
END INTERFACE
INTERFACE
SUBROUTINE four2_alt(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,,:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four2_alt
END INTERFACE
INTERFACE
SUBROUTINE four3(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
INTEGER(I4B),INTENT(IN) :: isign
END SUBROUTINE four3
END INTERFACE
INTERFACE
SUBROUTINE four3_alt(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four3_alt
END INTERFACE
INTERFACE
SUBROUTINE fourcol(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,,:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE fourcol
END INTERFACE
INTERFACE
SUBROUTINE fourcol_3d(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE fourcol_3d

```

```

END INTERFACE
INTERFACE
  SUBROUTINE fourn_gather(data,nn,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: nn
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourn_gather
END INTERFACE
INTERFACE fourrow
  SUBROUTINE fourrow_dp(data,isign)
    USE nrtype
    COMPLEX(DPC), DIMENSION(:,,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourrow_dp
!BL
  SUBROUTINE fourrow_sp(data,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourrow_sp
END INTERFACE
INTERFACE
  SUBROUTINE fourrow_3d(data,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourrow_3d
END INTERFACE
INTERFACE
  FUNCTION fpoly(x,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: fpoly
  END FUNCTION fpoly
END INTERFACE
INTERFACE
  SUBROUTINE fred2(a,b,t,f,w,g,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(OUT) :: t,f,w
  INTERFACE
    FUNCTION g(t)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: t
      REAL(SP), DIMENSION(size(t)) :: g
    END FUNCTION g
!BL
    FUNCTION ak(t,s)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: t,s
      REAL(SP), DIMENSION(size(t),size(s)) :: ak
    END FUNCTION ak
  END INTERFACE
END INTERFACE

```

```

END INTERFACE
END SUBROUTINE fred2
END INTERFACE
INTERFACE
  FUNCTION fredin(x,a,b,t,f,w,g,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,t,f,w
    REAL(SP), DIMENSION(size(x)) :: fredin
  INTERFACE
    FUNCTION g(t)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: t
      REAL(SP), DIMENSION(size(t)) :: g
    END FUNCTION g
  !BL
    FUNCTION ak(t,s)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: t,s
      REAL(SP), DIMENSION(size(t),size(s)) :: ak
    END FUNCTION ak
  END INTERFACE
END FUNCTION fredin
END INTERFACE
INTERFACE
  SUBROUTINE frenel(x,s,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: s,c
  END SUBROUTINE frenel
END INTERFACE
INTERFACE
  SUBROUTINE frprmn(p,ftol,iter,fret)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: iter
    REAL(SP), INTENT(IN) :: ftol
    REAL(SP), INTENT(OUT) :: fret
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
  END SUBROUTINE frprmn
END INTERFACE
INTERFACE
  SUBROUTINE ftest(data1,data2,f,prob)
    USE nrtype
    REAL(SP), INTENT(OUT) :: f,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
  END SUBROUTINE ftest
END INTERFACE
INTERFACE
  FUNCTION gamdev(ia)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: ia
    REAL(SP) :: gamdev
  END FUNCTION gamdev
END INTERFACE

```

```

INTERFACE gammln
  FUNCTION gammln_s(xx)
    USE nrtype
    REAL(SP), INTENT(IN) :: xx
    REAL(SP) :: gammln_s
  END FUNCTION gammln_s
!BL
  FUNCTION gammln_v(xx)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx
    REAL(SP), DIMENSION(size(xx)) :: gammln_v
  END FUNCTION gammln_v
END INTERFACE
INTERFACE gammp
  FUNCTION gammp_s(a,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP) :: gammp_s
  END FUNCTION gammp_s
!BL
  FUNCTION gammp_v(a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(size(a)) :: gammp_v
  END FUNCTION gammp_v
END INTERFACE
INTERFACE gammq
  FUNCTION gammq_s(a,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP) :: gammq_s
  END FUNCTION gammq_s
!BL
  FUNCTION gammq_v(a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(size(a)) :: gammq_v
  END FUNCTION gammq_v
END INTERFACE
INTERFACE gasdev
  SUBROUTINE gasdev_s(harvest)
    USE nrtype
    REAL(SP), INTENT(OUT) :: harvest
  END SUBROUTINE gasdev_s
!BL
  SUBROUTINE gasdev_v(harvest)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
  END SUBROUTINE gasdev_v
END INTERFACE
INTERFACE
  SUBROUTINE gaucof(a,b,amu0,x,w)
    USE nrtype
    REAL(SP), INTENT(IN) :: amu0

```

```

      REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
      REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
      END SUBROUTINE gaucof
END INTERFACE
INTERFACE
  SUBROUTINE gauher(x,w)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gauher
END INTERFACE
INTERFACE
  SUBROUTINE gaujac(x,w,alf,bet)
    USE nrtype
    REAL(SP), INTENT(IN) :: alf,bet
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gaujac
END INTERFACE
INTERFACE
  SUBROUTINE gaulag(x,w,alf)
    USE nrtype
    REAL(SP), INTENT(IN) :: alf
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gaulag
END INTERFACE
INTERFACE
  SUBROUTINE gauleg(x1,x2,x,w)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gauleg
END INTERFACE
INTERFACE
  SUBROUTINE gaussj(a,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a,b
    END SUBROUTINE gaussj
END INTERFACE
INTERFACE gcf
  FUNCTION gcf_s(a,x,gln)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP) :: gcf_s
    END FUNCTION gcf_s
!BL
  FUNCTION gcf_v(a,x,gln)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(:), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP), DIMENSION(size(a)) :: gcf_v
    END FUNCTION gcf_v
END INTERFACE
INTERFACE
  FUNCTION golden(ax,bx,cx,func,tol,xmin)

```

```

USE nrtype
REAL(SP), INTENT(IN) :: ax,bx,cx,tol
REAL(SP), INTENT(OUT) :: xmin
REAL(SP) :: golden
INTERFACE
  FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
  END FUNCTION func
END INTERFACE
END FUNCTION golden
END INTERFACE
INTERFACE gser
  FUNCTION gser_s(a,x,gln)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP) :: gser_s
  END FUNCTION gser_s
!BL
  FUNCTION gser_v(a,x,gln)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(:), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP), DIMENSION(size(a)) :: gser_v
  END FUNCTION gser_v
END INTERFACE
INTERFACE
  SUBROUTINE hqr(a,wr,wi)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: wr,wi
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
  END SUBROUTINE hqr
END INTERFACE
INTERFACE
  SUBROUTINE hunt(xx,x,jlo)
    USE nrtype
    INTEGER(I4B), INTENT(INOUT) :: jlo
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx
  END SUBROUTINE hunt
END INTERFACE
INTERFACE
  SUBROUTINE hypdrv(s,ry,rdyds)
    USE nrtype
    REAL(SP), INTENT(IN) :: s
    REAL(SP), DIMENSION(:), INTENT(IN) :: ry
    REAL(SP), DIMENSION(:), INTENT(OUT) :: rdyds
  END SUBROUTINE hypdrv
END INTERFACE
INTERFACE
  FUNCTION hypgeo(a,b,c,z)
    USE nrtype

```



```

        COMPLEX(SPC), INTENT(IN) :: a,b,c,z
        COMPLEX(SPC) :: hypgeo
    END FUNCTION hypgeo
END INTERFACE
INTERFACE
    SUBROUTINE hypser(a,b,c,z,series,deriv)
    USE nrtype
    COMPLEX(SPC), INTENT(IN) :: a,b,c,z
    COMPLEX(SPC), INTENT(OUT) :: series,deriv
    END SUBROUTINE hypser
END INTERFACE
INTERFACE
    FUNCTION icrc(crc,buf,jinit,jrev)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: buf
    INTEGER(I2B), INTENT(IN) :: crc,jinit
    INTEGER(I4B), INTENT(IN) :: jrev
    INTEGER(I2B) :: icrc
    END FUNCTION icrc
END INTERFACE
INTERFACE
    FUNCTION igray(n,is)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n,is
    INTEGER(I4B) :: igray
    END FUNCTION igray
END INTERFACE
INTERFACE
    RECURSIVE SUBROUTINE index_bypack(arr,index,partial)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: arr
    INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: index
    INTEGER, OPTIONAL, INTENT(IN) :: partial
    END SUBROUTINE index_bypack
END INTERFACE
INTERFACE indexx
    SUBROUTINE indexx_sp(arr,index)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: arr
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: index
    END SUBROUTINE indexx_sp
    SUBROUTINE indexx_i4b(iarr,index)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: iarr
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: index
    END SUBROUTINE indexx_i4b
END INTERFACE
INTERFACE
    FUNCTION interp(uc)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: uc
    REAL(DP), DIMENSION(2*size(uc,1)-1,2*size(uc,1)-1) :: interp
    END FUNCTION interp
END INTERFACE

```

```

INTERFACE
  FUNCTION rank(indx)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    INTEGER(I4B), DIMENSION(size(indx)) :: rank
  END FUNCTION rank
END INTERFACE
INTERFACE
  FUNCTION irbit1(iseed)
    USE nrtype
    INTEGER(I4B), INTENT(INOUT) :: iseed
    INTEGER(I4B) :: irbit1
  END FUNCTION irbit1
END INTERFACE
INTERFACE
  FUNCTION irbit2(iseed)
    USE nrtype
    INTEGER(I4B), INTENT(INOUT) :: iseed
    INTEGER(I4B) :: irbit2
  END FUNCTION irbit2
END INTERFACE
INTERFACE
  SUBROUTINE jacobi(a,d,v,nrot)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: nrot
    REAL(SP), DIMENSION(:), INTENT(OUT) :: d
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
  END SUBROUTINE jacobi
END INTERFACE
INTERFACE
  SUBROUTINE jacobn(x,y,dfdx,dfdy)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dfdx
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dfdy
  END SUBROUTINE jacobn
END INTERFACE
INTERFACE
  FUNCTION julday(mm,id,iyyy)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: mm,id,iyyy
    INTEGER(I4B) :: julday
  END FUNCTION julday
END INTERFACE
INTERFACE
  SUBROUTINE kendl1(data1,data2,tau,z,prob)
    USE nrtype
    REAL(SP), INTENT(OUT) :: tau,z,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
  END SUBROUTINE kendl1
END INTERFACE
INTERFACE

```

```

SUBROUTINE kendl2(tab,tau,z,prob)
USE nrtype
REAL(SP), DIMENSION(:,:), INTENT(IN) :: tab
REAL(SP), INTENT(OUT) :: tau,z,prob
END SUBROUTINE kendl2
END INTERFACE
INTERFACE
FUNCTION kermom(y,m)
USE nrtype
REAL(DP), INTENT(IN) :: y
INTEGER(I4B), INTENT(IN) :: m
REAL(DP), DIMENSION(m) :: kermom
END FUNCTION kermom
END INTERFACE
INTERFACE
SUBROUTINE ks2d1s(x1,y1,quadv1,d1,prob)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x1,y1
REAL(SP), INTENT(OUT) :: d1,prob
INTERFACE
SUBROUTINE quadv1(x,y,fa,fb,fc,fd)
USE nrtype
REAL(SP), INTENT(IN) :: x,y
REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
END SUBROUTINE quadv1
END INTERFACE
END SUBROUTINE ks2d1s
END INTERFACE
INTERFACE
SUBROUTINE ks2d2s(x1,y1,x2,y2,d,prob)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x1,y1,x2,y2
REAL(SP), INTENT(OUT) :: d,prob
END SUBROUTINE ks2d2s
END INTERFACE
INTERFACE
SUBROUTINE ksone(data,func,d,prob)
USE nrtype
REAL(SP), INTENT(OUT) :: d,prob
REAL(SP), DIMENSION(:), INTENT(INOUT) :: data
INTERFACE
FUNCTION func(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: func
END FUNCTION func
END INTERFACE
END SUBROUTINE ksone
END INTERFACE
INTERFACE
SUBROUTINE kstwo(data1,data2,d,prob)
USE nrtype
REAL(SP), INTENT(OUT) :: d,prob
REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2

```

```

        END SUBROUTINE kstwo
    END INTERFACE
INTERFACE
    SUBROUTINE laguer(a,x,its)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: its
    COMPLEX(SPC), INTENT(INOUT) :: x
    COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
    END SUBROUTINE laguer
END INTERFACE
INTERFACE
    SUBROUTINE lfit(x,y,sig,a,maska,covar,chisq,funcs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: covar
    REAL(SP), INTENT(OUT) :: chisq
    INTERFACE
        SUBROUTINE funcs(x,arr)
        USE nrtype
        REAL(SP),INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(OUT) :: arr
        END SUBROUTINE funcs
    END INTERFACE
    END SUBROUTINE lfit
END INTERFACE
INTERFACE
    SUBROUTINE linbcg(b,x,itol,tol,itmax,iter,err)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: b
    REAL(DP), DIMENSION(:), INTENT(INOUT) :: x
    INTEGER(I4B), INTENT(IN) :: itol,itmax
    REAL(DP), INTENT(IN) :: tol
    INTEGER(I4B), INTENT(OUT) :: iter
    REAL(DP), INTENT(OUT) :: err
    END SUBROUTINE linbcg
END INTERFACE
INTERFACE
    SUBROUTINE linmin(p,xi,fret)
    USE nrtype
    REAL(SP), INTENT(OUT) :: fret
    REAL(SP), DIMENSION(:), TARGET, INTENT(INOUT) :: p,xi
    END SUBROUTINE linmin
END INTERFACE
INTERFACE
    SUBROUTINE lnsrch(xold,fold,g,p,x,f,stpmax,check,func)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xold,g
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
    REAL(SP), INTENT(IN) :: fold,stpmax
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
    REAL(SP), INTENT(OUT) :: f
    LOGICAL(LGT), INTENT(OUT) :: check

```

```

INTERFACE
  FUNCTION func(x)
    USE nrtype
    REAL(SP) :: func
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
  END FUNCTION func
END INTERFACE
END SUBROUTINE lnsrch
END INTERFACE
INTERFACE
  FUNCTION locatenr(xx,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx
    REAL(SP), INTENT(IN) :: x
    INTEGER(I4B) :: locatenr
  END FUNCTION locatenr
END INTERFACE
INTERFACE
  FUNCTION lop(u)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: u
    REAL(DP), DIMENSION(size(u,1),size(u,1)) :: lop
  END FUNCTION lop
END INTERFACE
INTERFACE
  SUBROUTINE lubksb(a,indx,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:), INTENT(OUT) :: b
  END SUBROUTINE lubksb
END INTERFACE
INTERFACE
  SUBROUTINE ludcmp(a,indx,d)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: a
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: indx
    REAL(SP), INTENT(OUT) :: d
  END SUBROUTINE ludcmp
END INTERFACE
INTERFACE
  SUBROUTINE machar(ibeta,it,irnd,ngrd,machep,negep,iexp,minexp,&
    maxexp,eps,epsneg,xmin,xmax)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: ibeta,iexp,irnd,it,machep,maxexp,&
    minexp,negep,ngrd
    REAL(SP), INTENT(OUT) :: eps,epsneg,xmax,xmin
  END SUBROUTINE machar
END INTERFACE
INTERFACE
  SUBROUTINE medfit(x,y,a,b,abdev)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), INTENT(OUT) :: a,b,abdev

```

```

        END SUBROUTINE medfit
    END INTERFACE
INTERFACE
    SUBROUTINE memcof(data,xms,d)
    USE nrtype
    REAL(SP), INTENT(OUT) :: xms
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
    REAL(SP), DIMENSION(:), INTENT(OUT) :: d
    END SUBROUTINE memcof
END INTERFACE
INTERFACE
    SUBROUTINE mgfas(u,maxcyc)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    INTEGER(I4B), INTENT(IN) :: maxcyc
    END SUBROUTINE mgfas
END INTERFACE
INTERFACE
    SUBROUTINE mglin(u,ncycle)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    INTEGER(I4B), INTENT(IN) :: ncycle
    END SUBROUTINE mglin
END INTERFACE
INTERFACE
    SUBROUTINE midexp(funk,aa,bb,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: aa,bb
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION funk(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: funk
        END FUNCTION funk
    END INTERFACE
    END SUBROUTINE midexp
END INTERFACE
INTERFACE
    SUBROUTINE midinf(funk,aa,bb,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: aa,bb
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION funk(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: funk
        END FUNCTION funk
    END INTERFACE
    END SUBROUTINE midinf
END INTERFACE

```

```

INTERFACE
  SUBROUTINE midpnt(func,a,b,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: a,b
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE midpnt
END INTERFACE
INTERFACE
  SUBROUTINE midsql(funk,aa,bb,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: aa,bb
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION funk(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: funk
    END FUNCTION funk
  END INTERFACE
END SUBROUTINE midsql
END INTERFACE
INTERFACE
  SUBROUTINE midsqu(funk,aa,bb,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: aa,bb
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION funk(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: funk
    END FUNCTION funk
  END INTERFACE
END SUBROUTINE midsqu
END INTERFACE
INTERFACE
  RECURSIVE SUBROUTINE miser(func,regn,ndim,npts,dith,ave,var)
  USE nrtype
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP) :: func
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    END FUNCTION func
  END INTERFACE
END SUBROUTINE miser
END INTERFACE

```

```

END INTERFACE
REAL(SP), DIMENSION(:), INTENT(IN) :: regn
INTEGER(I4B), INTENT(IN) :: ndim,npts
REAL(SP), INTENT(IN) :: dith
REAL(SP), INTENT(OUT) :: ave,var
END SUBROUTINE miser
END INTERFACE
INTERFACE
  SUBROUTINE mmid(y,dydx,xs,htot,nstep,yout,derivs)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: nstep
  REAL(SP), INTENT(IN) :: xs,htot
  REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
  REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
END SUBROUTINE mmid
END INTERFACE
INTERFACE
  SUBROUTINE mnbrak(ax,bx,cx,fa,fb,fc,func)
  USE nrtype
  REAL(SP), INTENT(INOUT) :: ax,bx
  REAL(SP), INTENT(OUT) :: cx,fa,fb,fc
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE mnbrak
END INTERFACE
INTERFACE
  SUBROUTINE mnewt(ntrial,x,tolx,tolf,usrfun)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: ntrial
  REAL(SP), INTENT(IN) :: tolx,tolf
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
  INTERFACE
    SUBROUTINE usrfun(x,fvec,fjac)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: fvec
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: fjac
    END SUBROUTINE usrfun
  END INTERFACE
END SUBROUTINE mnewt
END INTERFACE

```



```

INTERFACE
  SUBROUTINE moment(data,ave,adev,sdev,var,skew,curt)
    USE nrtype
    REAL(SP), INTENT(OUT) :: ave,adev,sdev,var,skew,curt
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
  END SUBROUTINE moment
END INTERFACE
INTERFACE
  SUBROUTINE mp2dfr(a,s,n,m)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    INTEGER(I4B), INTENT(OUT) :: m
    CHARACTER(1), DIMENSION(:), INTENT(INOUT) :: a
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: s
  END SUBROUTINE mp2dfr
END INTERFACE
INTERFACE
  SUBROUTINE mpdiv(q,r,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: q,r
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: u,v
    INTEGER(I4B), INTENT(IN) :: n,m
  END SUBROUTINE mpdiv
END INTERFACE
INTERFACE
  SUBROUTINE mpinv(u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: u
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: v
    INTEGER(I4B), INTENT(IN) :: n,m
  END SUBROUTINE mpinv
END INTERFACE
INTERFACE
  SUBROUTINE mpmul(w,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: u,v
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: w
    INTEGER(I4B), INTENT(IN) :: n,m
  END SUBROUTINE mpmul
END INTERFACE
INTERFACE
  SUBROUTINE mppi(n)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
  END SUBROUTINE mppi
END INTERFACE
INTERFACE
  SUBROUTINE mprove(a,alud,indx,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:, :), INTENT(IN) :: a,alud
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:), INTENT(IN) :: b
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
  END SUBROUTINE mprove

```

```

END INTERFACE
INTERFACE
  SUBROUTINE mpsqrt(w,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: w,u
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: v
    INTEGER(I4B), INTENT(IN) :: n,m
  END SUBROUTINE mpsqrt
END INTERFACE
INTERFACE
  SUBROUTINE mrqcof(x,y,sig,a,maska,alpha,beta,chisq,funcs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,a,sig
    REAL(SP), DIMENSION(:), INTENT(OUT) :: beta
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: alpha
    REAL(SP), INTENT(OUT) :: chisq
    LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
  INTERFACE
    SUBROUTINE funcs(x,a,yfit,dyda)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
      REAL(SP), DIMENSION(:), INTENT(OUT) :: yfit
      REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
    END SUBROUTINE funcs
  END INTERFACE
END SUBROUTINE mrqcof
END INTERFACE
INTERFACE
  SUBROUTINE mrqmin(x,y,sig,a,maska,covar,alpha,chisq,funcs,alamda)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: covar,alpha
    REAL(SP), INTENT(OUT) :: chisq
    REAL(SP), INTENT(INOUT) :: alamda
    LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
  INTERFACE
    SUBROUTINE funcs(x,a,yfit,dyda)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
      REAL(SP), DIMENSION(:), INTENT(OUT) :: yfit
      REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
    END SUBROUTINE funcs
  END INTERFACE
END SUBROUTINE mrqmin
END INTERFACE
INTERFACE
  SUBROUTINE newt(x,check)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
    LOGICAL(LGT), INTENT(OUT) :: check
  END SUBROUTINE newt
END INTERFACE
INTERFACE

```

```

SUBROUTINE odeint(ystart,x1,x2,eps,h1,hmin,derivs,rkqs)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: ystart
REAL(SP), INTENT(IN) :: x1,x2,eps,h1,hmin
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
  USE nrtype
  REAL(SP), INTENT(IN) :: x
  REAL(SP), DIMENSION(:), INTENT(IN) :: y
  REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
!BL
  SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
  REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
  REAL(SP), INTENT(INOUT) :: x
  REAL(SP), INTENT(IN) :: htry,eps
  REAL(SP), INTENT(OUT) :: hdid,hnext
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
  END SUBROUTINE rkqs
END INTERFACE
END SUBROUTINE odeint
INTERFACE
  SUBROUTINE orthog(anu,alpha,beta,a,b)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: anu,alpha,beta
  REAL(SP), DIMENSION(:), INTENT(OUT) :: a,b
  END SUBROUTINE orthog
END INTERFACE
INTERFACE
  SUBROUTINE pade(cof,resid)
  USE nrtype
  REAL(DP), DIMENSION(:), INTENT(INOUT) :: cof
  REAL(SP), INTENT(OUT) :: resid
  END SUBROUTINE pade
END INTERFACE
INTERFACE
  FUNCTION pccheb(d)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: d
  REAL(SP), DIMENSION(size(d)) :: pccheb
  END FUNCTION pccheb
END INTERFACE
INTERFACE
  SUBROUTINE pcshft(a,b,d)

```

```

        USE nrtype
        REAL(SP), INTENT(IN) :: a,b
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
        END SUBROUTINE pcsht
END INTERFACE
INTERFACE
    SUBROUTINE pearsn(x,y,r,prob,z)
    USE nrtype
    REAL(SP), INTENT(OUT) :: r,prob,z
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    END SUBROUTINE pearsn
END INTERFACE
INTERFACE
    SUBROUTINE period(x,y,ofac,hifac,px,py,jmax,prob)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: jmax
    REAL(SP), INTENT(IN) :: ofac,hifac
    REAL(SP), INTENT(OUT) :: prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), DIMENSION(:), POINTER :: px,py
    END SUBROUTINE period
END INTERFACE
INTERFACE plgndr
    FUNCTION plgndr_s(l,m,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: l,m
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: plgndr_s
    END FUNCTION plgndr_s
!BL
    FUNCTION plgndr_v(l,m,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: l,m
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: plgndr_v
    END FUNCTION plgndr_v
END INTERFACE
INTERFACE
    FUNCTION poidev(xm)
    USE nrtype
    REAL(SP), INTENT(IN) :: xm
    REAL(SP) :: poidev
    END FUNCTION poidev
END INTERFACE
INTERFACE
    FUNCTION polcoe(x,y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), DIMENSION(size(x)) :: polcoe
    END FUNCTION polcoe
END INTERFACE
INTERFACE
    FUNCTION polcof(xa,ya)
    USE nrtype

```

```

REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
REAL(SP), DIMENSION(size(xa)) :: polcof
END FUNCTION polcof
END INTERFACE
INTERFACE
  SUBROUTINE poldiv(u,v,q,r)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: u,v
  REAL(SP), DIMENSION(:), INTENT(OUT) :: q,r
  END SUBROUTINE poldiv
END INTERFACE
INTERFACE
  SUBROUTINE polin2(x1a,x2a,ya,x1,x2,y,dy)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
  REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya
  REAL(SP), INTENT(IN) :: x1,x2
  REAL(SP), INTENT(OUT) :: y,dy
  END SUBROUTINE polin2
END INTERFACE
INTERFACE
  SUBROUTINE polint(xa,ya,x,y,dy)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
  REAL(SP), INTENT(IN) :: x
  REAL(SP), INTENT(OUT) :: y,dy
  END SUBROUTINE polint
END INTERFACE
INTERFACE
  SUBROUTINE powell(p,xi,ftol,iter,fret)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
  REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: xi
  INTEGER(I4B), INTENT(OUT) :: iter
  REAL(SP), INTENT(IN) :: ftol
  REAL(SP), INTENT(OUT) :: fret
  END SUBROUTINE powell
END INTERFACE
INTERFACE
  FUNCTION predic(data,d,nfut)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: data,d
  INTEGER(I4B), INTENT(IN) :: nfut
  REAL(SP), DIMENSION(nfut) :: predic
  END FUNCTION predic
END INTERFACE
INTERFACE
  FUNCTION probks(alam)
  USE nrtype
  REAL(SP), INTENT(IN) :: alam
  REAL(SP) :: probks
  END FUNCTION probks
END INTERFACE
INTERFACE psdes

```

```

SUBROUTINE psdes_s(lword,rword)
USE nrtype
INTEGER(I4B), INTENT(INOUT) :: lword,rword
END SUBROUTINE psdes_s
!BL
SUBROUTINE psdes_v(lword,rword)
USE nrtype
INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: lword,rword
END SUBROUTINE psdes_v
END INTERFACE
INTERFACE
SUBROUTINE pwt(a,isign)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE pwt
END INTERFACE
INTERFACE
SUBROUTINE pwtset(n)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n
END SUBROUTINE pwtset
END INTERFACE
INTERFACE pythag
FUNCTION pythag_dp(a,b)
USE nrtype
REAL(DP), INTENT(IN) :: a,b
REAL(DP) :: pythag_dp
END FUNCTION pythag_dp
!BL
FUNCTION pythag_sp(a,b)
USE nrtype
REAL(SP), INTENT(IN) :: a,b
REAL(SP) :: pythag_sp
END FUNCTION pythag_sp
END INTERFACE
INTERFACE
SUBROUTINE pzextr(iest,xest,yest,yz,dy)
USE nrtype
INTEGER(I4B), INTENT(IN) :: iest
REAL(SP), INTENT(IN) :: xest
REAL(SP), DIMENSION(:), INTENT(IN) :: yest
REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
END SUBROUTINE pzextr
END INTERFACE
!!! FB:
! INTERFACE
! FUNCTION qgaus(func,a,b)
! USE nrtype
! REAL(SP), INTENT(IN) :: a,b
! REAL(SP) :: qgaus
! INTERFACE
! FUNCTION func(x)
! USE nrtype

```

```

!      REAL(SP), DIMENSION(:), INTENT(IN) :: x
!      REAL(SP), DIMENSION(size(x)) :: func
!      END FUNCTION func
!      END INTERFACE
!      END FUNCTION qgaus
!      END INTERFACE
!!! /FB
INTERFACE
  SUBROUTINE qrdcmp(a,c,d,sing)
  USE nrtype
  REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
  REAL(SP), DIMENSION(:), INTENT(OUT) :: c,d
  LOGICAL(LGT), INTENT(OUT) :: sing
  END SUBROUTINE qrdcmp
END INTERFACE
INTERFACE
  FUNCTION qromb(func,a,b)
  USE nrtype
  REAL(SP), INTENT(IN) :: a,b
  REAL(SP) :: qromb
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
  END FUNCTION qromb
END INTERFACE
INTERFACE
  FUNCTION qromo(func,a,b,choose)
  USE nrtype
  REAL(SP), INTENT(IN) :: a,b
  REAL(SP) :: qromo
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END INTERFACE
INTERFACE
  SUBROUTINE choose(funk,aa,bb,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: aa,bb
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION funk(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: funk
    END FUNCTION funk
  END INTERFACE

```

```

        END SUBROUTINE choose
    END INTERFACE
    END FUNCTION qromo
END INTERFACE
INTERFACE
    SUBROUTINE qroot(p,b,c,eps)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: p
    REAL(SP), INTENT(INOUT) :: b,c
    REAL(SP), INTENT(IN) :: eps
    END SUBROUTINE qroot
END INTERFACE
INTERFACE
    SUBROUTINE qrsolv(a,c,d,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: c,d
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
    END SUBROUTINE qrsolv
END INTERFACE
INTERFACE
    SUBROUTINE grupdt(r,qt,u,v)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: r,qt
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: u
    REAL(SP), DIMENSION(:), INTENT(IN) :: v
    END SUBROUTINE grupdt
END INTERFACE
INTERFACE
    FUNCTION qsimp(func,a,b)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qsimp
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION qsimp
END INTERFACE
INTERFACE
    FUNCTION qtrap(func,a,b)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qtrap
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
END INTERFACE

```



```

        END FUNCTION qtrap
    END INTERFACE
    INTERFACE
        SUBROUTINE quadct(x,y,xx,yy,fa,fb,fc,fd)
            USE nrtype
            REAL(SP), INTENT(IN) :: x,y
            REAL(SP), DIMENSION(:), INTENT(IN) :: xx,yy
            REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
        END SUBROUTINE quadct
    END INTERFACE
    INTERFACE
        SUBROUTINE quadmx(a)
            USE nrtype
            REAL(SP), DIMENSION(:,:), INTENT(OUT) :: a
        END SUBROUTINE quadmx
    END INTERFACE
    INTERFACE
        SUBROUTINE quadvl(x,y,fa,fb,fc,fd)
            USE nrtype
            REAL(SP), INTENT(IN) :: x,y
            REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
        END SUBROUTINE quadvl
    END INTERFACE
    INTERFACE
        FUNCTION ran(idum)
            INTEGER(selected_int_kind(9)), INTENT(INOUT) :: idum
            REAL :: ran
        END FUNCTION ran
    END INTERFACE
    INTERFACE ran0
        SUBROUTINE ran0_s(harvest)
            USE nrtype
            REAL(SP), INTENT(OUT) :: harvest
        END SUBROUTINE ran0_s
!BL
        SUBROUTINE ran0_v(harvest)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
        END SUBROUTINE ran0_v
    END INTERFACE
    INTERFACE ran1
        SUBROUTINE ran1_s(harvest)
            USE nrtype
            REAL(SP), INTENT(OUT) :: harvest
        END SUBROUTINE ran1_s
!BL
        SUBROUTINE ran1_v(harvest)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
        END SUBROUTINE ran1_v
    END INTERFACE
    INTERFACE ran2
        SUBROUTINE ran2_s(harvest)
            USE nrtype

```

```

    REAL(SP), INTENT(OUT) :: harvest
END SUBROUTINE ran2_s
!BL
    SUBROUTINE ran2_v(harvest)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE ran2_v
END INTERFACE
INTERFACE ran3
    SUBROUTINE ran3_s(harvest)
    USE nrtype
    REAL(SP), INTENT(OUT) :: harvest
    END SUBROUTINE ran3_s
!BL
    SUBROUTINE ran3_v(harvest)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE ran3_v
END INTERFACE
INTERFACE
    SUBROUTINE ratint(xa,ya,x,y,dy)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: y,dy
    END SUBROUTINE ratint
END INTERFACE
INTERFACE
    SUBROUTINE ratlsq(func,a,b,mm,kk,cof,dev)
    USE nrtype
    REAL(DP), INTENT(IN) :: a,b
    INTEGER(I4B), INTENT(IN) :: mm,kk
    REAL(DP), DIMENSION(:), INTENT(OUT) :: cof
    REAL(DP), INTENT(OUT) :: dev
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(DP), DIMENSION(:), INTENT(IN) :: x
        REAL(DP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
    END SUBROUTINE ratlsq
END INTERFACE
INTERFACE ratval
    FUNCTION ratval_s(x,cof,mm,kk)
    USE nrtype
    REAL(DP), INTENT(IN) :: x
    INTEGER(I4B), INTENT(IN) :: mm,kk
    REAL(DP), DIMENSION(mm+kk+1), INTENT(IN) :: cof
    REAL(DP) :: ratval_s
    END FUNCTION ratval_s
!BL
    FUNCTION ratval_v(x,cof,mm,kk)
    USE nrtype

```

```

REAL(DP), DIMENSION(:), INTENT(IN) :: x
INTEGER(I4B), INTENT(IN) :: mm, kk
REAL(DP), DIMENSION(mm+kk+1), INTENT(IN) :: cof
REAL(DP), DIMENSION(size(x)) :: ratval_v
END FUNCTION ratval_v
END INTERFACE
INTERFACE rc
  FUNCTION rc_s(x,y)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y
    REAL(SP) :: rc_s
  END FUNCTION rc_s
!BL
  FUNCTION rc_v(x,y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), DIMENSION(size(x)) :: rc_v
  END FUNCTION rc_v
END INTERFACE
INTERFACE rd
  FUNCTION rd_s(x,y,z)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y,z
    REAL(SP) :: rd_s
  END FUNCTION rd_s
!BL
  FUNCTION rd_v(x,y,z)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z
    REAL(SP), DIMENSION(size(x)) :: rd_v
  END FUNCTION rd_v
END INTERFACE
INTERFACE realft
  SUBROUTINE realft_dp(data, isign, zdata)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    COMPLEX(DPC), DIMENSION(:), OPTIONAL, TARGET :: zdata
  END SUBROUTINE realft_dp
!BL
  SUBROUTINE realft_sp(data, isign, zdata)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    COMPLEX(SPC), DIMENSION(:), OPTIONAL, TARGET :: zdata
  END SUBROUTINE realft_sp
END INTERFACE
INTERFACE
  RECURSIVE FUNCTION recur1(a,b) RESULT(u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(size(a)) :: u
  END FUNCTION recur1
END INTERFACE

```

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INTERFACE
  FUNCTION recur2(a,b,c)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c
    REAL(SP), DIMENSION(size(a)) :: recur2
  END FUNCTION recur2
END INTERFACE
INTERFACE
  SUBROUTINE relax(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: rhs
  END SUBROUTINE relax
END INTERFACE
INTERFACE
  SUBROUTINE relax2(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: rhs
  END SUBROUTINE relax2
END INTERFACE
INTERFACE
  FUNCTION resid(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: u,rhs
    REAL(DP), DIMENSION(size(u,1),size(u,1)) :: resid
  END FUNCTION resid
END INTERFACE
INTERFACE rf
  FUNCTION rf_s(x,y,z)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y,z
    REAL(SP) :: rf_s
  END FUNCTION rf_s
!BL
  FUNCTION rf_v(x,y,z)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z
    REAL(SP), DIMENSION(size(x)) :: rf_v
  END FUNCTION rf_v
END INTERFACE
INTERFACE rj
  FUNCTION rj_s(x,y,z,p)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y,z,p
    REAL(SP) :: rj_s
  END FUNCTION rj_s
!BL
  FUNCTION rj_v(x,y,z,p)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z,p
    REAL(SP), DIMENSION(size(x)) :: rj_v
  END FUNCTION rj_v
END INTERFACE

```

```

INTERFACE
  SUBROUTINE rk4(y,dydx,x,h,yout,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
    REAL(SP), INTENT(IN) :: x,h
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
    INTERFACE
      SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
      END SUBROUTINE derivs
    END INTERFACE
  END SUBROUTINE rk4
END INTERFACE
INTERFACE
  SUBROUTINE rkck(y,dydx,x,h,yout,yerr,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
    REAL(SP), INTENT(IN) :: x,h
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout,yerr
    INTERFACE
      SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
      END SUBROUTINE derivs
    END INTERFACE
  END SUBROUTINE rkck
END INTERFACE
INTERFACE
  SUBROUTINE rkdump(vstart,x1,x2,nstep,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: vstart
    REAL(SP), INTENT(IN) :: x1,x2
    INTEGER(I4B), INTENT(IN) :: nstep
    INTERFACE
      SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
      END SUBROUTINE derivs
    END INTERFACE
  END SUBROUTINE rkdump
END INTERFACE
INTERFACE
  SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
    REAL(SP), INTENT(INOUT) :: x

```

```

REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE rkqs
END INTERFACE
INTERFACE
  SUBROUTINE rlft2(data,spec,speq,isign)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: data
    COMPLEX(SPC), DIMENSION(:,:), INTENT(OUT) :: spec
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: speq
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE rlft2
END INTERFACE
INTERFACE
  SUBROUTINE rlft3(data,spec,speq,isign)
    USE nrtype
    REAL(SP), DIMENSION(:,:,:), INTENT(INOUT) :: data
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(OUT) :: spec
    COMPLEX(SPC), DIMENSION(:,:), INTENT(OUT) :: speq
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE rlft3
END INTERFACE
INTERFACE
  SUBROUTINE rotate(r,qt,i,a,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), TARGET, INTENT(INOUT) :: r,qt
    INTEGER(I4B), INTENT(IN) :: i
    REAL(SP), INTENT(IN) :: a,b
  END SUBROUTINE rotate
END INTERFACE
INTERFACE
  SUBROUTINE rsolv(a,d,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: d
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
  END SUBROUTINE rsolv
END INTERFACE
INTERFACE
  FUNCTION rstrct(uf)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: uf
    REAL(DP), DIMENSION((size(uf,1)+1)/2,(size(uf,1)+1)/2) :: rstrct
  END FUNCTION rstrct
END INTERFACE
INTERFACE

```

```

FUNCTION rtbis(func,x1,x2,xacc)
USE nrtype
REAL(SP), INTENT(IN) :: x1,x2,xacc
REAL(SP) :: rtbis
INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
    END FUNCTION func
END INTERFACE
END FUNCTION rtbis
END INTERFACE
INTERFACE
    FUNCTION rtflsp(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtflsp
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION rtflsp
END INTERFACE
INTERFACE
    FUNCTION rtnewt(funcd,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtnewt
    INTERFACE
        SUBROUTINE funcd(x,fval,fderiv)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), INTENT(OUT) :: fval,fderiv
        END SUBROUTINE funcd
    END INTERFACE
    END FUNCTION rtnewt
END INTERFACE
INTERFACE
    FUNCTION rtsafe(funcd,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtsafe
    INTERFACE
        SUBROUTINE funcd(x,fval,fderiv)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), INTENT(OUT) :: fval,fderiv
        END SUBROUTINE funcd
    END INTERFACE
    END FUNCTION rtsafe

```

```

END INTERFACE
INTERFACE
  FUNCTION rtsec(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtsec
    INTERFACE
      FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END FUNCTION rtsec
END INTERFACE
INTERFACE
  SUBROUTINE rzextr(iest,xest,yest,yz,dy)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: iest
    REAL(SP), INTENT(IN) :: xest
    REAL(SP), DIMENSION(:), INTENT(IN) :: yest
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
  END SUBROUTINE rzextr
END INTERFACE
INTERFACE
  FUNCTION savgol(nl,nrr,ld,m)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: nl,nrr,ld,m
    REAL(SP), DIMENSION(nl+nrr+1) :: savgol
  END FUNCTION savgol
END INTERFACE
INTERFACE
  SUBROUTINE scrsho(func)
    USE nrtype
    INTERFACE
      FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END SUBROUTINE scrsho
END INTERFACE
INTERFACE
  FUNCTION select(k,arr)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: k
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
    REAL(SP) :: select
  END FUNCTION select
END INTERFACE
INTERFACE
  FUNCTION select_bypack(k,arr)
    USE nrtype

```



```

    INTEGER(I4B), INTENT(IN) :: k
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
    REAL(SP) :: select_bypack
    END FUNCTION select_bypack
END INTERFACE
INTERFACE
    SUBROUTINE select_heap(arr,heap)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: arr
    REAL(SP), DIMENSION(:), INTENT(OUT) :: heap
    END SUBROUTINE select_heap
END INTERFACE
INTERFACE
    FUNCTION select_inplace(k,arr)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: k
    REAL(SP), DIMENSION(:), INTENT(IN) :: arr
    REAL(SP) :: select_inplace
    END FUNCTION select_inplace
END INTERFACE
INTERFACE
    SUBROUTINE simplx(a,m1,m2,m3,icase,izrov,iposv)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    INTEGER(I4B), INTENT(IN) :: m1,m2,m3
    INTEGER(I4B), INTENT(OUT) :: icase
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: izrov,iposv
    END SUBROUTINE simplx
END INTERFACE
INTERFACE
    SUBROUTINE simpr(y,dydx,dfdx,dfdy,xs,htot,nstep,yout,derivs)
    USE nrtype
    REAL(SP), INTENT(IN) :: xs,htot
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx,dfdx
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: dfdy
    INTEGER(I4B), INTENT(IN) :: nstep
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE simpr
END INTERFACE
INTERFACE
    SUBROUTINE sinft(y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    END SUBROUTINE sinft
END INTERFACE
INTERFACE

```

```

SUBROUTINE slvsm2(u,rhs)
  USE nrtype
  REAL(DP), DIMENSION(3,3), INTENT(OUT) :: u
  REAL(DP), DIMENSION(3,3), INTENT(IN) :: rhs
END SUBROUTINE slvsm2
END INTERFACE
INTERFACE
  SUBROUTINE slvsml(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(3,3), INTENT(OUT) :: u
    REAL(DP), DIMENSION(3,3), INTENT(IN) :: rhs
  END SUBROUTINE slvsml
END INTERFACE
INTERFACE
  SUBROUTINE sncndn(uu,emmc,sn,cn,dn)
    USE nrtype
    REAL(SP), INTENT(IN) :: uu,emmc
    REAL(SP), INTENT(OUT) :: sn,cn,dn
  END SUBROUTINE sncndn
END INTERFACE
INTERFACE
  FUNCTION snrm(sx,itol)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: sx
    INTEGER(I4B), INTENT(IN) :: itol
    REAL(DP) :: snrm
  END FUNCTION snrm
END INTERFACE
INTERFACE
  SUBROUTINE sobseq(x,init)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
    INTEGER(I4B), OPTIONAL, INTENT(IN) :: init
  END SUBROUTINE sobseq
END INTERFACE
INTERFACE
  SUBROUTINE solvde(itmax,conv,slowc,scalv,indexv,nb,y)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: itmax,nb
    REAL(SP), INTENT(IN) :: conv,slowc
    REAL(SP), DIMENSION(:), INTENT(IN) :: scalv
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indexv
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: y
  END SUBROUTINE solvde
END INTERFACE
INTERFACE
  SUBROUTINE sor(a,b,c,d,e,f,u,rjac)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: a,b,c,d,e,f
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    REAL(DP), INTENT(IN) :: rjac
  END SUBROUTINE sor
END INTERFACE
INTERFACE

```

```

        SUBROUTINE sort(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort
    END INTERFACE
    INTERFACE
        SUBROUTINE sort2(arr,slave)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr,slave
        END SUBROUTINE sort2
    END INTERFACE
    INTERFACE
        SUBROUTINE sort3(arr,slave1,slave2)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr,slave1,slave2
        END SUBROUTINE sort3
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_bypack(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_bypack
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_byreshape(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_byreshape
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_heap(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_heap
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_pick(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_pick
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_radix(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_radix
    END INTERFACE
    INTERFACE
        SUBROUTINE sort_shell(arr)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
        END SUBROUTINE sort_shell
    END INTERFACE
    INTERFACE

```

```

SUBROUTINE spectrm(p,k,ovrlap,unit,n_window)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(OUT) :: p
INTEGER(I4B), INTENT(IN) :: k
LOGICAL(LGT), INTENT(IN) :: ovrlap
INTEGER(I4B), OPTIONAL, INTENT(IN) :: n_window,unit
END SUBROUTINE spectrm
END INTERFACE
INTERFACE
SUBROUTINE spear(data1,data2,d,zd,probd,rs,probrs)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
REAL(SP), INTENT(OUT) :: d,zd,probd,rs,probrs
END SUBROUTINE spear
END INTERFACE
INTERFACE sphbes
SUBROUTINE sphbes_s(n,x,sj,sy,sjp,syp)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), INTENT(IN) :: x
REAL(SP), INTENT(OUT) :: sj,sy,sjp,syp
END SUBROUTINE sphbes_s
!BL
SUBROUTINE sphbes_v(n,x,sj,sy,sjp,syp)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(OUT) :: sj,sy,sjp,syp
END SUBROUTINE sphbes_v
END INTERFACE
INTERFACE
SUBROUTINE splie2(x1a,x2a,ya,y2a)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: y2a
END SUBROUTINE splie2
END INTERFACE
INTERFACE
FUNCTION splin2(x1a,x2a,ya,y2a,x1,x2)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya,y2a
REAL(SP), INTENT(IN) :: x1,x2
REAL(SP) :: splin2
END FUNCTION splin2
END INTERFACE
INTERFACE
SUBROUTINE spline(x,y,yp1,ypn,y2)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
REAL(SP), INTENT(IN) :: yp1,ypn
REAL(SP), DIMENSION(:), INTENT(OUT) :: y2
END SUBROUTINE spline

```

```

END INTERFACE
INTERFACE
  FUNCTION splint(xa,ya,y2a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya,y2a
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: splint
  END FUNCTION splint
END INTERFACE
INTERFACE sprsax
  SUBROUTINE sprsax_dp(sa,x,b)
    USE nrtype
    TYPE(sprs2_dp), INTENT(IN) :: sa
    REAL(DP), DIMENSION (:), INTENT(IN) :: x
    REAL(DP), DIMENSION (:), INTENT(OUT) :: b
  END SUBROUTINE sprsax_dp
!BL
  SUBROUTINE sprsax_sp(sa,x,b)
    USE nrtype
    TYPE(sprs2_sp), INTENT(IN) :: sa
    REAL(SP), DIMENSION (:), INTENT(IN) :: x
    REAL(SP), DIMENSION (:), INTENT(OUT) :: b
  END SUBROUTINE sprsax_sp
END INTERFACE
INTERFACE sprsdiag
  SUBROUTINE sprsdiag_dp(sa,b)
    USE nrtype
    TYPE(sprs2_dp), INTENT(IN) :: sa
    REAL(DP), DIMENSION(:), INTENT(OUT) :: b
  END SUBROUTINE sprsdiag_dp
!BL
  SUBROUTINE sprsdiag_sp(sa,b)
    USE nrtype
    TYPE(sprs2_sp), INTENT(IN) :: sa
    REAL(SP), DIMENSION(:), INTENT(OUT) :: b
  END SUBROUTINE sprsdiag_sp
END INTERFACE
INTERFACE sprsin
  SUBROUTINE sprsin_sp(a,thresh,sa)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), INTENT(IN) :: thresh
    TYPE(sprs2_sp), INTENT(OUT) :: sa
  END SUBROUTINE sprsin_sp
!BL
  SUBROUTINE sprsin_dp(a,thresh,sa)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(DP), INTENT(IN) :: thresh
    TYPE(sprs2_dp), INTENT(OUT) :: sa
  END SUBROUTINE sprsin_dp
END INTERFACE
INTERFACE
  SUBROUTINE sprstp(sa)

```

```

        USE nrtype
        TYPE(sprs2_sp), INTENT(INOUT) :: sa
        END SUBROUTINE sprstp
    END INTERFACE
    INTERFACE sprstx
        SUBROUTINE sprstx_dp(sa,x,b)
            USE nrtype
            TYPE(sprs2_dp), INTENT(IN) :: sa
            REAL(DP), DIMENSION (:), INTENT(IN) :: x
            REAL(DP), DIMENSION (:), INTENT(OUT) :: b
        END SUBROUTINE sprstx_dp
!BL
        SUBROUTINE sprstx_sp(sa,x,b)
            USE nrtype
            TYPE(sprs2_sp), INTENT(IN) :: sa
            REAL(SP), DIMENSION (:), INTENT(IN) :: x
            REAL(SP), DIMENSION (:), INTENT(OUT) :: b
        END SUBROUTINE sprstx_sp
    END INTERFACE
    INTERFACE
        SUBROUTINE stifbs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
            REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
            REAL(SP), INTENT(IN) :: htry,eps
            REAL(SP), INTENT(INOUT) :: x
            REAL(SP), INTENT(OUT) :: hdid,hnext
        INTERFACE
            SUBROUTINE derivs(x,y,dydx)
                USE nrtype
                REAL(SP), INTENT(IN) :: x
                REAL(SP), DIMENSION(:), INTENT(IN) :: y
                REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
            END SUBROUTINE derivs
        END INTERFACE
    END SUBROUTINE stifbs
END INTERFACE
    INTERFACE
        SUBROUTINE stiff(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
            REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
            REAL(SP), INTENT(INOUT) :: x
            REAL(SP), INTENT(IN) :: htry,eps
            REAL(SP), INTENT(OUT) :: hdid,hnext
        INTERFACE
            SUBROUTINE derivs(x,y,dydx)
                USE nrtype
                REAL(SP), INTENT(IN) :: x
                REAL(SP), DIMENSION(:), INTENT(IN) :: y
                REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
            END SUBROUTINE derivs
        END INTERFACE
    END SUBROUTINE stiff

```

```

END INTERFACE
INTERFACE
  SUBROUTINE stoerm(y,d2y,xs,htot,nstep,yout,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,d2y
    REAL(SP), INTENT(IN) :: xs,htot
    INTEGER(I4B), INTENT(IN) :: nstep
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP), DIMENSION(:), INTENT(IN) :: y
      REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
END SUBROUTINE stoerm
END INTERFACE
INTERFACE svbksb
  SUBROUTINE svbksb_dp(u,w,v,b,x)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: u,v
    REAL(DP), DIMENSION(:), INTENT(IN) :: w,b
    REAL(DP), DIMENSION(:), INTENT(OUT) :: x
  END SUBROUTINE svbksb_dp
!BL
  SUBROUTINE svbksb_sp(u,w,v,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: u,v
    REAL(SP), DIMENSION(:), INTENT(IN) :: w,b
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
  END SUBROUTINE svbksb_sp
END INTERFACE
INTERFACE svdcmp
  SUBROUTINE svdcmp_dp(a,w,v)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(DP), DIMENSION(:), INTENT(OUT) :: w
    REAL(DP), DIMENSION(:,:), INTENT(OUT) :: v
  END SUBROUTINE svdcmp_dp
!BL
  SUBROUTINE svdcmp_sp(a,w,v)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: w
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
  END SUBROUTINE svdcmp_sp
END INTERFACE
INTERFACE
  SUBROUTINE svdfit(x,y,sig,a,v,w,chisq,funcs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
    REAL(SP), DIMENSION(:), INTENT(OUT) :: a,w
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v

```

```

REAL(SP), INTENT(OUT) :: chisq
INTERFACE
    FUNCTION funcs(x,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: funcs
    END FUNCTION funcs
END INTERFACE
END SUBROUTINE svdfit
END INTERFACE
INTERFACE
    SUBROUTINE svdvar(v,w,cvm)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: v
    REAL(SP), DIMENSION(:), INTENT(IN) :: w
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: cvm
    END SUBROUTINE svdvar
END INTERFACE
INTERFACE
    FUNCTION toeplz(r,y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: r,y
    REAL(SP), DIMENSION(size(y)) :: toeplz
    END FUNCTION toeplz
END INTERFACE
INTERFACE
    SUBROUTINE tpctest(data1,data2,t,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    REAL(SP), INTENT(OUT) :: t,prob
    END SUBROUTINE tpctest
END INTERFACE
INTERFACE
    SUBROUTINE tqli(d,e,z)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: d,e
    REAL(SP), DIMENSION(:,:), OPTIONAL, INTENT(INOUT) :: z
    END SUBROUTINE tqli
END INTERFACE
INTERFACE
    SUBROUTINE trapzd(func,a,b,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
END SUBROUTINE trapzd

```



```

END INTERFACE
INTERFACE
  SUBROUTINE tred2(a,d,e,novectors)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: d,e
    LOGICAL(LGT), OPTIONAL, INTENT(IN) :: novectors
  END SUBROUTINE tred2
END INTERFACE
! On a purely serial machine, for greater efficiency, remove
! the generic name tridag from the following interface,
! and put it on the next one after that.
INTERFACE tridag
  RECURSIVE SUBROUTINE tridag_par(a,b,c,r,u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
    REAL(SP), DIMENSION(:), INTENT(OUT) :: u
  END SUBROUTINE tridag_par
END INTERFACE
INTERFACE
  SUBROUTINE tridag_ser(a,b,c,r,u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
    REAL(SP), DIMENSION(:), INTENT(OUT) :: u
  END SUBROUTINE tridag_ser
END INTERFACE
INTERFACE
  SUBROUTINE ttest(data1,data2,t,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    REAL(SP), INTENT(OUT) :: t,prob
  END SUBROUTINE ttest
END INTERFACE
INTERFACE
  SUBROUTINE tutest(data1,data2,t,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    REAL(SP), INTENT(OUT) :: t,prob
  END SUBROUTINE tutest
END INTERFACE
INTERFACE
  SUBROUTINE twofft(data1,data2,fft1,fft2)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: fft1,fft2
  END SUBROUTINE twofft
END INTERFACE
INTERFACE
  FUNCTION vander(x,q)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: x,q
    REAL(DP), DIMENSION(size(x)) :: vander
  END FUNCTION vander
END INTERFACE

```

```

INTERFACE
  SUBROUTINE vegas(region,func,init,ncall,itmx,nprn,tgral,sd,chi2a)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: region
  INTEGER(I4B), INTENT(IN) :: init,ncall,itmx,nprn
  REAL(SP), INTENT(OUT) :: tgral,sd,chi2a
  INTERFACE
    FUNCTION func(pt,wgt)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: pt
    REAL(SP), INTENT(IN) :: wgt
    REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE vegas
END INTERFACE
INTERFACE
  SUBROUTINE voltra(t0,h,t,f,g,ak)
  USE nrtype
  REAL(SP), INTENT(IN) :: t0,h
  REAL(SP), DIMENSION(:), INTENT(OUT) :: t
  REAL(SP), DIMENSION(:,:), INTENT(OUT) :: f
  INTERFACE
    FUNCTION g(t)
    USE nrtype
    REAL(SP), INTENT(IN) :: t
    REAL(SP), DIMENSION(:), POINTER :: g
    END FUNCTION g
  END INTERFACE
!BL
  FUNCTION ak(t,s)
  USE nrtype
  REAL(SP), INTENT(IN) :: t,s
  REAL(SP), DIMENSION(:,:), POINTER :: ak
  END FUNCTION ak
END INTERFACE
END SUBROUTINE voltra
END INTERFACE
INTERFACE
  SUBROUTINE wt1(a,isign,wtstep)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
  INTEGER(I4B), INTENT(IN) :: isign
  INTERFACE
    SUBROUTINE wtstep(a,isign)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE wtstep
  END INTERFACE
END SUBROUTINE wt1
END INTERFACE
INTERFACE
  SUBROUTINE wtn(a,nn,isign,wtstep)
  USE nrtype

```

```

REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: nn
INTEGER(I4B), INTENT(IN) :: isign
INTERFACE
  SUBROUTINE wtstep(a,isign)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE wtstep
END INTERFACE
END SUBROUTINE wtn
END INTERFACE
INTERFACE
  FUNCTION wwghts(n,h,kermom)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: h
    REAL(SP), DIMENSION(n) :: wwghts
  INTERFACE
    FUNCTION kermom(y,m)
      USE nrtype
      REAL(DP), INTENT(IN) :: y
      INTEGER(I4B), INTENT(IN) :: m
      REAL(DP), DIMENSION(m) :: kermom
    END FUNCTION kermom
  END INTERFACE
END FUNCTION wwghts
END INTERFACE
INTERFACE
  SUBROUTINE zbrac(func,x1,x2,succes)
    USE nrtype
    REAL(SP), INTENT(INOUT) :: x1,x2
    LOGICAL(LGT), INTENT(OUT) :: succes
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE zbrac
END INTERFACE
INTERFACE
  SUBROUTINE zbrak(func,x1,x2,n,xb1,xb2,nb)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    INTEGER(I4B), INTENT(OUT) :: nb
    REAL(SP), INTENT(IN) :: x1,x2
    REAL(SP), DIMENSION(:), POINTER :: xb1,xb2
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE zbrak
END INTERFACE

```

```

        END FUNCTION func
    END INTERFACE
    END SUBROUTINE zbrak
END INTERFACE
INTERFACE
    FUNCTION zbrent(func,x1,x2,tol)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,tol
    REAL(SP) :: zbrent
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION zbrent
END INTERFACE
INTERFACE
    SUBROUTINE zrhqr(a,rtr,rti)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: rtr,rti
    END SUBROUTINE zrhqr
END INTERFACE
INTERFACE
    FUNCTION zriddr(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: zriddr
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION zriddr
END INTERFACE
INTERFACE
    SUBROUTINE zroots(a,roots,polish)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: roots
    LOGICAL(LGT), INTENT(IN) :: polish
    END SUBROUTINE zroots
END INTERFACE
END MODULE nr

```

```

SUBROUTINE rkck(y,dydx,x,h,yout,yerr,derivs)
USE nrtype; USE nrutil, ONLY : assert_eq
IMPLICIT NONE

```

```

REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
REAL(SP), INTENT(IN) :: x,h
REAL(SP), DIMENSION(:), INTENT(OUT) :: yout,yerr
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B) :: ndum
REAL(SP), DIMENSION(size(y)) :: ak2,ak3,ak4,ak5,ak6,ytemp
REAL(SP), PARAMETER :: A2=0.2_sp,A3=0.3_sp,A4=0.6_sp,A5=1.0_sp,&
  A6=0.875_sp,B21=0.2_sp,B31=3.0_sp/40.0_sp,B32=9.0_sp/40.0_sp,&
  B41=0.3_sp,B42=-0.9_sp,B43=1.2_sp,B51=-11.0_sp/54.0_sp,&
  B52=2.5_sp,B53=-70.0_sp/27.0_sp,B54=35.0_sp/27.0_sp,&
  B61=1631.0_sp/55296.0_sp,B62=175.0_sp/512.0_sp,&
  B63=575.0_sp/13824.0_sp,B64=44275.0_sp/110592.0_sp,&
  B65=253.0_sp/4096.0_sp,C1=37.0_sp/378.0_sp,&
  C3=250.0_sp/621.0_sp,C4=125.0_sp/594.0_sp,&
  C6=512.0_sp/1771.0_sp,DC1=C1-2825.0_sp/27648.0_sp,&
  DC3=C3-18575.0_sp/48384.0_sp,DC4=C4-13525.0_sp/55296.0_sp,&
  DC5=-277.0_sp/14336.0_sp,DC6=C6-0.25_sp
ndum=assert_eq(size(y),size(dydx),size(yout),size(yerr),'rkck')
ytemp=y+B21*h*dydx
call derivs(x+A2*h,ytemp,ak2)
ytemp=y+h*(B31*dydx+B32*ak2)
call derivs(x+A3*h,ytemp,ak3)
ytemp=y+h*(B41*dydx+B42*ak2+B43*ak3)
call derivs(x+A4*h,ytemp,ak4)
ytemp=y+h*(B51*dydx+B52*ak2+B53*ak3+B54*ak4)
call derivs(x+A5*h,ytemp,ak5)
ytemp=y+h*(B61*dydx+B62*ak2+B63*ak3+B64*ak4+B65*ak5)
call derivs(x+A6*h,ytemp,ak6)
yout=y+h*(C1*dydx+C3*ak3+C4*ak4+C6*ak6)
yerr=h*(DC1*dydx+DC3*ak3+DC4*ak4+DC5*ak5+DC6*ak6)
END SUBROUTINE rkck

SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
  USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
  USE nr, ONLY : rkck
  IMPLICIT NONE
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
  REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
  REAL(SP), INTENT(INOUT) :: x
  REAL(SP), INTENT(IN) :: htry,eps
  REAL(SP), INTENT(OUT) :: hdid,hnext
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
      USE nrtype
      IMPLICIT NONE
      REAL(SP), INTENT(IN) :: x

```

```

    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B) :: ndum
REAL(SP) :: errmax,h,htemp,xnew
REAL(SP), DIMENSION(size(y)) :: yerr,ytemp
REAL(SP), PARAMETER :: SAFETY=0.9_sp,PGROW=-0.2_sp,PSHRNK=-0.25_sp,&
    ERRCON=1.89e-4
ndum=assert_eq(size(y),size(dydx),size(yscal),'rkqs')
h=htry
do
    call rkck(y,dydx,x,h,ytemp,yerr,derivs)
    errmax=maxval(abs(yerr(:)/yscal(:)))/eps
    if (errmax <= 1.0) exit
    htemp=SAFETY*h*(errmax**PSHRNK)
    h=sign(max(abs(htemp),0.1_sp*abs(h)),h)
    xnew=x+h
    if (xnew == x) call nrerror('stepsize underflow in rkqs')
end do
if (errmax > ERRCON) then
    hnext=SAFETY*h*(errmax**PGROW)
else
    hnext=5.0_sp*h
end if
hdid=h
x=x+h
y(:)=ytemp(:)
END SUBROUTINE rkqs

SUBROUTINE mmid(y,dydx,xs,htot,nstep,yout,derivs)
USE nrtype; USE nrutil, ONLY : assert_eq,swap
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: nstep
REAL(SP), INTENT(IN) :: xs,htot
REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B) :: n,ndum
REAL(SP) :: h,h2,x
REAL(SP), DIMENSION(size(y)) :: ym,yn
ndum=assert_eq(size(y),size(dydx),size(yout),'mmid')
h=htot/nstep
ym=y
yn=y+h*dydx
x=xs+h

```

```

call derivs(x,yn,yout)
h2=2.0_sp*h
do n=2,nstep
    call swap(ym,yn)
    yn=yn+h2*yout
    x=x+h
    call derivs(x,yn,yout)
end do
yout=0.5_sp*(ym+yn+h*yout)
END SUBROUTINE mmid

SUBROUTINE pzextr(iest,xest,yest,yz,dy)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: iest
REAL(SP), INTENT(IN) :: xest
REAL(SP), DIMENSION(:), INTENT(IN) :: yest
REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
INTEGER(I4B), PARAMETER :: IEST_MAX=16
INTEGER(I4B) :: j,nv
INTEGER(I4B), SAVE :: nvold=-1
REAL(SP) :: delta,f1,f2
REAL(SP), DIMENSION(size(yz)) :: d,tmp,q
REAL(SP), DIMENSION(IEST_MAX), SAVE :: x
REAL(SP), DIMENSION(:,:), ALLOCATABLE, SAVE :: qcol
nv=assert_eq(size(yz),size(yest),size(dy),'pzextr')
if (iest > IEST_MAX) call &
    nrerror('pzextr: probable misuse, too much extrapolation')
if (nv /= nvold) then
    if (allocated(qcol)) deallocate(qcol)
    allocate(qcol(nv,IEST_MAX))
    nvold=nv
end if
x(iest)=xest
dy(:)=yest(:)
yz(:)=yest(:)
if (iest == 1) then
    qcol(:,1)=yest(:)
else
    d(:)=yest(:)
    do j=1,iest-1
        delta=1.0_sp/(x(iest-j)-xest)
        f1=xest*delta
        f2=x(iest-j)*delta
        q(:)=qcol(:,j)
        qcol(:,j)=dy(:)
        tmp(:)=d(:)-q(:)
        dy(:)=f1*tmp(:)
        d(:)=f2*tmp(:)
        yz(:)=yz(:)+dy(:)
    end do
    qcol(:,iest)=dy(:)
end if
END SUBROUTINE pzextr

```

```

SUBROUTINE bsstep(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype; USE nrutil, ONLY : arth,assert_eq,cumsum,iminloc,nrerror,&
    outerdiff,outerprod,upper_triangle
USE nr, ONLY : mmid,pzextr
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B), PARAMETER :: IMAX=9, KMAXX=IMAX-1
REAL(SP), PARAMETER :: SAFE1=0.25_sp,SAFE2=0.7_sp,REDMAX=1.0e-5_sp,&
    REDMIN=0.7_sp,TINY=1.0e-30_sp,SCALMX=0.1_sp
INTEGER(I4B) :: k,km,ndum
INTEGER(I4B), DIMENSION(IMAX) :: nseq = (/ 2,4,6,8,10,12,14,16,18 /)
INTEGER(I4B), SAVE :: kopt,kmax
REAL(SP), DIMENSION(KMAXX,KMAXX), SAVE :: alf
REAL(SP), DIMENSION(KMAXX) :: err
REAL(SP), DIMENSION(IMAX), SAVE :: a
REAL(SP), SAVE :: epsold = -1.0_sp,xnew
REAL(SP) :: eps1,errmax,fact,h,red,scale,wrkmin,xest
REAL(SP), DIMENSION(size(y)) :: yerr,ysav,yseq
LOGICAL(LGT) :: reduct
LOGICAL(LGT), SAVE :: first=.true.
ndum=assert_eq(size(y),size(dydx),size(yscal),'bsstep')
if (eps /= epsold) then
    hnext=-1.0e29_sp
    xnew=-1.0e29_sp
    eps1=SAFE1*eps
    a(:)=cumsum(nseq,1)
    where (upper_triangle(KMAXX,KMAXX)) alf=eps1** &
        (outerdiff(a(2:),a(2:))/outerprod(arth( &
            3.0_sp,2.0_sp,KMAXX),(a(2:)-a(1)+1.0_sp)))
    epsold=eps
    do kopt=2,KMAXX-1
        if (a(kopt+1) > a(kopt)*alf(kopt-1,kopt)) exit
    end do
    kmax=kopt
end if
h=htry
ysav(:)=y(:)
if (h /= hnext .or. x /= xnew) then
    first=.true.
    kopt=kmax

```



```

end if
reduct=.false.
main_loop: do
  do k=1,kmax
    xnew=x+h
    if (xnew == x) call nrerror('step size underflow in bsstep')
    call mmid(ysav,dydx,x,h,nseq(k),yseq,derivs)
    xest=(h/nseq(k))**2
    call pzextr(k,xest,yseq,y,yerr)
    if (k /= 1) then
      errmax=maxval(abs(yerr(:)/yscal(:)))
      errmax=max(TINY,errmax)/eps
      km=k-1
      err(km)=(errmax/SAFE1)**(1.0_sp/(2*km+1))
    end if
    if (k /= 1 .and. (k >= kopt-1 .or. first)) then
      if (errmax < 1.0) exit main_loop
      if (k == kmax .or. k == kopt+1) then
        red=SAFE2/err(km)
        exit
      else if (k == kopt) then
        if (alf(kopt-1,kopt) < err(km)) then
          red=1.0_sp/err(km)
          exit
        end if
      else if (kopt == kmax) then
        if (alf(km,kmax-1) < err(km)) then
          red=alf(km,kmax-1)*SAFE2/err(km)
          exit
        end if
      else if (alf(km,kopt) < err(km)) then
        red=alf(km,kopt-1)/err(km)
        exit
      end if
    end if
  end do
  red=max(min(red,REDMIN),REDMAX)
  h=h*red
  reduct=.true.
end do main_loop
x=xnew
hdid=h
first=.false.
kopt=1+iminloc(a(2:km+1)*max(err(1:km),SCALMX))
scale=max(err(kopt-1),SCALMX)
wrkmin=scale*a(kopt)
hnext=h/scale
if (kopt >= k .and. kopt /= kmax .and. .not. reduct) then
  fact=max(scale/alf(kopt-1,kopt),SCALMX)
  if (a(kopt+1)*fact <= wrkmin) then
    hnext=h/fact
    kopt=kopt+1
  end if
end if
end if

```

```

END SUBROUTINE bsstep

FUNCTION hypgeo(a,b,c,z)
  USE nrtype
  USE hypgeo_info
  USE nr, ONLY : bsstep,hypdrv,hypser,odeint
  IMPLICIT NONE
  COMPLEX(SPC), INTENT(IN) :: a,b,c,z
  COMPLEX(SPC) :: hypgeo
  REAL(SP), PARAMETER :: EPS=1.0e-6_sp
  COMPLEX(SPC), DIMENSION(2) :: y
  REAL(SP), DIMENSION(4) :: ry
  if (real(z)**2+aimag(z)**2 <= 0.25) then
    call hypser(a,b,c,z,hypgeo,y(2))
    RETURN
  else if (real(z) < 0.0) then
    hypgeo_z0=cplx(-0.5_sp,0.0_sp,kind=spc)
  else if (real(z) <= 1.0) then
    hypgeo_z0=cplx(0.5_sp,0.0_sp,kind=spc)
  else
    hypgeo_z0=cplx(0.0_sp,sign(0.5_sp,aimag(z)),kind=spc)
  end if
  hypgeo_aa=a
  hypgeo_bb=b
  hypgeo_cc=c
  hypgeo_dz=z-hypgeo_z0
  call hypser(hypgeo_aa,hypgeo_bb,hypgeo_cc,hypgeo_z0,y(1),y(2))
  ry(1:4:2)=real(y)
  ry(2:4:2)=aimag(y)
!  call odeint(ry,0.0_sp,1.0_sp,EPS,0.1_sp,0.0001_sp,hypdrv,bsstep)
  call odeint(ry,0.0_sp,1.0_sp,EPS,0.1_sp,0.000001_sp,hypdrv,bsstep) !!! FB
  y=cplx(ry(1:4:2),ry(2:4:2),kind=spc)
  hypgeo=y(1)
END FUNCTION hypgeo

SUBROUTINE hypdrv(s,ry,rdyds)
  USE nrtype
  USE hypgeo_info
  IMPLICIT NONE
  REAL(SP), INTENT(IN) :: s
  REAL(SP), DIMENSION(:), INTENT(IN) :: ry
  REAL(SP), DIMENSION(:), INTENT(OUT) :: rdyds
  COMPLEX(SPC), DIMENSION(2) :: y,dyds
  COMPLEX(SPC) :: z
  y=cplx(ry(1:4:2),ry(2:4:2),kind=spc)
  z=hypgeo_z0+s*hypgeo_dz
  dyds(1)=y(2)*hypgeo_dz
  dyds(2)=((hypgeo_aa*hypgeo_bb)*y(1)-(hypgeo_cc-&
    ((hypgeo_aa+hypgeo_bb)+1.0_sp)*z)*y(2))*hypgeo_dz/(z*(1.0_sp-z))
  rdyds(1:4:2)=real(dyds)
  rdyds(2:4:2)=aimag(dyds)
END SUBROUTINE hypdrv

SUBROUTINE hypser(a,b,c,z,series,deriv)

```

```

USE nrtype; USE nrutil, ONLY : nrerror
IMPLICIT NONE
COMPLEX(SPC), INTENT(IN) :: a,b,c,z
COMPLEX(SPC), INTENT(OUT) :: series,deriv
INTEGER(I4B) :: n
INTEGER(I4B), PARAMETER :: MAXIT=1000
COMPLEX(SPC) :: aa,bb,cc,fac,temp
deriv=cmplx(0.0_sp,0.0_sp,kind=spc)
fac=cmplx(1.0_sp,0.0_sp,kind=spc)
temp=fac
aa=a
bb=b
cc=c
do n=1,MAXIT
    fac=((aa*bb)/cc)*fac
    deriv=deriv+fac
    fac=fac*z/n
    series=temp+fac
    if (series == temp) RETURN
    temp=series
    aa=aa+1.0
    bb=bb+1.0
    cc=cc+1.0
end do
call nrerror('hypser: convergence failure')
END SUBROUTINE hypser

SUBROUTINE odeint(ystart,x1,x2,eps,h1,hmin,derivs,rkqs)
USE nrtype; USE nrutil, ONLY : nrerror,reallocate
USE ode_path
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: ystart
REAL(SP), INTENT(IN) :: x1,x2,eps,h1,hmin
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
!BL
    SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
    REAL(SP), INTENT(INOUT) :: x
    REAL(SP), INTENT(IN) :: htry,eps
    REAL(SP), INTENT(OUT) :: hdid,hnext
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        IMPLICIT NONE

```

```

        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE rkqs
END INTERFACE
REAL(SP), PARAMETER :: TINY=1.0e-30_sp
INTEGER(I4B), PARAMETER :: MAXSTP=10000
INTEGER(I4B) :: nstp
REAL(SP) :: h,hdid,hnext,x,xsav
REAL(SP), DIMENSION(size(ystart)) :: dydx,y,yscal
x=x1
h=sign(h1,x2-x1)
nok=0
nbad=0
kount=0
y(:)=ystart(:)
nullify(xp,yp)
if (save_steps) then
    xsav=x-2.0_sp*dxsav
    allocate(xp(256))
    allocate(yp(size(ystart),size(xp)))
end if
do nstp=1,MAXSTP
    call derivs(x,y,dydx)
    yscal(:)=abs(y(:))+abs(h*dydx(:))+TINY
    if (save_steps .and. (abs(x-xsav) > abs(dxsav))) &
        call save_a_step
    if ((x+h-x2)*(x+h-x1) > 0.0) h=x2-x
    call rkqs(y,dydx,x,h,eps,yscal,hdid,hnext,derivs)
    if (hdid == h) then
        nok=nok+1
    else
        nbad=nbad+1
    end if
    if ((x-x2)*(x2-x1) >= 0.0) then
        ystart(:)=y(:)
        if (save_steps) call save_a_step
        RETURN
    end if
    if (abs(hnext) < hmin) then
print *, "abs(hnext) = ", abs(hnext)
print *, "hmin = ", hmin
        call nrerror('stepsize smaller than minimum in odeint')
    end if
    h=hnext
end do
call nrerror('too many steps in odeint')
CONTAINS
!BL
SUBROUTINE save_a_step
kount=kount+1
if (kount > size(xp)) then

```

```

        xp=>reallocate(xp,2*size(xp))
        yp=>reallocate(yp,size(yp,1),size(xp))
    end if
    xp(kount)=x
    yp(:,kount)=y(:)
    xsav=x
END SUBROUTINE save_a_step
END SUBROUTINE odeint

FUNCTION gammln_s(xx)
USE nrtype; USE nrutil, ONLY : arth,assert
IMPLICIT NONE
REAL(SP), INTENT(IN) :: xx
REAL(SP) :: gammln_s
REAL(DP) :: tmp,x
REAL(DP) :: stp = 2.5066282746310005_dp
REAL(DP), DIMENSION(6) :: coef = (/76.18009172947146_dp,&
    -86.50532032941677_dp,24.01409824083091_dp,&
    -1.231739572450155_dp,0.1208650973866179e-2_dp,&
    -0.5395239384953e-5_dp/)
call assert(xx > 0.0, 'gammln_s arg')
x=xx
tmp=x+5.5_dp
tmp=(x+0.5_dp)*log(tmp)-tmp
gammln_s=tmp+log(stp*(1.000000000190015_dp+&
    sum(coef(:)/arth(x+1.0_dp,1.0_dp,size(coef))))/x)
END FUNCTION gammln_s

FUNCTION gammln_v(xx)
USE nrtype; USE nrutil, ONLY: assert
IMPLICIT NONE
INTEGER(I4B) :: i
REAL(SP), DIMENSION(:), INTENT(IN) :: xx
REAL(SP), DIMENSION(size(xx)) :: gammln_v
REAL(DP), DIMENSION(size(xx)) :: ser,tmp,x,y
REAL(DP) :: stp = 2.5066282746310005_dp
REAL(DP), DIMENSION(6) :: coef = (/76.18009172947146_dp,&
    -86.50532032941677_dp,24.01409824083091_dp,&
    -1.231739572450155_dp,0.1208650973866179e-2_dp,&
    -0.5395239384953e-5_dp/)
if (size(xx) == 0) RETURN
call assert(all(xx > 0.0), 'gammln_v arg')
x=xx
tmp=x+5.5_dp
tmp=(x+0.5_dp)*log(tmp)-tmp
ser=1.000000000190015_dp
y=x
do i=1,size(coef)
    y=y+1.0_dp
    ser=ser+coef(i)/y
end do
gammln_v=tmp+log(stp*ser/x)
END FUNCTION gammln_v

```

```

!   FUNCTION qgaus(func,a,b)
!   USE nrtype
!   REAL(SP), INTENT(IN) :: a,b
!   REAL(SP) :: qgaus
!   INTERFACE
!     FUNCTION func(x)
!     USE nrtype
!     REAL(SP), DIMENSION(:), INTENT(IN) :: x
!     REAL(SP), DIMENSION(size(x)) :: func
!     END FUNCTION func
!   END INTERFACE
!   REAL(SP) :: xm,xr
!   REAL(SP), DIMENSION(5) :: dx, w = (/ 0.2955242247_sp,0.2692667193_sp,&
!     0.2190863625_sp,0.1494513491_sp,0.0666713443_sp /),&
!     x = (/ 0.1488743389_sp,0.4333953941_sp,0.6794095682_sp,&
!     0.8650633666_sp,0.9739065285_sp /)
!   xm=0.5_sp*(b+a)
!   xr=0.5_sp*(b-a)
!   dx(:)=xr*x(:)
!   qgaus=xr*sum(w(:)*(func(xm+dx)+func(xm-dx)))
!   END FUNCTION qgaus

FUNCTION locatenr(xx,x)
USE nrtype
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: xx
REAL(SP), INTENT(IN) :: x
INTEGER(I4B) :: locatenr
INTEGER(I4B) :: n,jl,jm,ju
LOGICAL :: ascnd
n=size(xx)
ascnd = (xx(n) >= xx(1))
jl=0
ju=n+1
do
  if (ju-jl <= 1) exit
  jm=(ju+jl)/2
  if (ascnd .eqv. (x >= xx(jm))) then
    jl=jm
  else
    ju=jm
  end if
end do
if (x == xx(1)) then
  locatenr=1
else if (x == xx(n)) then
  locatenr=n-1
else
  locatenr=jl
end if
END FUNCTION locatenr

SUBROUTINE tridag_ser(a,b,c,r,u)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror

```

```

IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
REAL(SP), DIMENSION(:), INTENT(OUT) :: u
REAL(SP), DIMENSION(size(b)) :: gam
INTEGER(I4B) :: n,j
REAL(SP) :: bet
n=assert_eq((/size(a)+1,size(b),size(c)+1,size(r),size(u)/),'tridag_ser')
bet=b(1)
if (bet == 0.0) call nrerror('tridag_ser: Error at code stage 1')
u(1)=r(1)/bet
do j=2,n
    gam(j)=c(j-1)/bet
    bet=b(j)-a(j-1)*gam(j)
    if (bet == 0.0) &
        call nrerror('tridag_ser: Error at code stage 2')
    u(j)=(r(j)-a(j-1)*u(j-1))/bet
end do
do j=n-1,1,-1
    u(j)=u(j)-gam(j+1)*u(j+1)
end do
END SUBROUTINE tridag_ser

RECURSIVE SUBROUTINE tridag_par(a,b,c,r,u)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
USE nr, ONLY : tridag_ser
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
REAL(SP), DIMENSION(:), INTENT(OUT) :: u
INTEGER(I4B), PARAMETER :: NPAR_TRIDAG=4
INTEGER(I4B) :: n,n2,nm,nx
REAL(SP), DIMENSION(size(b)/2) :: y,q,piva
REAL(SP), DIMENSION(size(b)/2-1) :: x,z
REAL(SP), DIMENSION(size(a)/2) :: pivc
n=assert_eq((/size(a)+1,size(b),size(c)+1,size(r),size(u)/),'tridag_par')
if (n < NPAR_TRIDAG) then
    call tridag_ser(a,b,c,r,u)
else
    if (maxval(abs(b(1:n))) == 0.0) &
        call nrerror('tridag_par: possible singular matrix')
    n2=size(y)
    nm=size(pivc)
    nx=size(x)
    piva = a(1:n-1:2)/b(1:n-1:2)
    pivc = c(2:n-1:2)/b(3:n:2)
    y(1:nm) = b(2:n-1:2)-piva(1:nm)*c(1:n-2:2)-pivc*a(2:n-1:2)
    q(1:nm) = r(2:n-1:2)-piva(1:nm)*r(1:n-2:2)-pivc*r(3:n:2)
    if (nm < n2) then
        y(n2) = b(n)-piva(n2)*c(n-1)
        q(n2) = r(n)-piva(n2)*r(n-1)
    end if
    x = -piva(2:n2)*a(2:n-2:2)
    z = -pivc(1:nx)*c(3:n-1:2)
    call tridag_par(x,y,z,q,u(2:n:2))
    u(1) = (r(1)-c(1)*u(2))/b(1)

```

```

      u(3:n-1:2) = (r(3:n-1:2)-a(2:n-2:2)*u(2:n-2:2) &
                   -c(3:n-1:2)*u(4:n:2))/b(3:n-1:2)
      if (nm == n2) u(n)=(r(n)-a(n-1)*u(n-1))/b(n)
    end if
  END SUBROUTINE tridag_par

  SUBROUTINE spline(x,y,yp1,ypn,y2)
  USE nrtype; USE nrutil, ONLY : assert_eq
  USE nr, ONLY : tridag
  IMPLICIT NONE
  REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
  REAL(SP), INTENT(IN) :: yp1,ypn
  REAL(SP), DIMENSION(:), INTENT(OUT) :: y2
  INTEGER(I4B) :: n
  REAL(SP), DIMENSION(size(x)) :: a,b,c,r
  n=assert_eq(size(x),size(y),size(y2),'spline')
  c(1:n-1)=x(2:n)-x(1:n-1)
  r(1:n-1)=6.0_sp*((y(2:n)-y(1:n-1))/c(1:n-1))
  r(2:n-1)=r(2:n-1)-r(1:n-2)
  a(2:n-1)=c(1:n-2)
  b(2:n-1)=2.0_sp*(c(2:n-1)+a(2:n-1))
  b(1)=1.0
  b(n)=1.0
  if (yp1 > 0.99e30_sp) then
    r(1)=0.0
    c(1)=0.0
  else
    r(1)=(3.0_sp/(x(2)-x(1)))*((y(2)-y(1))/(x(2)-x(1))-yp1)
    c(1)=0.5
  end if
  if (ypn > 0.99e30_sp) then
    r(n)=0.0
    a(n)=0.0
  else
    r(n)=(-3.0_sp/(x(n)-x(n-1)))*((y(n)-y(n-1))/(x(n)-x(n-1))-ypn)
    a(n)=0.5
  end if
  call tridag(a(2:n),b(1:n),c(1:n-1),r(1:n),y2(1:n))
  END SUBROUTINE spline

  FUNCTION splint(xa,ya,y2a,x)
  USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
  USE nr, ONLY: locatenr
  IMPLICIT NONE
  REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya,y2a
  REAL(SP), INTENT(IN) :: x
  REAL(SP) :: splint
  INTEGER(I4B) :: khi,klo,n
  REAL(SP) :: a,b,h
  n=assert_eq(size(xa),size(ya),size(y2a),'splint')
  klo=max(min(locatenr(xa,x),n-1),1)
  khi=klo+1
  h=xa(khi)-xa(klo)
  if (h == 0.0) call nrerror('bad xa input in splint')

```



```

a=(xa(khi)-x)/h
b=(x-xa(klo))/h
splint=a*ya(klo)+b*ya(khi)+((a**3-a)*y2a(klo)+(b**3-b)*y2a(khi))*(h**2)/6.0_sp
END FUNCTION splint

```

```

SUBROUTINE sort(arr)
USE nrtype; USE nrutil, ONLY : swap,nrerror
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
INTEGER(I4B), PARAMETER :: NN=15, NSTACK=50
REAL(SP) :: a
INTEGER(I4B) :: n,k,i,j,jstack,l,r
INTEGER(I4B), DIMENSION(NSTACK) :: istack
n=size(arr)
jstack=0
l=1
r=n
do
  if (r-l < NN) then
    do j=l+1,r
      a=arr(j)
      do i=j-1,l,-1
        if (arr(i) <= a) exit
        arr(i+1)=arr(i)
      end do
      arr(i+1)=a
    end do
    if (jstack == 0) RETURN
    r=istack(jstack)
    l=istack(jstack-1)
    jstack=jstack-2
  else
    k=(l+r)/2
    call swap(arr(k),arr(l+1))
    call swap(arr(l),arr(r),arr(l)>arr(r))
    call swap(arr(l+1),arr(r),arr(l+1)>arr(r))
    call swap(arr(l),arr(l+1),arr(l)>arr(l+1))
    i=l+1
    j=r
    a=arr(l+1)
    do
      do
        i=i+1
        if (arr(i) >= a) exit
      end do
      do
        j=j-1
        if (arr(j) <= a) exit
      end do
      if (j < i) exit
      call swap(arr(i),arr(j))
    end do
    arr(l+1)=arr(j)
    arr(j)=a
  end if
end do

```

```

        jstack=jstack+2
        if (jstack > NSTACK) call nrerror('sort: NSTACK too small')
        if (r-i+1 >= j-1) then
            istack(jstack)=r
            istack(jstack-1)=i
            r=j-1
        else
            istack(jstack)=j-1
            istack(jstack-1)=1
            l=i
        end if
    end if
end do
END SUBROUTINE sort

```

```

!!! Whizard wrapper for NR tools
module nr_tools
    use kinds, only: default !NODEP!
    use nrtype, only: i4b, sp, spc !NODEP!
    use nr, only: gammln, hypgeo, locatenr, sort, spline, splint !NODEP!
    implicit none
    save
    private

    public :: nr_hypgeo, nr_gamma, nr_locate, nr_sort, nr_spline_t

    type :: nr_spline_t
        real(sp), dimension(:), allocatable :: xa, ya_re, ya_im, y2a_re, y2a_im
    contains
        procedure :: init => nr_spline_init
        procedure :: interpolate => nr_spline_interpolate
        procedure :: dealloc => nr_spline_dealloc
    end type nr_spline_t

contains

    function nr_hypgeo (a, b, c, d) result (h)
        complex(default), intent(in) :: a, b, c, d
        complex(default) :: h
        complex(spc) :: a_sp, b_sp, c_sp, d_sp
        a_sp = cmplx(a,kind=sp)
        b_sp = cmplx(b,kind=sp)
        c_sp = cmplx(c,kind=sp)
        d_sp = cmplx(d,kind=sp)
        h = cmplx( hypgeo (a_sp, b_sp, c_sp, d_sp) , kind=default )
    end function nr_hypgeo

    function nr_gamma (x) result (y)
        real(default), intent(in) :: x
        real(default) :: y
        y = real( exp(gammln(real(x,kind=sp))) , kind=default )
    end function nr_gamma

```

```

function nr_locate (xa, x) result (pos)
    real(default), dimension(:), intent(in) :: xa
    real(default), intent(in) :: x
    integer :: pos
    pos = locatenr (real(xa,kind=sp), real(x,kind=sp))
end function

! function nr_qgaus (fun, pts) result (res)
!     real(default), dimension(:), intent(in) :: pts
!     complex(default) :: res
!     integer :: i_pts
!     real(sp) :: lo, hi, re, im
!     interface
!         function fun (x)
!             use kinds, only: default !NODEP!
!             real(default), intent(in) :: x
!             complex(default) :: fun
!         end function fun
!     end interface
!     res = 0.0_default
!     if ( size(pts) < 2 ) return
!     do i_pts=1, size(pts)-1
!         lo = real(pts(i_pts ),kind=sp)
!         hi = real(pts(i_pts+1),kind=sp)
!         re = qgaus (fun_re, lo, hi)
!         im = qgaus (fun_im, lo, hi)
!         res = res + cmplx(re,im,kind=default)
!     end do
!     contains
!     function fun_re (xa_sp)
!         use kinds, only: default !NODEP!
!         use nrtype, only: sp !NODEP!
!         real(sp), dimension(:), intent(in) :: xa_sp
!         real(sp), dimension(size(xa_sp)) :: fun_re
!         real(default), dimension(size(xa_sp)) :: xa
!         integer :: ix
!         xa = real(xa_sp,kind=default)
!         fun_re = (/ (real(fun(xa(ix))),kind=sp), ix=1, size(xa)) /)
!     end function fun_re
!     function fun_im (xa_sp)
!         use kinds, only: default !NODEP!
!         use nrtype, only: sp !NODEP!
!         real(sp), dimension(:), intent(in) :: xa_sp
!         real(sp), dimension(size(xa_sp)) :: fun_im
!         real(default), dimension(size(xa_sp)) :: xa
!         integer :: ix
!         xa = real(xa_sp,kind=default)
!         fun_im = (/ (real(aimag(fun(xa(ix)))),kind=sp), ix=1, size(xa)) /)
!     end function fun_im
! end function nr_qgaus

subroutine nr_sort (array)
    real(default), dimension(:), intent(inout) :: array

```

```

    real(sp), dimension(size(array)) :: array_sp
    array_sp = real(array,kind=sp)
    call sort (array_sp)
    array = real(array_sp,kind=default)
end subroutine nr_sort

subroutine nr_spline_init (spl, xa_in, ya_in)
    class(nr_spline_t), intent(inout) :: spl
    real(default), dimension(:), intent(in) :: xa_in
    complex(default), dimension(:), intent(in) :: ya_in
    integer :: n
    if ( allocated(spl%xa) ) then
        print *, "ERROR: nr_spline: init: already initialized!"
        stop
    end if
    n = size(xa_in)
    allocate( spl%xa(n) )
    allocate( spl%ya_re(n) )
    allocate( spl%ya_im(n) )
    allocate( spl%y2a_re(n) )
    allocate( spl%y2a_im(n) )
    spl%xa = real(xa_in,kind=sp)
    spl%ya_re = real(ya_in,kind=sp)
    spl%ya_im = real(aimag(ya_in),kind=sp)
    call spline (spl%xa, spl%ya_re, 1.e30, 1.e30, spl%y2a_re)
    call spline (spl%xa, spl%ya_im, 1.e30, 1.e30, spl%y2a_im)
end subroutine nr_spline_init

function nr_spline_interpolate (spl, x) result (y)
    complex(default) :: y
    class(nr_spline_t), intent(in) :: spl
    real(default), intent(in) :: x
    real(sp) :: y_re, y_im
    if ( .not.allocated(spl%xa) ) then
        print *, "ERROR: nr_spline: interpolate: not initialized!"
        stop
    end if
    y_re = splint (spl%xa, spl%ya_re, spl%y2a_re, real(x,kind=sp))
    y_im = splint (spl%xa, spl%ya_im, spl%y2a_im, real(x,kind=sp))
    y = cmplx(y_re,y_im,kind=default)
end function nr_spline_interpolate

subroutine nr_spline_dealloc (spl)
    class(nr_spline_t), intent(inout) :: spl
    if ( .not.allocated(spl%xa) ) then
        print *, "ERROR: nr_spline: dealloc: not initialized!"
        stop
    end if
    deallocate( spl%xa )
    deallocate( spl%ya_re )
    deallocate( spl%ya_im )
    deallocate( spl%y2a_re )
    deallocate( spl%y2a_im )
end subroutine nr_spline_dealloc

```

```

end module nr_tools

<toppik.f>≡
! WHIZARD <Version> <Date>

! TOPPIK code by M. Jezabek, T. Teubner (v1.1, 1992), T. Teubner (1998)
!
! FB: -commented out numerical recipes code for hypergeometric 2F1
!      included in hypgeo.f90;
!      -commented out unused function 'ZAPVQ1';
!      -replaced function 'cdabs' by 'abs';
!      -replaced function 'dimag' by 'aimag';
!      -replaced function 'dcmplx(,)' by 'cmplx(,kind=kind(0d0))';
!      -replaced function 'dreal' by 'real';
!      -replaced function 'cdlog' by 'log';
!      -replaced PAUSE by PRINT statement to avoid compiler warning;
!      -initialized 'idum' explicitly as real to avoid compiler warning.
!      -modified 'adglg1', 'adglg2' and 'tttoppik' to catch unstable runs.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

c *****
c
c Working version with all the different original potentials
c like (p^2+q^2)/|p-q|^2, not transformed in terms of delta and 1/r^2;
c accuracy eps=1.d-3 possible (only), but should be save, 13.8.'98, tt.
c
c *****
c
      subroutine tttoppik(xenergy,xtm,xtg,xalphas,xscale,xcutn,xcutv,
u      xc0,xc1,xc2,xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,
u      xkincm,xkinca,jknflg,jgcflg,
u      xkincv,jvflg,xim,xdi,np,xpp,xww,xdsdp,zvfct)
c
c *****
c
c !! THIS IS NOT A PUBLIC VERSION !!
c
c - Calculation of the Green function in momentum space by solving the
c   Lippmann-Schwinger equation
c    $G(p) = G_0(p) + G_0(p) \int_0^{xcutn} V(p,q) G(q) dq$ 
c
c - Written by Thomas Teubner, Hamburg, November 1998
c   * Based on TOPPIK Version 1.1
c     from M. Jezabek and TT, Karlsruhe, June 1992
c   * Version originally for non-constant top-width
c   * Constant width supplied here
c   * No generator included
c
c - Use of double precision everywhere
c
c - All masses, momenta, energies, widths in GeV
c
c - Input parameters:
c

```

```

c   xenergy : E=Sqrt[s]-2*topmass
c   xtm      : topmass (in the Pole scheme)
c   xtg      : top-width
c   xalphas  : alpha_s^{MSbar,n_f=5}(xscale)
c   xscale   : soft scale mu_{soft}
c   xcutn    : numerical UV cutoff on all momenta
c              (UV cutoff of the Gauss-Legendre grid)
c   xcutv    : renormalization cutoff on the
c              delta-, the (p^2+q^2)/(p-q)^2-, and the
c              1/r^2-[1/|p-q|]-potential:
c              if (max(p,q).ge.xcutv) then the three potentials
c              are set to zero in the Lippmann-Schwinger equation
c   xc0      : 0th order coefficient for the Coulomb potential,
c              see calling example above
c   xc1      : 1st order coefficient for the Coulomb potential
c   xc2      : 2nd order coefficient for the Coulomb potential
c   xcdeltc  : constant of the delta(r)-
c              [= constant in momentum space-] potential
c   xcdeletl : constant for the additional log(q^2/mu^2)-part of the
c              delta-potential:
c              xcdeltc*1 + xcdeletl*log(q^2/mu^2)
c   xcfullc  : constant of the (p^2+q^2)/(p-q)^2-potential
c   xcfulll  : constant for the additional log(q^2/mu^2)-part of the
c              (p^2+q^2)/(p-q)^2-potential
c   xcrm2    : constant of the 1/r^2-[1/|p-q|]-potential
c   xkincm   : } kinetic corrections in the 0th order Green-function:
c   xkinca   : } G_0(p):=1/[E+iGamma_t-p^2/m_t]*(1+xkincm)+xkinca
c              !!! WATCH THE SIGN IN G_0 !!!
c   jknflg   : flag for these kinetic corrections:
c              0 : no kinetic corrections applied
c              1 : kinetic corrections applied with cutoff xcutv
c                  for xkinca only
c              2 : kinetic corrections applied with cutoff xcutv
c                  for xkinca AND xkincm
c   jgcflg   : flag for G_0(p) in the LS equation:
c              0 (standard choice) : G_0(p) as given above
c              1 (for TIPT)         : G_0(p) = G_c^{0}(p) the 0th
c                                      order Coulomb-Green-function
c                                      in analytical form; not for
c                                      momenta p > 1000*topmass
c   xkincv   : additional kinematic vertexcorrection in G_0, see below:
c   jvflg    : flag for the additional vertexcorrection xkincv in the
c              "zeroth order" G_0(p) in the LS-equation:
c              0 : no correction, means G = G_0 + G_0 int V G
c                  with G_0=1/[E+iGamma_t-p^2/m_t]*(1+xkincm)+xkinca
c              1 : apply the correction in the LS equation as
c                  G = G_0 + xkincv*p^2/m_t^2/[E+iGamma_t-p^2/m_t] +
c                  G_0 int V G
c              and correct the integral over Im[G(p)] to get sigma_tot
c              from the optical theorem by the same factor.
c              The cutoff xcutv is applied for these corrections.
c
c - Output:
c

```

```

c      xim      :  R_{ttbar} from the imaginary part of the green
c                  function
c      xdi      :  R_{ttbar} form the integral over the momentum
c                  distribution (no cutoff but the numerical one here!!)
c      np       :  number of points used for the grid; fixed in tttoppik
c      xpp      :  1-dim array (max. 900 elements) giving the momenta of
c                  the Gauss-Legendre grid (pp(i) in the code)
c      xww      :  1-dim array (max. 900 elements) giving the corresponding
c                  Gauss-Legendre weights for the grid
c      xdsdp    :  1-dim array (max. 900 elements) giving the
c                  momentum distribution of top: d\sigma/dp,
c                  normalized to R,
c                  at the momenta of the Gauss-Legendre grid xpp(i)
c      zvfct    :  1-dim array (max. 900 elements) of COMPLEX*16 numbers
c                  giving the vertex function K(p), G(p)=K(p)*G_0(p)
c                  at the momenta of the grid
c
c *****
c
c
c      implicit none
c      real*8
c      u      pi,energy,vzero,eps,
c      u      pp,
c      u      tmass,tgamma,zmass,alphas,alamb5,
c      u      wmass,wgamma,bmass,GFERMI,
c      u      xx,critp,consde,
c      u      w1,w2,sig1,sig2,const,
c      u      gtpcor,etot,
c      u      xenergy,xtm,xtg,xalphas,xscale,xc0,xc1,xc2,xim,xdi,
c      u      xdsdp,xpp,xww,
c      u      cplas,scale,c0,c1,c2,cdeltc,cdeltl,cfullc,cfulll,crm2,
c      u      xcutn,dcut,xcutv,
c      u      xp,xpmax,hmass,
c      u      kincom,kincoa,kincov,xkincm,xkinca,xkincv,
c      u      xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,chiggs
c      complex*16 bb,gg,a1,a,g0,g0c,zvfct
c      integer i,n,nmax,npot,np,gcflg,kinflg,jknflg,jgcflg,
c      u      jvflg,vflag
c      parameter (nmax=900)
c      dimension pp(nmax), bb(nmax), xx(nmax), gg(nmax),
c      u      w1(nmax), w2(nmax), a1(nmax),
c      u      xdsdp(nmax),xpp(nmax),xww(nmax),zvfct(nmax)
c
c      external a,gtpcor,g0,g0c
c
c      common/ovalco/ pi, energy, vzero, eps, npot
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/cplcns/cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c      common/mom/ xp,xpmax,dcut
c      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c

```

```

pi=3.141592653589793238d0
c
c Number of points to evaluate on the integral equation
c (<=900 and n mod 3 = 0 !!):
c     n=66
c     n=600
c     np=n
c
c For second order potential with free parameters:
c
c     npot=5
c Internal accuracy for TOPPIK, the reachable limit may be smaller,
c depending on the parameters. But increase in real accuracy only
c in combination with large number of points.
c     eps=1.d-3
c Some physical parameters:
c     wgamma=2.07d0
c     zmass=91.187d0
c     wmass=80.33d0
c     bmass=4.7d0
c
c Input:
c     energy=xenergy
c     tmass=xtm
c     tgamma=xtg
c     cplas=xalphas
c     scale=xscale
c     c0=xc0
c     c1=xc1
c     c2=xc2
c     cdeltc=xcdeltc
c     cdeltl=xcdeltl
c     cfullc=xcfullc
c     cfulll=xcfulll
c     crm2=xcrm2
c     kincom=xkincom
c     kincoa=xkinca
c     kincov=xkincv
c     kinflg=jknflg
c     gcflg=jgcflg
c     vflag=jvflg
c
c     alphas=xalphas
c
c Cut for divergent potential-terms for large momenta in the function vhat
c and in the integrals a(p):
c     dcut=xcutv
c
c Numerical Cutoff of all momenta (maximal momenta of the grid):
c     xpmay=xcutn
c     if (dcut.gt.xpmay) then
c         write(*,*) ' dcut > xpmay makes no sense! Stop.'
c         stop
c     endif

```



```

c
c Not needed for the fixed order potentials:
      alamb5=0.2d0
c
c      WRITE(*,*) 'INPUT TGAMMA=',TGAMMA
c Needed in subroutine GAMMAT:
      GFERMI=1.16637d-5
c      CALL GAMMAT
c      WRITE(*,*) 'CALCULATED TGAMMA=',TGAMMA
c
      etot=2.d0*tmass+energy
c
      if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
         u (npot.eq.5)) then
c For pure coulomb and fixed order potentials there is no delta-part:
      consde = 0.d0
      else if (npot.eq.2) then
c Initialize QCD-potential common-blocks and calculate constant multiplying
c the delta-part of the 'qcutted' potential in momentum-space:
      call iniphc(1)
      call vqdelt(consde)
      else
        write (*,*) ' Potential not implemented! Stop.'
        stop
      endif
c Delta-part of potential is absorbed by subtracting vzero from the
c original energy (shift from the potential to the free Hamiltonian):
      vzero = consde / (2.d0*pi)**3
c      write (*,*) 'vzero=', vzero
c
c Find x-values pp(i) and weigths w1(i) for the gaussian quadrature;
c care about large number of points in the important intervals:
c      if (energy-vzero.le.0.d0) then
cc      call gauleg(0.d0, 1.d0, pp, w1, n/3)
cc      call gauleg(1.d0, 5.d0, pp(n/3+1), w1(n/3+1), n/3)
cc      call gauleg(0.d0, 0.2d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      call gauleg(0.d0, 5.d0, pp, w1, n/3)
c      call gauleg(5.d0, 20.d0, pp(n/3+1), w1(n/3+1), n/3)
c      call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      else
cc Avoid numerical singular points in the inner of the intervals:
c      critp = dsqrt((energy-vzero)*tmass)
c      if (critp.le.1.d0) then
cc Gauss-Legendre is symmetric => automatically principal-value prescription:
c      call gauleg(0.d0, 2.d0*critp, pp, w1, n/3)
c      call gauleg(2.d0*critp, 20.d0, pp(n/3+1),
         u w1(n/3+1), n/3)
c      call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      else
cc Better behaviour at the border of the intervals:
c      call gauleg(0.d0, critp, pp, w1, n/3)
c      call gauleg(critp, 2.d0*critp, pp(n/3+1),
         u w1(n/3+1), n/3)
c      call gauleg(0.d0, 1.d0/(2.d0*critp), pp(2*n/3+1),

```

```

c      u      w1(2*n/3+1), n/3)
c      endif
c      endif
c
c Or different (simpler) method, good for V_JKT:
      if (energy.le.0.d0) then
        critp=tmass/3.d0
      else
        critp=max(tmass/3.d0,2.d0*dsqrt(energy*tmass))
      endif
      call gauleg(0.d0, critp, pp, w1, 2*n/3)
      call gauleg(1.d0/xpmax, 1.d0/critp, pp(2*n/3+1),
u      w1(2*n/3+1), n/3)
c
c Do substitution p => 1/p for the last interval explicitly:
      do 10 i=2*n/3+1,n
        pp(i) = 1.d0/pp(i)
10      continue
c
c Reorder the arrays for the third interval:
      do 20 i=1,n/3
        xx(i) = pp(2*n/3+i)
        w2(i) = w1(2*n/3+i)
20      continue
      do 30 i=1,n/3
        pp(n-i+1) = xx(i)
        w1(n-i+1) = w2(i)
30      continue
c
c Calculate the integrals a(p) for the given momenta pp(i)
c and store weights and momenta for the output arrays:
      do 40 i=1,n
        a1(i) = a(pp(i)) !!! FB: can get stuck in original Toppik!
        !!! FB: abuse 'np' as a flag to communicate unstable runs
        if ( abs(a1(i)) .gt. 1d10 ) then
          np = -1
          return
        endif
        xpp(i)=pp(i)
        xww(i)=w1(i)
40      continue
      do 41 i=n+1,nmax
        xpp(i)=0.d0
        xww(i)=0.d0
41      continue
c
c Solve the integral-equation by solving a system of algebraic equations:
      call sae(pp, w1, bb, a1, n)
c
c (The substitution for the integration to infinity pp => 1/pp
c is done already.)
      do 50 i=1,n
        zvft(i)=bb(i)
        gg(i) = bb(i)*g0c(pp(i))

```

```

cc          gg(i) = (1.d0 + bb(i))*g0c(pp(i))
cc Urspruenglich anderes (Minus) VZ hier, dafuer kein Minus mehr bei der
cc Definition des WQs ueber Im G, 2.6.1998, tt.
cc          gg(i) = - (1.d0 + bb(i))*g0c(pp(i))
50          continue
c
c
c Normalisation on R:
          const = 8.d0*pi/tmass**2
c
c Proove of the optical theorem for the output values of sae:
c Simply check if sig1 = sig2.
          sig1 = 0.d0
          sig2 = 0.d0
          do 60 i=1,n*2/3
c          write(*,*) 'check! p(',i,') = ',pp(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
              sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i)
cc          u          *(1.d0+kincov*(pp(i)/tmass)**2)
u          *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u          )
          else
              sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i))
          endif
          if (pp(i).lt.dcut.and.kinflg.ne.0) then
              sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              *(1.d0-pp(i)**2/2.d0/tmass**2)
cc          u              *tmass/dsqrt(tmass**2+pp(i)**2)
u              xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              *(1.d0-pp(i)**2/2.d0/tmass**2)
u              /(2.d0*pi**2)*const
          else
              sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              /(2.d0*pi**2)*const
          endif
c          write(*,*) 'xdsdp = ',xdsdp(i)
c          write(*,*) 'zvfct = ',zvfct(i)
60          continue
c '*p**2' because of substitution p => 1/p in the integration of p**2*G(p)
c to infinity
          do 70 i=n*2/3+1,n
c          write(*,*) 'check! p(',i,') = ',pp(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
              sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i)
cc          u          *(1.d0+kincov*(pp(i)/tmass)**2)
u          *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u          )
          else

```

```

        sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i))
    endif
    if (pp(i).lt.dcut.and.kinflg.ne.0) then
        sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u          *tmass/dsqrt(tmass**2+pp(i)**2)
        xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
u          /(2.d0*pi**2)*const
    else
        sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
        xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          /(2.d0*pi**2)*const
    endif
    endif

c
c      write(*,*) 'xdsdp = ',xdsdp(i)
c      write(*,*) 'zvfct = ',zvfct(i)
70      continue
      do 71 i=n+1,nmax
          xdsdp(i)=0.d0
          zvfct(i)=(0.d0,0.d0)
71      continue
c
c
c Normalisation on R:
      sig1 = sig1 / (2.d0*pi**2) * const
      sig2 = sig2 / (2.d0*pi**2) * const
c
c The results from the momentum space approach finally are:
cc Jetzt Minus hier, 2.6.98, tt.
      xim=-sig1
      xdi=sig2
c
      end
c
c
c      complex*16 function g0(p)
c
c      implicit none
c      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi,energy,vzero,eps,
u      p,gtpcor,hmass
      integer npot
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      external gtpcor
      save
      g0=1.d0/cmplx(energy-vzero-p**2/tmass,

```

```

u          tgamma*gtpcor(p,2.d0*tmass+energy),
u          kind=kind(0d0))
      end
c
      complex*16 function g0c(p)
c
      implicit none
      complex*16 hypgeo,green,zk,zi,amd2k,aa,bb,cc,zzp,zzm,
u          hypp,hypm,g0
      real*8
u          tmass,tgamma,zmass,alphas,alamb5,
u          wmass,wgamma,bmass,GFERMI,
u          pi,energy,vzero,eps,
u          p,gtpcor,hmass,
u          kincom,kincoa,kincov,xp,xpmax,dcut
      integer npot,kinflg,gcflg,vflag
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
      common/mom/ xp,xpmax,dcut
      external hypgeo,gtpcor,g0
      save
c
      if (gcflg.eq.0) then
      if (kinflg.eq.0) then
      g0c=g0(p)
      else if (kinflg.eq.1.and.p.lt.dcut) then
      g0c=g0(p)*(1.d0+kincom)+kincoa
      else if (kinflg.eq.1.and.p.ge.dcut) then
      g0c=g0(p)*(1.d0+kincom)
      else if (kinflg.eq.2.and.p.lt.dcut) then
      g0c=g0(p)*(1.d0+kincom)+kincoa
      else if (kinflg.eq.2.and.p.ge.dcut) then
      g0c=g0(p)
      else
      write(*,*) ' kinflg wrong! Stop.'
      stop
      endif
      else if (gcflg.eq.1) then
      zi=(0.d0,1.d0)
      zk=-tmass*cmplx(energy,tgamma
u          *gtpcor(p,2.d0*tmass+energy),
u          kind=kind(0d0))
      zk=sqrt(zk)
      amd2k=4.d0/3.d0*alphas*tmass/2.d0/zk
      aa=(2.d0,0.d0)
      bb=(1.d0,0.d0)
      cc=2.d0-amd2k
      zzp=(1.d0+zi*p/zk)/2.d0
      zzm=(1.d0-zi*p/zk)/2.d0
      if (abs(zzp).gt.20.d0) then
      hypp=(1.d0-zzp)**(-aa)*
u          hypgeo(aa,cc-bb,cc,zzp/(zzp-1.d0))

```



```

c
u      if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
          (npot.eq.5)) then
c
          xp=p
          buf=0.d0
c
          a1=0.d0
          a2=0.d0
          a3=0.d0
          a4=0.d0
          a5=0.d0
          a6=0.d0
          if (gcflg.eq.0) then
              ddcut=xpmax
          else if (gcflg.eq.1) then
              ddcut=dcut
          else
              write(*,*) ' gcflg wrong! Stop.'
              stop
          endif
c
          if (2.d0*xp.lt.ddcut) then
              xb1=xp
              xb2=2.d0*xp
c
c More stable for logarithmically divergent fixed order potentials:
c
              a1=adglg1(fretil1, buf, xb1, eps) !!! FB: can get stuck!
              a2=adglg1(fimtil1, buf, xb1, eps)
c Slightly unstable:
              a3=adglg2(fretil1,xb1,xb2,eps) !!! FB: can get stuck!
c No good:
              a3=adglg1(fretil1,xb1,xb2,eps)
c Not better:
              call adqua(xb1,xb2,fretil1,xerg,eps)
              a3=xerg
c Also not better:
              a1=adglg1(fretil1, buf, xb2, eps)
c
              a4=adglg2(fimtil1,xb1,xb2,eps)
c
              a5 = adglg2(fretil1, xb2, ddcut, eps)
c
              a6 = adglg2(fimtil1, xb2, ddcut, eps)
              a5 = adglg2(fretil2, 1.d0/ddcut, 1.d0/xb2, eps)
              a6 = adglg2(fimtil2, 1.d0/ddcut, 1.d0/xb2, eps)
          else if (xp.lt.ddcut) then
              xb1=xp
              xb2=ddcut
              a1=adglg1(fretil1, buf, xb1, eps)
              a2=adglg1(fimtil1, buf, xb1, eps)
              a3=adglg2(fretil1,xb1,xb2,eps)
              a4=adglg2(fimtil1,xb1,xb2,eps)
          else if (ddcut.le.xp) then
              else

```

```

        write(*,*) ' Constellation not possible! Stop.'
        stop
    endif
c
    a = 1.d0/(4.d0*pi**2)*cmplx(a1+a3+a5,a2+a4+a6,
u                                kind=kind(0d0))
c
    else if (npot.eq.2) then
PCUT=QCUT
ETOT=ENERGY+2*TMASS
        a = ZAPVGP(P,ETOT,VZERO-ENERGY,PCUT,EPS)
c        acomp = zapvq1(ALEFVQ, p, vzero-energy, gtpcor, eps)
c        a = zapvq1(ALEFVQ, p, vzero-energy, gtpcor, eps)
c        acomp = acomp/a
c        if (abs(acomp-1.d0).gt.1.d-3) then
c            write (*,*) 'p=', p
c            write (*,*) 'acomp/a=', acomp
c        endif
        else
            write (*,*) ' Potential not implemented! Stop.'
            stop
        endif
c
    end
c
    real*8 function fretil1(xk)
        implicit none
        real*8 xk, freal
        external freal
        fretil1 = freal(xk)
    end
c
    real*8 function fretil2(xk)
        implicit none
        real*8 xk, freal
        external freal
        fretil2 = freal(1.d0/xk) * xk**(-2)
    end
c
    real*8 function fimtil1(xk)
        implicit none
        real*8 xk, fim
        external fim
        fimtil1 = fim(xk)
    end
c
    real*8 function fimtil2(xk)
        implicit none
        real*8 xk, fim
        external fim
        fimtil2 = fim(1.d0/xk) * xk**(-2)
    end
c
    real*8 function freal(xk)

```



```

        implicit none
        complex*16 vhat
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
        complex*16 g0,g0c
        integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot
        common/mom/ p,pmax,dcut
        external vhat, g0, g0c, gtpcor
c
        freal = real(g0c(xk)*vhat(p, xk)) !!! FB: NaN?
        end
c
        real*8 function fim(xk)
        implicit none
        complex*16 vhat
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
        complex*16 g0,g0c
        integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot
        common/mom/ p,pmax,dcut
        external vhat, g0, g0c, gtpcor
        fim = aimag(g0c(xk)*vhat(p, xk))
        end
c
c
        complex*16 function vhat(p, xk)
c
        implicit none
        complex*16 zi
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p, xk,
u      cnspot, phiint, phfqcd, AD8GLE,
u      pm, xkm, ALPHEF,
u      zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
u      cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,
u      xkpln1st,xkpln2nd,xkpln3rd,
u      pp,pmax,dcut,hmass,chiggs
        integer npot

```

```

parameter(zi=(0.d0,1.d0))
parameter(zeta3=1.20205690316d0,
u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
u      xnf=5.d0)
c
external AD8GLE, phfqcd, ALPHEF
c
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
common/ovalco/ pi, energy, vzero, eps, npot
common/pmaxkm/ pm, xkm
common/mom/ pp,pmax,dcut
common/cplcns/cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
b0=11.d0-2.d0/3.d0*xf
b1=102.d0-38.d0/3.d0*xf
c
a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xf
a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
u      22.d0/3.d0*zeta3)*ca**2-
u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xf-
u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xf+
u      (20.d0/9.d0*tf*xf)**2
c
pm=p
xkm=xk
cnspt=-4.d0/3.d0*4.d0*pi
c
if (p/xk.le.1.d-5.and.p.le.1.d-5) then
xkpln1st=2.d0
xkpln2nd=-4.d0*dlog(scale/xk)
xkpln3rd=-6.d0*dlog(scale/xk)**2
else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
xkpln1st=2.d0*(xk/p)**2
xkpln2nd=-4.d0*(xk/p)**2*dlog(scale/p)
xkpln3rd=-6.d0*(xk/p)**2*dlog(scale/p)**2
else
c      xkpln1st=xk/p*dlog(dabs((p+xk)/(p-xk)))
xkpln1st=xk/p*(dlog(p+xk)-dlog(dabs(p-xk)))
xkpln2nd=xk/p*(-1.d0)*(dlog(scale/(p+xk))**2-
u      dlog(scale/dabs(p-xk))**2)
xkpln3rd=xk/p*(-4.d0/3.d0)*(dlog(scale/(p+xk))**3-
u      dlog(scale/dabs(p-xk))**3)
endif
c
if (npot.eq.2) then
if (p/xk.le.1.d-5.and.p.le.1.d-5) then
vhat = 2.d0 * cnspt * ALPHEF(xk)
else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
vhat = 2.d0 * cnspt * xk**2 / p**2 * ALPHEF(p)
else
phiint = cnspt * (AD8GLE(phfqcd, 0.d0, 0.3d0, 1.d-5)
u      +AD8GLE(phfqcd, 0.3d0, 1.d0, 1.d-5))

```

```

        vhat = xk / p * dlog(dabs((p+xk)/(p-xk))) * phiint
    endif
else
    if (npot.eq.1) then
        c0=1.d0
        c1=0.d0
        c2=0.d0
    else if (npot.eq.3) then
        c0=1.d0+alphas/(4.d0*pi)*a1
        c1=alphas/(4.d0*pi)*b0
        c2=0
    else if (npot.eq.4) then
        c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
        c1=alphas/(4.d0*pi)*b0+
u        (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
        c2=(alphas/(4.d0*pi))**2*b0**2
    else if (npot.eq.5) then
    else
        write(*,*) ' Potential not implemented! Stop.'
        stop
    endif
    phiint=cnspt*alphas
c
c    if ((xk+p).le.dcut) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c            -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c            *(pi*cf*alphas)**2/tmass
c            *xk/p*(p+xk-dabs(xk-p))
c    else if (dabs(xk-p).lt.dcut) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c            -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c            *(pi*cf*alphas)**2/tmass
c            *xk/p*(dcut-dabs(xk-p))
c    else if (dcut.le.dabs(xk-p)) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c    else
c        write(*,*) ' Not possible! Stop.'
c        stop
c    endif
c
c    if (max(xk,p).lt.dcut) then
c Coulomb + first + second order corrections:
        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c All other potentials:
u        +cdeltc*2.d0*xk**2
u        +cdeltl*xk/p/2.d0*(
u            (p+xk)**2*(dlog(((p+xk)/scale)**2)-1.d0)-
u            (p-xk)**2*(dlog(((p-xk)/scale)**2)-1.d0))
u        +cfullc*(p**2+xk**2)*xkpln1st
u        +cfulll*(p**2+xk**2)*xk/p/4.d0*
u            (dlog(((p+xk)/scale)**2)**2-
u            dlog(((p-xk)/scale)**2)**2)
u        +crm2*xk/p*(p+xk-dabs(xk-p))
    else

```

```

        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
    endif
endif
c
    end
c
c
c
c -- Routines needed for use of phenomenological potentials --
c
    SUBROUTINE INIPHC(INIFLG)
    implicit real*8(a-h,o-z)
    save
    COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
    common/ovalco/ pi, energy, vzero, eps, npot
    COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
    CHARACTER QCTCHR,QMTCHR,ALFCHR
    DATA QCUTO/.100d0/,QMT1S/5.0d0/
c
    zmass= 91.187d0
    if(INIFLG.eq.0) then
c
    standard set of parameters
        ilflag= 1
        alphas=.12d0
        qcut= qcut0
        qmat1= qmt1s
    else
c
    Parameters of QCD potential specified by USER
    5   write(*,*) 'QCD coupling at M_z:  ALPHAS  or  LAMBDA  ?'
        write(*,*) 'A/L  :'
        read(*,895) ALFCHR
        if(ALFCHR.eq.'A'.or.ALFCHR.eq.'a') then
            ilflag= 1
            write(*,*) 'alpha_s(M_z)= ?'
            read(*,*) alphas
        elseif(ALFCHR.eq.'L'.or.ALFCHR.eq.'l') then
            write(*,*) 'Lambda(nf=5) =?'
            read(*,*) alamb5
            ilflag= 0
        else
            write(*,*) '!!! PLEASE TYPE: A OR L  !!!'
            goto 5
        endif
    10  write(*,896) qcut0
        read(*,895) QCTCHR
        if(QCTCHR.eq.'Y'.or.QCTCHR.eq.'y') then
            qcut=qcut0
        elseif(QCTCHR.eq.'N'.or.QCTCHR.eq.'n') then
            write(*,*) 'QCUT (GeV) = ?'
            read(*,*) qcut
        else
            write(*,*) '!!! PLEASE TYPE: Y OR N  !!!'
            goto 10

```

```

        endif
15  write(*,902) qmt1s
    read(*,895) QMTCHR
        if(QMTCHR.eq.'Y'.or.QMTCHR.eq.'y') then
            qmat1=qmt1s
        elseif(QMTCHR.eq.'N'.or.QMTCHR.eq.'n') then
            write(*,*) 'QMAT1 (GeV) = ?'
            read(*,*) qmat1
        else
            write(*,*) '!!! PLEASE TYPE: Y OR N !!!'
            goto 15
        endif
    endif
895 format(1A)
896 format(1x,'Long distance cut off for QCD potential'/
    $ 1x,'QCUT = ',f5.4,' GeV. OK ? Y/N')
902 format(1x,
    $ 'Matching QCD for NF=5 and Richardson for NF=3 at QMAT1 =',
    $ f5.2,' GeV.'/1x,' OK ? Y/N')
    end

c
c
    real*8 function phfqcd(x)
c  integrand over k ?
        real*8 pm, xkm, x, ALPHEF
        external ALPHEF
        common/pmaxkm/ pm, xkm
        phfqcd = ALPHEF((pm+xkm)*(dabs(pm-xkm)/(pm+xkm))**x)
    end

c
c
    FUNCTION ALEFVQ(x)
    implicit real*8(a-h,o-z)
    external ALPHEF
    common/xtr101/ p0
    data pi/3.1415926535897930d0/
    q= p0*x
    ALEFVQ= - 4d0/3* 4*pi*ALPHEF(q)
    return
    end

C
C
C
C
    COMPLEX*16 FUNCTION ZAPVGP(P,ETOT,VME,PCUT,ACC)

C
C  A(p,E)= ZAPVGP(P,ETOT,VME,PCUT,ACC)
C  for QCD potential VQGBAR(q) and GAMTPE(P,E) - momentum
C  dependent width of top quark in t-tbar system.
C  2-dimensional integration
C  P - intrinsic momentum of t quark, ETOT - total energy of t-tbar,
C  VME=V0-E, where V0-potential at spatial infinity, E=ETOT-2*TMASS,
C  PCUT - cut off in momentum space; e.g. for QCD potential
C  given by ALPHEF PCUT=QCUT in COMMON/parflg/,

```

```

C      ACC - accuracy
C      external functions: VQGBAR,GAMTPE,ADQUA,AD8GLE,ADGLG1,ADGLG2
C
      IMPLICIT REAL*8(A-Z)
      EXTERNAL FIN01P,FIN02P,FIN03P,FIN04P,AD8GLE,ADGLG1,ADGLG2
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$      WMASS,WGAMMA,BMASS,GFERMI,hmass
      COMMON/XTR102/ PO,E0,VMEM,TM,ACCO
      DATA PI/3.14159265/,BUF/1D-10/,SMALL/1D-2/
C For Testing only
      small = 1.d-1
C
      CONST= -TMASS/(8*PI**2*P)
      TM= TMASS
      ACCO=ACC*SMALL
      PO=P
      E0=ETOT
      VMEM=VME*TMASS
      IF(PCUT.LE.P) THEN
          XXRE=AD8GLE(FIN01P,BUF,PCUT,ACC)+ADGLG1(FIN01P,PCUT,P,ACC)+
$          ADGLG1(FIN02P,BUF,1/P,ACC)
          XXIM=AD8GLE(FIN03P,BUF,PCUT,ACC)+ADGLG1(FIN03P,PCUT,P,ACC)+
$          ADGLG1(FIN04P,BUF,1/P,ACC)
      ELSE
          XXRE=ADGLG1(FIN01P,BUF,P,ACC)+ADGLG2(FIN01P,P,PCUT,ACC)+
$          AD8GLE(FIN02P,BUF,1/PCUT,ACC)
          XXIM=ADGLG1(FIN03P,BUF,P,ACC)+ADGLG2(FIN03P,P,PCUT,ACC)+
$          AD8GLE(FIN04P,BUF,1/PCUT,ACC)
      ENDIF
      ZAPVGP=CONST*CMPLX(XXRE,XXIM,KIND=KIND(0d0))
      END
C
      REAL*8 FUNCTION FIN01P(Q)
C      this segment contains FIN01P,FIN02P,FIN03P,FIN04P
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL VQGBAR,FIN11P, FIN12P
      COMMON/XTR102/ PO,E0,VMEM,TM,ACCO
      DATA PI/3.14159265/,BUF/1d-10/
      Q0=Q
      XL=(PO-Q0)**2
      XU=(PO+Q0)**2
      CALL ADQUA(XL,XU,FIN11P,Y,ACCO)
      FIN01P= VQGBAR(Q0)*Q0*Y
      RETURN
      ENTRY FIN02P(Q)
      Q0=1/Q
      XL=(PO-Q0)**2
      XU=(PO+Q0)**2
      CALL ADQUA(XL,XU,FIN11P,Y,ACCO)
      FIN02P= VQGBAR(Q0)*Q0**3*Y
      RETURN
      ENTRY FIN03P(Q)
      Q0=Q
      XL=(PO-Q0)**2

```

```

XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN12P,Y,ACCO)
FINO3P= VQQBAR(Q0)*Q0*Y
RETURN
ENTRY FINO4P(Q)
Q0=1/Q
XL=(P0-Q0)**2
XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN12P,Y,ACCO)
FINO4P= VQQBAR(Q0)*Q0**3*Y
END
REAL*8 FUNCTION FIN11P(T)
C this segment contains FIN11P,FIN12P
IMPLICIT REAL*8(A-C,D-H,O-Z)
EXTERNAL GAMTPE
COMMON/XTR102/ P0,E0,VMEM,TM,ACCO
T1= T+VMEM
TSQRT= SQRT(T)
GAMMA= TM*GAMTPE(TSQRT,E0)
FIN11P= T1/(T1**2+GAMMA**2)
RETURN
ENTRY FIN12P(T)
T1= T+VMEM
TSQRT= SQRT(T)
GAMMA= TM*GAMTPE(TSQRT,E0)
FIN12P= GAMMA/(T1**2+GAMMA**2)
END
C
C
SUBROUTINE VQDELT(VQ)
C
C evaluates constants multiplying Dirac delta in potentials VQCUT
C calls: ADQUA
C
implicit real*8(a-h,o-z)
external alphef,fncqct
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
data pi/3.141592653589793238D0/
C
call adqua(1d-8,1d4,fncqct,y,1d-4)
v=-4d0/3*2/pi*y
VQ=(-.25-v)*(2*pi)**3
end
C
function fncqct(q)
implicit real*8(a-h,o-z)
fncqct=sin(q)/q*alphef(q)
end
C
C
REAL*8 FUNCTION VQQBAR(P)
C

```

```

C      interquark potential for q- qbar singlet state
C
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL ALPHEF
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      DATA PI/3.14159265/
      VQGBAR = -4D0/3*4*PI*ALPHEF(P)/P**2
      END

C
      FUNCTION ALPHEF(q)

c
c      V(q) = -4/3 * 4*pi*ALPHEF(q)/q**2
c      input: alphas or alamb5 in COMMON/PHCONS/. If:
c      ILFLAG.EQ.0   alamb5= \Lambda_{\bar{MS}}^{(5)} at M_z
c      ILFLAG.EQ.1   alphas = alpha_{strong} at M_z (91.161)
c
c      effective coupling ALPHEF is defined as follows:
c      for q > qmat1=m_b:
c          alphas*( 1 +(31/3-10*nf/9)*alphas/(4*pi) )
c          where alphas=\alpha_{\bar{MS}} for nf=5, i.e.
c          alpha=4*pi/( b0(nf=5)*x + b1(5)/b0(5)*ln(x) )
c          and x = ln(q**2/alamb5**2)
c      for qmat1 > q > qcut:
c          4*pi/b0(nf=3)*(alfmt+1/log(1+q**2/alr**2))
c          where alr=.4 GeV, nefr=3, and continuity -> alfmt
c      below qcut: alphrc*2*q**2/(q**2+qcut**2) (cont.->alphrc)
c
      implicit real*8(a-h,o-z)
      SAVE
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
      common/parpot/ a5,b5,c5,alfmt,d,alphrc
      data pi/3.141592653589793238D0/,
$ zold/-1d0/,qctold/-1d0/,alfold/-1d0/,
$ olmbd/-1d0/

c
      if(zmass.le.0d0 .or. qcut.le.0d0) STOP 10001
      if(zold.ne.zmass .or. qcut.ne.qctold) num=0
      if(ilflag.eq.0 .and. olmbd.ne.alamb5) num=0
      if(ilflag.eq.1 .and. alfold.ne.alphas) num=0
      if(num.eq.0)then
          num=num+1
          zold=zmass
          qctold=qcut
          call potpar
          alfold= alphas
          olmbd= alamb5
      endif
      if(q.le.qcut) then
          alphef=alphrc*(2*q**2)/(qcut**2+q**2)
      elseif(q.le.qmat1) then
          alphef=alfmt+d/log(1+q**2/alr**2)

```



```

        else
            x=2*log(q/alamb5)
            alfas5=1/(a5*x+b5*log(x))
            alphef=alfas5*(1+c5*alfas5)
        endif
    end

c
c Only called by ALPHEF:
    SUBROUTINE POTPAR
        implicit real*8(a-h,o-z)
        COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
        common/parpot/ a5,b5,c5,alfmt,d,alphrc
        data pi/3.141592653589793238D0/,nefr/3/
        b0(nf)=11-2./3*nf
        b1(nf)=102-38./3*nf
        cn(nf)=31./3-10./9*nf
        alr=400d-3
        a5=b0(5)/(4*pi)
        b5=b1(5)/b0(5)/(4*pi)
        c5=cn(5)/(4*pi)
        d=4*pi/b0(nefr)
        if(ilflag.eq.0) then
            if(alamb5.le.0d0) STOP 10002
            xa=2*log(zmass/alamb5)
            alphas= 1/(a5*xa + b5*log(xa))
        else
            if(alphas.le.0d0) STOP 10003
            t0=0
            t1=max(1d0,alphas*a5)
10      tm=(t0+t1)/2
            fm=tm/alphas+b5*tm*log(tm)-a5
            if(fm.lt.-1d-10) then
                t0=tm
                goto 10
            elseif(fm.gt.1d-10) then
                t1=tm
                goto 10
            endif
            alamb5=zmass*exp(-5d-1/tm)
        endif
        x=2*log(qmat1/alamb5)
        alfas=1/(a5*x+b5*log(x))
        alfmt=alfas*(1+c5*alfas)-d/log(1+qmat1**2/alr**2)
        alphrc=alfmt+ d/log(1+qcut**2/alr**2)
        return
    end

c
c -- End of routines for phenomenological potentials --
c
c
c -- Routines for Gamma_top --
C

```

```

SUBROUTINE GAMMAT
C
C   on shell width of top quark including QCD corrections, c.f.
C   M.Jezabek and J.H. Kuhn, Nucl. Phys. B314(1989)1
C
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL DILOGG
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      DATA PI/3.14159265/
      F(X)= PI**2+2*DILOGG(X)-2*DILOGG(1-X)+( 4*X*(1-X-2*X**2)*LOG(X)+
$ 2*(1-X)**2*(5+4*X)*LOG(1-X) - (1-X)*(5+9*X-6*X**2) ) /
$ (2*(1-X)**2*(1+2*X))
      Y= (WMASS/TMASS)**2
cc alpha_s(M_t) corresponding to alpha_s(M_Z)=0.118:
cc   alphas=0.107443d0
cc   write(*,*) 'alphas=',alphas
c Usage of alpha_s as given as input for the potential.. better use
c alpha_s at a scale close to m_t..
      TGAMMA= GFERMI*TMASS**3/(8*SQRT(2D0)*PI)*(1-Y)**2*(1+2*Y)*
$ (1- 2D0/3*ALPHAS/PI*F(Y))
      END

C
C
      REAL*8 FUNCTION GAMTPE(P,ETOT)

C
C   momentum dependent width of top quark in t-tbar system
C   GAMTPE = TGAMMA*GTPCOR(P,E), where TGAMMA includes
C   QCD corrections, see JKT, eq.(8), and
C   GTPCOR - correction factor for bound t quark
C
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL GTPCOR
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      GAMTPE= TGAMMA*GTPCOR(P,ETOT)
      END

C
C
C   GTPCOR and GTPCOR1 should be merged (M.J.) !!!!
C
      real*8 function gtpcor(topp,etot)
      real*8 topp,etot,
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,hmass
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      if (topp.ge.tmass/2.d0) then
c      gtpcor1=0.001d0
c      else
c      gtpcor=1.d0
c      endif
c      end
c

```

```

c
c Correction function for non-constant (energy and momentum dependent) width:
  FUNCTION GTPCOR1(TOPP,ETOT)
c
c   TOPP - momentum of t quark = - momentum of tbar
c   ETOT - total energy of t-tbar system
c   calls: GENWDS, RAN2
c
c   Evaluates a correction factor to the width of t-tbar system.
c   in future has to be replaced by a function evaluating
c   width including radiative corrections and GTPCOR.
c   I include two factors reducing the width:
c   a - time dilatation: for decay in flight lifetime
c       increased accordingly to relativistic kinematics
c   b - overall energy-momentum conservation: I assume that
c       t and tbar decay in flight and in this decays energies
c       of Ws follow from 2-body kinematics. Then I calculate
c       effective mass squared of b-bar system (it may be
c       negative!) from en-momentum conservation.
c       If effective mass is < 2*Mb + 2 GeV configuration
c       is rejected. The weight is acceptance.
c
  IMPLICIT REAL*8(A-H,O-Z)
  real ran2
  external ran2
  PARAMETER(NG=20,NC=4)
  dimension gamma(0:NG),pw1(0:3),pw2(0:3),AIJ(NC,NC),BJ(NC),
$AI(NC),SIG2IN(0:NG),XIK(0:NG,NC),INDX(NC)
  COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
  SAVE NUM,EOLD,TOLD,AI
  data nevent/10000/, num/0/, eold/-1d5/, told/-1d0/

c
C   for test runs!!
C   nevent=1000
C
  if(etot.ne.eold) num=0
  if(tmass.ne.told) num=0
5  if(num.eq.0) then
c
c       xdumm= ran2(-2)
c       do 10 itp=0,NG
c       tp=itp*tmass/NG*2
c       gamma(itp)=0
c       do 10 ix=1,nevent
c       call GENWDS(tp,etot,pw1,pw2,efmsq)
c       if(efmsq.gt.0d0) then
c       efms=sqrt(efmsq)
c       if(efms.ge. 2*bmass+2) gamma(itp)=gamma(itp)+1
c       endif
10      continue
c       do 15 ix=0,NG
15      SIG2IN(IX)= MAX(1D0,GAMMA(IX))
c       DO 17 JX=1,NC
c       IF(JX.EQ.1)THEN

```

```

        XIK(0,JX)= .5D0
      ELSE
        XIK(0,JX)= 0D0
      ENDIF
      DO 17 IX=1,NG
        tp= 2D0*ix/NG
17      XIK(IX,JX)= tp**(JX-1)/(1+EXP(tp*3))
        DO 20 I=1,NC
          BJ(I)=0
          DO 20 J=1,NC
20          AIJ(I,J)=0
            DO 30 I=1,NC
              DO 25 IX=0,NG
25              BJ(I)= BJ(I)+GAMMA(IX)*XIK(IX,I)*SIG2IN(IX)
                DO 30 J=1,I
                  DO 30 IX=0,NG
30                  AIJ(I,J)= AIJ(I,J)+XIK(IX,I)*XIK(IX,J)*SIG2IN(IX)
                    DO 35 I=1,NC
                      DO 35 J=I,NC
35                      AIJ(I,J)= AIJ(J,I)
                        CALL LUDCMP(AIJ,NC,NC,INDX,D)
                        CALL LUBKSB(AIJ,NC,NC,INDX,BJ)
                        DO 40 I=1,NC
70                      AI(I)= BJ(I)/NEVENT
                          do 42 i=1,nc
42                          write(*,*)'a(',i,')=',ai(i)
                            do 100 ix=0,NG
100                            gamma(ix)= gamma(ix)/nevent
                              eold=etot
                              told=tmass
                              num= 1
                            endif
                          SUM=AI(1)
                          DO 110 I=2,NC
110                          SUM= SUM+AI(I)*(TOPP/TMASS)**(I-1)
C                          CORRF2= SUM/(1+ EXP(TOPP/TMASS*3))
C                          CORRF2= SUM/(1+ EXP(MIN(1d1,TOPP/TMASS*3)))
C                          if(topp.gt. 2d0*tmass) then
C                            corrf1= 0.001d0
C                          else
C                            ip= NG*topp/tmass/2
C                            corrf1= gamma(ip)
C                          endif
C                          write(*,*)'ratio=',corrf1/corrf2
C                          GTPCOR1 = CORRF2
C                          GTPCOR1 = CORRF2*SQRT(1-TOPP**2/(TOPP**2+TMASS**2))
C                          END
C
C Generator: only called by GTPCOR1
      SUBROUTINE GENWDS(tp,etot,pw1,pw2,efm2)
C
C   generates 4-momenta of W's and effective mass of b-bbar
C   from t and tbar quarks decays at flight (tp = momentum of t
C   = - momentum of tbar (in GeV) ) in Oz direction

```

```

c      implicit real*8(a-h,o-z)
c      real ran2
c      real ranf
c      external ran2
c      external ranf
c      dimension pw1(0:3),pw2(0:3)
c      save
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      data PI/3.141592653589793238D0/
c      real idum
c 3      s1= wmass**2+wmass*wgamma*TAN((2*ran2(idum)-1)*pi/2)
3      s1= wmass**2+wmass*wgamma*TAN((2*ranf(idum)-1)*pi/2)
c      if(s1.le.0d0) goto 3
c      wmass1= sqrt(s1)
c      if(abs(wmass1-wmass).ge.3*wgamma) goto 3
c 4      s2= wmass**2+wmass*wgamma*TAN((2*ran2(idum)-1)*pi/2)
4      s2= wmass**2+wmass*wgamma*TAN((2*ranf(idum)-1)*pi/2)
c      if(s2.le.0d0) goto 4
c      wmass2= sqrt(s2)
c      if(abs(wmass2-wmass).ge.3*wgamma) goto 4
c      ew1= (tmass**2+wmass1**2-bmass**2)/(2*tmass)
c      pwt1= sqrt(ew1**2-wmass1**2)
c      ew2= (tmass**2+wmass2**2-bmass**2)/(2*tmass)
c      pwt2= sqrt(ew2**2-wmass2**2)
c 5      p=tp
c      u1= 2*ran2(idum)-1
c      u1= 2*ranf(idum)-1
c      pw1z= pwt1*u1
c      u2= 2*ran2(idum)-1
c      u2= 2*ranf(idum)-1
c      pw2z= pwt2*u2
c      et= sqrt(tmass**2+p**2)
c      bet= p/et
c      gam= et/tmass
c      pw1(0)= gam*(ew1+bet*pw1z)
c      pw1(3)= gam*(pw1z+bet*ew1)
c      pw2(0)= gam*(ew2-bet*pw2z)
c      pw2(3)= gam*(pw2z-bet*ew2)
c      pw1tr= sqrt(pw1(0)**2-pw1(3)**2-wmass1**2)
c      pw2tr= sqrt(pw2(0)**2-pw2(3)**2-wmass2**2)
c      phi1= 2*pi*ran2(idum)
c      phi1= 2*pi*ranf(idum)
c      phi2= 2*pi*ran2(idum)
c      phi2= 2*pi*ranf(idum)
c      pw1(1)= pw1tr*cos(phi1)
c      pw1(2)= pw1tr*sin(phi1)
c      pw2(1)= pw2tr*cos(phi2)
c      pw2(2)= pw2tr*sin(phi2)
c      prec2= (pw1(1)+pw2(1))**2+(pw1(2)+pw2(2))**2+(pw1(3)+pw2(3))**2
c      erest=etot-pw1(0)-pw2(0)
c      efm2= erest*abs(erest)-prec2

```

```

      END
c
c -- End of routines for Gamma_top --
c
c -- Routines for solving linear equations and matrix inversion (complex) --
c
      subroutine sae(pp, w1, bb, a1, n)
c
      implicit none
      complex*16 vhat
      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      d, pp, w1, gtpcor,hmass,
u      xp,xpmax,dcut,kincom,kincoa,kincov
      complex*16 a, a1, bb, ff, cw, svw, g0, g0c
      integer i, j, npot, n, nmax, indx,kinflg,gcflg,vflag
      parameter (nmax=900)
      dimension bb(nmax), ff(nmax,nmax), pp(nmax), w1(nmax),
u      indx(nmax), cw(nmax), a1(nmax)
c
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/mom/ xp,xpmax,dcut
      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
      external a, vhat, gtpcor, g0, g0c
c
      do 10 i=1,n*2/3
        cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i))
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),
c      u      kind=kind(0d0))-pp(i)**2/tmass))
10      continue
      do 20 i=n*2/3+1,n
        cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i)) * pp(i)**2
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),
c      u      kind=kind(0d0)) /
c      u      pp(i)**2 - 1.d0/tmass))
20      continue
c
      do 30 i=1,n
cc      bb(i) = a1(i)
cvv
      if (pp(i).lt.dcut.and.vflag.eq.1) then
c      bb(i) = cmplx(1.d0+kincov*(pp(i)/tmass)**2,0.d0,
c      u      kind=kind(0d0))
u      bb(i)=1.d0+kincov*
u      g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i))

```

```

        else
            bb(i) = (1.d0,0.d0)
        endif
        svw = (0.d0,0.d0)
        do 40 j=1,n
            if (i.ne.j) then
                ff(i,j) = - vhat(pp(i),pp(j)) * cw(j)
                svw = svw + ff(i,j)
            endif
40          continue
            ff(i,i) = 1.d0 - a1(i) - svw
30          continue
c
            call zldcmp(ff, n, nmax, indx, d)
            call zlbksb(ff, n, nmax, indx, bb)
c
        end
c
c
c
        SUBROUTINE ZLBKSB(A,N,NP,INDX,B)
C complex version of lubksb
        IMPLICIT NONE
        INTEGER I, II, INDX, J, LL, N, NP
        COMPLEX*16 A, B, SUM
        DIMENSION A(NP,NP),INDX(N),B(N)
        II=0
        DO 12 I=1,N
            LL=INDX(I)
            SUM=B(LL)
            B(LL)=B(I)
            IF (II.NE.0)THEN
                DO 11 J=II,I-1
                    SUM=SUM-A(I,J)*B(J)
11              CONTINUE
                ELSE IF (SUM.NE.(0.DO,0.DO)) THEN
                    II=I
                ENDIF
            B(I)=SUM
12          CONTINUE
        DO 14 I=N,1,-1
            SUM=B(I)
            IF(I.LT.N)THEN
                DO 13 J=I+1,N
                    SUM=SUM-A(I,J)*B(J)
13              CONTINUE
                ENDIF
            B(I)=SUM/A(I,I)
14          CONTINUE
        RETURN
        END
c
        SUBROUTINE ZLDCMP(A,N,NP,INDX,D)
C complex version of ludcmp
        IMPLICIT NONE

```

```

      INTEGER I, IMAX, INDX, J, K, N, NP, NMAX
      REAL*8 AAMAX, D, TINY, VV
      COMPLEX*16 A, DUM, SUM
      PARAMETER (NMAX=900)
      DIMENSION A(NP,NP), INDX(N), VV(NMAX)

c
      tiny=1.d-5
c
      D=1.DO
      DO 12 I=1,N
        AAMAX=0.DO
        DO 11 J=1,N
          IF (ABS(A(I,J)).GT.AAMAX) AAMAX=ABS(A(I,J))
11      CONTINUE
c      IF (AAMAX.EQ.0.DO) PAUSE 'Singular matrix.'
      IF (AAMAX.EQ.0.DO) print *, "Singular matrix."
      VV(I)=1.DO/AAMAX
12      CONTINUE
      DO 19 J=1,N
        IF (J.GT.1) THEN
          DO 14 I=1,J-1
            SUM=A(I,J)
            IF (I.GT.1) THEN
              DO 13 K=1,I-1
                SUM=SUM-A(I,K)*A(K,J)
13          CONTINUE
              A(I,J)=SUM
            ENDIF
14          CONTINUE
        ENDIF
        AAMAX=0.DO
        DO 16 I=J,N
          SUM=A(I,J)
          IF (J.GT.1) THEN
            DO 15 K=1,J-1
              SUM=SUM-A(I,K)*A(K,J)
15          CONTINUE
              A(I,J)=SUM
            ENDIF
            DUM=VV(I)*ABS(SUM)
            IF (ABS(DUM).GE.AAMAX) THEN
              IMAX=I
              AAMAX=DUM
            ENDIF
16          CONTINUE
          IF (J.NE.IMAX) THEN
            DO 17 K=1,N
              DUM=A(IMAX,K)
              A(IMAX,K)=A(J,K)
              A(J,K)=DUM
17          CONTINUE
            D=-D
            VV(IMAX)=VV(J)
          ENDIF

```



```

      INDX(J)=IMAX
      IF (J.NE.N) THEN
        IF (A(J,J).EQ.(0.D0,0.D0)) A(J,J)=cplx(TINY, 0.d0,
u          kind=kind(0d0))
        DUM=1.D0/A(J,J)
        DO 18 I=J+1,N
          A(I,J)=A(I,J)*DUM
18      CONTINUE
        ENDIF
19      CONTINUE
        IF(A(N,N).EQ.(0.D0,0.D0)) A(N,N)=cplx(TINY, 0.d0,
u          kind=kind(0d0))
        RETURN
      END
C
C
C *** TOOLS ***
C
C
C ***** ROUTINES FOR GAUSSIAN INTEGRATIONS
C
C
C      SUBROUTINE GAULEG(X1,X2,X,W,N)
C
C      Given the lower and upper limits of integration X1 and X2
C      and given N, this routine returns arrays X(N) and W(N)
C      containing the abscissas and weights of the Gauss-Legendre
C      N-point quadrature formula
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      REAL*8 X1,X2,X(N),W(N)
C      PARAMETER (EPS=3.D-14)
C      save
C      M=(N+1)/2
C      XM=0.5D0*(X2+X1)
C      XL=0.5D0*(X2-X1)
C      DO 12 I=1,M
C        Z=DCOS(3.141592653589793238D0*(I-.25D0)/(N+.5D0))
1      CONTINUE
        P1=1.D0
        P2=0.D0
        DO 11 J=1,N
          P3=P2
          P2=P1
          P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
11      CONTINUE
        PP=N*(Z*P1-P2)/(Z*Z-1.D0)
        Z1=Z
        Z=Z1-P1/PP
        IF(DABS(Z-Z1).GT.EPS)GO TO 1
        X(I)=XM-XL*Z
        X(N+1-I)=XM+XL*Z
        W(I)=2.D0*XL/((1.D0-Z*Z)*PP*PP)
        W(N+1-I)=W(I)

```

```

12  CONTINUE
    RETURN
    END

C
C
    DOUBLE PRECISION FUNCTION AD8GLE(F,A,B,EPS)
    implicit double precision (a-h,o-z)
    EXTERNAL F
    DIMENSION W(12),X(12)
c    SAVE W, X
    SAVE

C
C *****
C
C    ADAPTIVE GAUSSIAN QUADRATURE.
C
C    AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C    THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C    EPS.
C
C *****
C
    DATA W / 0.10122 85362 90376 25915 25313 543D0,
$           0.22238 10344 53374 47054 43559 944D0,
$           0.31370 66458 77887 28733 79622 020D0,
$           0.36268 37833 78361 98296 51504 493D0,
$           0.27152 45941 17540 94851 78057 246D-1,
$           0.62253 52393 86478 92862 84383 699D-1,
$           0.95158 51168 24927 84809 92510 760D-1,
$           0.12462 89712 55533 87205 24762 822D0,
$           0.14959 59888 16576 73208 15017 305D0,
$           0.16915 65193 95002 53818 93120 790D0,
$           0.18260 34150 44923 58886 67636 680D0,
$           0.18945 06104 55068 49628 53967 232D0/

C
    DATA X / 0.96028 98564 97536 23168 35608 686D0,
$           0.79666 64774 13626 73959 15539 365D0,
$           0.52553 24099 16328 98581 77390 492D0,
$           0.18343 46424 95649 80493 94761 424D0,
$           0.98940 09349 91649 93259 61541 735D0,
$           0.94457 50230 73232 57607 79884 155D0,
$           0.86563 12023 87831 74388 04678 977D0,
$           0.75540 44083 55003 03389 51011 948D0,
$           0.61787 62444 02643 74844 66717 640D0,
$           0.45801 67776 57227 38634 24194 430D0,
$           0.28160 35507 79258 91323 04605 015D0,
$           0.95012 50983 76374 40185 31933 543D-1/

C
C *****
C
    GAUSS=0.0D0
    AD8GLE=GAUSS
    IF(B.EQ.A) RETURN
    CONST=EPS/(B-A)

```

```

      BB=A
C
C  COMPUTATIONAL LOOP.
  1  AA=BB
      BB=B
  2  C1=0.5D0*(BB+AA)
      C2=0.5D0*(BB-AA)
      S8=0.0D0
      DO 3 I=1,4
          U=C2*X(I)
          S8=S8+W(I)*(F(C1+U)+F(C1-U))
  3  CONTINUE
      S8=C2*S8
      S16=0.0D0
      DO 4 I=5,12
          U=C2*X(I)
          S16=S16+W(I)*(F(C1+U)+F(C1-U))
  4  CONTINUE
      S16=C2*S16
      IF( ABS(S16-S8) .LE. EPS*(abs(s8)+ABS(S16))*0.5D0 ) GO TO 5
      BB=C1
      IF( 1.D0+ABS(CONST*C2) .NE. 1.D0) GO TO 2
      AD8GLE=0.0D0
      write(*,*)'too high accuracy required in function ad8gle!'
      RETURN
  5  GAUSS=GAUSS+S16
      IF(BB.NE.B) GO TO 1
      AD8GLE=GAUSS
      RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION ADGLG1(F,A,B,EPS)
      IMPLICIT REAL*8 (A-H,O-Z)
      EXTERNAL F,AD8GLE,adqua
      DIMENSION W(6),X(6),xx(6)
c      SAVE W, XX, NUM
      SAVE
C
C  *****
C
C  ADAPTIVE GAUSSIAN QUADRATURE.
C  For x->b   f(x) = 0 (ln^k (b-x) )
C  A - lower limit, B - upper limit (integrable singularity)
C  AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C  THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C  EPS.
C
C  *****
C
      DATA W / 4.58964 673950d-1,
$           4.17000 830772d-1,
$           1.13373 382074d-1,
$           1.03991 974531d-2,
$           2.61017 202815d-4,

```

```

$          8.98547 906430d-7/
C
  DATA X / 0.22284 66041 79d0,
$          1.18893 21016 73d0,
$          2.99273 63260 59d0,
$          5.77514 35691 05d0,
$          9.83746 74183 83d0,
$          15.98287 39806 02d0/
  DATA NUM/0/
  IF(NUM.eq.0d0) then
do 1 ix=1,6
1  xx(ix)= EXP(-x(ix))
  ENDIF
  num=num+1
  sum=0d0
  c=b-a
  sum6=0d0
do 10 in=1,6
10  sum6= sum6+ w(in)*f(b-c*xx(in))
  sum6=sum6*c
  a1=a
15  a2= (a1+b)/2
  c=b-a2
  sumn=0d0
do 20 in=1,6
  !!! FB: catch NaN
  if ( c/b .lt. 1d-9 ) then
    adglg1 = 1d15
    return
  endif
20  sumn= sumn+ w(in)*f(b-c*xx(in)) !!! FB: f(b) = NaN !
  sumn=sumn*c
ctt
c    call adqua(a1,a2,f,sum1,eps)
c    sum1=sum1+sum
  sum1=AD8GLE(F,A1,A2,eps)+sum
  IF(ABS( (sum+sum6)/(sum1+sumn)-1d0 ).lt.EPS) THEN
ctt
c    call adqua(a,a2,f,sum2,eps)
  sum2=AD8GLE(F,A,A2,eps)
  IF(ABS( (sum2+sumn)/(sum1+sumn)-1d0 ).gt.EPS) THEN
    sum=sum2
    a1=a2
    sum6=sumn
    goto 15
  ENDIF
  ADGLG1= SUM1+SUMN
  RETURN
ELSE
  sum=sum1
  a1=a2
  sum6=sumn
  goto 15
ENDIF

```

```

      END
C
      DOUBLE PRECISION FUNCTION ADGLG2(F,A,B,EPS)
      IMPLICIT REAL*8 (A-H,O-Z)
      EXTERNAL F,AD8GLE
      DIMENSION W(6),X(6),xx(6)
C      SAVE W,XX,NUM
      SAVE
C
C      *****
C
C      ADAPTIVE GAUSSIAN QUADRATURE.
C      For x->A   f(x) = 0 (lnk (x-a) )
C      A - lower limit (integrable singularity), B - upper limit
C      AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C      THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C      EPS.
C
C      *****
      DATA W / 4.58964 673950d-1,
$           4.17000 830772d-1,
$           1.13373 382074d-1,
$           1.03991 974531d-2,
$           2.61017 202815d-4,
$           8.98547 906430d-7/
C
      DATA X / 0.22284 66041 79d0,
$           1.18893 21016 73d0,
$           2.99273 63260 59d0,
$           5.77514 35691 05d0,
$           9.83746 74183 83d0,
$           15.98287 39806 02d0/
      DATA NUM/0/
      IF(NUM.eq.0d0) then
        do 1 ix=1,6
1      xx(ix)= EXP(-x(ix))
        ENDIF
        num=num+1
        sum=0d0
        c=b-a
        sum6=0d0
        do 10 in=1,6
10      sum6= sum6+ w(in)*f(A+c*xx(in))
        sum6=sum6*c
        b1=b
15      b2= (a+b1)/2
        c=b2-a
        sumn=0d0
        do 20 in=1,6
          !!! FB: catch NaN
          if ( c/a .lt. 1d-9 ) then
            adglg2 = 1d15
            return
          endif
20

```

```

20  sumn= sumn+ w(in)*f(a+c*xx(in)) !!! FB: f(a) = NaN !
    sumn=sumn*c
    sum1=AD8GLE(F,b2,b1,eps)+sum
    IF(ABS( (sum+sum6)/(sum1+sumn)-1d0 ).lt.EPS) THEN
        sum2=AD8GLE(F,b2,b,eps)
        IF(ABS( (sum2+sumn)/(sum1+sumn)-1d0 ).gt.EPS) THEN
            sum=sum2
            b1=b2
            sum6=sumn
            goto 15
        ENDIF
        ADGLG2= SUM1+SUMN
        RETURN
    ELSE
        sum=sum1
        b1=b2
        sum6=sumn
        goto 15
    ENDIF
END
C
C
C-----
C INTEGRATION ROUTINE ADQUA written by M. Jezabek      ---
C-----
C
    SUBROUTINE ADQUA(XL,XU,F,Y,ACC)
C
C    ADAPTIVE GAUSS-LEGENDRE + SIMPSON'S RULE QUADRATURE
C    XL - LOWER LIMIT, XU - UPPER LIMIT, F - FUNCTION TO INTEGRATE
C    Y - INTEGRAL
C    ACC - ACCURACY (IF .LE. 0. ACC=1.D-6)
C    ***** new constants, 1 error removed, Oct '92
C
C    CALLS: SIMPSA
C
C    PARAMETERS: NSUB > NO OF SUBDIVISION LEVELS IN GAUSS INTEGRATION
C                100*2**IMAX > NO OF POINTS IN SIMPSON INTEGRATION
C
    IMPLICIT REAL*8 (A-H,O-Z)
    EXTERNAL F
    DIMENSION VAL(25,2), BOUND(25,2,2), LEV(25),SING(25,3)
    DIMENSION W8(4),X8(4)
    DATA W8
    $/0.101228536290376D0, 0.222381034453374D0, 0.313706645877887D0,
    $ 0.362683783378362D0/
    DATA X8
    $/0.960289856497536D0, 0.796666477413627D0, 0.525532409916329D0,
    $ 0.183434642495650D0/
    save
C
    IF(ACC.LE.0.D0) ACC=1.D-6
    NSUB=24
    NSG=25

```

```

NSC=0
A=XL
B=XU
C1=0.5d0*(A+B)
C2=C1-A
S8=0d0
DO 1 I=1,4
U=X8(I)*C2
1 S8=S8+W8(I)*(F(C1+U)+F(C1-U))
S8=S8*C2
XM=(XL+XU)/2.d0
BOUND(1,1,1)=XL
BOUND(1,1,2)=XM
BOUND(1,2,1)=XM
BOUND(1,2,2)=XU
NC=1
DO 3 IX=1,2
A=BOUND(NC,IX,1)
B=BOUND(NC,IX,2)
C1=0.5d0*(A+B)
C2=C1-A
VAL(NC,IX)=0.d0
DO 2 I=1,4
U=X8(I)*C2
2 VAL(NC,IX)=VAL(NC,IX)+W8(I)*(F(C1+U)+F(C1-U))
3 VAL(NC,IX)=VAL(NC,IX)*C2
S16=VAL(NC,1)+VAL(NC,2)
IF(DABS(S8-S16).GT.ACC*DABS(S16)) GOTO 4
Y=S16
RETURN
4 DO 5 I=1,NSUB
5 LEV(I)=0
NC1= NC+1
11 XM=(BOUND(NC,1,1)+BOUND(NC,1,2))/2.d0
BOUND(NC1,1,1)=BOUND(NC,1,1)
BOUND(NC1,1,2)=XM
BOUND(NC1,2,1)=XM
BOUND(NC1,2,2)=BOUND(NC,1,2)
DO 13 IX=1,2
A=BOUND(NC1,IX,1)
B=BOUND(NC1,IX,2)
C1=0.5d0*(A+B)
C2=C1-A
VAL(NC1,IX)=0.d0
DO 12 I=1,4
U=X8(I)*C2
12 VAL(NC1,IX)=VAL(NC1,IX)+W8(I)*(F(C1+U)+F(C1-U))
13 VAL(NC1,IX)=VAL(NC1,IX)*C2
S16=VAL(NC1,1)+VAL(NC1,2)
S8=VAL(NC,1)
IF(DABS(S8-S16).LE.ACC*DABS(S16)) GOTO 20
NC=NC1
NC1= NC+1
IF(NC1.LE.NSUB) GOTO 11

```

```

C      NC=NSUB   USE SIMPSON'S RULE
      NSC=NSC+1
      IF(NSC.LE.NSG) GOTO 15
      WRITE(*,911)
911  FORMAT(1X,'ADQUA: TOO MANY SINGULARITIES')
      STOP
15  SING(NSC,1)=BOUND(NC,1,1)
      SING(NSC,2)=BOUND(NC,2,2)
      SING(NSC,3)=S16
      S16=0.d0
      NC=NC-1
20  VAL(NC,1)= S16
121 LEV(NC)=1
21  XM=(BOUND(NC,2,1)+BOUND(NC,2,2))/2.d0
      BOUND(NC1,1,1)=BOUND(NC,2,1)
      BOUND(NC1,1,2)=XM
      BOUND(NC1,2,1)=XM
      BOUND(NC1,2,2)=BOUND(NC,2,2)
      DO 23 IX=1,2
      A=BOUND(NC1,IX,1)
      B=BOUND(NC1,IX,2)
      C1=0.5d0*(A+B)
      C2=C1-A
      VAL(NC1,IX)=0.d0
      DO 22 I=1,4
      U=X8(I)*C2
22  VAL(NC1,IX)=VAL(NC1,IX)+W8(I)*(F(C1+U)+F(C1-U))
23  VAL(NC1,IX)=VAL(NC1,IX)*C2
      S16=VAL(NC1,1)+VAL(NC1,2)
      S8=VAL(NC,2)
      IF(DABS(S8-S16).LE.ACC*DABS(S16)) GOTO 40
      NC=NC+1
      NC1=NC+1
      IF(NC1.LE.NSUB) GOTO 11
C      NC=NSUB   USE SIMPSON'S RULE
      NSC=NSC+1
      IF(NSC.LE.NSG) GOTO 35
      WRITE(*,911)
      STOP
35  SING(NSC,1)=BOUND(NC,1,1)
      SING(NSC,2)=BOUND(NC,2,2)
      SING(NSC,3)=S16
      S16=0.d0
      NC=NC-1
40  VAL(NC,2)= S16
45  IF(NC.GT.1) GOTO 50
      Y1=VAL(1,1)+VAL(1,2)
      GOTO 100
50  NC0=NC-1
      IF(LEV(NC0).EQ.0) IX=1
      IF(LEV(NC0).EQ.1) IX=2
      LEV(NC)=0
      NC1=NC
      VAL(NC0,IX)=VAL(NC,1)+VAL(NC,2)

```



```

        NC=NC0
        IF(IX.EQ.1) GOTO 121
        GOTO 45
100 CONTINUE
        IF(NSC.GT.0) GOTO 101
        Y=Y1
        RETURN
101 FSUM=0.d0
        DO 102 IK=1,NSC
102 FSUM=FSUM+DABS(SING(IK,3))
        ACCR=ACC*DMAX1(FSUM,DABS(Y1))/FSUM/10.d0
        DO 104 IK=1,NSC
104 CALL SIMPSA(SING(IK,1),SING(IK,2),F,SING(IK,3),ACCR)
        DO 106 IK=1,NSC
106 Y1=Y1+SING(IK,3)
        Y=Y1
        RETURN
        END
C
        SUBROUTINE SIMPSA(A,B,F,F0,ACC)
C
        SIMPSON'S ADAPTIVE QUADRATURE
        IMPLICIT REAL*8 (A-H,O-Z)
        save
        EXTERNAL F
        IMAX=5
        NO=100
        H=(B-A)/NO
        NO2=NO/2
        S2=0.d0
        IC=1
        S0=F(A)+F(B)
        DO 5 K=1,NO2
5 S2=S2+F(A+2.d0*K*H)
        DO 7 S1=0.d0
        DO 10 K=1,NO2
10 S1=S1+F(A+(2.d0*K-1.d0)*H)
        Y=H/3.d0*(S0+4.d0*S1+2.d0*S2)
        IF(DABS(F0/Y-1.d0).GT.ACC) GOTO 20
        RETURN
20 NO2=NO
        NO=2*NO
        S2=S1+S2
        H=H/2.d0
        IF(IC.GT.IMAX) GOTO 30
        F0=Y
        IC=IC+1
        GOTO 7
30 ACCO=DABS(Y/F0-1.d0)
        WRITE(*,900) A,B,ACCO
        STOP
900 FORMAT(1H , 'SIMPSA: TOO HIGH ACCURACY REQUIRED' /
/1X, 29HSINGULARITY IN THE INTERVAL ,D20.12,1X,D20.12/
/1X, 29HACCURACY ACHIEVED ,D20.12)
        END

```

```

C
C
C ***** matrix-inversion-routines
C
      SUBROUTINE LUDCMP(A,N,NP,INDX,D)
      IMPLICIT REAL*8(A-H,O-Z)
      PARAMETER (NMAX=100,TINY=1.0E-20)
      DIMENSION A(NP,NP),INDX(N),VV(NMAX)
      D=1.
      DO 12 I=1,N
        AAMAX=0.
        DO 11 J=1,N
          IF (ABS(A(I,J)).GT.AAMAX) AAMAX=ABS(A(I,J))
11      CONTINUE
      !      IF (AAMAX.EQ.0.) PAUSE 'Singular matrix.'
          IF (AAMAX.EQ.0.) print *, 'Singular matrix.'
          VV(I)=1./AAMAX
12      CONTINUE
      DO 19 J=1,N
        IF (J.GT.1) THEN
          DO 14 I=1,J-1
            SUM=A(I,J)
            IF (I.GT.1) THEN
              DO 13 K=1,I-1
                SUM=SUM-A(I,K)*A(K,J)
13          CONTINUE
              A(I,J)=SUM
            ENDIF
14          CONTINUE
          ENDIF
          AAMAX=0.
          DO 16 I=J,N
            SUM=A(I,J)
            IF (J.GT.1) THEN
              DO 15 K=1,J-1
                SUM=SUM-A(I,K)*A(K,J)
15          CONTINUE
              A(I,J)=SUM
            ENDIF
            DUM=VV(I)*ABS(SUM)
            IF (DUM.GE.AAMAX) THEN
              IMAX=I
              AAMAX=DUM
            ENDIF
16          CONTINUE
          IF (J.NE.IMAX) THEN
            DO 17 K=1,N
              DUM=A(IMAX,K)
              A(IMAX,K)=A(J,K)
              A(J,K)=DUM
17          CONTINUE
            D=-D
            VV(IMAX)=VV(J)
          ENDIF

```

```

      INDX(J)=IMAX
      IF(J.NE.N)THEN
        IF(A(J,J).EQ.O.)A(J,J)=TINY
        DUM=1./A(J,J)
        DO 18 I=J+1,N
          A(I,J)=A(I,J)*DUM
18      CONTINUE
        ENDIF
19      CONTINUE
      IF(A(N,N).EQ.O.)A(N,N)=TINY
      RETURN
      END
C
      SUBROUTINE LUBKSB(A,N,NP,INDX,B)
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION A(NP,NP),INDX(N),B(N)
      II=0
      DO 12 I=1,N
        LL=INDX(I)
        SUM=B(LL)
        B(LL)=B(I)
        IF (II.NE.O)THEN
          DO 11 J=II,I-1
            SUM=SUM-A(I,J)*B(J)
11          CONTINUE
          ELSE IF (SUM.NE.O.) THEN
            II=I
          ENDIF
        B(I)=SUM
12      CONTINUE
      DO 14 I=N,1,-1
        SUM=B(I)
        IF(I.LT.N)THEN
          DO 13 J=I+1,N
            SUM=SUM-A(I,J)*B(J)
13          CONTINUE
          ENDIF
        B(I)=SUM/A(I,I)
14      CONTINUE
      RETURN
      END
C
C
C      *****  RANDOM NUMBER GENERATORS
C
C      FUNCTION RANF(DUMMY)
C
C      RANDOM NUMBER FUNCTION TAKEN FROM KNUTH
C      (SEMINUMERICAL ALGORITHMS).
C      METHOD IS  $X(N)=MOD(X(N-55)-X(N-24),1/FMODUL)$ 
C      NO PROVISION YET FOR CONTROL OVER THE SEED NUMBER.
C
C      RANF GIVES ONE RANDOM NUMBER BETWEEN 0 AND 1.

```

```

C   IRN55 GENERATES 55 RANDOM NUMBERS BETWEEN 0 AND 1/FMODUL.
C   IN55  INITIALIZES THE 55 NUMBERS AND WARMS UP THE SEQUENCE.
C
      PARAMETER (FMODUL=1.E-09)
      SAVE /CIRN55/
      COMMON /CIRN55/NCALL,MCALL,IA(55)
      INTEGER IA
      CALL RANDAT
      IF( NCALL.EQ.0 ) THEN
        CALL IN55 ( IA,234612947 )
        MCALL = 55
        NCALL = 1
      ENDIF
      IF ( MCALL.EQ.0 ) THEN
        CALL IRN55(IA)
        MCALL=55
      ENDIF
      RANF=IA(MCALL)*FMODUL
      MCALL=MCALL-1
      RETURN
      END

C
      SUBROUTINE RANDAT
C
C   INITIALISES THE NUMBER NCALL TO 0 TO FLAG THE FIRST CALL
C   OF THE RANDOM NUMBER GENERATOR
C
      SAVE /CIRN55/
      SAVE FIRST
      SAVE
      COMMON /CIRN55/NCALL,MCALL,IA(55)
      INTEGER IA
      LOGICAL FIRST
      DATA FIRST /.TRUE./
      IF(FIRST)THEN
        FIRST=.FALSE.
        NCALL=0
      ENDIF
      RETURN
      END

C
      SUBROUTINE IN55(IA,IX)
      PARAMETER (MODULO=1000000000)
      INTEGER IA(55)
C
      IA(55)=IX
      J=IX
      K=1
      DO 10 I=1,54
        II=MOD(21*I,55)
        IA(II)=K
        K=J-K
        IF(K.LT.0)K=K+MODULO
        J=IA(II)

```

```

10  CONTINUE
    DO 20 I=1,10
        CALL IRN55(IA)
20  CONTINUE
    RETURN
    END

C
    SUBROUTINE IRN55(IA)
    PARAMETER (MODULO=1000000000)
    INTEGER IA(55)
    DO 10 I=1,24
        J=IA(I)-IA(I+31)
        IF(J.LT.0)J=J+MODULO
        IA(I)=J
10  CONTINUE
    DO 20 I=25,55
        J=IA(I)-IA(I-24)
        IF(J.LT.0)J=J+MODULO
        IA(I)=J
20  CONTINUE
    RETURN
    END

C
C
    FUNCTION RAN2(IDUM)
C *****
    REAL RDM(31)
    DATA IWARM/0/

C
    IF (IDUM.LT.0.OR.IWARM.EQ.0) THEN
C INITIALIZATION OR REINITIALISATION
        IWARM=1
        IA1=      1279
        IC1=      351762
        M1=      1664557
        IA2=      2011
        IC2=      221592
        M2=      1048583
        IA3=      15091
        IC3=      6171
        M3=      29201
        IX1=MOD(-IDUM,M1)
        IX1=MOD(IA1*IX1+IC1,M1)
        IX2=MOD(IX1,M2)
        IX1=MOD(IA1*IX1+IC1,M1)
        IX3=MOD(IX1,M3)
        RM1=1./FLOAT(M1)
        RM2=1./FLOAT(M2)
        DO 10 J=1,31
            IX1=MOD(IA1*IX1+IC1,M1)
            IX2=MOD(IA2*IX2+IC2,M2)
10      RDM(J)=(FLOAT(IX1)+FLOAT(IX2)*RM2)*RM1
        ENDIF
C

```

```

C GENERATE NEXT NUMBER IN SEQUENCE
  IF(IWARM.EQ.0) GOTO 901
  IX1=MOD(IA1*IX1+IC1,M1)
  IX2=MOD(IA2*IX2+IC2,M2)
  IX3=MOD(IA3*IX3+IC3,M3)
  J=1+(31*IX3)/M3
  RAN2=RDM(J)
  RDM(J)=(FLOAT(IX1)+FLOAT(IX2)*RM2)*RM1
  RETURN
901  PRINT 9010
9010  FORMAT('  RAN2: LACK OF ITINIALISATION')
      STOP
      END

C
C
C ***** SPECIAL FUNCTIONS
C
C
C DOUBLE PRECISION FUNCTION DILOGG(X)
C
C SPENCE'S DILOGARITHM IN DOUBLE PRECISION
C
  IMPLICIT REAL*8 (A-H,O-Z)
  Z=-1.644934066848226
  IF(X .LT. -1.0) GO TO 1
  IF(X .LE. 0.5) GO TO 2
  IF(X .EQ. 1.0) GO TO 3
  IF(X .LE. 2.0) GO TO 4
  Z=3.289868133696453
1  T=1.0/X
  S=-0.5
  Z=Z-0.5*DLOG(DABS(X))**2
  GO TO 5
2  T=X
  S=0.5
  Z=0.
  GO TO 5
3  DILOGG=1.644934066848226
  RETURN
4  T=1.0-X
  S=-0.5
  Z=1.644934066848226-DLOG(X)*DLOG(DABS(T))
5  Y=2.666666666666667*T+0.666666666666667
  B= 0.00000 00000 00001
  A=Y*B +0.00000 00000 00004
  B=Y*A-B+0.00000 00000 00011
  A=Y*B-A+0.00000 00000 00037
  B=Y*A-B+0.00000 00000 00121
  A=Y*B-A+0.00000 00000 00398
  B=Y*A-B+0.00000 00000 01312
  A=Y*B-A+0.00000 00000 04342
  B=Y*A-B+0.00000 00000 14437
  A=Y*B-A+0.00000 00000 48274
  B=Y*A-B+0.00000 00001 62421

```

```

A=Y*B-A+0.00000 00005 50291
B=Y*A-B+0.00000 00018 79117
A=Y*B-A+0.00000 00064 74338
B=Y*A-B+0.00000 00225 36705
A=Y*B-A+0.00000 00793 87055
B=Y*A-B+0.00000 02835 75385
A=Y*B-A+0.00000 10299 04264
B=Y*A-B+0.00000 38163 29463
A=Y*B-A+0.00001 44963 00557
B=Y*A-B+0.00005 68178 22718
A=Y*B-A+0.00023 20021 96094
B=Y*A-B+0.00100 16274 96164
A=Y*B-A+0.00468 63619 59447
B=Y*A-B+0.02487 93229 24228
A=Y*B-A+0.16607 30329 27855
A=Y*A-B+1.93506 43008 69969
DILOGG=S*T*(A-B)+Z
RETURN
END

```

c

```

SUBROUTINE pzext0(iest,xest,yest,yz,dy,nv)
implicit none
INTEGER iest,nv,IMAX,NMAX
REAL*8 xest,dy(nv),yest(nv),yz(nv)
PARAMETER (IMAX=13,NMAX=50)
INTEGER j,k1
REAL*8 delta,f1,f2,q,d(NMAX),qcol(NMAX,IMAX),x(IMAX)
SAVE qcol,x
x(iest)=xest
do 11 j=1,nv
    dy(j)=yest(j)
    yz(j)=yest(j)
11 continue
if(iest.eq.1) then
    do 12 j=1,nv
        qcol(j,1)=yest(j)
12 continue
else
    do 13 j=1,nv
        d(j)=yest(j)
13 continue
    do 15 k1=1,iest-1
        delta=1.d0/(x(iest-k1)-xest)
        f1=xest*delta
        f2=x(iest-k1)*delta
        do 14 j=1,nv
            q=qcol(j,k1)
            qcol(j,k1)=dy(j)
            delta=d(j)-q
            dy(j)=f1*delta
            d(j)=f2*delta
            yz(j)=yz(j)+dy(j)
14 continue
15 continue

```

```

        do 16 j=1,nv
            qcol(j,iest)=dy(j)
16        continue
        endif
        return
        END

c
c
        complex*16 function zdigamma(z)
        implicit none
        complex*16 z,psi,psipr1,psipr2
        call mkpsi(z,psi,psipr1,psipr2)
        zdigamma=psi
        end

c
        subroutine mkpsi(z,psi,psipr1,psipr2)
        implicit none
        complex*16 tmp,tmps2,tmps3,tmp0,tmp1,tmp2,ser0,ser1,ser2,ser3,
        .          zz,z,psi,psipr1,psipr2,off0,off1,off2,zcf,ser02,ser12,
        .          z1,z2
        real*8 cof(6),re1
        integer i
        data cof/76.18009173d0,-86.50532033d0,24.01409822d0,
        .      -1.231739516d0,.120858003d-2,-.536382d-5/
        save
        zz=z
        off0=cmlpx(0.d0,0.d0,kind=kind(0d0))
        off1=cmlpx(0.d0,0.d0,kind=kind(0d0))
        off2=cmlpx(0.d0,0.d0,kind=kind(0d0))
5      re1=real(zz)
        if (re1.le.0.d0) then
            off0=off0+1.d0/zz
            z1=zz*zz
            off1=off1-1.d0/z1
            z2=z1*zz
            off2=off2+2.d0/z2
            zz=zz+(1.d0,0.d0)
            goto 5
        endif
        tmp=zz+cmlpx(4.5d0,0.d0,kind=kind(0d0))
        tmps2=tmp*tmp
        tmps3=tmp*tmps2
        tmp0=(zz-cmlpx(0.5d0,0.d0,kind=kind(0d0)))/tmp+log(tmp)
u      -cmlpx(1.d0,0.d0,kind=kind(0d0))
        tmp1=(5.d0,0.d0)/tmps2+1.d0/tmp
        tmp2=(-10.0d0,0.d0)/tmps3-1.d0/tmps2
        ser0=cmlpx(1.d0,0.d0,kind=kind(0d0))
        ser1=cmlpx(0.d0,0.d0,kind=kind(0d0))
        ser2=cmlpx(0.d0,0.d0,kind=kind(0d0))
        ser3=cmlpx(0.d0,0.d0,kind=kind(0d0))
        do 10 i=1,6
            zcf=cof(i)/zz
            ser0=ser0+zcf
            zcf=zcf/zz

```



```

        ser1=ser1+zcf
        zcf=zcf/zz
        ser2=ser2+zcf
        zcf=zcf/zz
        ser3=ser3+zcf
        zz=zz+(1.d0,0.d0)
10 continue
    ser1=-ser1
    ser2=2.d0*ser2
    ser3=-6.d0*ser3
    ser02=ser0*ser0
    ser12=ser1*ser1
    psi=tmp0+ser1/ser0-off0
    psipr1=tmp1+(ser2*ser0-ser12)/ser02-off1
    psipr2=tmp2+(ser3*ser02-3.d0*ser2*ser1*ser0+2.d0*ser12*ser1)
    .      /ser02/ser0-off2
    return
end

<toppik_axial.f>≡
! WHIZARD <Version> <Date>

! TOPPIK code by M. Jezabek, T. Teubner (v1.1, 1992), T. Teubner (1998)
!
! NOTE: axial part (p-wave) only
!
! FB: -commented out numerical recipes code for hypergeometric 2F1
!      included in hypgeo.f90;
!      -replaced function 'cdabs' by 'abs';
!      -replaced function 'dabs' by 'abs';
!      -replaced function 'dimag' by 'aimag';
!      -replaced function 'dcmplx(,)' by 'cmplx(,kind=kind(0d0))';
!      -replaced function 'dreal' by 'real';
!      -replaced function 'dlog' by 'log';
!      -replaced function 'dsqrt' by 'sqrt';
!      -renamed function 'a' to 'aax'
!      -renamed function 'fretil1' to 'fretil1ax'
!      -renamed function 'fretil2' to 'fretil2ax'
!      -renamed function 'fimtil1' to 'fimtil1ax'
!      -renamed function 'fimtil2' to 'fimtil2ax'
!      -renamed function 'freal' to 'frealax'
!      -renamed function 'fim' to 'fimax'
!      -renamed subroutine 'vhat' to 'vhatax'
!      -renamed subroutine 'sae' to 'saeax'
!      -commented out many routines identically defined in 'toppik.f'
!      -modified 'tttoppikaxial' to catch unstable runs.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

c *****
c      Version tuned to provide 0(1%) relative accuracy for Coulomb axial
c      vertex function at first and second order (search for 'cctt'):
c      - integrals A(p), Vhat, Vhhat provided analytically w/out cut-off
c      - grid range fixed to 0.1 ... 10**6 absolut
c      - and grid size enhanced to 600 points (900 foreseen in arrays).

```

```

c
c      This provides a compromise between stability and accuracy:
c      We need a relatively high momentum resolution and large maximal
c      momenta to achieve a ~1 percent accuracy, but the method of
c      direct inversion of the discretised integral equation for objects
c      whose integral is divergent induces instabilities at small
c      momenta. As the behaviour there is known, they can be cut off and
c      the vertex function fixed by hand; but limiting the grid
c      further would impact on the accuracy.
c      22.3.2017, tt
c *****
c
c Working version with all the different original potentials
c like (p^2+q^2)/|p-q|^2, not transformed in terms of delta and 1/r^2;
c accuracy eps=1.d-3 possible (only), but should be save, 13.8.'98, tt.
c cleaned up a bit, 24.2.1999, tt.
c
c *****
c
c
c      subroutine tttoppikaxial(xenergy,xtm,xtg,xalphas,xscale,xcutn,
u      xcutv,
u      xc0,xc1,xc2,xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,
u      xkincm,xkinca,jknflg,jgcflg,xkincv,jvflg,
u      xim,xdi,np,xpp,xww,xsdp,zftild)
c
c *****
c
c !! THIS IS NOT A PUBLIC VERSION !!
c
c !!! Only P wave result given as output!!! 9.4.1999, tt.
c
c - Calculation of the Green function in momentum space by solving the
c   Lippmann-Schwinger equation
c   
$$F(p) = G_0(p) + G_0(p) \int_0^{xcutn} V(p,q) q.p/p^2 F(q) dq$$

c
c - Written by Thomas Teubner, Hamburg, November 1998
c   * Based on TOPPIK Version 1.1
c     from M. Jezabek and TT, Karlsruhe, June 1992
c   * Version originally for non-constant top-width
c   * Constant width supplied here
c   * No generator included
c
c - Use of double precision everywhere
c
c - All masses, momenta, energies, widths in GeV
c
c - Input parameters:
c
c   xenergy : E=Sqrt[s]-2*topmass
c   xtm      : topmass (in the Pole scheme)
c   xtg      : top-width
c   xalphas  :  $\alpha_s^{\{MSbar,n_f=5\}}$ (xscale)
c   xscale   : soft scale  $\mu_{\{soft\}}$ 

```

```

c   xcutn      : numerical UV cutoff on all momenta
c               (UV cutoff of the Gauss-Legendre grid)
c   xcutv      : renormalization cutoff on the
c               delta-, the  $(p^2+q^2)/(p-q)^2$ -, and the
c                $1/r^2-[1/|p-q|]$ -potential:
c               if (max(p,q).ge.xcutv) then the three potentials
c               are set to zero in the Lippmann-Schwinger equation
c   xc0        : 0th order coefficient for the Coulomb potential,
c               see calling example above
c   xc1        : 1st order coefficient for the Coulomb potential
c   xc2        : 2nd order coefficient for the Coulomb potential
c   xcdeltc    : constant of the delta(r)-
c               [= constant in momentum space-] potential
c   xcdeltl    : constant for the additional  $\log(q^2/\mu^2)$ -part of the
c               delta-potential:
c               xcdeltc*1 + xcdeltl*log( $q^2/\mu^2$ )
c   xcfullc    : constant of the  $(p^2+q^2)/(p-q)^2$ -potential
c   xcfulll    : constant for the additional  $\log(q^2/\mu^2)$ -part of the
c                $(p^2+q^2)/(p-q)^2$ -potential
c   xcrm2      : constant of the  $1/r^2-[1/|p-q|]$ -potential
c   xkincm     : } kinetic corrections in the 0th order Green function:
c   xkinca     : }  $G_0(p) = 1/[E+i\Gamma_t-p^2/m_t]*(1+xkincm)+xkinca$ 
c               !!! WATCH THE SIGN IN  $G_0$  !!!
c   jknflg     : flag for these kinetic corrections:
c               0 : no kinetic corrections applied
c               1 : kinetic corrections applied with cutoff xcutv
c                   for xkinca only
c               2 : kinetic corrections applied with cutoff xcutv
c                   for xkinca AND xkincm
c   jgcflg     : flag for  $G_0(p)$  in the LS equation:
c               0 (standard choice) :  $G_0(p)$  as given above
c               1 (for TIPT)         :  $G_0(p) = G_c^{(0)}(p)$  the 0th
c                                   order Coulomb Green function
c                                   in analytical form; not for
c                                   momenta  $p > 1000*topmass$ 
c   xkincv     : additional kinematic vertexcorrection in  $G_0$ , see below:
c   jvflg      : flag for the additional vertexcorrection xkincv in the
c               "zeroth order"  $G_0(p)$  in the LS-equation:
c               0 : no correction, means  $G = G_0 + G_0 \text{ int } V G$ 
c                   with  $G_0 = 1/[E+i\Gamma_t-p^2/m_t]*(1+xkincm)+xkinca$ 
c               1 : apply the correction in the LS equation as
c                    $G = G_0 + xkincv*p^2/m_t^2/[E+i\Gamma_t-p^2/m_t] +$ 
c                    $G_0 \text{ int } V G$ 
c               and correct the integral over  $\text{Im}[G(p)]$  to get  $\sigma_{tot}$ 
c               from the optical theorem by the same factor.
c               The cutoff xcutv is applied for these corrections.
c
c - Output:
c
c   xim        :  $R^{\{P \text{ wave}\}}_{\{ttbar\}}$  from the imaginary part of the Green
c               function
c   xdi        :  $R^{\{P \text{ wave}\}}_{\{ttbar\}}$  from the integral over the momentum
c               distribution:  $\text{int}_0^{\sim xcutv} dp \, p^3/m_t*|F(p,E)|^2$ 
c   np         : number of points used for the grid; fixed in tttoppik

```

```

c   xpp      : 1-dim array (max. 900 elements) giving the momenta of
c               the Gauss-Legendre grid (pp(i) in the code)
c   xww      : 1-dim array (max. 900 elements) giving the corresponding
c               Gauss-Legendre weights for the grid
c   xdsdp    : 1-dim array (max. 900 elements) giving the
c               momentum distribution of top:  $d\sigma^{\{P \text{ wave}\}}/dp$ ,
c               normalized to R,
c               at the momenta of the Gauss-Legendre grid xpp(i)
c   zftild   : 1-dim array (max. 900 elements) of COMPLEX*16 numbers
c               giving the vertex function K_A for the P-wave
c               at the momenta of the grid.
c               Then  $F(p)=K_A(p)*G_0(p)$  corresponding to  $G=K_V*G_0$ .
c
c *****
c
c
c       implicit none
c       real*8
c
c       u      pi,energy,vzero,eps,
c       u      pp,
c       u      tmass,tgamma,zmass,alphas,alamb5,
c       u      wmass,wgamma,bmass,GFERMI,hmass,
c       u      xx,critp,consde,
c       u      w1,w2,sig1,sig2,const,
c       u      gtpcor,etot,
c       u      xenergy,xtm,xtg,xalphas,xscale,xc0,xc1,xc2,xim,xdi,
c       u      xaai,xaad,xdsdp,xpp,xww,
c       u      cplas,scale,c0,c1,c2,cdeltc,cdeltl,cfullc,cfllll,crm2,
c       u      chiggs,xcutn,dcut,xcutv,
c       u      xp,xpmax,
c       u      kincom,kincoa,kincov,xkincm,xkinca,xkincv,
c       u      xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2
c       complex*16 bb,vec,gg,a1,aax,g0,g0c,zvfct,zftild
c       integer i,n,nmax,npot,np,gcflg,kinflg,jknflg,jgcflg,
c       u      jvflg,vflag
c       parameter (nmax=900)
c       dimension pp(nmax),bb(nmax),vec(nmax),xx(nmax),gg(nmax),
c       u      w1(nmax),w2(nmax),a1(nmax),
c       u      xdsdp(nmax),xpp(nmax),xww(nmax),
c       u      zvfct(nmax),zftild(nmax)
c
c       external aax,gtpcor,g0,g0c
c
c       common/ovalco/ pi, energy, vzero, eps, npot
c       COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c       $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c       common/cplcns/cplas,scale,c0,c1,c2,
c       u      cdeltc,cdeltl,cfullc,cfllll,crm2,chiggs
c       common/mom/ xp,xpmax,dcut
c       common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
c       pi=3.141592653589793238d0
c
c       c Number of points to evaluate on the integral equation

```

```

c  (<=900 and n mod 3 = 0 !!):
      n=600
      np=n
c
c  For second order potential with free parameters:
c
      npot=5
c  Internal accuracy for TOPPIK, the reachable limit may be smaller,
c  depending on the parameters. But increase in real accuracy only
c  in combination with large number of points.
      eps=1.d-3
c  Some physical parameters:
      wgamma=2.07d0
      zmass=91.187d0
      wmass=80.33d0
      bmass=4.7d0
c
c  Input:
      tmass=xm
      energy=xenergy
      tgamma=xtg
      cplas=xalphas
      scale=xscale
      c0=xc0
      c1=xc1
      c2=xc2
      cdeltc=xcdeltc
      cdeltl=xcdeltl
      cfullc=xcfullc
      cfulll=xcfulll
      crm2=xcrm2
      kincom=xkincom
      kincoa=xkincoa
      kincov=xkincov
      kinflg=jknflg
      gcflg=jgcflg
      vflag=jvflg
c
      alphas=xalphas
c
c  Cut for divergent potential-terms for large momenta in the function vhatax
c  and in the integrals aax(p):
      dcut=xcutv
c
c  Numerical Cutoff of all momenta (maximal momenta of the grid):
      xpmx=xcutn
      if (dcut.gt.xpmx) then
        write(*,*) ' dcut > xpmx  makes no sense! Stop.'
        stop
      endif
c
c  Not needed for the fixed order potentials:
      alamb5=0.2d0
c

```

```

c      WRITE(*,*) 'INPUT TGAMMA=',TGAMMA
c Needed in subroutine GAMMAT:
      GFERMI=1.16637d-5
c      CALL GAMMAT
c      WRITE(*,*) 'CALCULATED TGAMMA=',TGAMMA
c
      etot=2.d0*tmass+energy
c
      if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
u      (npot.eq.5)) then
c For pure coulomb and fixed order potentials there is no delta-part:
      consde = 0.d0
      else if (npot.eq.2) then
c Initialize QCD-potential common-blocks and calculate constant multiplying
c the delta-part of the 'qcutted' potential in momentum-space:
      call iniphc(1)
c      call vqdelt(consde)
c      write(*,*) ' Not supplied with this version. Stop.'
      stop
      else
      write (*,*) ' Potential not implemented! Stop. 1'
      stop
      endif
c Delta-part of potential is absorbed by subtracting vzero from the
c original energy (shift from the potential to the free Hamiltonian):
      vzero = consde / (2.d0*pi)**3
c      write (*,*) 'vzero=', vzero
c
c Find x-values pp(i) and weigths w1(i) for the gaussian quadrature;
c care about large number of points in the important intervals:
c      if (energy-vzero.le.0.d0) then
cc      call gauleg(0.d0, 1.d0, pp, w1, n/3)
cc      call gauleg(1.d0, 5.d0, pp(n/3+1), w1(n/3+1), n/3)
cc      call gauleg(0.d0, 0.2d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      call gauleg(0.d0, 5.d0, pp, w1, n/3)
c      call gauleg(5.d0, 20.d0, pp(n/3+1), w1(n/3+1), n/3)
c      call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      else
cc Avoid numerical singular points in the inner of the intervals:
c      critp = sqrt((energy-vzero)*tmass)
c      if (critp.le.1.d0) then
cc Gauss-Legendre is symmetric => automatically principal-value prescription:
c      call gauleg(0.d0, 2.d0*critp, pp, w1, n/3)
c      call gauleg(2.d0*critp, 20.d0, pp(n/3+1),
c      u      w1(n/3+1), n/3)
c      call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c      else
cc Better behaviour at the border of the intervals:
c      call gauleg(0.d0, critp, pp, w1, n/3)
c      call gauleg(critp, 2.d0*critp, pp(n/3+1),
c      u      w1(n/3+1), n/3)
c      call gauleg(0.d0, 1.d0/(2.d0*critp), pp(2*n/3+1),
c      u      w1(2*n/3+1), n/3)
c      endif

```

```

c      endif
c
c Or different (simpler) method, good for V_JKT:
      if (energy.le.0.d0) then
        critp=tmass/3.d0
      else
        critp=max(tmass/3.d0,2.d0*sqrt(energy*tmass))
      endif
c      call gauleg(0.d0, critp, pp, w1, 2*n/3)
c      call gauleg(1.d0/xpmax, 1.d0/critp, pp(2*n/3+1),
c      u      w1(2*n/3+1), n/3)
cctt Tuned March 2017 for best possible numerical behaviour of P-wave
      call gauleg(0.1d0, 2.d0, pp, w1, 10)
      call gauleg(2.d0, critp, pp(11), w1(11), 2*n/3-10)
      call gauleg(1.d-6, 1.d0/critp, pp(2*n/3+1),
c      u      w1(2*n/3+1), n/3)
c
c Do substitution  $p \Rightarrow 1/p$  for the last interval explicitly:
      do 10 i=2*n/3+1,n
        pp(i) = 1.d0/pp(i)
10      continue
c
c Reorder the arrays for the third interval:
      do 20 i=1,n/3
        xx(i) = pp(2*n/3+i)
        w2(i) = w1(2*n/3+i)
20      continue
      do 30 i=1,n/3
        pp(n-i+1) = xx(i)
        w1(n-i+1) = w2(i)
30      continue
c
c Calculate the integrals aax(p) for the given momenta pp(i)
c and store weights and momenta for the output arrays:
      do 40 i=1,n
        a1(i) = aax(pp(i)) !!! FB: can get stuck in original Toppik!
        !!! FB: abuse 'np' as a flag to communicate unstable runs
        if ( abs(a1(i)) .gt. 1d10 ) then
          np = -1
          return
        endif
        xpp(i)=pp(i)
        xww(i)=w1(i)
40      continue
      do 41 i=n+1,nmax
        xpp(i)=0.d0
        xww(i)=0.d0
41      continue
c
c Solve the integral-equation by solving a system of algebraic equations:
      call saeax(pp, w1, bb, vec, a1, n)
c
c (The substitution for the integration to infinity  $pp \Rightarrow 1/pp$ 
c is done already.)

```

```

do 50 i=1,n
  zvfct(i)=bb(i)
  zftild(i)=vec(i)
  gg(i) = bb(i)*g0c(pp(i))
cc      gg(i) = (1.d0 + bb(i))*g0c(pp(i))
cc Urspruenglich anderes (Minus) VZ hier, dafuer kein Minus mehr bei der
cc Definition des WQs ueber Im G, 2.6.1998, tt.
cc      gg(i) = - (1.d0 + bb(i))*g0c(pp(i))
50      continue
c
c Normalisation on R:
      const = 8.d0*pi/tmass**2
c
c Proove of the optical theorem for the output values of saeax:
c Simply check if sig1 = sig2.
      sig1 = 0.d0
      sig2 = 0.d0
      xaai = 0.d0
      xaad = 0.d0
      do 60 i=1,n*2/3
c        write(*,*) 'check! p(',i,') = ',pp(i)
cvv
        if (pp(i).lt.dcut.and.vflag.eq.1) then
          sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i)
cc      u      *(1.d0+kincov*(pp(i)/tmass)**2)
u      *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u      )
          else
            sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i))
          endif
          if (pp(i).lt.dcut.and.kinflg.ne.0) then
            sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
cc      u      tgamma*gtpcor(pp(i),etot)
u      *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u      *tmass/sqrt(tmass**2+pp(i)**2)
c      xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u      tgamma*gtpcor(pp(i),etot)
c      u      *(1.d0-pp(i)**2/2.d0/tmass**2)
c      u      /(2.d0*pi**2)*const
          else
            sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
cc      u      tgamma*gtpcor(pp(i),etot)
c      xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u      tgamma*gtpcor(pp(i),etot)
c      u      /(2.d0*pi**2)*const
          endif
          xdsdp(i)=pp(i)**4/tmass**2*abs(zftild(i)*g0c(pp(i)))**2
u      *tgamma*gtpcor(pp(i),etot)
u      /(2.d0*pi**2)*const
          xaai=xaai+w1(i)*pp(i)**4/tmass**2*
u      aimag(zftild(i)*g0c(pp(i)))
          xaad=xaad+w1(i)*pp(i)**4/tmass**2*
u      abs(zftild(i)*g0c(pp(i)))**2 *
u      tgamma*gtpcor(pp(i),etot)

```



```

c          write(*,*) 'xdsdp = ',xdsdp(i)
c          write(*,*) 'zvfct = ',zvfct(i)
c          write(*,*) 'zftild = ',zftild(i)
60      continue
c '*p**2' because of substitution p => 1/p in the integration of p**2*G(p)
c to infinity
      do 70 i=n*2/3+1,n
c          write(*,*) 'check! p(',i,') = ',pp(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
              sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i)
cc      u          *(1.d0+kincov*(pp(i)/tmass)**2)
u          *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u          )
              else
                  sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i))
              endif
          if (pp(i).lt.dcut.and.kinflg.ne.0) then
              sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u              *tmass/sqrt(tmass**2+pp(i)**2)
c          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u          tgamma*gtpcor(pp(i),etot)
c      u          *(1.d0-pp(i)**2/2.d0/tmass**2)
c      u          /(2.d0*pi**2)*const
              else
                  sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u                  tgamma*gtpcor(pp(i),etot)
c          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u          tgamma*gtpcor(pp(i),etot)
c      u          /(2.d0*pi**2)*const
              endif
          xdsdp(i)=pp(i)**4/tmass**2*abs(zftild(i)*g0c(pp(i)))**2
u          *tgamma*gtpcor(pp(i),etot)
u          /(2.d0*pi**2)*const
          xaai=xaai+w1(i)*pp(i)**6/tmass**2*
u          aimag(zftild(i)*g0c(pp(i)))
          xaad=xaad+w1(i)*pp(i)**6/tmass**2*
u          abs(zftild(i)*g0c(pp(i)))**2 *
u          tgamma*gtpcor(pp(i),etot)
c          write(*,*) 'xdsdp = ',xdsdp(i)
c          write(*,*) 'zvfct = ',zvfct(i)
c          write(*,*) 'zftild = ',zftild(i)
70      continue
      do 71 i=n+1,nmax
          xdsdp(i)=0.d0
          zvfct(i)=(0.d0,0.d0)
          zftild(i)=(0.d0,0.d0)
71      continue
c
c Normalisation on R:
      sig1 = sig1 / (2.d0*pi**2) * const
      sig2 = sig2 / (2.d0*pi**2) * const

```

```

c
c The results from the momentum space approach finally are:
cc Jetzt Minus hier, 2.6.98, tt.
c      xim=-sig1
c      xdi=sig2
c      xaai=-xaai / (2.d0*pi**2) * const
c      xaad=xaad / (2.d0*pi**2) * const
c Output of P wave part only:
c      xim=xaai
c      xdi=xaad
c      write(*,*) 'vvi = ', -sig1, ' . vvd = ', sig2
c      write(*,*) 'aai = ', xim, ' . aad = ', xdi
c
c      end
c
c
c
c      complex*16 function aax(p)
c
c Neue Funktion fuer die Integrale aax(p), die hier im Falle Cutoff -> infinity
c fuer reine Coulombpotentiale vollstaendig analytisch loesbar sind.
c 22.3.2001, tt.
c
c      implicit none
c      complex*16 zi,zb,zlp,zlm,zalo,zanlo,zannlo,zahig,za
c      real*8
c      u      tmass,tgamma,zmass,alphas,alamb5,
c      u      wmass,wgamma,bmass,GFERMI,hmass,
c      u      pi,energy,vzero,eps,
c      u      p,zeta3,cf,ca,tf,xnf,b0,b1,a1,a2,cnspot,phiint,
c      u      cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c      integer npot
c      parameter(zi=(0.d0,1.d0),zeta3=1.20205690316d0,
c      u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,xnf=5.d0)
c
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/ovalco/ pi, energy, vzero, eps, npot
c      common/cplcns/cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
c      b0=11.d0-2.d0/3.d0*xnf
c      b1=102.d0-38.d0/3.d0*xnf
c
c      a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
c      a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
c      u      22.d0/3.d0*zeta3)*ca**2-
c      u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
c      u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
c      u      (20.d0/9.d0*tf*xnf)**2
c
c      cnspot=-4.d0/3.d0*4.d0*pi

```

```

        phiint=cnspt*alphas
c
        zb=sqrt(tmass*cmplx(energy,tgamma,kind=kind(0d0)))
        zlp=log(zb+p)
        zlm=log(zb-p)
c L0: no log in z-integral
        zalo=zi*pi/2.d0/p*(zlp-zlm)
c from NLO: log in the z-integral
        zanlo=pi/2.d0/p*(zlp-zlm)*(pi+zi*(zlp+zlm))
c from NNLO: log**2 in the z-integral
        zannlo=pi/3.d0/p*(zlp-zlm)
        u      *(3.d0*pi*(zlp+zlm)+2.d0*zi*(zlm**2+zlm*zlp+zlp**2))
c Sum of the Coulomb contributions:
        za=c0*zalo-c1*(zanlo-2.d0*dlog(scale)*zalo)
        u      +c2*(zannlo-4.d0*dlog(scale)*zanlo)
        u      +4.d0*dlog(scale)**2*zalo)
c (Higgs) Yukawa contribution
cctt      zahig=zi*pi/2.d0/p*log((zb+p+zi*hmass)/(zb-p+zi*hmass))
c Alltogether:
cctt      aax=-tmass/(4.d0*pi**2)*(phiint*za+chiggs*zahig)
        aax=-tmass/(4.d0*pi**2)*phiint*za
c
c      write(*,*) 'aax(',p,')= ',aax
c      end
c
c      real*8 function fretillax(xk)
c      implicit none
c      real*8 xk, frealax
c      external frealax
c      fretillax = frealax(xk)
c      end
c
c      real*8 function fretil2ax(xk)
c      implicit none
c      real*8 xk, frealax
c      external frealax
c      fretil2ax = frealax(1.d0/xk) * xk**(-2)
c      end
c
c      real*8 function fimtillax(xk)
c      implicit none
c      real*8 xk, fimax
c      external fimax
c      fimtillax = fimax(xk)
c      end
c
c      real*8 function fimtil2ax(xk)
c      implicit none
c      real*8 xk, fimax
c      external fimax
c      fimtil2ax = fimax(1.d0/xk) * xk**(-2)
c      end
c
c      real*8 function frealax(xk)

```

```

        implicit none
        complex*16 vhatax
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
        complex*16 g0,g0c
        integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot
        common/mom/ p,pmax,dcut
        external vhatax, g0, g0c, gtpcor
c
        frealax = real(g0c(xk)*vhatax(p, xk))
end
c
        real*8 function fimax(xk)
        implicit none
        complex*16 vhatax
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
        complex*16 g0,g0c
        integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot
        common/mom/ p,pmax,dcut
        external vhatax, g0, g0c, gtpcor
        fimax = aimag(g0c(xk)*vhatax(p, xk))
end
c
c
        complex*16 function vhatax(p, xk)
c
        implicit none
        complex*16 zi
        real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p, xk,
u      cnspot, phiint, AD8GLE,
u      pm, xkm,
c  u      phfqcd, ALPHEF,
u      zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
u      cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,
u      xkpln1st,xkpln2nd,xkpln3rd,
u      pp,pmax,dcut,hmass,chiggs

```

```

integer npot
parameter(zi=(0.d0,1.d0))
parameter(zeta3=1.20205690316d0,
u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
u      xnf=5.d0)
c
      external AD8GLE
c      u      , phfqcd, ALPHEF
c
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/pmaxkm/ pm, xkm
      common/mom/ pp,pmax,dcut
      common/cplcns/cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
      b0=11.d0-2.d0/3.d0*xf
      b1=102.d0-38.d0/3.d0*xf
c
      a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xf
      a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
u      22.d0/3.d0*zeta3)*ca**2-
u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xf-
u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xf+
u      (20.d0/9.d0*tf*xf)**2
c
      pm=p
      xkm=xk
      cnspot=-4.d0/3.d0*4.d0*pi
c
      if (p/xk.le.1.d-5.and.p.le.1.d-5) then
        xkpln1st=2.d0
        xkpln2nd=-4.d0*log(scale/xk)
        xkpln3rd=-6.d0*log(scale/xk)**2
      else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
        xkpln1st=2.d0*(xk/p)**2
        xkpln2nd=-4.d0*(xk/p)**2*log(scale/p)
        xkpln3rd=-6.d0*(xk/p)**2*log(scale/p)**2
      else
c        xkpln1st=xk/p*log(abs((p+xk)/(p-xk)))
        xkpln1st=xk/p*(log(p+xk)-log(abs(p-xk)))
cctt sign checked again, 2.2.2017, tt.
        xkpln2nd=xk/p*(-1.d0)*(log(scale/(p+xk))**2-
u          log(scale/abs(p-xk))**2)
        xkpln3rd=xk/p*(-4.d0/3.d0)*(log(scale/(p+xk))**3-
u          log(scale/abs(p-xk))**3)
      endif
c
c      if (npot.eq.2) then
c        if (p/xk.le.1.d-5.and.p.le.1.d-5) then
c          vhatx = 2.d0 * cnspot * ALPHEF(xk)
c        else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
c          vhatx = 2.d0 * cnspot * xk**2 / p**2 * ALPHEF(p)

```

```

c      else
c          phiint = cnspt * (AD8GLE(phfqcd, 0.d0, 0.3d0, 1.d-5)
c      u          +AD8GLE(phfqcd, 0.3d0, 1.d0, 1.d-5))
c          vhatx = xk / p * log(abs((p+xk)/(p-xk))) * phiint
c      endif
c      else
c          if (npot.eq.1) then
c              c0=1.d0
c              c1=0.d0
c              c2=0.d0
c          else if (npot.eq.3) then
c              c0=1.d0+alphas/(4.d0*pi)*a1
c              c1=alphas/(4.d0*pi)*b0
c              c2=0
c          else if (npot.eq.4) then
c              c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
c              c1=alphas/(4.d0*pi)*b0+
c      u          (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
c              c2=(alphas/(4.d0*pi))**2*b0**2
c          else if (npot.eq.5) then
c          else
c              write(*,*) ' Potential not implemented! Stop. 3'
c              stop
c          endif
c          phiint=cnspt*alphas
c
c      if ((xk+p).le.dcut) then
c          vhatx=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      u          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c      u          *(pi*cf*alphas)**2/tmass
c      u          *xk/p*(p+xk-abs(xk-p))
c      else if (abs(xk-p).lt.dcut) then
c          vhatx=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      u          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c      u          *(pi*cf*alphas)**2/tmass
c      u          *xk/p*(dcut-abs(xk-p))
c      else if (dcut.le.abs(xk-p)) then
c          vhatx=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      else
c          write(*,*) ' Not possible! Stop.'
c          stop
c      endif
c
c      ctt
c      Cut not applied here, should be left hard-wired in gauleg for stability of axial part. March 201
c      if (max(xk,p).lt.dcut) then
c      Coulomb + first + second order corrections:
c          vhatx=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      All other potentials:
c      u          +cdeltc*2.d0*xk**2
c      u          +cdeltl*xk/p/2.d0*(
c      u          (p+xk)**2*(log(((p+xk)/scale)**2)-1.d0)-
c      u          (p-xk)**2*(log(((p-xk)/scale)**2)-1.d0))
c      u          +cfullc*(p**2+xk**2)*xkpln1st

```

```

c      u      +cfulll*(p**2+xk**2)*xk/p/4.d0*
c      u      (log(((p+xk)/scale)**2)**2-
c      u      log(((p-xk)/scale)**2)**2)
c      u      +crm2*xk/p*(p+xk-abs(xk-p))
c      else
c      vhatx=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      endif
c      endif
c
c      end
c
c
c      complex*16 function vhat(p, xk)
c
c      implicit none
c      complex*16 zi
c      real*8
c      u      tmass,tgamma,zmass,alphas,alamb5,
c      u      wmass,wgamma,bmass,GFERMI,
c      u      pi, energy, vzero, eps,
c      u      p, xk,
c      u      cnspot, phiint, AD8GLE,
c      u      pm, xkm,
c      u      zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
c      u      cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,
c      u      xkpln1st,xkpln2nd,
c      u      pp,pmax,dcut,hmass,chiggs
c      integer npot
c      parameter(zi=(0.d0,1.d0))
c      parameter(zeta3=1.20205690316d0,
c      u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
c      u      xnf=5.d0)
c
c      external AD8GLE
c
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/ovalco/ pi, energy, vzero, eps, npot
c      common/pmaxkm/ pm, xkm
c      common/mom/ pp,pmax,dcut
c      common/cplcns/cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
c      b0=11.d0-2.d0/3.d0*xnf
c      b1=102.d0-38.d0/3.d0*xnf
c
c      a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
c      a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
c      u      22.d0/3.d0*zeta3)*ca**2-
c      u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
c      u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
c      u      (20.d0/9.d0*tf*xnf)**2
c

```

```

      pm=p
      xkm=xk
      cnspot=-4.d0/3.d0*4.d0*pi
c
      if (npot.eq.1) then
        c0=1.d0
        c1=0.d0
        c2=0.d0
      else if (npot.eq.3) then
        c0=1.d0+alphas/(4.d0*pi)*a1
        c1=alphas/(4.d0*pi)*b0
        c2=0
      else if (npot.eq.4) then
        write(*,*) '2nd order Coulomb in Vhhat not implemented yet.'
        stop
        c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
        c1=alphas/(4.d0*pi)*b0+
u          (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
        c2=(alphas/(4.d0*pi))**2*b0**2
      else if (npot.eq.5) then
        else
          write(*,*) ' Potential not implemented! Stop. 4'
          stop
        endif
        phiint=cnspot*alphas
c
cctt No cut-off description used here either.
c      if (max(xk,p).lt.dcut) then
cctt Pure Coulomb in first order and second order only:
c
      xkpln1st=-(xk/p)**2*(1.d0+(xk**2+p**2)/(2.d0*xk*p)*
u          (dlog(dabs(p-xk))-dlog(p+xk)))
c      xkpln1st=-(xk/p)**2*(1.d0+(xk**2+p**2)/(4.d0*xk*p)*
c      u          (dlog((p-xk)**2)-2.d0*dlog(p+xk)))
c
      xkpln2nd=((xk/p)**2/2.d0+xk*(xk**2+p**2)/8.d0/p**3*
u          (dlog((p-xk)**2)-2.d0*dlog(p+xk)))*
u          (-2.d0+dlog((xk-p)**2/scale**2)
u          +dlog((xk+p)**2/scale**2))
c
cctt 3rd order not yet.      xkpln3rd=
      if (c2.ne.0.d0) then
        write(*,*) ' Vhhat: 2nd order not implemented yet. Stop.'
        stop
      endif
c
cctt      vhat=dcmplx(phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd),
cctt      u          0.d0)
      vhat=cmplx(phiint*(c0*xkpln1st+c1*xkpln2nd),
u          0.d0,kind=kind(0d0))
c      else
c      vhat=(0.d0,0.d0)
c      endif
c

```



```

end

c
c
c
c
c -- Routines for solving linear equations and matrix inversion (complex) --
c
      subroutine saeax(pp, w1, bb, vec, a1, n)
c
      implicit none
      complex*16 vhatax,vhhat
      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      d, d1, pp, w1, gtpcor,hmass,
u      xp,xpmax,dcut,kincom,kincoa,kincov
      complex*16 aax, a1, bb, vec, ff, kk, cw, svw, g0, g0c
      integer i, j, npot, n, nmax, indx,kinflg,gcflg,vflag
      parameter (nmax=900)
      dimension bb(nmax),vec(nmax),ff(nmax,nmax),kk(nmax,nmax),
u      pp(nmax),w1(nmax),indx(nmax),cw(nmax),a1(nmax)
c
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/mom/ xp,xpmax,dcut
      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
      external aax, vhatax, gtpcor, g0, g0c, vhhat
c
      do 10 i=1,n*2/3
        cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i))
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),
c      u      kind=kind(0d0))-pp(i)**2/tmass))
10      continue
      do 20 i=n*2/3+1,n
        cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i)) * pp(i)**2
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),kind=kind(0d0)) /
c      u      pp(i)**2 - 1.d0/tmass))
20      continue
c
      do 30 i=1,n
cc      bb(i) = a1(i)
cvv
      if (pp(i).lt.dcut.and.vflag.eq.1) then
c      bb(i) = cmplx(1.d0+kincov*(pp(i)/tmass)**2,0.d0,
c      u      kind=kind(0d0))
      bb(i)=1.d0+kincov*
u      g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i))

```

```

        else
            bb(i) = (1.d0,0.d0)
        endif
c
c Without extra kinematic corrections:
        vec(i)=(1.d0,0.d0)
c
        svw = (0.d0,0.d0)
        do 40 j=1,n
            if (i.ne.j) then
                ff(i,j) = - vhatx(pp(i),pp(j)) * cw(j)
                kk(i,j) = - vhhath(pp(i),pp(j)) * cw(j)
                svw = svw + ff(i,j)
            endif
40          continue
            ff(i,i) = 1.d0 - a1(i) - svw
            kk(i,i) = ff(i,i)
30          continue
c
        call zldcmp(ff, n, nmax, indx, d)
        call zldcmp(kk, n, nmax, indx, d1)
        call zlbksb(ff, n, nmax, indx, bb)
        call zlbksb(kk, n, nmax, indx, vec)
c
        end
c
c

```

29.1 Top threshold form factor code

This module contains the infrastructure for the resummed form factors for the top threshold simulation as well as the calculation of the top mass and width etc.

```
<ttv_formfactors.f90>≡  
  <File header>  
  
  module ttv_formfactors  
  
    use, intrinsic :: iso_fortran_env !NODEP!  
  
    use kinds  
    <Use strings>  
    <Use debug>  
    use constants  
    use sm_physics  
    use lorentz  
    use interpolation  
    use nr_tools  
    use diagnostics  
  
    <Standard module head>  
    save  
  
    <TTV formfactors: public>  
  
    <TTV formfactors: public parameters>  
  
    <TTV formfactors: types>  
  
    <TTV formfactors: global variables>  
  
    interface  
    <TTV formfactors: sub interfaces>  
    end interface  
  
  end module ttv_formfactors  
<ttv_formfactors_sub.f90>≡  
  <File header>  
  
  submodule (ttv_formfactors) ttv_formfactors_s  
  
    use numeric_utils  
    use string_utils  
    use physics_defs, only: CF, CA, TR  
    use io_units  
    use system_dependencies  
  
    implicit none  
  
    <TTV formfactors: parameters>
```

```

    <TTV formfactors: interfaces>

contains

    <TTV formfactors: procedures>

end submodule ttv_formfactors_s

<TTV formfactors: public>≡
    public :: onshell_projection_t

<TTV formfactors: types>≡
    type :: onshell_projection_t
        logical :: production
        logical :: decay
        logical :: width
        logical :: boost_decay
contains
    <TTV formfactors: onshell projection: TBP>
end type onshell_projection_t

<TTV formfactors: onshell projection: TBP>≡
    procedure :: debug_write => onshell_projection_debug_write

<TTV formfactors: sub interfaces>≡
    module subroutine onshell_projection_debug_write (onshell_projection)
        class(onshell_projection_t), intent(in) :: onshell_projection
    end subroutine onshell_projection_debug_write

<TTV formfactors: procedures>≡
    module subroutine onshell_projection_debug_write (onshell_projection)
        class(onshell_projection_t), intent(in) :: onshell_projection
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%production", &
            onshell_projection%production)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%decay", &
            onshell_projection%decay)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%width", &
            onshell_projection%width)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%boost_decay", &
            onshell_projection%boost_decay)
    end subroutine onshell_projection_debug_write

<TTV formfactors: onshell projection: TBP>+≡
    procedure :: set_all => onshell_projection_set_all

<TTV formfactors: sub interfaces>+≡
    pure module subroutine onshell_projection_set_all (onshell_projection, flag)
        class(onshell_projection_t), intent(inout) :: onshell_projection
        logical, intent(in) :: flag
    end subroutine onshell_projection_set_all

<TTV formfactors: procedures>+≡
    pure module subroutine onshell_projection_set_all (onshell_projection, flag)
        class(onshell_projection_t), intent(inout) :: onshell_projection
        logical, intent(in) :: flag

```

```

        onshell_projection%production = flag
        onshell_projection%decay = flag
    end subroutine onshell_projection_set_all

<TTV formfactors: onshell projection: TBP>+≡
    procedure :: active => onshell_projection_active

<TTV formfactors: sub interfaces>+≡
    pure module function onshell_projection_active (onshell_projection) result (active)
        logical :: active
        class(onshell_projection_t), intent(in) :: onshell_projection
    end function onshell_projection_active

<TTV formfactors: procedures>+≡
    pure module function onshell_projection_active (onshell_projection) result (active)
        logical :: active
        class(onshell_projection_t), intent(in) :: onshell_projection
        active = onshell_projection%production .or. &
            onshell_projection%decay
    end function onshell_projection_active

<TTV formfactors: types>+≡
    type :: helicity_approximation_t
        logical :: simple = .false.
        logical :: extra = .false.
        logical :: ultra = .false.
    contains
    <TTV formfactors: helicity approximation: TBP>
    end type helicity_approximation_t

<TTV formfactors: public>+≡
    public :: settings_t

<TTV formfactors: types>+≡
    type :: settings_t
        ! look what is set by initialized_parameters, bundle them in a class and rename to initialize
        logical :: initialized_parameters
        ! this belongs to init_threshold_phase_space_grid in phase_space_grid_t
        logical :: initialized_ps
        ! this belongs to the ff_grid_t, its usefulness is doubtful
        logical :: initialized_ff
        logical :: mpole_dynamic
        integer :: offshell_strategy
        logical :: factorized_computation
        logical :: interference
        logical :: only_interference_term
        logical :: nlo
        logical :: no_nlo_width_in_signal_propagators
        logical :: force_minus_one
        logical :: flip_relative_sign
        integer :: sel_hel_top = 0
        integer :: sel_hel_topbar = 0
        logical :: Z_disabled
        type(onshell_projection_t) :: onshell_projection

```

```

        type(helicity_approximation_t) :: helicity_approximation
contains
    <TTV formfactors: settings: TBP>
end type settings_t

<TTV formfactors: settings: TBP>≡
    procedure :: setup_flags => settings_setup_flags

<TTV formfactors: sub interfaces>+≡
    module subroutine settings_setup_flags (settings, ff_in, offshell_strategy_in, &
        top_helicity_selection)
        class(settings_t), intent(inout) :: settings
        integer, intent(in) :: ff_in, offshell_strategy_in, top_helicity_selection
    end subroutine settings_setup_flags

<TTV formfactors: procedures>+≡
    ! TODO: (bcn 2016-03-21) break this up into a part regarding the
    ! FF grid and a part regarding the settings
    module subroutine settings_setup_flags (settings, ff_in, offshell_strategy_in, &
        top_helicity_selection)
        class(settings_t), intent(inout) :: settings
        integer, intent(in) :: ff_in, offshell_strategy_in, top_helicity_selection
        logical :: bit_top, bit_topbar
        !!! RESUMMED_SWITCHOFF = - 2
        !!! MATCHED = -1, &
        SWITCHOFF_RESUMMED = ff_in < 0
        TOPPIK_RESUMMED = ff_in <= 1
        settings%nlo = btest(offshell_strategy_in, 0)
        settings%factorized_computation = btest(offshell_strategy_in, 1)
        settings%interference = btest(offshell_strategy_in, 2)
        call settings%onshell_projection%set_all(btest(offshell_strategy_in, 3))
        settings%no_nlo_width_in_signal_propagators = btest(offshell_strategy_in, 4)
        settings%helicity_approximation%simple = btest(offshell_strategy_in, 5)
        if (.not. settings%onshell_projection%active ()) then
            settings%onshell_projection%production = btest(offshell_strategy_in, 6)
            settings%onshell_projection%decay = btest(offshell_strategy_in, 7)
        end if
        settings%onshell_projection%width = .not. btest(offshell_strategy_in, 8)
        settings%onshell_projection%boost_decay = btest(offshell_strategy_in, 9)
        settings%helicity_approximation%extra = btest(offshell_strategy_in, 10)
        settings%force_minus_one = btest(offshell_strategy_in, 11)
        settings%flip_relative_sign = btest(offshell_strategy_in, 12)
        if (top_helicity_selection > -1) then
            settings%helicity_approximation%ultra = .true.
            bit_top = btest (top_helicity_selection, 0)
            bit_topbar = btest (top_helicity_selection, 1)
            if (bit_top) then
                settings%sel_hel_top = 1
            else
                settings%sel_hel_top = -1
            end if
            if (bit_topbar) then
                settings%sel_hel_topbar = 1
            else
                settings%sel_hel_topbar = -1
            end if
        end if
    end subroutine settings_setup_flags

```

```

        end if
    end if
    settings%only_interference_term = btest(offshell_strategy_in, 14)
    settings%Z_disabled = btest(offshell_strategy_in, 15)
    if (ff_in == MATCHED .or. ff_in == MATCHED_NOTSOHARD) then
        settings%onshell_projection%width = .true.
        settings%onshell_projection%production = .true.
        settings%onshell_projection%decay = .true.
        settings%factorized_computation = .true.
        settings%interference = .true.
        settings%onshell_projection%boost_decay = .true.
    end if
    if (debug_on) call msg_debug (D_THRESHOLD, "SWITCHOFF_RESUMMED", SWITCHOFF_RESUMMED)
    if (debug_on) call msg_debug (D_THRESHOLD, "TOPPIK_RESUMMED", TOPPIK_RESUMMED)
    if (debug_active (D_THRESHOLD)) &
        call settings%write ()
end subroutine settings_setup_flags

```

<TTV formfactors: settings: TBP>+≡

```

    procedure :: write => settings_write

```

<TTV formfactors: sub interfaces>+≡

```

    module subroutine settings_write (settings, unit)
        class(settings_t), intent(in) :: settings
        integer, intent(in), optional :: unit
    end subroutine settings_write

```

<TTV formfactors: procedures>+≡

```

    module subroutine settings_write (settings, unit)
        class(settings_t), intent(in) :: settings
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, '(A,L1)') "settings%helicity_approximation%simple = ", &
            settings%helicity_approximation%simple
        write (u, '(A,L1)') "settings%helicity_approximation%extra = ", &
            settings%helicity_approximation%extra
        write (u, '(A,L1)') "settings%helicity_approximation%ultra = ", &
            settings%helicity_approximation%ultra
        write (u, '(A,L1)') "settings%initialized_parameters = ", &
            settings%initialized_parameters
        write (u, '(A,L1)') "settings%initialized_ps = ", &
            settings%initialized_ps
        write (u, '(A,L1)') "settings%initialized_ff = ", &
            settings%initialized_ff
        write (u, '(A,L1)') "settings%mpole_dynamic = ", &
            settings%mpole_dynamic
        write (u, '(A,I5)') "settings%offshell_strategy = ", &
            settings%offshell_strategy
        write (u, '(A,L1)') "settings%factorized_computation = ", &
            settings%factorized_computation
        write (u, '(A,L1)') "settings%interference = ", settings%interference
        write (u, '(A,L1)') "settings%only_interference_term = ", &
            settings%only_interference_term
        write (u, '(A,L1)') "settings%Z_disabled = ", &

```

```

        settings%Z_disabled
write (u, '(A,L1)') "settings%nlo = ", settings%nlo
write (u, '(A,L1)') "settings%no_nlo_width_in_signal_propagators = ", &
        settings%no_nlo_width_in_signal_propagators
write (u, '(A,L1)') "settings%force_minus_one = ", settings%force_minus_one
write (u, '(A,L1)') "settings%flip_relative_sign = ", settings%flip_relative_sign
call settings%onshell_projection%debug_write ()
end subroutine settings_write

<TTV formfactors: settings: TBP>+≡
    procedure :: use_nlo_width => settings_use_nlo_width

<TTV formfactors: sub interfaces>+≡
    pure module function settings_use_nlo_width (settings, ff) result (nlo)
        logical :: nlo
        class(settings_t), intent(in) :: settings
        integer, intent(in) :: ff
    end function settings_use_nlo_width

<TTV formfactors: procedures>+≡
    pure module function settings_use_nlo_width (settings, ff) result (nlo)
        logical :: nlo
        class(settings_t), intent(in) :: settings
        integer, intent(in) :: ff
        nlo = settings%nlo
    end function settings_use_nlo_width

<TTV formfactors: public>+≡
    public :: formfactor_t

<TTV formfactors: types>+≡
    type :: formfactor_t
        logical :: active
    contains
        <TTV formfactors: formfactor: TBP>
    end type formfactor_t

<TTV formfactors: formfactor: TBP>≡
    procedure :: activate => formfactor_activate

<TTV formfactors: sub interfaces>+≡
    pure module subroutine formfactor_activate (formfactor)
        class(formfactor_t), intent(inout) :: formfactor
    end subroutine formfactor_activate

<TTV formfactors: procedures>+≡
    pure module subroutine formfactor_activate (formfactor)
        class(formfactor_t), intent(inout) :: formfactor
        formfactor%active = .true.
    end subroutine formfactor_activate

<TTV formfactors: formfactor: TBP>+≡
    procedure :: disable => formfactor_disable

```



```

<TTV formfactors: sub interfaces>+≡
  pure module subroutine formfactor_disable (formfactor)
    class(formfactor_t), intent(inout) :: formfactor
  end subroutine formfactor_disable

```

```

<TTV formfactors: procedures>+≡
  pure module subroutine formfactor_disable (formfactor)
    class(formfactor_t), intent(inout) :: formfactor
    formfactor%active = .false.
  end subroutine formfactor_disable

```

This function actually returns \tilde{F} , i.e. $F - 1$.

```

<TTV formfactors: formfactor: TBP>+≡

```

```

  procedure :: compute => formfactor_compute

```

```

<TTV formfactors: sub interfaces>+≡

```

```

  module function formfactor_compute (formfactor, ps, vec_type, FF_mode) result (FF)
    complex(default) :: FF
    class(formfactor_t), intent(in) :: formfactor
    type(phase_space_point_t), intent(in) :: ps
    integer, intent(in) :: vec_type, FF_mode
  end function formfactor_compute

```

```

<TTV formfactors: procedures>+≡

```

```

  module function formfactor_compute (formfactor, ps, vec_type, FF_mode) result (FF)
    complex(default) :: FF
    class(formfactor_t), intent(in) :: formfactor
    type(phase_space_point_t), intent(in) :: ps
    integer, intent(in) :: vec_type, FF_mode
    real(default) :: f
    if (threshold%settings%initialized_parameters .and. formfactor%active) then
      select case (FF_mode)
        case (MATCHED, MATCHED_NOTSOHARD, RESUMMED, RESUMMED_SWITCHOFF)
          FF = resummed_formfactor (ps, vec_type) - one
        case (MATCHED_EXPANDED)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = - expanded_formfactor (f * AS_HARD, f * AS_HARD, ps, vec_type) &
            + resummed_formfactor (ps, vec_type)
        case (MATCHED_EXPANDED_NOTSOHARD)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = - expanded_formfactor (f * alphas_notsohard (ps%sqrts), f * &
            alphas_notsohard (ps%sqrts), ps, vec_type) &
            + resummed_formfactor (ps, vec_type)
        case (EXPANDED_HARD)
          FF = expanded_formfactor (AS_HARD, AS_HARD, ps, vec_type) - one
        case (EXPANDED_NOTSOHARD)
          FF = expanded_formfactor (alphas_notsohard (ps%sqrts), &
            alphas_notsohard (ps%sqrts), ps, vec_type) - one
        case (EXPANDED_SOFT)
          FF = expanded_formfactor (AS_HARD, alphas_soft (ps%sqrts), ps, &
            vec_type) - one
        case (EXPANDED_SOFT_SWITCHOFF)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = expanded_formfactor (f * AS_HARD, &
            f * alphas_soft (ps%sqrts), ps, vec_type) - one
      end select
    end if
  end function formfactor_compute

```

```

        case (RESUMMED_ANALYTIC_LL)
            FF = formfactor_LL_analytic (alphas_soft (ps%sqrts), ps%sqrts, &
                ps%p, vec_type) - one
        case (TREE)
            FF = zero
        case default
            FF = zero
        end select
    else
        FF = zero
    end if
    if (debug2_active (D_THRESHOLD)) then
        call update_global_sqrts_dependent_variables (ps%sqrts)
        call msg_debug2 (D_THRESHOLD, "threshold%settings%initialized_parameters", &
            threshold%settings%initialized_parameters)
        call msg_debug2 (D_THRESHOLD, "formfactor%active", formfactor%active)
        call msg_debug2 (D_THRESHOLD, "FF_mode", FF_mode)
        call msg_debug2 (D_THRESHOLD, "FF", FF)
        call msg_debug2 (D_THRESHOLD, "v", sqrts_to_v (ps%sqrts, GAM))
        call msg_debug2 (D_THRESHOLD, "vec_type", vec_type)
        call ps%write ()
    end if
end function formfactor_compute

```

<TTV formfactors: public>+≡

```
public :: width_t
```

<TTV formfactors: types>+≡

```

type :: width_t
    real(default) :: aem
    real(default) :: sw
    real(default) :: mw
    real(default) :: mb
    real(default) :: vtb
    real(default) :: gam_inv

```

contains

<TTV formfactors: width: TBP>

```
end type width_t
```

<TTV formfactors: width: TBP>≡

```
procedure :: init => width_init
```

<TTV formfactors: sub interfaces>+≡

```

pure module subroutine width_init (width, aemi, sw, mw, mb, vtb, gam_inv)
    class(width_t), intent(inout) :: width
    real(default), intent(in) :: aemi, sw, mw, mb, vtb, gam_inv
end subroutine width_init

```

<TTV formfactors: procedures>+≡

```

pure module subroutine width_init (width, aemi, sw, mw, mb, vtb, gam_inv)
    class(width_t), intent(inout) :: width
    real(default), intent(in) :: aemi, sw, mw, mb, vtb, gam_inv
    width%aem = one / aemi
    width%sw = sw
    width%mw = mw

```

```

width%mb = mb
width%vtb = vtb
width%gam_inv = gam_inv
end subroutine width_init

```

```

<TTV formfactors: width: TBP>+≡
  procedure :: compute => width_compute

<TTV formfactors: sub interfaces>+≡
  pure module function width_compute (width, top_mass, sqrts, initial) result (gamma)
    real(default) :: gamma
    class(width_t), intent(in) :: width
    real(default), intent(in) :: top_mass, sqrts
    logical, intent(in), optional :: initial
  end function width_compute

<TTV formfactors: procedures>+≡
  pure module function width_compute (width, top_mass, sqrts, initial) result (gamma)
    real(default) :: gamma
    class(width_t), intent(in) :: width
    real(default), intent(in) :: top_mass, sqrts
    logical, intent(in), optional :: initial
    real(default) :: alphas
    logical :: ini
    ini = .false.; if (present (initial)) ini = initial
    if (ini) then
      alphas = AS_HARD
    else
      alphas = alphas_notsohard (sqrts)
    end if
    if (threshold%settings%nlo) then
      gamma = top_width_sm_qcd_nlo_jk (width%aem, width%sw, width%vtb, &
        top_mass, width%mw, width%mb, alphas) + width%gam_inv
    else
      gamma = top_width_sm_lo (width%aem, width%sw, width%vtb, top_mass, &
        width%mw, width%mb) + width%gam_inv
    end if
  end function width_compute

```

Use singleton pattern instead of global variables. At least shows where the variables are from.

```

<TTV formfactors: public>+≡
  public :: threshold

<TTV formfactors: public>+≡
  public :: threshold_t

<TTV formfactors: global variables>≡
  type(threshold_t) :: threshold

<TTV formfactors: types>+≡
  type :: threshold_t
    type(settings_t) :: settings
    type(formfactor_t) :: formfactor
    type(width_t) :: width

```

```

contains
  <TTV formfactors: threshold: TBP>
end type threshold_t

<TTV formfactors: public parameters>≡
  integer, parameter, public :: &
    MATCHED_EXPANDED_NOTSOHARD = -5, &
    MATCHED_NOTSOHARD = -4, &
    MATCHED_EXPANDED = - 3, &
    RESUMMED_SWITCHOFF = - 2, &
    MATCHED = -1, &
    RESUMMED = 1, &
    EXPANDED_HARD = 4, &
    EXPANDED_SOFT = 5, &
    EXPANDED_SOFT_SWITCHOFF = 6, &
    RESUMMED_ANALYTIC_LL = 7, &
    EXPANDED_NOTSOHARD = 8, &
    TREE = 9

<TTV formfactors: parameters>≡
  integer, parameter :: VECTOR = 1
  integer, parameter :: AXIAL = 2
  real(default), parameter :: NF = 5.0_default

  real(default), parameter :: z3 = 1.20205690315959428539973816151_default
  real(default), parameter :: A1 = 31./9.*CA - 20./9.*TR*NF
  real(default), parameter :: A2 = (4343./162. + 4.*pi**2 - pi**4/4. + &
    22./3.*z3)*CA**2 - (1798./81. + 56./3.*z3)*CA*TR*NF - &
    (55./3. - 16.*z3)*CF*TR*NF + (20./9.*TR*NF)**2
  complex(default), parameter :: ieps = imago*tiny_10

gam_m1s is only used for the scale nustar
<TTV formfactors: public>+≡
  public :: GAM, GAM_M1S

<TTV formfactors: global variables>+≡
  real(default) :: M1S, GAM, GAM_M1S
  integer :: NRQCD_ORDER
  real(default) :: MTPOLE = - one
  real(default) :: mtpole_init
  real(default) :: RESCALE_H, MU_HARD, AS_HARD
  real(default) :: AS_MZ, MASS_Z
  real(default) :: MU_USOFT, AS_USOFT

NUSTAR_FIXED is normally not used
<TTV formfactors: public>+≡
  public :: AS_SOFT
  public :: AS_LL_SOFT
  public :: AS_USOFT
  public :: AS_HARD
  public :: SWITCHOFF_RESUMMED
  public :: TOPPIK_RESUMMED

```

```

<TTV formfactors: global variables>+≡
  real(default) :: RESCALE_F, MU_SOFT, AS_SOFT, AS_LL_SOFT, NUSTAR_FIXED
  logical :: NUSTAR_DYNAMIC, SWITCHOFF_RESUMMED, TOPPIK_RESUMMED
  real(default) :: B0
  real(default) :: B1

  real(default), dimension(2) :: aa2, aa3, aa4, aa5, aa8, aa0
  character(len=200) :: parameters_ref
  type(nr_spline_t) :: ff_p_spline
  real(default) :: v1, v2

  integer :: POINTS_SQ, POINTS_P, POINTS_PO, n_q
  real(default), dimension(:), allocatable :: sq_grid, p_grid, p0_grid, q_grid
  complex(default), dimension(:,:,:), allocatable :: ff_grid
  complex(single), dimension(:,:,:), allocatable :: Vmatrix

```

Explicit range and step size of the sqrts-grid relative to 2*M1S:

```

<TTV formfactors: global variables>+≡
  real(default) :: sqrts_min, sqrts_max, sqrts_it

<TTV formfactors: interfaces>≡
  interface char
    module procedure int_to_char, real_to_char, complex_to_char, logical_to_char
  end interface char

<TTV formfactors: public>+≡
  public :: m1s_to_mpole

<TTV formfactors: public>+≡
  public :: phase_space_point_t

<TTV formfactors: types>+≡
  type :: phase_space_point_t
    real(default) :: p2 = 0, k2 = 0, q2 = 0
    real(default) :: sqrts = 0, p = 0, p0 = 0
    real(default) :: mpole = 0, en = 0
    logical :: inside_grid = .false., onshell = .false.
  contains
    <TTV formfactors: phase space point: TBP>
  end type phase_space_point_t

<TTV formfactors: phase space point: TBP>≡
  procedure :: init => phase_space_point_init_rel

<TTV formfactors: sub interfaces>+≡
  pure module subroutine phase_space_point_init_rel (ps_point, p2, k2, q2, m)
    class(phase_space_point_t), intent(inout) :: ps_point
    real(default), intent(in) :: p2
    real(default), intent(in) :: k2
    real(default), intent(in) :: q2
    real(default), intent(in), optional :: m
  end subroutine phase_space_point_init_rel

```

<TTV formfactors: procedures>+≡

```

pure module subroutine phase_space_point_init_rel (ps_point, p2, k2, q2, m)
  class(phase_space_point_t), intent(inout) :: ps_point
  real(default), intent(in) :: p2
  real(default), intent(in) :: k2
  real(default), intent(in) :: q2
  real(default), intent(in), optional :: m
  ps_point%p2 = p2
  ps_point%k2 = k2
  ps_point%q2 = q2
  call rel_to_nonrel (p2, k2, q2, ps_point%sqrts, ps_point%p, ps_point%p0)
  ps_point%mpole = mls_to_mpole (ps_point%sqrts)
  ps_point%en = sqrts_to_en (ps_point%sqrts)
  ps_point%inside_grid = sqrts_within_range (ps_point%sqrts)
  if ( present(m) ) ps_point%onshell = ps_point%is_onshell (m)
end subroutine phase_space_point_init_rel

```

<TTV formfactors: phase space point: TBP>+≡

```

procedure :: init_nonrel => phase_space_point_init_nonrel

```

<TTV formfactors: sub interfaces>+≡

```

pure module subroutine phase_space_point_init_nonrel (ps_point, sqrts, p, p0, m)
  class(phase_space_point_t), intent(inout) :: ps_point
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: p
  real(default), intent(in) :: p0
  real(default), intent(in), optional :: m
end subroutine phase_space_point_init_nonrel

```

<TTV formfactors: procedures>+≡

```

pure module subroutine phase_space_point_init_nonrel (ps_point, sqrts, p, p0, m)
  class(phase_space_point_t), intent(inout) :: ps_point
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: p
  real(default), intent(in) :: p0
  real(default), intent(in), optional :: m
  ps_point%sqrts = sqrts
  ps_point%p = p
  ps_point%p0 = p0
  call nonrel_to_rel (sqrts, p, p0, ps_point%p2, ps_point%k2, ps_point%q2)
  ps_point%mpole = mls_to_mpole (sqrts)
  ps_point%en = sqrts_to_en (sqrts, ps_point%mpole)
  ps_point%inside_grid = sqrts_within_range (sqrts)
  if ( present(m) ) ps_point%onshell = ps_point%is_onshell (m)
end subroutine phase_space_point_init_nonrel

```

<TTV formfactors: procedures>+≡

```

!!! convert squared 4-momenta into sqrts, p0 = E_top-sqrts/2 and abs. 3-momentum p
pure subroutine rel_to_nonrel (p2, k2, q2, sqrts, p, p0)
  real(default), intent(in) :: p2
  real(default), intent(in) :: k2
  real(default), intent(in) :: q2
  real(default), intent(out) :: sqrts
  real(default), intent(out) :: p

```

```

    real(default), intent(out) :: p0
    sqrts = sqrt(q2)
    p0 = abs(p2 - k2) / (2. * sqrts)
    p = sqrt (0.5_default * (- p2 - k2 + sqrts**2/2. + 2.* p0**2))
end subroutine rel_to_nonrel

<TTV formfactors: procedures>+≡
!!! convert sqrts, p0 = E_top-sqrts/2 and abs. 3-momentum p into squared 4-momenta
pure subroutine nonrel_to_rel (sqrts, p, p0, p2, k2, q2)
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: p
    real(default), intent(in) :: p0
    real(default), intent(out) :: p2
    real(default), intent(out) :: k2
    real(default), intent(out) :: q2
    p2 = (sqrts/2.+p0)**2 - p**2
    k2 = (sqrts/2.-p0)**2 - p**2
    q2 = sqrts**2
end subroutine nonrel_to_rel

<TTV formfactors: procedures>+≡
pure function complex_m2 (m, w) result (m2c)
    real(default), intent(in) :: m
    real(default), intent(in) :: w
    complex(default) :: m2c
    m2c = m**2 - imago*m*w
end function complex_m2

<TTV formfactors: phase space point: TBP>+≡
procedure :: is_onshell => phase_space_point_is_onshell

<TTV formfactors: sub interfaces>+≡
pure module function phase_space_point_is_onshell (ps_point, m) result (flag)
    logical :: flag
    class(phase_space_point_t), intent(in) :: ps_point
    real(default), intent(in) :: m
end function phase_space_point_is_onshell

<TTV formfactors: procedures>+≡
pure module function phase_space_point_is_onshell (ps_point, m) result (flag)
    logical :: flag
    class(phase_space_point_t), intent(in) :: ps_point
    real(default), intent(in) :: m
    flag = nearly_equal (ps_point%p2 , m**2, rel_smallness=1E-5_default) .and. &
        nearly_equal (ps_point%k2 , m**2, rel_smallness=1E-5_default)
end function phase_space_point_is_onshell

<TTV formfactors: phase space point: TBP>+≡
procedure :: write => phase_space_point_write

<TTV formfactors: sub interfaces>+≡
module subroutine phase_space_point_write (psp, unit)
    class(phase_space_point_t), intent(in) :: psp
    integer, intent(in), optional :: unit
end subroutine phase_space_point_write

```

<TTV formfactors: procedures>+≡

```

module subroutine phase_space_point_write (psp, unit)
  class(phase_space_point_t), intent(in) :: psp
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, '(A)') char ("p2 = " // str (psp%p2))
  write (u, '(A)') char ("k2 = " // str (psp%k2))
  write (u, '(A)') char ("q2 = " // str (psp%q2))
  write (u, '(A)') char ("sqrts = " // str (psp%sqrts))
  write (u, '(A)') char ("p = " // str (psp%p))
  write (u, '(A)') char ("p0 = " // str (psp%p0))
  write (u, '(A)') char ("mpole = " // str (psp%mpole))
  write (u, '(A)') char ("en = " // str (psp%en))
  write (u, '(A)') char ("inside_grid = " // str (psp%inside_grid))
  write (u, '(A)') char ("onshell = " // str (psp%onshell))
end subroutine phase_space_point_write

```

<TTV formfactors: procedures>+≡

```

function set_nrqcd_order (nrqcd_order_in) result (nrqcdorder)
  integer :: nrqcdorder
  real(default), intent(in) :: nrqcd_order_in
  nrqcdorder = 1
  if ( int(nrqcd_order_in) > nrqcdorder ) then
    call msg_warning ("reset to highest available NRQCD_ORDER = " // char(nrqcdorder))
  else
    nrqcdorder = int(nrqcd_order_in)
  end if
end function set_nrqcd_order

```

<TTV formfactors: public>+≡

public :: init_parameters

<TTV formfactors: sub interfaces>+≡

```

module subroutine init_parameters (mpole_out, gam_out, m1s_in, Vtb, gam_inv, &
  aemi, sw, az, mz, mw, mb, h_in, f_in, nrqcd_order_in, ff_in, &
  offshell_strategy_in, v1_in, v2_in, scan_sqrts_min, &
  scan_sqrts_max, scan_sqrts_stepsize, mpole_fixed, top_helicity_selection)
  real(default), intent(out) :: mpole_out
  real(default), intent(out) :: gam_out
  real(default), intent(in) :: m1s_in
  real(default), intent(in) :: Vtb
  real(default), intent(in) :: gam_inv
  real(default), intent(in) :: aemi
  real(default), intent(in) :: sw
  real(default), intent(in) :: az
  real(default), intent(in) :: mz
  real(default), intent(in) :: mw
  real(default), intent(in) :: mb
  real(default), intent(in) :: h_in
  real(default), intent(in) :: f_in
  real(default), intent(in) :: nrqcd_order_in
  real(default), intent(in) :: ff_in
  real(default), intent(in) :: offshell_strategy_in

```



```

    real(default), intent(in) :: v1_in
    real(default), intent(in) :: v2_in
    real(default), intent(in) :: scan_sqrts_min
    real(default), intent(in) :: scan_sqrts_max
    real(default), intent(in) :: scan_sqrts_stepsize
    logical, intent(in) :: mpole_fixed
    real(default), intent(in) :: top_helicity_selection
end subroutine init_parameters

<TTV formfactors: procedures>+≡
module subroutine init_parameters (mpole_out, gam_out, m1s_in, Vtb, gam_inv, &
    aemi, sw, az, mz, mw, mb, h_in, f_in, nrqcd_order_in, ff_in, &
    offshell_strategy_in, v1_in, v2_in, scan_sqrts_min, &
    scan_sqrts_max, scan_sqrts_stepsize, mpole_fixed, top_helicity_selection)
    real(default), intent(out) :: mpole_out
    real(default), intent(out) :: gam_out
    real(default), intent(in) :: m1s_in
    real(default), intent(in) :: Vtb
    real(default), intent(in) :: gam_inv
    real(default), intent(in) :: aemi
    real(default), intent(in) :: sw
    real(default), intent(in) :: az
    real(default), intent(in) :: mz
    real(default), intent(in) :: mw
    real(default), intent(in) :: mb
    real(default), intent(in) :: h_in
    real(default), intent(in) :: f_in
    real(default), intent(in) :: nrqcd_order_in
    real(default), intent(in) :: ff_in
    real(default), intent(in) :: offshell_strategy_in
    real(default), intent(in) :: v1_in
    real(default), intent(in) :: v2_in
    real(default), intent(in) :: scan_sqrts_min
    real(default), intent(in) :: scan_sqrts_max
    real(default), intent(in) :: scan_sqrts_stepsize
    logical, intent(in) :: mpole_fixed
    real(default), intent(in) :: top_helicity_selection
    if (debug_active (D_THRESHOLD)) call show_input()
    threshold%settings%initialized_parameters = .false.
    M1S = m1s_in
    threshold%settings%mpole_dynamic = .not. mpole_fixed
    threshold%settings%offshell_strategy = int (offshell_strategy_in)
    call threshold%settings%setup_flags (int(ff_in), &
        threshold%settings%offshell_strategy, &
        int (top_helicity_selection))
    NRQCD_ORDER = set_nrqcd_order (nrqcd_order_in)
    v1 = v1_in
    v2 = v2_in
    sqrts_min = scan_sqrts_min
    sqrts_max = scan_sqrts_max
    sqrts_it = scan_sqrts_stepsize
    !!! global hard parameters incl. hard alphas used in all form factors
    RESCALE_H = h_in
    MU_HARD   = M1S * RESCALE_H
    AS_MZ     = az

```

```

MASS_Z      = mz
AS_HARD     = running_as (MU_HARD, az, mz, 2, NF)
call threshold%width%init (aemi, sw, mw, mb, vtb, gam_inv)
GAM_M1S = threshold%width%compute (M1S, zero, initial=.true.)
call compute_global_auxiliary_numbers ()
!!! soft parameters incl. mtpole
!!! (depend on sqrts: initialize with sqrts ~ 2*M1S)
NUSTAR_FIXED = - one
NUSTAR_DYNAMIC = NUSTAR_FIXED < zero
RESCALE_F = f_in
call update_global_sqrts_dependent_variables (2. * M1S)
mtpole_init = MTPOLE
mpole_out = mtpole_init
gam_out = GAM
threshold%settings%initialized_parameters = .true.
contains
  <TTV formfactors: init parameters: subroutines>
end subroutine init_parameters

```

<TTV formfactors: init parameters: subroutines>≡

```

subroutine show_input()
  if (debug_on) call msg_debug (D_THRESHOLD, "init_parameters")
  if (debug_on) call msg_debug (D_THRESHOLD, "m1s_in", m1s_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "Vtb", Vtb)
  if (debug_on) call msg_debug (D_THRESHOLD, "gam_inv", gam_inv)
  if (debug_on) call msg_debug (D_THRESHOLD, "aemi", aemi)
  if (debug_on) call msg_debug (D_THRESHOLD, "sw", sw)
  if (debug_on) call msg_debug (D_THRESHOLD, "az", az)
  if (debug_on) call msg_debug (D_THRESHOLD, "mz", mz)
  if (debug_on) call msg_debug (D_THRESHOLD, "mw", mw)
  if (debug_on) call msg_debug (D_THRESHOLD, "mb", mb)
  if (debug_on) call msg_debug (D_THRESHOLD, "h_in", h_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "f_in", f_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "nrqcd_order_in", nrqcd_order_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "ff_in", ff_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "offshell_strategy_in", offshell_strategy_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "top_helicity_selection", top_helicity_selection)
  if (debug_on) call msg_debug (D_THRESHOLD, "v1_in", v1_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "v2_in", v2_in)
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_min", scan_sqrts_min)
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_max", scan_sqrts_max)
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_stepsize", scan_sqrts_stepsize)
  if (debug_on) call msg_debug (D_THRESHOLD, "AS_HARD", AS_HARD)
end subroutine show_input

```

<TTV formfactors: procedures>+≡

```

subroutine compute_global_auxiliary_numbers ()
  !!! auxiliary numbers needed later
  !!! current coefficients Ai(S,L,J), cf. arXiv:hep-ph/0609151, Eqs. (63)-(64)
  !!! 3S1 coefficients (s-wave, vector current)
  B0 = coeff_b0(NF) * (4.*pi)
  B1 = coeff_b1(NF) * (4.*pi)**2
  aa2(1) = (CF*(CA*CF*(9.*CA - 100.*CF) - &

```

```

      B0*(26.*CA**2 + 19.*CA*CF - 32.*CF**2)))/(26.*B0**2 *CA)
aa3(1) = CF**2/( B0**2 *(6.*B0 - 13.*CA)*(B0 - 2.*CA)) * &
      (CA**2 *(9.*CA - 100.*CF) + B0*CA*(74.*CF - CA*16.) - &
      6.*B0**2 *(2.*CF - CA))
aa4(1) = (24.*CF**2 * (11.*CA - 3.*B0)*(5.*CA + 8.*CF)) / &
      (13.*CA*(6.*B0 - 13.*CA)**2)
aa5(1) = (CF**2 * (CA*(15.-28) + B0*5.))/(6.*(B0-2.*CA)**2)
aa8(1) = zero
aa0(1) = -((8.*CF*(CA + CF)*(CA + 2.*CF))/(3.*B0**2))
!!! 3P1 coefficients (p-wave, axial vector current)
aa2(2) = -1./3. * (CF*(CA+2.*CF)/B0 - CF**2/(4.*B0) )
aa3(2) = zero
aa4(2) = zero
aa5(2) = 1./3. * CF**2/(4.*(B0-2.*CA))
aa8(2) = -1./3. * CF**2/(B0-CA)
aa0(2) = -1./3. * 8.*CA*CF*(CA+4.*CF)/(3.*B0**2)
end subroutine compute_global_auxiliary_numbers

```

<TTV formfactors: public>+≡

```
public :: init_threshold_grids
```

<TTV formfactors: sub interfaces>+≡

```

module subroutine init_threshold_grids (test)
  real(default), intent(in) :: test
end subroutine init_threshold_grids

```

<TTV formfactors: procedures>+≡

```

module subroutine init_threshold_grids (test)
  real(default), intent(in) :: test
  if (debug_active (D_THRESHOLD)) then
    call msg_debug (D_THRESHOLD, "init_threshold_grids")
    call msg_debug (D_THRESHOLD, "TOPPIK_RESUMMED", TOPPIK_RESUMMED)
  end if
  if (test > zero) then
    call msg_message ("TESTING ONLY: Skip threshold initialization and use tree-level SM.")
    return
  end if
  if (.not. threshold%settings%initialized_parameters) &
    call msg_fatal ("init_threshold_grid: parameters not initialized!")
  !!! !!! !!! MAC OS X and BSD don't load the global module with parameter values stored
  !!! if (parameters_ref == parameters_string ()) return
  call dealloc_grids ()
  if (TOPPIK_RESUMMED) call init_formfactor_grid ()
  parameters_ref = parameters_string ()
end subroutine init_threshold_grids

```

<TTV formfactors: procedures>+≡

```

!!! LL/NLL resummation of nonrelativistic Coulomb potential
pure function resummed_formfactor (ps, vec_type) result (c)
  type(phase_space_point_t), intent(in) :: ps
  integer, intent(in) :: vec_type
  complex(default) :: c
  c = one
  if (.not. threshold%settings%initialized_ff .or. .not. ps%inside_grid) return

```

```

if (POINTS_SQ > 1) then
  call interpolate_linear (sq_grid, p_grid, ff_grid(:, :, 1, vec_type), ps%sqrts, ps%p, c)
else
  call interpolate_linear (p_grid, ff_grid(1, :, 1, vec_type), ps%p, c)
end if
end function resummed_formfactor

```

(TTV formfactors: procedures)+≡

```

!!! leading nonrelativistic  $O(\alpha_s^1)$  contribution (-> expansion of resummation)
function expanded_formfactor (alphas_hard, alphas_soft, ps, vec_type) result (FF)
  complex(default) :: FF
  real(default), intent(in) :: alphas_hard, alphas_soft
  type(phase_space_point_t), intent(in) :: ps
  integer, intent(in) :: vec_type
  real(default) :: shift_from_hard_current
  complex(default) :: v, contrib_from_potential
  FF = one
  if (.not. threshold%settings%initialized_parameters) return
  call update_global_sqrts_dependent_variables (ps%sqrts)
  v = sqrts_to_v (ps%sqrts, GAM)
  if (NRQCD_ORDER == 1) then
    if (vec_type == AXIAL) then
      shift_from_hard_current = - CF / pi
    else
      shift_from_hard_current = - two * CF / pi
    end if
  else
    shift_from_hard_current = zero
  end if
  if (ps%onshell) then
    contrib_from_potential = CF * ps%mpole * Pi / (4 * ps%p)
  else
    if (vec_type == AXIAL) then
      contrib_from_potential = - CF * ps%mpole / (two * ps%p) * &
        (imago * ps%mpole * v / ps%p + &
        (ps%mpole**2 * v**2 + (ps%p)**2) / (4 * Pi * (ps%p)**2) * ( &
        (log (- ps%mpole * v - ps%p))**2 - &
        (log (- ps%mpole * v + ps%p))**2 + &
        (log (ps%mpole * v - ps%p))**2 - &
        (log (ps%mpole * v + ps%p))**2 ))
    else
      contrib_from_potential = imago * CF * ps%mpole * &
        log ((ps%p + ps%mpole * v) / &
        (-ps%p + ps%mpole * v) + ieps) / (two * ps%p)
    end if
  end if
  FF = one + alphas_soft * contrib_from_potential + &
    alphas_hard * shift_from_hard_current
end function expanded_formfactor

```

(TTV formfactors: procedures)+≡

```

subroutine init_formfactor_grid ()
  type(string_t) :: ff_file

```

```

if (debug_on) call msg_debug (D_THRESHOLD, "init_formfactor_grid")
threshold%settings%initialized_ff = .false.
ff_file = "SM_tt_threshold.grid"
call msg_message ()
call msg_message ("%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%")
call msg_message (" Initialize e+e- => ttbar threshold resummation:")
call msg_message (" Use analytic (LL) or TOPPIK (NLL) form factors for ttA/ttZ vector")
call msg_message (" and axial vector couplings (S/P-wave) in the threshold region.")
call msg_message (" Cf. threshold shapes from A. Hoang et al.: [arXiv:hep-ph/0107144],")
call msg_message (" [arXiv:1309.6323].")
if (NRQCD_ORDER > 0) then
    call msg_message (" Numerical NLL solutions calculated with TOPPIK [arXiv:hep-ph/9904468]")
    call msg_message (" by M. Jezabek, T. Teubner.")
end if
call msg_message ("%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%")
call msg_message ()
call read_formfactor_grid (ff_file)
if (.not. threshold%settings%initialized_ff) then
    if (.not. threshold%settings%initialized_ps) call init_threshold_phase_space_grid ()
    call scan_formfactor_over_phase_space_grid ()
    call write_formfactor_grid (ff_file)
end if
end subroutine init_formfactor_grid

```

(TTV formfactors: procedures)+≡

```

subroutine read_formfactor_grid (ff_file)
    type(string_t), intent(in) :: ff_file
    complex(single), dimension(:, :, :, :), allocatable :: ff_grid_sp
    character(len(parameters_ref)) :: parameters
    integer :: u, st
    logical :: ex
    integer, dimension(4) :: ff_shape
    if (debug_on) call msg_debug (D_THRESHOLD, "read_formfactor_grid")
    inquire (file=char(ff_file), exist=ex)
    if (.not. ex) return
    u = free_unit ()
    call msg_message ("Opening grid file: " // char(ff_file))
    open (unit=u, status='old', file=char(ff_file), form='unformatted', iostat=st)
    if (st /= 0) call msg_fatal ("iostat = " // char(st))
    read (u) parameters
    read (u) ff_shape
    if (ff_shape(4) /= 2) call msg_fatal ("read_formfactor_grid: i = " // char(ff_shape(4)))
    if (parameters /= parameters_string ()) then
        call msg_message ("Threshold setup has changed: recalculate threshold grid.")
        close (unit=u, status='delete')
        return
    end if
    call msg_message ("Threshold setup unchanged: reusing existing threshold grid.")
    POINTS_SQ = ff_shape(1)
    POINTS_P = ff_shape(2)
    if (debug_active (D_THRESHOLD)) then
        call msg_debug (D_THRESHOLD, "ff_shape(1) (POINTS_SQ)", ff_shape(1))
        call msg_debug (D_THRESHOLD, "ff_shape(2)", ff_shape(2))
        call msg_debug (D_THRESHOLD, "ff_shape(3) (POINTS_P0)", ff_shape(3))
    end if
end subroutine read_formfactor_grid

```

```

        call msg_debug (D_THRESHOLD, "ff_shape(4) (==2)", ff_shape(4))
    end if
    allocate (sq_grid(POINTS_SQ))
    read (u) sq_grid
    allocate (p_grid(POINTS_P))
    read (u) p_grid
    POINTS_PO = ff_shape(3)
    allocate (ff_grid_sp(POINTS_SQ,POINTS_P,POINTS_PO,2))
    read (u) ff_grid_sp
    allocate (ff_grid(POINTS_SQ,POINTS_P,POINTS_PO,2))
    ff_grid = cmplx (ff_grid_sp, kind=default)
    close (u, iostat=st)
    if (st > 0) call msg_fatal ("close " // char(ff_file) // ": iostat = " // char(st))
    threshold%settings%initialized_ps = .true.
    threshold%settings%initialized_ff = .true.
end subroutine read_formfactor_grid

```

<TTV formfactors: procedures>+≡

```

subroutine write_formfactor_grid (ff_file)
    type(string_t), intent(in) :: ff_file
    integer :: u, st
    if (.not. threshold%settings%initialized_ff) then
        call msg_warning ("write_formfactor_grid: no grids initialized!")
        return
    end if
    u = free_unit ()
    open (unit=u, status='replace', file=char(ff_file), form='unformatted', iostat=st)
    if (st /= 0) call msg_fatal ("open " // char(ff_file) // ": iostat = " // char(st))
    write (u) parameters_string ()
    write (u) shape(ff_grid)
    write (u) sq_grid
    write (u) p_grid
    write (u) cmplx(ff_grid, kind=single)
    close (u, iostat=st)
    if (st > 0) call msg_fatal ("close " // char(ff_file) // ": iostat = " // char(st))
end subroutine write_formfactor_grid

```

<TTV formfactors: procedures>+≡

```

pure function parameters_string () result (str)
    character(len(parameters_ref)) :: str
    str = char(M1S) // " " // char(GAM_M1S) &
        // " " // char(NRQCD_ORDER) &
        // " " // char(RESCALE_H) &
        // " " // char(RESCALE_F) &
        // " " // char(sqrts_min) &
        // " " // char(sqrts_max) &
        // " " // char(sqrts_it)
end function parameters_string

```

<TTV formfactors: procedures>+≡

```

subroutine update_global_sqrts_dependent_variables (sqrts)
    real(default), intent(in) :: sqrts
    real(default) :: nu_soft, f

```

```

logical :: only_once_for_fixed_nu, already_done
real(default), save :: last_sqrts = - one
if (debug_on) call msg_debug (D_THRESHOLD, "update_global_sqrts_dependent_variables")
if (debug_on) call msg_debug (D_THRESHOLD, "sqrts", sqrts)
if (debug_on) call msg_debug (D_THRESHOLD, "last_sqrts", last_sqrts)
already_done = threshold%settings%initialized_parameters .and. &
    nearly_equal (sqrts, last_sqrts, rel_smallness=1E-6_default)
if (debug_on) call msg_debug (D_THRESHOLD, "already_done", already_done)
only_once_for_fixed_nu = .not. NUSTAR_DYNAMIC .and. MTPOLE > zero
if (debug_on) call msg_debug (D_THRESHOLD, "only_once_for_fixed_nu", only_once_for_fixed_nu)
if (only_once_for_fixed_nu .or. already_done) return
last_sqrts = sqrts
nu_soft = RESCALE_F * nustar (sqrts)
MU_SOFT = M1S * RESCALE_H * nu_soft
MU_USOFT = M1S * RESCALE_H * nu_soft**2
AS_SOFT = running_as (MU_SOFT, AS_HARD, MU_HARD, NRQCD_ORDER, NF)
AS_LL_SOFT = running_as (MU_SOFT, AS_HARD, MU_HARD, 0, NF)
AS_USOFT = running_as (MU_USOFT, AS_HARD, MU_HARD, 0, NF) !!! LL here
if (SWITCHOFF_RESUMMED) then
    f = f_switch_off (v_matching (sqrts, GAM_M1S))
    AS_SOFT = AS_SOFT * f
    AS_LL_SOFT = AS_LL_SOFT * f
    AS_USOFT = AS_USOFT * f
end if
MTPOLE = m1s_to_mpole (sqrts)
GAM = threshold%width%compute (MTPOLE, sqrts)
if (debug_on) call msg_debug (D_THRESHOLD, "GAM", GAM)
if (debug_on) call msg_debug (D_THRESHOLD, "nu_soft", nu_soft)
if (debug_on) call msg_debug (D_THRESHOLD, "MTPOLE", MTPOLE)
if (debug_on) call msg_debug (D_THRESHOLD, "AS_SOFT", AS_SOFT)
if (debug_on) call msg_debug (D_THRESHOLD, "AS_LL_SOFT", AS_LL_SOFT)
if (debug_on) call msg_debug (D_THRESHOLD, "AS_USOFT", AS_USOFT)
end subroutine update_global_sqrts_dependent_variables

!!! Coulomb potential coefficients needed by TOPPIK
pure function xc (a_soft, i_xc) result (xci)
    real(default), intent(in) :: a_soft
    integer, intent(in) :: i_xc
    real(default) :: xci
    xci = zero
    select case (i_xc)
        case (0)
            xci = one
            if ( NRQCD_ORDER>0 ) xci = xci + a_soft/(4.*pi) * A1
            if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * A2
        case (1)
            if ( NRQCD_ORDER>0 ) xci = xci + a_soft/(4.*pi) * B0
            if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * (B1 + 2*B0*A1)
        case (2)
            if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * B0**2
        case default
            return
    end select
end function xc

```

<TTV formfactors: procedures>+≡

```
function current_coeff (a_hard, a_soft, a_usoft, i) result (coeff)
  real(default), intent(in) :: a_hard, a_soft, a_usoft
  integer, intent(in) :: i
  real(default) :: coeff
  real(default) :: matching_c, c1
  real(default) :: z, w
  if (debug_on) call msg_debug (D_THRESHOLD, "current_coeff")
  coeff = one
  if (NRQCD_ORDER == 0) return
  z = a_soft / a_hard
  w = a_usoft / a_soft
  !!! hard s/p-wave 1-loop matching coefficients, cf. arXiv:hep-ph/0604072
  select case (i)
    case (1)
      matching_c = one - 2.*(CF/pi) * a_hard
    case (2)
      matching_c = one - (CF/pi) * a_hard
    case default
      call msg_fatal ("current_coeff: unknown coeff i = " // char(i))
  end select
  !!! current coefficient c1, cf. arXiv:hep-ph/0609151, Eq. (62)
  c1 = exp( a_hard * pi * ( aa2(i)*(1.-z) + aa3(i)*log(z) + &
    aa4(i)*(1.-z**(1.-13.*CA/(6.*B0))) + aa5(i)*(1.-z**(1.-2.*CA/B0)) + &
    aa8(i)*(1.-z**(1.-CA/B0)) + aa0(i)*(z-1.-log(w)/w) ))
  coeff = matching_c * c1
end function current_coeff
```

<TTV formfactors: public>+≡

```
public :: v_matching
```

<TTV formfactors: sub interfaces>+≡

```
pure module function v_matching (sqrts, gamma) result (v)
  real(default) :: v
  real(default), intent(in) :: sqrts, gamma
end function v_matching
```

<TTV formfactors: procedures>+≡

```
pure module function v_matching (sqrts, gamma) result (v)
  real(default) :: v
  real(default), intent(in) :: sqrts, gamma
  v = abs (sqrts_to_v_1S (sqrts, gamma))
end function v_matching
```

Smooth transition from f1 to f2 between v1 and v2 (simplest polynomial).

<TTV formfactors: public>+≡

```
public :: f_switch_off
```

<TTV formfactors: sub interfaces>+≡

```
pure module function f_switch_off (v) result (fval)
  real(default), intent(in) :: v
  real(default) :: fval
end function f_switch_off
```


<TTV formfactors: procedures>+≡

```

pure module function f_switch_off (v) result (fval)
  real(default), intent(in) :: v
  real(default) :: fval
  real(default) :: vm, f1, f2, x
  f1 = one
  f2 = zero + tiny_10
  vm = (v1+v2) / 2.
  if ( v < v1 ) then
    fval = f1
  else if (v < v2) then
    x = (v - v1) / (v2 - v1)
    fval = 1 - x**2 * (3 - 2 * x)
  else
    fval = f2
  end if
end function f_switch_off

```

<TTV formfactors: procedures>+≡

```

function formfactor_LL_analytic (a_soft, sqrts, p, vec_type) result (c)
  real(default), intent(in) :: a_soft
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: p
  integer, intent(in) :: vec_type
  complex(default) :: c
  real(default) :: en
  c = one
  if (.not. threshold%settings%initialized_parameters) return
  call update_global_sqrts_dependent_variables (sqrts)
  en = sqrts_to_en (sqrts, MTPOLE)
  select case (vec_type)
    case (1)
      c = G0p (CF*a_soft, en, p, MTPOLE, GAM) / G0p_tree (en, p, MTPOLE, GAM)
    case (2)
      c = G0p_ax (CF*a_soft, en, p, MTPOLE, GAM) / G0p_tree (en, p, MTPOLE, GAM)
    case default
      call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
  end select
end function formfactor_LL_analytic

```

<TTV formfactors: procedures>+≡

```

!!! Max's LL nonrelativistic threshold Green's function
function G0p (a, en, p, m, w) result (c)
  real(default), intent(in) :: a
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  complex(default) :: k, ipk, la, z1, z2
  complex(default) :: one, two, cc, dd
  k = sqrt( -m*en -imago*m*w )
  ipk = imago * p / k

```

```

la = a * m / 2. / k
one = cmplx (1., kind=default)
two = cmplx (2., kind=default)
cc = 2. - la
dd = ( 1. + ipk ) / 2.
z1 = nr_hypgeo (two, one, cc, dd)
dd = ( 1. - ipk ) / 2.
z2 = nr_hypgeo (two, one, cc, dd)
c = - imago * m / (4.*p*k) / (1.-la) * ( z1 - z2 )
end function G0p

```

<TTV formfactors: procedures>+≡

```

!!! tree level version: a_soft -> 0
pure function G0p_tree (en, p, m, w) result (c)
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  c = m / (p**2 - m*(en+imago*w))
end function G0p_tree

```

<TTV formfactors: procedures>+≡

```

!!! Peter Poier's LL nonrelativistic axial threshold Green's function
function G0p_ax (a, en, p, m, w) result (c)
  real(default), intent(in) :: a
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  complex(default) :: k, ipk, la, z1, z2, z3, z4
  complex(default) :: zero, two, three, cc, ddp, ddm
  k = sqrt( -m*en -imago*m*w )
  ipk = imago * p / k
  la = a * m / 2. / k
  zero = cmplx (0., kind=default)
  two = cmplx (2., kind=default)
  three = cmplx (3., kind=default)
  cc = 1. - la
  ddp = ( 1. + ipk ) / 2.
  ddm = ( 1. - ipk ) / 2.
  z1 = nr_hypgeo (zero, two, cc, ddp)
  z2 = nr_hypgeo (zero, two, cc, ddm)
  cc = 2. - la
  z3 = nr_hypgeo (zero, three, cc, ddm)
  z4 = nr_hypgeo (zero, three, cc, ddp)
  c = m / 2. / p**3 * ( 2.*p + imago*k*(1.-la)*(z1-z2) + imago*k*(z3-z4) )
end function G0p_ax

```

<TTV formfactors: procedures>+≡

```

pure function nustar (sqrts) result (nu)
  real(default), intent(in) :: sqrts

```

```

real(default) :: nu
real(default), parameter :: nustar_offset = 0.05_default
complex(default) :: arg
if (NUSTAR_DYNAMIC) then
  !!! from [arXiv:1309.6323], Eq. (3.2) (other definitions possible)
  arg = ( sqrts - 2.*M1S + imago*GAM_M1S ) / M1S
  nu = nustar_offset + abs(sqrt(arg))
else
  nu = NUSTAR_FIXED
end if
end function nustar

```

We recompute `alpha_soft` for form factors that do not call `update_global_parameters` (it is called in the scan for the (N)LL grid).

```

<TTV formfactors: procedures>+≡
pure function alphas_soft (sqrts) result (a_soft)
  real(default) :: a_soft
  real(default), intent(in) :: sqrts
  real(default) :: mu_soft, nusoft
  nusoft = RESCALE_F * nustar (sqrts)
  mu_soft = RESCALE_H * M1S * nusoft
  a_soft = running_as (mu_soft, AS_HARD, MU_HARD, NRQCD_ORDER, NF)
end function alphas_soft

<TTV formfactors: public>+≡
public :: alphas_notsohard

<TTV formfactors: sub interfaces>+≡
pure module function alphas_notsohard (sqrts) result (a_soft)
  real(default) :: a_soft
  real(default), intent(in) :: sqrts
end function alphas_notsohard

<TTV formfactors: procedures>+≡
pure module function alphas_notsohard (sqrts) result (a_soft)
  real(default) :: a_soft
  real(default), intent(in) :: sqrts
  real(default) :: mu_notsohard
  ! complex(default) :: v
  ! v = sqrts_to_v_1S (sqrts, GAM_M1S)
  ! mu_notsohard = RESCALE_H * M1S * sqrt(abs(v))
  mu_notsohard = RESCALE_H * M1S * sqrt(nustar (sqrts))
  a_soft = running_as (mu_notsohard, AS_MZ, MASS_Z, 2, NF)
end function alphas_notsohard

<TTV formfactors: sub interfaces>+≡
pure module function m1s_to_mpole (sqrts) result (mpole)
  real(default), intent(in) :: sqrts
  real(default) :: mpole
end function m1s_to_mpole

<TTV formfactors: procedures>+≡
pure module function m1s_to_mpole (sqrts) result (mpole)
  real(default), intent(in) :: sqrts

```

```

real(default) :: mpole
mpole = mtpole_init
if (threshold%settings%mpole_dynamic) then
    mpole = M1S * ( 1. + deltaM(sqrts) )
else
    mpole = M1S
end if
end function m1s_to_mpole

```

<TTV formfactors: procedures>+≡

```

!pure
!function mpole_to_M1S (mpole, sqrts, nl) result (m)
    !real(default), intent(in) :: mpole
    !real(default), intent(in) :: sqrts
    !integer, intent(in) :: nl
    !real(default) :: m
    !m = mpole * ( 1. - deltaM(sqrts, nl) )
!end function mpole_to_M1S

```

<TTV formfactors: procedures>+≡

```

pure function deltaM (sqrts) result (del)
    real(default), intent(in) :: sqrts
    real(default) :: del
    real(default) :: ac
    ac = CF * alphas_soft (sqrts)
    del = ac**2 / 8.
    if (NRQCD_ORDER > 0) then
        del = del + ac**3 / (8. * pi * CF) * &
            (B0 * (log (RESCALE_H * RESCALE_F * nustar (sqrts) / ac) + one) + A1 / 2.)
    end if
end function deltaM

```

<TTV formfactors: procedures>+≡

```

pure function sqrts_within_range (sqrts) result (flag)
    real(default), intent(in) :: sqrts
    logical :: flag
    flag = ( sqrts >= sqrts_min - tiny_07 .and. sqrts <= sqrts_max + tiny_07 )
end function

```

<TTV formfactors: procedures>+≡

```

! The mapping is such that even for min=max, we get three points:
! min - it , min, min + it
pure function sqrts_iter (i_sq) result (sqrts)
    integer, intent(in) :: i_sq
    real(default) :: sqrts
    if (POINTS_SQ > 1) then
        sqrts = sqrts_min - sqrts_it + &
            (sqrts_max - sqrts_min + two * sqrts_it) * &
            real(i_sq - 1) / real(POINTS_SQ - 1)
    else
        sqrts = sqrts_min
    end if
end function

```

```
end function sqrts_iter
```

(TTV formfactors: procedures)+≡

```
function scan_formfactor_over_p_LL_analytic (a_soft, sqrts, vec_type) result (ff_analytic)
  real(default), intent(in) :: a_soft
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  complex(default), dimension(POINTS_P) :: ff_analytic
  integer :: i_p
  ff_analytic = [(formfactor_LL_analytic (a_soft, sqrts, p_grid(i_p), vec_type), i_p=1, POINTS_P)
end function scan_formfactor_over_p_LL_analytic
```

(TTV formfactors: procedures)+≡

```
!!! tttoppik wrapper
subroutine scan_formfactor_over_p_TOPPIK (a_soft, sqrts, vec_type, p_grid_out, mpole_in, ff_toppik)
  real(default), intent(in) :: a_soft
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  real(default), dimension(POINTS_P), intent(out), optional :: p_grid_out
  real(default), intent(in), optional :: mpole_in
  complex(default), dimension(POINTS_P), optional :: ff_toppik
  integer :: i_p
  real(default) :: mpole, alphas_hard, f
  real(default), dimension(POINTS_P) :: p_toppik
  type(nr_spline_t) :: toppik_spline
  real*8 :: xenergy, xtm, xtg, xalphas, xscale, xc0, xc1, xc2, xim, xdi, &
    xcutn, xcutv, xkincm, xkinca, xkincv, xcdeltc, &
    xcdeltl, xcfullc, xcfulll, xcrm2
  integer, parameter :: nmax=900
  real*8 :: xdsdp(nmax), xpp(nmax), xww(nmax)
  complex*16 :: zff(nmax)
  integer :: np, jknflg, jgcfllg, jvflg
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_p_TOPPIK")
  if (POINTS_P > nmax-40) call msg_fatal ("TOPPIK: POINTS_P must be <=" // char(nmax-40))
  if (debug_on) call msg_debug (D_THRESHOLD, "POINTS_P", POINTS_P)
  if (present (ff_toppik)) ff_toppik = zero
  mpole = MTPOLE; if (present (mpole_in)) mpole = mpole_in
  xenergy = sqrts_to_en (sqrts, MTPOLE)
  xtm      = mpole
  xtg      = GAM
  xalphas  = a_soft
  xscale   = MU_SOFT
  xcutn    = 175.E6
  xcutv    = 175.E6
  xc0      = xc (a_soft, 0)
  xc1      = xc (a_soft, 1)
  xc2      = xc (a_soft, 2)
  xcdeltc  = 0.
  xcdeltl  = 0.
  xcfullc  = 0.
  xcfulll  = 0.
  xcrm2    = 0.
  xkincm   = 0.
```

```

xkinca = 0.
jknflg = 0
jgcflg = 0
xkincv = 0.
jvflg = 0
select case (vec_type)
  case (VECTOR)
    if (debug_on) call msg_debug (D_THRESHOLD, "calling tttoppik")
    call tttoppik &
      (xenergy,xtm,xtg,xalphas,xscale,xcutn,xcutv,xc0,xc1,xc2, &
       xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,xkinca,jknflg, &
       jgcflg, xkincv,jvflg,xim,xdi,np,xpp,xww,xsdsp,zff)
  case (AXIAL)
    if (debug_on) call msg_debug (D_THRESHOLD, "calling tttoppikaxial")
    call tttoppikaxial &
      (xenergy,xtm,xtg,xalphas,xscale,xcutn,xcutv,xc0,xc1,xc2, &
       xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,xkinca,jknflg, &
       jgcflg, xkincv,jvflg,xim,xdi,np,xpp,xww,xsdsp,zff)
    !!! 1st ~10 TOPPIK p-wave entries are ff_unstable: discard them
    zff(1:10) = [(zff(11), i_p=1, 10)]
  case default
    call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
end select
if (present (p_grid_out)) p_grid_out = xpp(1:POINTS_P)
if (.not. present (ff_toppik)) return
!!! keep track of TOPPIK instabilities and try to repair later
if (np < 0) then
  ff_toppik(1) = 2.d30
  if (debug_active (D_THRESHOLD)) then
    call msg_warning ("caught TOPPIK instability at sqrts = " // char(sqrts))
  end if
  return
end if
p_toppik = xpp(1:POINTS_P)
ff_toppik = zff(1:POINTS_P)
!!! TOPPIK output p-grid scales with en above ~ 4 GeV:
!!! interpolate for global sqrts/p grid
if (.not. nearly_equal (p_toppik(42), p_grid(42), rel_smallness=1E-6_default)) then
  call toppik_spline%init (p_toppik, ff_toppik)
  ff_toppik(2:POINTS_P) = [(toppik_spline%interpolate (p_grid(i_p)), i_p=2, POINTS_P)]
  call toppik_spline%dealloc ()
end if
!!! TOPPIK output includes tree level ~ 1, a_soft @ LL in current coefficient!
if (SWITCHOFF_RESUMMED) then
  f = f_switch_off (v_matching (sqrts, GAM_M1S))
  alphas_hard = AS_HARD * f
else
  alphas_hard = AS_HARD
end if
ff_toppik = ff_toppik * current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type)
if (debug_on) call msg_debug (D_THRESHOLD, &
  "current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type)", &
  current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type))
end subroutine scan_formfactor_over_p_TOPPIK

```

(TTV formfactors: procedures)+≡

```
function scan_formfactor_over_p (sqrts, vec_type) result (ff)
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  complex(default), dimension(POINTS_P) :: ff
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_p")
  select case (NRQCD_ORDER)
    case (0)
      ! ff = scan_formfactor_over_p_LL_analytic (AS_SOFT, sqrts, vec_type)
      call scan_formfactor_over_p_TOPPIK (AS_SOFT, sqrts, vec_type, ff_toppik=ff)
    case (1)
      call scan_formfactor_over_p_TOPPIK (AS_SOFT, sqrts, vec_type, ff_toppik=ff)
    case default
      call msg_fatal ("NRQCD_ORDER = " // char(NRQCD_ORDER))
  end select
end function scan_formfactor_over_p
```

(TTV formfactors: procedures)+≡

```
subroutine scan_formfactor_over_phase_space_grid ()
  integer :: i_sq, vec_type, unstable_loop
  logical, dimension(:, :), allocatable :: ff_unstable
  real(default) :: t1, t2, t3, t_toppik, t_p0_dep
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_phase_space_grid")
  allocate (ff_grid(POINTS_SQ, POINTS_P, POINTS_P0, 2))
  allocate (ff_unstable(POINTS_SQ, 2))
  t_toppik = zero
  t_p0_dep = zero
  write (msg_buffer, "(3(A,F7.3,1X),A)") "Scanning from ", &
    sqrts_min - sqrts_it, "GeV to ", &
    sqrts_max + sqrts_it, "GeV in steps of ", sqrts_it, "GeV"
  call msg_message ()
  ENERGY_SCAN: do i_sq = 1, POINTS_SQ
    if (signal_is_pending ()) return
    call update_global_sqrts_dependent_variables (sq_grid(i_sq))
    !!! vector and axial vector
    do vec_type = VECTOR, AXIAL
      call cpu_time (t1)
      unstable_loop = 0
      UNTIL_STABLE: do
        ff_grid(i_sq, :, 1, vec_type) = scan_formfactor_over_p (sq_grid(i_sq), vec_type)
        ff_unstable(i_sq, vec_type) = abs(ff_grid(i_sq, 1, 1, vec_type)) > 1.d30
        unstable_loop = unstable_loop + 1
        if (ff_unstable(i_sq, vec_type) .and. unstable_loop < 10) then
          cycle
        else
          exit
        end if
      end do UNTIL_STABLE
    end do
    call cpu_time (t2)
    !!! include p0 dependence by an integration over the p0-independent FF
    call cpu_time (t3)
    t_toppik = t_toppik + t2 - t1
  end do
```

```

        t_p0_dep = t_p0_dep + t3 - t2
    end do
    call msg_show_progress (i_sq, POINTS_SQ)
end do ENERGY_SCAN
if (debug_active (D_THRESHOLD)) then
    print *, "time for TOPPIK call: ", t2 - t1, " seconds."
    print *, "time for p0 dependence: ", t3 - t2, " seconds."
end if
if (any (ff_unstable)) call handle_TOPPIK_instabilities (ff_grid, ff_unstable)
if (allocated(Vmatrix)) deallocate(Vmatrix)
if (allocated(q_grid)) deallocate(q_grid)
threshold%settings%initialized_ff = .true.
end subroutine scan_formfactor_over_phase_space_grid

```

<TTV formfactors: procedures>+≡

```

subroutine init_threshold_phase_space_grid ()
    integer :: i_sq
    if (debug_on) call msg_debug (D_THRESHOLD, "init_threshold_phase_space_grid")
    if (sqrts_it > tiny_07) then
        POINTS_SQ = int ((sqrts_max - sqrts_min) / sqrts_it + tiny_07) + 3
    else
        POINTS_SQ = 1
    end if
    if (debug_on) call msg_debug (D_THRESHOLD, "Number of sqrts grid points: POINTS_SQ", POINTS_SQ)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_max", sqrts_max)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_min", sqrts_min)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_it", sqrts_it)
    allocate (sq_grid(POINTS_SQ))
    sq_grid = [(sqrts_iter (i_sq), i_sq=1, POINTS_SQ)]
    POINTS_P = 600
    allocate (p_grid(POINTS_P))
    p_grid = p_grid_from_TOPPIK ()
    POINTS_P0 = 1
    threshold%settings%initialized_ps = .true.
end subroutine init_threshold_phase_space_grid

```

<TTV formfactors: procedures>+≡

```

subroutine init_p0_grid (p_in, n)
    real(default), dimension(:), allocatable, intent(in) :: p_in
    integer, intent(in) :: n
    if (debug_on) call msg_debug (D_THRESHOLD, "init_p0_grid")
    if (debug_on) call msg_debug (D_THRESHOLD, "n", n)
    if (debug_on) call msg_debug (D_THRESHOLD, "size(p_in)", size(p_in))
    if (.not. allocated (p_in)) call msg_fatal ("init_p0_grid: p_in not allocated!")
    if (allocated (p0_grid)) deallocate (p0_grid)
    allocate (p0_grid(n))
    p0_grid(1) = zero
    p0_grid(2:n) = p_in(1:n-1)
end subroutine init_p0_grid

```

<TTV formfactors: procedures>+≡

```

!!! Andre's procedure to refine an existing grid
pure subroutine finer_grid (gr, fgr, n_in)

```



```

real(default), dimension(:), intent(in) :: gr
real(default), dimension(:), allocatable, intent(inout) :: fgr
integer, intent(in), optional :: n_in
integer :: n, i, j
real(default), dimension(:), allocatable :: igr
n = 4
if ( present(n_in) ) n = n_in
allocate( igr(n) )
if ( allocated(fgr) ) deallocate( fgr )
allocate( fgr(n*(size(gr)-1)+1) )
do i=1, size(gr)-1
  do j=0, n-1
    igr(j+1) = gr(i) + real(j)*(gr(i+1)-gr(i))/real(n)
  end do
  fgr((i-1)*n+1:i*n) = igr
end do
fgr(size(fgr)) = gr(size(gr))
deallocate( igr )
end subroutine finer_grid

```

(TTV formfactors: procedures)+≡

```

subroutine dealloc_grids ()
  if ( allocated(sq_grid) ) deallocate( sq_grid )
  if ( allocated( p_grid) ) deallocate( p_grid )
  if ( allocated(p0_grid) ) deallocate( p0_grid )
  if ( allocated(ff_grid) ) deallocate( ff_grid )
  threshold%settings%initialized_ps = .false.
  threshold%settings%initialized_ff = .false.
end subroutine dealloc_grids

```

(TTV formfactors: procedures)+≡

```

subroutine trim_p_grid (n_p_new)
  integer, intent(in) :: n_p_new
  real(default), dimension(n_p_new) :: p_save
  complex(default), dimension(POINTS_SQ,n_p_new,POINTS_P0,2) :: ff_save
  if (n_p_new > POINTS_P) then
    call msg_fatal ("trim_p_grid: new size larger than old size.")
    return
  end if
  p_save = p_grid(1:n_p_new)
  ff_save = ff_grid(:,1:n_p_new,:,:)
  deallocate( p_grid, ff_grid )
  allocate( p_grid(n_p_new), ff_grid(POINTS_SQ,n_p_new,POINTS_P0,2) )
  p_grid = p_save
  ff_grid = ff_save
end subroutine trim_p_grid

```

(TTV formfactors: procedures)+≡

```

!!! try to repair TOPPIK instabilities by interpolation of adjacent sq_grid points
subroutine handle_TOPPIK_instabilities (ff, nan)
  complex(default), dimension(:,:,:), intent(inout) :: ff
  logical, dimension(:,:), intent(in) :: nan
  integer :: i, i_sq, n_nan

```

```

logical :: interrupt
n_nan = sum (merge ([1, i=1, 2*POINTS_SQ]), &
                [(0, i=1, 2*POINTS_SQ)], reshape (nan, [2*POINTS_SQ])) )
interrupt = n_nan > 3
do i = 1, 2
  if (interrupt ) exit
  if (.not. any (nan(:,i))) cycle
  do i_sq = 2, POINTS_SQ - 1
    if (.not. nan(i_sq,i)) cycle
    if (nan(i_sq+1,i) .or. nan(i_sq-1,i)) then
      interrupt = .true.
      exit
    end if
    ff(i_sq,::,i) = (ff(i_sq-1,::,i) + ff(i_sq+1,::,i)) / two
  end do
end do
if (.not. interrupt) return
call msg_fatal ("Too many TOPPIK instabilities! Check your parameter setup " &
               // "or slightly vary the scales sh and/or sf.")
end subroutine handle_TOPPIK_instabilities

```

<TTV formfactors: procedures>+≡

```

pure function sqrts_to_v (sqrts, gamma) result (v)
  complex(default) :: v
  real(default), intent(in) :: sqrts, gamma
  real(default) :: m
  m = m1s_to_mpole (sqrts)
  v = sqrt ((sqrts - two * m + imago * gamma) / m)
end function sqrts_to_v

```

<TTV formfactors: procedures>+≡

```

pure function sqrts_to_v_1S (sqrts, gamma) result (v)
  complex(default) :: v
  real(default), intent(in) :: sqrts, gamma
  v = sqrt ((sqrts - two * M1S + imago * gamma) / M1S)
end function sqrts_to_v_1S

```

<TTV formfactors: procedures>+≡

```

pure function v_to_sqrts (v) result (sqrts)
  real(default), intent(in) :: v
  real(default) :: sqrts
  real(default) :: m
  m = mtpole_init
  sqrts = 2.*m + m*v**2
end function v_to_sqrts

```

<TTV formfactors: procedures>+≡

```

!!! -q^2 times the Coulomb potential V at L0 resp. NLO
function minus_q2_V (a, q, p, pOr, vec_type) result (v)
  real(default), intent(in) :: a
  real(default), intent(in) :: q
  real(default), intent(in) :: p

```

```

real(default), intent(in) :: p0r
integer, intent(in) :: vec_type
complex(default) :: p0, log_mppp, log_mmpm, log_mu_s, v
p0 = abs(p0r) + ieps
log_mppp = log( (p-p0+q) * (p+p0+q) )
log_mmpm = log( (p-p0-q) * (p+p0-q) )
select case (vec_type)
case (1)
select case (NRQCD_ORDER)
case (0)
v = CF*a * 2.*pi*(log_mppp-log_mmpm) * q/p
case (1)
log_mu_s = 2.*log(MU_SOFT)
v = CF*a * (2.*(4.*pi+A1*a)*(log_mppp-log_mmpm) &
+ B0*a*((log_mmpm-log_mu_s)**2-(log_mppp-log_mu_s)**2)) * q/(4.*p)
case default
call msg_fatal ("NRQCD_ORDER = " // char(NRQCD_ORDER))
end select
case (2)
!!! not implemented yet
v = zero
case default
call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
end select
end function minus_q2_V

```

<TTV formfactors: procedures>+≡

```

!!! compute support points (~> q-grid) for numerical integration: trim p-grid and
!!! merge with singular points of integrand: q = p, |p-p0|, p+p0, sqrt(mpole*E)
subroutine compute_support_points (en, i_p, i_p0, n_trim)
real(default), intent(in) :: en
integer, intent(in) :: i_p
integer, intent(in) :: i_p0
integer, intent(in) :: n_trim
real(default) :: p, p0
real(default), dimension(4) :: sing_vals
integer :: n_sing, i_q
if (mod (POINTS_P, n_trim) /= 0) call msg_fatal ("trim p-grid for q-integration: POINTS_P = "
// char(POINTS_P) // " and n_trim = " // char(n_trim))
n_q = POINTS_P / n_trim + merge(0,1,n_trim==1)
p = p_grid(i_p)
p0 = p0_grid(i_p0)
n_sing = 0
if ( i_p /= 1 .and. mod(i_p,n_trim) /= 0 ) then
n_sing = n_sing+1
sing_vals(n_sing) = p
end if
if ( i_p0 /= 1 ) then
n_sing = n_sing+1
sing_vals(n_sing) = p0 + p
if ( i_p0 /= i_p+1 ) then
n_sing = n_sing+1
sing_vals(n_sing) = abs( p0 - p )
end if
end if

```

```

end if
if ( en > 0. ) then
    n_sing = n_sing+1
    sing_vals(n_sing) = sqrt( MTPOLE * en )
end if
if ( allocated(q_grid) ) deallocate( q_grid )
allocate( q_grid(n_q+n_sing) )
q_grid(1) = p_grid(1)
q_grid(2:n_q) = [(p_grid(i_q), i_q=max(n_trim,2), POINTS_P, n_trim)]
if (n_sing > 0 ) q_grid(n_q+1:n_q+n_sing) = sing_vals(1:n_sing)
call nr_sort (q_grid)
end subroutine compute_support_points

```

(TTV formfactors: procedures)+≡

```

!!! cf. arXiv:hep-ph/9503238, validated against arXiv:hep-ph/0008171
pure function formfactor_ttv_relativistic_nlo (alphas, ps, J0) result (c)
    real(default), intent(in) :: alphas
    type(phase_space_point_t), intent(in) :: ps
    complex(default), intent(in) :: J0
    complex(default) :: c
    real(default) :: p2, k2, q2, kp, pq, kq
    complex(default) :: D2, chi, ln1, ln2, L1, L2, z, S, m2, m
    complex(default) :: JA, JB, JC, JD, JE, IA, IB, IC, ID, IE
    complex(default) :: CCmsbar
    complex(default) :: dF1, dF2, dM1, dM2
    complex(default), dimension(12) :: P1
    complex(default), parameter :: ximo = zero
    p2 = ps%p2
    k2 = ps%k2
    q2 = ps%q2
    m2 = complex_m2 (ps%mpole, GAM)
    !!! kinematic abbreviations
    kp = 0.5_default * (-q2 + p2 + k2)
    pq = 0.5_default * ( k2 - p2 - q2)
    kq = 0.5_default * (-p2 + k2 + q2)
    D2 = kp**2 - k2*p2
    chi = p2*k2*q2 + 2.*m2*((p2 + k2)*kp - 2.*p2*k2) + m2**2 * q2
    ln1 = log( (1. - p2/m2)*(1,0) + ieps )
    ln2 = log( (1. - k2/m2)*(1,0) + ieps )
    L1 = (1. - m2/p2) * ln1
    L2 = (1. - m2/k2) * ln2
    z = sqrt( (1.-4.*m2/q2)*(1,0) )
    S = 0.5_default * z * log( (z+1.)/(z-1.) + ieps )
    m = sqrt(m2)

    !!! loop integrals in terms of J0
    JA = 1./D2 * (J0/2.*(-m2*pq - p2*kq) + kp*L2 - p2*L1 - 2.*pq*S)
    JB = 1./D2 * (J0/2.*( m2*kq + k2*pq) + kp*L1 - k2*L2 + 2.*kq*S)
    JC = 1/(4.*D2) * (2.*p2 + 2*kp*m2/k2 - 4.*kp*S + 2.*kp*(1. - m2/k2)*L2 + &
        (2.*kp*(p2 - m2) + 3.*p2*(m2 - k2))*JA + p2*(m2 - p2)*JB)
    JD = 1./(4.*D2) * (2.*kp*((k2 - m2)*JA + (p2 - m2)*JB - 1.) - k2*(2.*m2/k2 &
        - 2.*S + (1. - m2/k2)*L2 + (p2 - m2)*JA) - p2*(-2.*S + (1. - &
        m2/p2)*L1 + (k2 - m2)*JB))
    JE = 1./(4.*D2) * (2.*k2 + 2*kp*m2/p2 - 4.*kp*S + 2.*kp*(1. - m2/p2)*L1 + &

```

```

      (2.*kp*(k2 - m2) + 3.*k2*(m2 - p2))*JB + k2*(m2 - k2)*JA)
IA = 1./D2 * (-(kq/2.)*J0 - 2.*q2/chi *((m2 - p2)*k2 - (m2 - k2)*kp)*S + &
      1./(m2 - p2)*(p2 - kp + p2*q2/chi *(k2 - m2)*(m2 + kp))*L1 + &
      k2*q2/chi *(m2 + kp)*L2)
IB = 1./D2 * ( (pq/2.)*J0 - 2.*q2/chi *((m2 - k2)*p2 - (m2 - p2)*kp)*S + &
      1./(m2 - k2)*(k2 - kp + k2*q2/chi *(p2 - m2)*(m2 + kp))*L2 + &
      p2*q2/chi *(m2 + kp)*L1)
IC = 1./(4.*D2) * (2.*p2*J0 - 4.*kp/k2*(1. + m2/(k2 - m2)*L2) + (2.*kp - &
      3.*p2)*JA - p2*JB + (-2.*kp*(m2 - p2) + 3.*p2*(m2 - k2))*IA + &
      p2*(m2 - p2)*IB)
ID = 1./(4.*D2) * (-2.*kp*J0 + 2.*(1. + m2/(k2 - m2)*L2) + 2.*(1. + &
      m2/(p2 - m2)*L1) + (2.*kp - k2)*JA + (2.*kp - p2)*JB + (k2*(m2 - &
      p2) - 2.*kp*(m2 - k2))*IA + (p2*(m2 - k2) - 2.*kp*(m2 - p2))*IB)
IE = 1./(4.*D2) * (2.*k2*J0 - 4.*kp/p2*(1. + m2/(p2 - m2)*L1) + (2.*kp - &
      3.*k2)*JB - k2*JA + (-2.*kp*(m2 - k2) + 3.*k2*(m2 - p2))*IB + &
      k2*(m2 - k2)*IA)

!!! divergent part ~ 1/epsilon: depends on subtraction scheme
CCmsbar = -2.0_default * log(RESCALE_H)

! real top mass in the loop numerators
! m2 = cmplx(real(m2), kind=default)
! m = sqrt(m2)

!!! quark self energies
dF1 = - (ximo+1.) * (CCmsbar + (1.+m2/p2)*(1.-L1))
dF2 = - (ximo+1.) * (CCmsbar + (1.+m2/k2)*(1.-L2))
dM1 = m/p2 * ( (ximo+1.)*(1.+m2/p2*ln1) - 3.*ln1 )
dM2 = m/k2 * ( (ximo+1.)*(1.+m2/k2*ln2) - 3.*ln2 )

!!! coefficient list: vertex function Gamma_mu (k,p) = sum_i( Vi_mu * Pi )
P1(1) = 2.*JA - 2.*JC + ximo*(m2*IC + p2*ID)
P1(2) = 2.*JB - 2.*JE + ximo*(k2*ID + m2*IE)
P1(3) = -2.*J0 + 2.*JA + 2.*JB - 2.*JD + ximo*(-J0/2. - k2/2.*IC - &
      kp*ID + m2*ID + p2/2.*IE + JA)
P1(4) = -2.*JD + ximo*(k2*IC + m2*ID - JA)
P1(5) = J0 - JA - JB + ximo*(J0/4. + k2/4.*IC + kp/2.*ID + p2/4.*IE - &
      1./2.*JA - 1./2.*JB)
P1(6) = -m2*J0 - k2*JA - p2*JB + k2/2.*JC + kp*JD + p2/2.*JE + &
      (1./2. + CCmsbar - 2.*S) &
      + ximo*(-m2*J0/4. - m2/4.*k2*IC - m2/2.*kp*ID - m2/4.*p2*IE &
      - k2/2.*JA - p2/2.*JB + (CCmsbar + 2.))
P1(7) = 2.*m*J0 - 4.*m*JA + ximo*m*(J0/2. - 2.*kp*IC + k2/2.*IC - &
      p2*ID - kp*ID - p2/2.*IE - JA)
P1(8) = 2.*m*J0 - 4.*m*JB + ximo*m*(J0/2. + k2/2.*IC - kp*ID + k2*ID - &
      p2/2.*IE - JB)
P1(9) = ximo*m*(ID + IE)
P1(10) = ximo*m*(ID + IC)
P1(11) = ximo*m*( p2*ID + kp*IC + p2/2.*IE - k2/2.*IC) + dM2
      !!! self energy contribution: ~ gamma_mu.k_slash = V11
P1(12) = ximo*m*(-k2*ID - kp*IE + p2/2.*IE - k2/2.*IC) + dM1
      !!! self energy contribution: ~ gamma_mu.p_slash = V12

!!! leading form factor: V6 = gamma_mu, V5 = gamma_mu.k_slash.p_slash ~> -m^2*gamma_mu

```

```

c = one + alphas * CF / (4.*pi) * ( P1(6) - m2*P1(5) &
!!! self energy contributions ~ gamma^mu
+ dF1 + dF2 + m*( dM1 + dM2 ) )
!!! on-shell subtraction: UV divergence cancels
! + 0.5_default*( dF1 + dF2 + m*( dM1 + dM2 ) )
end function formfactor_ttv_relativistic_nlo

```

<TTV formfactors: procedures>+≡

```

pure function sqrts_to_en (sqrts, mpole_in) result (en)
real(default), intent(in) :: sqrts
real(default), intent(in), optional :: mpole_in
real(default) :: mpole, en
if (present (mpole_in)) then
mpole = mpole_in
else
mpole = m1s_to_mpole (sqrts)
end if
en = sqrts - two * mpole
end function sqrts_to_en

```

<TTV formfactors: procedures>+≡

```

function p_grid_from_TOPPIK (mpole_in) result (p_topplik)
real(default), intent(in), optional :: mpole_in
real(default), dimension(POINTS_P) :: p_topplik
real(default) :: mpole
if (debug_on) call msg_debug (D_THRESHOLD, "p_grid_from_TOPPIK")
mpole = MTPOLE; if (present (mpole_in)) mpole = mpole_in
call scan_formfactor_over_p_TOPPIK &
(alphas_soft(2. * M1S), 2. * M1S, 1, p_topplik, mpole)
if (.not. strictly_monotonous (p_topplik)) &
call msg_fatal ("p_grid NOT strictly monotonous!")
end function p_grid_from_TOPPIK

```

<TTV formfactors: sub interfaces>+≡

```

pure module function int_to_char (i) result (c)
integer, intent(in) :: i
character(len=len(trim(int2fixed(i)))) :: c
end function int_to_char

```

<TTV formfactors: procedures>+≡

```

pure module function int_to_char (i) result (c)
integer, intent(in) :: i
character(len=len(trim(int2fixed(i)))) :: c
c = int2char (i)
end function int_to_char

```

<TTV formfactors: sub interfaces>+≡

```

pure module function real_to_char (r) result (c)
real(default), intent(in) :: r
character(len=len(trim(real2fixed(r)))) :: c
end function real_to_char

```

```

<TTV formfactors: procedures>+≡
  pure module function real_to_char (r) result (c)
    real(default), intent(in) :: r
    character(len=len(trim(real2fixed(r)))) :: c
    c = real2char (r)
  end function real_to_char

<TTV formfactors: sub interfaces>+≡
  pure module function complex_to_char (z) result (c)
    complex(default), intent(in) :: z
    character(len=len(trim(real2fixed(real(z))))+len(trim(real2fixed(aimag(z))))+5) :: c
  end function complex_to_char

<TTV formfactors: procedures>+≡
  pure module function complex_to_char (z) result (c)
    complex(default), intent(in) :: z
    character(len=len(trim(real2fixed(real(z))))+len(trim(real2fixed(aimag(z))))+5) :: c
    character(len=len(trim(real2fixed(real(z)))) :: re
    character(len=len(trim(real2fixed(aimag(z)))) :: im
    re = real_to_char (real(z))
    im = real_to_char (aimag(z))
    if (nearly_equal (aimag(z), zero)) then
      c = re
    else
      c = re // " + " // im // "*I"
    end if
  end function complex_to_char

<TTV formfactors: sub interfaces>+≡
  pure module function logical_to_char (l) result (c)
    logical, intent(in) :: l
    character(len=1) :: c
  end function logical_to_char

<TTV formfactors: procedures>+≡
  pure module function logical_to_char (l) result (c)
    logical, intent(in) :: l
    character(len=1) :: c
    write (c, '(l1)') l
  end function logical_to_char

<TTV formfactors: procedures>+≡
  subroutine get_rest_frame (p1_in, p2_in, p1_out, p2_out)
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(out) :: p1_out, p2_out
    type(lorentz_transformation_t) :: L
    L = inverse (boost (p1_in + p2_in, (p1_in + p2_in)**1))
    p1_out = L * p1_in; p2_out = L * p2_in
  end subroutine get_rest_frame

  function shift_momentum (p_in, E, p) result (p_out)
    type(vector4_t) :: p_out
    type(vector4_t), intent(in) :: p_in

```

```

real(default), intent(in) :: E, p
type(vector3_t) :: vec
vec = p_in%p(1:3) / space_part_norm (p_in)
p_out = vector4_moving (E, p * vec)
end function shift_momentum

subroutine evaluate_one_to_two_splitting_threshold (p_origin, &
    p1_in, p2_in, p1_out, p2_out, msq_in, jac)
    type(vector4_t), intent(in) :: p_origin
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(inout) :: p1_out, p2_out
    real(default), intent(in), optional :: msq_in
    real(default), intent(inout), optional :: jac
    type(lorentz_transformation_t) :: L
    type(vector4_t) :: p1_rest, p2_rest
    real(default) :: msq, msq1, msq2
    real(default) :: m
    real(default) :: E1, E2, E_max
    real(default) :: p, lda
    real(default), parameter :: E_offset = 0.001_default
    !!! (TODO-cw-2016-10-13) Find a better way to get masses
    real(default), parameter :: mb = 4.2_default
    real(default), parameter :: mw = 80.419_default

    call get_rest_frame (p1_in, p2_in, p1_rest, p2_rest)

    msq = p_origin**2; m = sqrt(msq)
    msq1 = p1_in**2
    msq2 = m * (m - two * p1_rest%p(0))
    E1 = (msq + msq1 - msq2) / (two * m)
    E_max = (msq - (mb + mw)**2) / (two * m)
    E_max = E_max - E_offset
    if (E1 > E_max) then
        E1 = E_max
        msq2 = m * (m - two * E_max)
    end if

    lda = lambda (msq, msq1, msq2)
    if (lda < zero) call msg_fatal &
        ("Threshold Splitting: lambda < 0 encountered! Use a higher offset.")
    p = sqrt(lda) / (two * m)

    E1 = sqrt (msq1 + p**2)
    E2 = sqrt (msq2 + p**2)

    p1_out = shift_momentum (p1_rest, E1, p)
    p2_out = shift_momentum (p2_rest, E2, p)

    L = boost (p_origin, p_origin**1)
    p1_out = L * p1_out
    p2_out = L * p2_out
end subroutine evaluate_one_to_two_splitting_threshold

```

(TTV formfactors: public)+≡


```

    public :: generate_on_shell_decay_threshold
<TTV formfactors: sub interfaces>+≡
    module subroutine generate_on_shell_decay_threshold (p_decay, p_top, p_decay_onshell)
        !!! Gluon must be on first position in this array
        type(vector4_t), intent(in), dimension(:) :: p_decay
        type(vector4_t), intent(inout) :: p_top
        type(vector4_t), intent(inout), dimension(:) :: p_decay_onshell
    end subroutine generate_on_shell_decay_threshold

<TTV formfactors: procedures>+≡
    module subroutine generate_on_shell_decay_threshold (p_decay, p_top, p_decay_onshell)
        !!! Gluon must be on first position in this array
        type(vector4_t), intent(in), dimension(:) :: p_decay
        type(vector4_t), intent(inout) :: p_top
        type(vector4_t), intent(inout), dimension(:) :: p_decay_onshell
        procedure(evaluate_one_to_two_splitting_special), pointer :: ppointer
        ppointer => evaluate_one_to_two_splitting_threshold
        call generate_on_shell_decay (p_top, p_decay, p_decay_onshell, 1, &
            evaluate_special = ppointer)
    end subroutine generate_on_shell_decay_threshold

```

29.1.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<ttv_formfactors_ut.f90>≡
<File header>

    module ttv_formfactors_ut
        use unit_tests
        use ttv_formfactors_uti

<Standard module head>

<TTV formfactors: public test>

contains

<TTV formfactors: test driver>

    end module ttv_formfactors_ut
<ttv_formfactors_uti.f90>≡
<File header>

    module ttv_formfactors_uti

<Use kinds>
<Use debug>
        use constants
        use ttv_formfactors
        use diagnostics
        use sm_physics, only: running_as
        use numeric_utils

```

```

    <Standard module head>

    <TTV formfactors: test declarations>

contains

    <TTV formfactors: tests>

    end module ttv_formfactors_util
API: driver for the unit tests below.
    <TTV formfactors: public test>≡
        public ::ttv_formfactors_test
    <TTV formfactors: test driver>≡
        subroutine ttv_formfactors_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <TTV formfactors: execute tests>
        end subroutine ttv_formfactors_test

```

Basic setup

```

    <TTV formfactors: execute tests>≡
        call test(ttv_formfactors_1, "ttv_formfactors_1", &
            "Basic setup", u, results)
    <TTV formfactors: test declarations>≡
        public :: ttv_formfactors_1
    <TTV formfactors: tests>≡
        subroutine ttv_formfactors_1 (u)
            integer, intent(in) :: u
            real(default) :: m1s, Vtb, wt_inv, alphaemi, sw, alphas_mz, mz, &
                mw, mb, sh, sf, NRQCD_ORDER, FF, offshell_strategy, v1, v2, &
                scan_sqrts_max, sqrts, scan_sqrts_min, scan_sqrts_stepsize, &
                test, gam_out, mpole
            type(formfactor_t) :: formfactor
            type(phase_space_point_t) :: ps
            logical :: mpole_fixed
            integer :: top_helicity_selection
            write (u, "(A)")  "* Test output: ttv_formfactors_1"
            write (u, "(A)")  "* Purpose: Basic setup"
            write (u, "(A)")

            m1s = 172.0_default
            Vtb = one
            wt_inv = zero
            alphaemi = 125.0_default
            alphas_mz = 0.118_default
            mz = 91.1876_default
            mw = 80.399_default
            sw = sqrt(one - mw**2 / mz**2)
            mb = 4.2_default

```

```

sh = one
sf = one
NRQCD_ORDER = one
FF = MATCHED
offshell_strategy = 0
top_helicity_selection = -1
v1 = 0.3_default
v2 = 0.5_default
scan_sqrts_stepsize = 0.0_default
test = - one
write (u, "(A)") "Check high energy behavior"
sqrts = 500.0_default
scan_sqrts_min = sqrts
scan_sqrts_max = sqrts
write (u, "(A)") "Check that the mass is not fixed"
mpole_fixed = .false.

<(re)start grid>
call threshold%formfactor%activate ()
call formfactor%activate ()
call assert (u, m1s_to_mpole (350.0_default) > m1s + 0.1_default, &
  "m1s_to_mpole (350.0_default) > m1s")
write (u, "(A)")

! For simplicity we test on-shell back-to-back tops
call ps%init (m1s**2, m1s**2, sqrts**2, mpole)
call assert_equal (u, f_switch_off (v_matching (ps%sqrts, GAM_M1S)), tiny_10, &
  "f_switch_off (v_matching (ps%sqrts, GAM_M1S))")
call assert (u, &
  abs (formfactor%compute (ps, 1, EXPANDED_HARD)) > &
  abs (formfactor%compute (ps, 1, RESUMMED)), &
  "expansion with hard alphas should be larger " // &
  "than resummed (with switchoff)")
call assert_equal (u, &
  abs (formfactor%compute (ps, 1, RESUMMED)), zero, &
  "resummed (with switchoff) should be zero", abs_smallness=tiny_10)
call assert_equal (u, &
  abs (formfactor%compute (ps, 1, EXPANDED_SOFT_SWITCHOFF)), zero, &
  "expanded (with switchoff) should be zero", abs_smallness=tiny_10)
write (u, "(A)") ""

write (u, "(A)") "Check global variables"
call assert_equal (u, AS_HARD, &
  running_as (m1s, alphas_mz, mz, 2, 5.0_default), "hard alphas")
call assert_equal (u, AS_SOFT, zero, "soft alphas", abs_smallness=tiny_10)
call assert_equal (u, AS_USOFT, zero, "ultrasoft alphas", abs_smallness=tiny_10)
call assert_equal (u, AS_LL_SOFT, zero, "LL soft alphas", abs_smallness=tiny_10)

!!! care: the formfactor contains the tree level that we usually subtract again
write (u, "(A)") "Check low energy behavior"
sqrts = 2 * m1s + 0.01_default
scan_sqrts_min = sqrts
scan_sqrts_max = sqrts
write (u, "(A)") "Check that the mass is fixed"

```

```

    mpole_fixed = .true.
  <(re)start grid>

    call ps%init (m1s**2, m1s**2, sqrts**2, mpole)
    call assert_equal (u, m1s_to_mpole (350.0_default), m1s, &
      "m1s_to_mpole (350.0_default) == m1s")
    call assert_equal (u, m1s_to_mpole (550.0_default), m1s, &
      "m1s_to_mpole (550.0_default) == m1s")
    write (u, "(A)") ""
    call assert_equal (u, f_switch_off (v_matching (ps%sqrts, GAM_M1S)), &
      one, "f_switch_off (v_matching (ps%sqrts, GAM_M1S))")
    call formfactor%disable ()
    call assert_equal (u, &
      abs(formfactor%compute (ps, 1, 1)), &
      zero, &
      "disabled formfactor should return zero")
    call formfactor%activate ()
    call assert_equal (u, &
      formfactor%compute (ps, 1, EXPANDED_SOFT_SWITCHOFF), &
      formfactor%compute (ps, 1, EXPANDED_SOFT), &
      "switchoff function should do nothing here")
    write (u, "(A)") ""

    write (u, "(A)") "* Test output end: ttv_formfactors_1"
  end subroutine ttv_formfactors_1

  <(re)start grid>≡
    call init_parameters &
      (mpole, gam_out, m1s, Vtb, wt_inv, &
        alphaemi, sw, alphas_mz, mz, mw, &
        mb, sh, sf, NRQCD_ORDER, FF, offshell_strategy, &
        v1, v2, scan_sqrts_min, scan_sqrts_max, &
        scan_sqrts_stepsize, mpole_fixed, real(top_helicity_selection, default))
    call init_threshold_grids (test)

```

Test flags

```

  <TTV formfactors: execute tests>+≡
    call test(ttv_formfactors_2, "ttv_formfactors_2", &
      "Test flags", u, results)

  <TTV formfactors: test declarations>+≡
    public :: ttv_formfactors_2

  <TTV formfactors: tests>+≡
    subroutine ttv_formfactors_2 (u)
      integer, intent(in) :: u
      write (u, "(A)") "* Test output: ttv_formfactors_2"
      write (u, "(A)") "* Purpose: Test flags"
      write (u, "(A)")

      write (u, "(A)") "RESUMMED_SWITCHOFF + NLO"
      call threshold%settings%setup_flags (-2, 1, -1)
      call assert (u, SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
      call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")

```

```

call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
".not. threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, &
".not. threshold%settings%interference")
call assert (u, .not. threshold%settings%no_nlo_width_in_signal_propagators, &
".not. threshold%settings%no_nlo_width_in_signal_propagators")

write (u, "(A)") "MATCHED + FACTORIZATION"
call threshold%settings%setup_flags (-1, 0+2, -1)
call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")
call assert (u, threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")

write (u, "(A)") "RESUMMED + INTERFERENCE"
call threshold%settings%setup_flags (1, 0+0+4, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
".not. threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, "threshold%settings%interference")

write (u, "(A)") "EXPANDED_HARD"
call threshold%settings%setup_flags (4, 0+2+4, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, "threshold%settings%interference")

write (u, "(A)") "EXPANDED_SOFT"
call threshold%settings%setup_flags (5, 1+2+4, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, &
"threshold%settings%interference")

write (u, "(A)") "EXPANDED_SOFT_SWITCHOFF"
call threshold%settings%setup_flags (6, 0+0+0+8, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, &
"threshold%settings%interference")

write (u, "(A)") "RESUMMED_ANALYTIC_LL"

```

```

call threshold%settings%setup_flags (7, 0+0+4+8, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, "threshold%settings%interference")
call assert (u, threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")

write (u, "(A)") "EXPANDED_SOFT_HARD"
call threshold%settings%setup_flags (8, 0+2+0+128, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, "threshold%settings%interference")
call assert (u, .not. threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")
call assert (u, threshold%settings%onshell_projection%decay, &
"threshold%settings%onshell_projection%decay")

write (u, "(A)") "EXTRA_TREE"
call threshold%settings%setup_flags (9, 1+0+0+16+64, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, "threshold%settings%interference")
call assert (u, threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")
call assert (u, .not. threshold%settings%onshell_projection%decay, &
"threshold%settings%onshell_projection%decay")
call assert (u, threshold%settings%no_nlo_width_in_signal_propagators, &
"threshold%settings%no_nlo_width_in_signal_propagators")

write (u, "(A)") "test projection of width"
call threshold%settings%setup_flags (9, 0+0+0+0+256, -1)
call assert (u, .not. threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")
call assert (u, .not. threshold%settings%onshell_projection%decay, &
"threshold%settings%onshell_projection%decay")
call assert (u, .not. threshold%settings%onshell_projection%width, &
"threshold%settings%onshell_projection%width")

write (u, "(A)") "test boost of decay momenta"
call threshold%settings%setup_flags (9, 512, -1)
if (debug_on) call msg_debug (D_THRESHOLD, &
"threshold%settings%onshell_projection%boost_decay", &
threshold%settings%onshell_projection%boost_decay)
call threshold%settings%setup_flags (9, 0, -1)
if (debug_on) call msg_debug (D_THRESHOLD, &

```

```

        ".not. threshold%settings%onshell_projection%boost_decay", &
        ".not. threshold%settings%onshell_projection%boost_decay")

write (u, "(A)") "test helicity approximations"
call threshold%settings%setup_flags (9, 32, -1)
call assert (u, threshold%settings%helicity_approximation%simple, &
    "threshold%settings%helicity_approximation%simple")
call assert (u, .not. threshold%settings%helicity_approximation%extra, &
    ".not. threshold%settings%helicity_approximation%extra")
call assert (u, .not. threshold%settings%helicity_approximation%ultra, &
    ".not. threshold%settings%helicity_approximation%ultra")
call threshold%settings%setup_flags (9, 1024, -1)
call assert (u, .not. threshold%settings%helicity_approximation%simple, &
    ".not. threshold%settings%helicity_approximation%simple")
call assert (u, threshold%settings%helicity_approximation%extra, &
    "threshold%settings%helicity_approximation%extra")

write (u, "(A)")
write (u, "(A)")  "* Test output end: ttv_formfactors_2"
end subroutine ttv_formfactors_2

```

Chapter 30

Integration and Process Objects

This is the central part of the **WHIZARD** package. It provides the functionality for evaluating structure functions, kinematics and matrix elements, integration and event generation. It combines the various parts that deal with those tasks individually and organizes the data transfer between them.

subevt_expr This enables process observables as (abstract) expressions, to be evaluated for each process call.

parton_states A **parton_state_t** object represents an elementary partonic interaction. There are two versions: one for the isolated elementary process, one for the elementary process convoluted with the structure-function chain. The parton state is an effective state. It needs not coincide with the seed-kinematics state which is used in evaluating phase space.

process Here, all pieces are combined for the purpose of evaluating the elementary processes. The whole algorithm is coded in terms of abstract data types as defined in the appropriate modules: **prc_core** for matrix-element evaluation, **prc_core_def** for the associated configuration and driver, **sf_base** for beams and structure-functions, **phs_base** for phase space, and **mci_base** for integration and event generation.

process_config

process_counter Very simple object for statistics

process_mci

pcm

kinematics

instances While the above modules set up all static information, the instances have the changing event data. There are term and process instances but no component instances.

process_stacks Process stacks collect process objects.

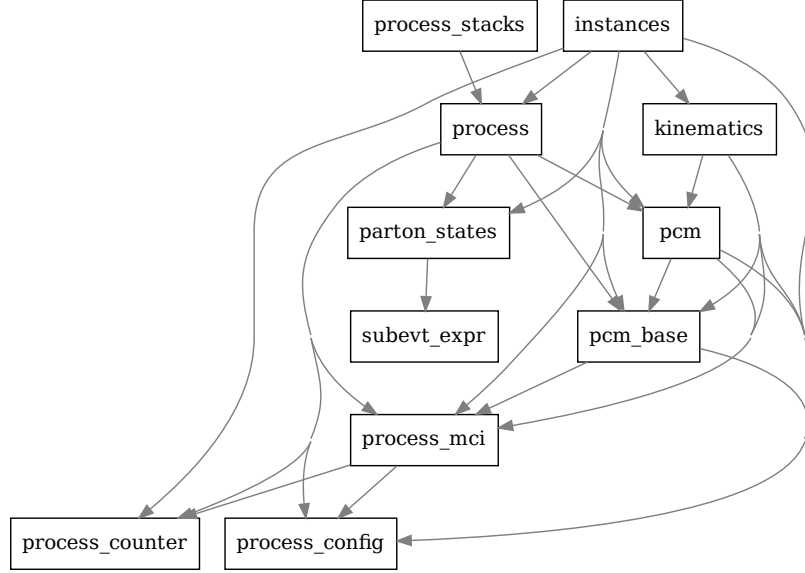


Figure 30.1: Module dependencies in `src/process_integration`.

We combine here hard interactions, phase space, and (for scatterings) structure functions and interfaces them to the integration module.

The process object implements the combination of a fixed beam and structure-function setup with a number of elementary processes. The latter are called process components. The process object represents an entity which is supposedly observable. It should be meaningful to talk about the cross section of a process.

The individual components of a process are, technically, processes themselves, but they may have unphysical cross sections which have to be added for a physical result. Process components may be exclusive tree-level elementary processes, dipole subtraction term, loop corrections, etc.

The beam and structure function setup is common to all process components. Thus, there is only one instance of this part.

The process may be a scattering process or a decay process. In the latter case, there are no structure functions, and the beam setup consists of a single particle. Otherwise, the two classes are treated on the same footing.

Once a sampling point has been chosen, a process determines a set of partons with a correlated density matrix of quantum numbers. In general, each sampling point will generate, for each process component, one or more distinct parton configurations. This is the **computed** state. The computed state is the subject of the multi-channel integration algorithm.

For NLO computations, it is necessary to project the computed states onto another set of parton configurations (e.g., by recombining certain pairs). This is the **observed** state. When computing partonic observables, the information

is taken from the observed state.

For the purpose of event generation, we will later select one parton configuration from the observed state and collapse the correlated quantum state. This configuration is then dressed by applying parton shower, decays and hadronization. The decay chain, in particular, combines a scattering process with possible subsequent decay processes on the parton level, which are full-fledged process objects themselves.

30.1 Process observables

We define an abstract `subvt_expr_t` object as an extension of the `subvt_t` type. The object contains a local variable list, variable instances (as targets for pointers in the variable list), and evaluation trees. The evaluation trees reference both the variables and the `subvt`.

There are two instances of the abstract type: one for process instances, one for physical events. Both have a common logical expression `selection` which determines whether the object passes user-defined cuts.

The intention is that we fill the `subvt_t` base object and compute the variables once we have evaluated a kinematical phase space point (or a complete event). We then evaluate the expressions and can use the results in further calculations.

The `process_expr_t` extension contains furthermore scale and weight expressions. The `event_expr_t` extension contains a reweighting-factor expression and a logical expression for event analysis. In practice, we will link the variable list of the `event_obs` object to the variable list of the currently active `process_obs` object, such that the process variables are available to both objects. Event variables are meaningful only for physical events.

Note that there are unit tests, but they are deferred to the `expr_tests` module.

```

<subvt_expr.f90>≡
  <File header>
  module subvt_expr

    <Use kinds>
    <Use strings>
    use lorentz
    use subevents
    use variables
    use flavors
    use quantum_numbers
    use interactions
    use particles
    use expr_base

    <Standard module head>

    <Subvt expr: public>

    <Subvt expr: types>

    <Subvt expr: interfaces>

```

```

        interface
        <Subvt expr: sub interfaces>
        end interface

    end module subvt_expr

<subvt_expr_sub.f90>≡
    <File header>

    submodule (subvt_expr) subvt_expr_s

        use constants, only: zero, one
        use io_units
        use format_utils, only: write_separator
        use diagnostics

        implicit none

    contains

    <Subvt expr: procedures>

    end submodule subvt_expr_s

```

30.1.1 Abstract base type

```

<Subvt expr: types>≡
    type, extends (subvt_t), abstract :: subvt_expr_t
        logical :: subvt_filled = .false.
        type(var_list_t) :: var_list
        real(default) :: sqrts_hat = 0
        integer :: n_in = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        logical :: has_selection = .false.
        class(expr_t), allocatable :: selection
        logical :: colorize_subvt = .false.
    contains
    <Subvt expr: subvt expr: TBP>
    end type subvt_expr_t

```

Output: Base and extended version. We already have a `write` routine for the `subvt_t` parent type.

```

<Subvt expr: subvt expr: TBP>≡
    procedure :: base_write => subvt_expr_write

<Subvt expr: sub interfaces>≡
    module subroutine subvt_expr_write (object, unit, pacified)
        class(subvt_expr_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacified
    end subroutine subvt_expr_write

```

```

<Subevt expr: procedures>≡
module subroutine subevt_expr_write (object, unit, pacified)
  class(subevt_expr_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacified
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Local variables:"
  call write_separator (u)
  call object%var_list%write (u, follow_link=.false., &
    pacified = pacified)
  call write_separator (u)
  if (object%subevt_filled) then
    call object%subevt_t%write (u, pacified = pacified)
    if (object%has_selection) then
      call write_separator (u)
      write (u, "(1x,A)") "Selection expression:"
      call write_separator (u)
      call object%selection%write (u)
    end if
  else
    write (u, "(1x,A)") "subevt: [undefined]"
  end if
end subroutine subevt_expr_write

```

Finalizer.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure (subevt_expr_final), deferred :: final
  procedure :: base_final => subevt_expr_final

<Subevt expr: sub interfaces>+≡
  module subroutine subevt_expr_final (object)
    class(subevt_expr_t), intent(inout) :: object
  end subroutine subevt_expr_final

<Subevt expr: procedures>+≡
module subroutine subevt_expr_final (object)
  class(subevt_expr_t), intent(inout) :: object
  call object%var_list%final ()
  if (object%has_selection) then
    call object%selection%final ()
  end if
end subroutine subevt_expr_final

```

30.1.2 Initialization

Initialization: define local variables and establish pointers.

The common variables are `sqrts` (the nominal beam energy, fixed), `sqrts_hat` (the actual energy), `n_in`, `n_out`, and `n_tot` for the subevt. With the exception of `sqrts`, all are implemented as pointers to subobjects.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure (subevt_expr_setup_vars), deferred :: setup_vars
  procedure :: base_setup_vars => subevt_expr_setup_vars

```

```

<Subevt expr: sub interfaces>+≡
  module subroutine subevt_expr_setup_vars (expr, sqrts)
    class(subevt_expr_t), intent(inout), target :: expr
    real(default), intent(in) :: sqrts
  end subroutine subevt_expr_setup_vars

<Subevt expr: procedures>+≡
  module subroutine subevt_expr_setup_vars (expr, sqrts)
    class(subevt_expr_t), intent(inout), target :: expr
    real(default), intent(in) :: sqrts
    call expr%var_list%final ()
    call expr%var_list%append_real (var_str ("sqrts"), sqrts, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call expr%var_list%append_real_ptr (var_str ("sqrts_hat"), &
      expr%sqrts_hat, is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call expr%var_list%append_int_ptr (var_str ("n_in"), expr%n_in, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call expr%var_list%append_int_ptr (var_str ("n_out"), expr%n_out, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call expr%var_list%append_int_ptr (var_str ("n_tot"), expr%n_tot, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
  end subroutine subevt_expr_setup_vars

```

Append the subevent expr (its base-type core) itself to the variable list, if it is not yet present.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure :: setup_var_self => subevt_expr_setup_var_self

<Subevt expr: sub interfaces>+≡
  module subroutine subevt_expr_setup_var_self (expr)
    class(subevt_expr_t), intent(inout), target :: expr
  end subroutine subevt_expr_setup_var_self

<Subevt expr: procedures>+≡
  module subroutine subevt_expr_setup_var_self (expr)
    class(subevt_expr_t), intent(inout), target :: expr
    if (.not. expr%var_list%contains (var_str ("@evt"))) then
      call expr%var_list%append_subevt_ptr &
        (var_str ("@evt"), expr%subevt_t, &
          is_known = expr%subevt_filled, &
          locked = .true., verbose = .false., intrinsic=.true.)
    end if
  end subroutine subevt_expr_setup_var_self

```

Link a variable list to the local one. This could be done event by event, but before evaluating expressions.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure :: link_var_list => subevt_expr_link_var_list

```

```

<Subvt expr: sub interfaces>+≡
    module subroutine subvt_expr_link_var_list (expr, var_list)
        class(subvt_expr_t), intent(inout) :: expr
        type(var_list_t), intent(in), target :: var_list
    end subroutine subvt_expr_link_var_list

```

```

<Subvt expr: procedures>+≡
    module subroutine subvt_expr_link_var_list (expr, var_list)
        class(subvt_expr_t), intent(inout) :: expr
        type(var_list_t), intent(in), target :: var_list
        call expr%var_list%link (var_list)
    end subroutine subvt_expr_link_var_list

```

Compile the selection expression. If there is no expression, the build method will not allocate the expression object.

```

<Subvt expr: subvt expr: TBP>+≡
    procedure :: setup_selection => subvt_expr_setup_selection

<Subvt expr: sub interfaces>+≡
    module subroutine subvt_expr_setup_selection (expr, ef_cuts)
        class(subvt_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_cuts
    end subroutine subvt_expr_setup_selection

<Subvt expr: procedures>+≡
    module subroutine subvt_expr_setup_selection (expr, ef_cuts)
        class(subvt_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_cuts
        call ef_cuts%build (expr%selection)
        if (allocated (expr%selection)) then
            call expr%setup_var_self ()
            call expr%selection%setup_lexpr (expr%var_list)
            expr%has_selection = .true.
        end if
    end subroutine subvt_expr_setup_selection

```

(De)activate color storage and evaluation for the expression. The subevent particles will have color information.

```

<Subvt expr: subvt expr: TBP>+≡
    procedure :: colorize => subvt_expr_colorize

<Subvt expr: sub interfaces>+≡
    module subroutine subvt_expr_colorize (expr, colorize_subvt)
        class(subvt_expr_t), intent(inout), target :: expr
        logical, intent(in) :: colorize_subvt
    end subroutine subvt_expr_colorize

<Subvt expr: procedures>+≡
    module subroutine subvt_expr_colorize (expr, colorize_subvt)
        class(subvt_expr_t), intent(inout), target :: expr
        logical, intent(in) :: colorize_subvt
        expr%colorize_subvt = colorize_subvt
    end subroutine subvt_expr_colorize

```

30.1.3 Evaluation

Reset to initial state, i.e., mark the subevt as invalid.

```
<Subevt expr: subevt expr: TBP>+≡
  procedure :: reset_contents => subevt_expr_reset_contents
  procedure :: base_reset_contents => subevt_expr_reset_contents

<Subevt expr: sub interfaces>+≡
  module subroutine subevt_expr_reset_contents (expr)
    class(subevt_expr_t), intent(inout) :: expr
  end subroutine subevt_expr_reset_contents

<Subevt expr: procedures>+≡
  module subroutine subevt_expr_reset_contents (expr)
    class(subevt_expr_t), intent(inout) :: expr
    expr%subevt_filled = .false.
  end subroutine subevt_expr_reset_contents
```

Evaluate the selection expression and return the result. There is also a deferred version: this should evaluate the remaining expressions if the event has passed.

```
<Subevt expr: subevt expr: TBP>+≡
  procedure :: base_evaluate => subevt_expr_evaluate

<Subevt expr: sub interfaces>+≡
  module subroutine subevt_expr_evaluate (expr, passed)
    class(subevt_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
  end subroutine subevt_expr_evaluate

<Subevt expr: procedures>+≡
  module subroutine subevt_expr_evaluate (expr, passed)
    class(subevt_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
    if (expr%has_selection) then
      call expr%selection%evaluate ()
      if (expr%selection%is_known ()) then
        passed = expr%selection%get_log ()
      else
        call msg_error ("Evaluate selection expression: result undefined")
        passed = .false.
      end if
    else
      passed = .true.
    end if
  end subroutine subevt_expr_evaluate
```

30.1.4 Implementation for partonic events

This implementation contains the expressions that we can evaluate for the partonic process during integration.

```
<Subevt expr: public>≡
  public :: parton_expr_t
```

```

<Subvt expr: types>+=
  type, extends (subvt_expr_t) :: parton_expr_t
    integer, dimension(:), allocatable :: i_beam
    integer, dimension(:), allocatable :: i_in
    integer, dimension(:), allocatable :: i_out
    logical :: has_scale = .false.
    logical :: has_fac_scale = .false.
    logical :: has_ren_scale = .false.
    logical :: has_weight = .false.
    class(expr_t), allocatable :: scale
    class(expr_t), allocatable :: fac_scale
    class(expr_t), allocatable :: ren_scale
    class(expr_t), allocatable :: weight
  contains
    <Subvt expr: parton expr: TBP>
  end type parton_expr_t

```

Finalizer.

```

<Subvt expr: parton expr: TBP>=
  procedure :: final => parton_expr_final

<Subvt expr: sub interfaces>+=
  module subroutine parton_expr_final (object)
    class(parton_expr_t), intent(inout) :: object
  end subroutine parton_expr_final

<Subvt expr: procedures>+=
  module subroutine parton_expr_final (object)
    class(parton_expr_t), intent(inout) :: object
    call object%base_final ()
    if (object%has_scale) then
      call object%scale%final ()
    end if
    if (object%has_fac_scale) then
      call object%fac_scale%final ()
    end if
    if (object%has_ren_scale) then
      call object%ren_scale%final ()
    end if
    if (object%has_weight) then
      call object%weight%final ()
    end if
  end subroutine parton_expr_final

```

Output: continue writing the active expressions, after the common selection expression.

Note: the `prefix` argument is declared in the `write` method of the `subvt_t` base type. Here, it is unused.

```

<Subvt expr: parton expr: TBP>+=
  procedure :: write => parton_expr_write

<Subvt expr: sub interfaces>+=
  module subroutine parton_expr_write (object, unit, prefix, pacified)
    class(parton_expr_t), intent(in) :: object

```



```

integer, intent(in), optional :: unit
character(*), intent(in), optional :: prefix
logical, intent(in), optional :: pacified
end subroutine parton_expr_write

<Subevt expr: procedures>+≡
module subroutine parton_expr_write (object, unit, prefix, pacified)
class(parton_expr_t), intent(in) :: object
integer, intent(in), optional :: unit
character(*), intent(in), optional :: prefix
logical, intent(in), optional :: pacified
integer :: u
u = given_output_unit (unit)
call object%base_write (u, pacified = pacified)
if (object%subevt_filled) then
if (object%has_scale) then
call write_separator (u)
write (u, "(1x,A)") "Scale expression:"
call write_separator (u)
call object%scale%write (u)
end if
if (object%has_fac_scale) then
call write_separator (u)
write (u, "(1x,A)") "Factorization scale expression:"
call write_separator (u)
call object%fac_scale%write (u)
end if
if (object%has_ren_scale) then
call write_separator (u)
write (u, "(1x,A)") "Renormalization scale expression:"
call write_separator (u)
call object%ren_scale%write (u)
end if
if (object%has_weight) then
call write_separator (u)
write (u, "(1x,A)") "Weight expression:"
call write_separator (u)
call object%weight%write (u)
end if
end if
end subroutine parton_expr_write

```

Define variables.

```

<Subevt expr: parton expr: TBP>+≡
procedure :: setup_vars => parton_expr_setup_vars

<Subevt expr: sub interfaces>+≡
module subroutine parton_expr_setup_vars (expr, sqrts)
class(parton_expr_t), intent(inout), target :: expr
real(default), intent(in) :: sqrts
end subroutine parton_expr_setup_vars

<Subevt expr: procedures>+≡
module subroutine parton_expr_setup_vars (expr, sqrts)
class(parton_expr_t), intent(inout), target :: expr

```

```

    real(default), intent(in) :: sqrts
    call expr%base_setup_vars (sqrts)
end subroutine parton_expr_setup_vars

```

Compile the scale expressions. If a pointer is disassociated, there is no expression.

```

<Subevt expr: parton expr: TBP>+≡
  procedure :: setup_scale => parton_expr_setup_scale
  procedure :: setup_fac_scale => parton_expr_setup_fac_scale
  procedure :: setup_ren_scale => parton_expr_setup_ren_scale
<Subevt expr: sub interfaces>+≡
  module subroutine parton_expr_setup_scale (expr, ef_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_scale
  end subroutine parton_expr_setup_scale
  module subroutine parton_expr_setup_fac_scale (expr, ef_fac_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_fac_scale
  end subroutine parton_expr_setup_fac_scale
  module subroutine parton_expr_setup_ren_scale (expr, ef_ren_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_ren_scale
  end subroutine parton_expr_setup_ren_scale
<Subevt expr: procedures>+≡
  module subroutine parton_expr_setup_scale (expr, ef_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_scale
    call ef_scale%build (expr%scale)
    if (allocated (expr%scale)) then
      call expr%setup_var_self ()
      call expr%scale%setup_expr (expr%var_list)
      expr%has_scale = .true.
    end if
  end subroutine parton_expr_setup_scale

  module subroutine parton_expr_setup_fac_scale (expr, ef_fac_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_fac_scale
    call ef_fac_scale%build (expr%fac_scale)
    if (allocated (expr%fac_scale)) then
      call expr%setup_var_self ()
      call expr%fac_scale%setup_expr (expr%var_list)
      expr%has_fac_scale = .true.
    end if
  end subroutine parton_expr_setup_fac_scale

  module subroutine parton_expr_setup_ren_scale (expr, ef_ren_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_ren_scale
    call ef_ren_scale%build (expr%ren_scale)
    if (allocated (expr%ren_scale)) then
      call expr%setup_var_self ()
      call expr%ren_scale%setup_expr (expr%var_list)

```

```

        expr%has_ren_scale = .true.
    end if
end subroutine parton_expr_setup_ren_scale

```

Compile the weight expression.

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: setup_weight => parton_expr_setup_weight

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_setup_weight (expr, ef_weight)
        class(parton_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_weight
    end subroutine parton_expr_setup_weight

<Subevt expr: procedures>+≡
    module subroutine parton_expr_setup_weight (expr, ef_weight)
        class(parton_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_weight
        call ef_weight%build (expr%weight)
        if (allocated (expr%weight)) then
            call expr%setup_var_self ()
            call expr%weight%setup_expr (expr%var_list)
            expr%has_weight = .true.
        end if
    end subroutine parton_expr_setup_weight

```

Filling the partonic state consists of two parts. The first routine prepares the subevt without assigning momenta. It takes the particles from an `interaction_t`. It needs the indices and flavors for the beam, incoming, and outgoing particles.

We can assume that the particle content of the subevt does not change. Therefore, we set the event variables `n_in`, `n_out`, `n_tot` already in this initialization step.

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: setup_subevt => parton_expr_setup_subevt

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_setup_subevt (expr, int, &
        i_beam, i_in, i_out, f_beam, f_in, f_out)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
        integer, dimension(:), intent(in) :: i_beam, i_in, i_out
        type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
    end subroutine parton_expr_setup_subevt

<Subevt expr: procedures>+≡
    module subroutine parton_expr_setup_subevt (expr, int, &
        i_beam, i_in, i_out, f_beam, f_in, f_out)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
        integer, dimension(:), intent(in) :: i_beam, i_in, i_out
        type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
        allocate (expr%i_beam (size (i_beam)))
        allocate (expr%i_in (size (i_in)))
        allocate (expr%i_out (size (i_out)))

```

```

expr%i_beam = i_beam
expr%i_in = i_in
expr%i_out = i_out
call interaction_to_subevt (int, &
    expr%i_beam, expr%i_in, expr%i_out, expr%subevt_t)
call expr%set_pdg_beam (f_beam%get_pdg ())
call expr%set_pdg_incoming (f_in%get_pdg ())
call expr%set_pdg_outgoing (f_out%get_pdg ())
call expr%set_p2_beam (f_beam%get_mass () ** 2)
call expr%set_p2_incoming (f_in%get_mass () ** 2)
call expr%set_p2_outgoing (f_out%get_mass () ** 2)
expr%n_in = size (i_in)
expr%n_out = size (i_out)
expr%n_tot = expr%n_in + expr%n_out
end subroutine parton_expr_setup_subevt

```

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: renew_flv_content_subevt => parton_expr_renew_flv_content_subevt

```

```

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_renew_flv_content_subevt (expr, int, &
        i_beam, i_in, i_out, f_beam, f_in, f_out)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
        integer, dimension(:), intent(in) :: i_beam, i_in, i_out
        type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
    end subroutine parton_expr_renew_flv_content_subevt

```

```

<Subevt expr: procedures>+≡
    module subroutine parton_expr_renew_flv_content_subevt (expr, int, &
        i_beam, i_in, i_out, f_beam, f_in, f_out)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
        integer, dimension(:), intent(in) :: i_beam, i_in, i_out
        type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
        expr%i_beam = i_beam
        expr%i_in = i_in
        expr%i_out = i_out
        call expr%set_pdg_beam (f_beam%get_pdg ())
        call expr%set_pdg_incoming (f_in%get_pdg ())
        call expr%set_pdg_outgoing (f_out%get_pdg ())
        expr%n_in = size (i_in)
        expr%n_out = size (i_out)
        expr%n_tot = expr%n_in + expr%n_out
    end subroutine parton_expr_renew_flv_content_subevt

```

Transfer PDG codes, masses (initialization) and momenta to a predefined subevent. We use the flavor assignment of the first branch in the interaction state matrix. Only incoming and outgoing particles are transferred. Switch momentum sign for incoming particles.

```

<Subevt expr: interfaces>≡
    interface interaction_momenta_to_subevt
        module procedure interaction_momenta_to_subevt_id
        module procedure interaction_momenta_to_subevt_tr
    end interface

```

```
end interface
```

(Subevt expr: sub interfaces)+≡

```
module subroutine interaction_momenta_to_subevt_id &
  (int, j_beam, j_in, j_out, subevt)
  type(interaction_t), intent(in) :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(inout) :: subevt
end subroutine interaction_momenta_to_subevt_id
module subroutine interaction_momenta_to_subevt_tr &
  (int, j_beam, j_in, j_out, lt, subevt)
  type(interaction_t), intent(in) :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(inout) :: subevt
  type(lorentz_transformation_t), intent(in) :: lt
end subroutine interaction_momenta_to_subevt_tr
```

(Subevt expr: procedures)+≡

```
subroutine interaction_to_subevt (int, j_beam, j_in, j_out, subevt)
  type(interaction_t), intent(in), target :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(out) :: subevt
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: n_beam, n_in, n_out, i, j
  allocate (flv (int%get_n_tot ()))
  flv = quantum_numbers_get_flavor (int%get_quantum_numbers (1))
  n_beam = size (j_beam)
  n_in = size (j_in)
  n_out = size (j_out)
  call subevt_init (subevt, n_beam + n_in + n_out)
  do i = 1, n_beam
    j = j_beam(i)
    call subevt%set_beam (i, flv(j)%get_pdg (), &
      vector4_null, flv(j)%get_mass () ** 2)
  end do
  do i = 1, n_in
    j = j_in(i)
    call subevt%set_incoming (n_beam + i, flv(j)%get_pdg (), &
      vector4_null, flv(j)%get_mass () ** 2)
  end do
  do i = 1, n_out
    j = j_out(i)
    call subevt%set_outgoing (n_beam + n_in + i, &
      flv(j)%get_pdg (), vector4_null, &
      flv(j)%get_mass () ** 2)
  end do
end subroutine interaction_to_subevt

module subroutine interaction_momenta_to_subevt_id &
  (int, j_beam, j_in, j_out, subevt)
  type(interaction_t), intent(in) :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(inout) :: subevt
  call subevt%set_p_beam (- int%get_momenta (j_beam))
```

```

    call subevt%set_p_incoming (- int%get_momenta (j_in))
    call subevt%set_p_outgoing (int%get_momenta (j_out))
end subroutine interaction_momenta_to_subevt_id

module subroutine interaction_momenta_to_subevt_tr &
    (int, j_beam, j_in, j_out, lt, subevt)
    type(interaction_t), intent(in) :: int
    integer, dimension(:), intent(in) :: j_beam, j_in, j_out
    type(subevt_t), intent(inout) :: subevt
    type(lorentz_transformation_t), intent(in) :: lt
    call subevt%set_p_beam (- lt * int%get_momenta (j_beam))
    call subevt%set_p_incoming (- lt * int%get_momenta (j_in))
    call subevt%set_p_outgoing (lt * int%get_momenta (j_out))
end subroutine interaction_momenta_to_subevt_tr

```

The second part takes the momenta from the interaction object and thus completes the subevt. The partonic energy can then be computed.

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: fill_subevt => parton_expr_fill_subevt

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_fill_subevt (expr, int)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
    end subroutine parton_expr_fill_subevt

<Subevt expr: procedures>+≡
    module subroutine parton_expr_fill_subevt (expr, int)
        class(parton_expr_t), intent(inout) :: expr
        type(interaction_t), intent(in), target :: int
        call interaction_momenta_to_subevt (int, &
            expr%i_beam, expr%i_in, expr%i_out, expr%subevt_t)
        expr%sqrts_hat = expr%get_sqrts_hat ()
        expr%subevt_filled = .true.
    end subroutine parton_expr_fill_subevt

```

Evaluate, if the event passes the selection. For absent expressions we take default values.

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: evaluate => parton_expr_evaluate

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_evaluate (expr, passed, scale, fac_scale, &
        ren_scale, weight, scale_forced, force_evaluation)
        class(parton_expr_t), intent(inout) :: expr
        logical, intent(out) :: passed
        real(default), intent(out) :: scale
        real(default), allocatable, intent(out) :: fac_scale
        real(default), allocatable, intent(out) :: ren_scale
        real(default), intent(out) :: weight
        real(default), intent(in), allocatable, optional :: scale_forced
        logical, intent(in), optional :: force_evaluation
    end subroutine parton_expr_evaluate

```

<Subevt expr: procedures>+≡

```

module subroutine parton_expr_evaluate (expr, passed, scale, fac_scale, &
    ren_scale, weight, scale_forced, force_evaluation)
    class(parton_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
    real(default), intent(out) :: scale
    real(default), allocatable, intent(out) :: fac_scale
    real(default), allocatable, intent(out) :: ren_scale
    real(default), intent(out) :: weight
    real(default), intent(in), allocatable, optional :: scale_forced
    logical, intent(in), optional :: force_evaluation
    logical :: force_scale, force_eval
    force_scale = .false.; force_eval = .false.
    if (present (scale_forced)) force_scale = allocated (scale_forced)
    if (present (force_evaluation)) force_eval = force_evaluation
    call expr%base_evaluate (passed)
    if (passed .or. force_eval) then
        if (force_scale) then
            scale = scale_forced
        else if (expr%has_scale) then
            call expr%scale%evaluate ()
            if (expr%scale%is_known ()) then
                scale = expr%scale%get_real ()
            else
                call msg_error ("Evaluate scale expression: result undefined")
                scale = zero
            end if
        else
            scale = expr%sqrts_hat
        end if
        if (expr%has_fac_scale) then
            call expr%fac_scale%evaluate ()
            if (expr%fac_scale%is_known ()) then
                if (.not. allocated (fac_scale)) then
                    allocate (fac_scale, source = expr%fac_scale%get_real ())
                else
                    fac_scale = expr%fac_scale%get_real ()
                end if
            else
                call msg_error ("Evaluate factorization scale expression: &
                    &result undefined")
            end if
        end if
        if (expr%has_ren_scale) then
            call expr%ren_scale%evaluate ()
            if (expr%ren_scale%is_known ()) then
                if (.not. allocated (ren_scale)) then
                    allocate (ren_scale, source = expr%ren_scale%get_real ())
                else
                    ren_scale = expr%ren_scale%get_real ()
                end if
            else
                call msg_error ("Evaluate renormalization scale expression: &
                    &result undefined")
            end if
        end if
    end if
end subroutine

```

```

        end if
    end if
    if (expr%has_weight) then
        call expr%weight%evaluate ()
        if (expr%weight%is_known ()) then
            weight = expr%weight%get_real ()
        else
            call msg_error ("Evaluate weight expression: result undefined")
            weight = zero
        end if
    else
        weight = one
    end if
else
    weight = zero
end if
end subroutine parton_expr_evaluate

```

Return the beam/incoming parton indices.

```

<Subevt expr: parton expr: TBP>+≡
    procedure :: get_beam_index => parton_expr_get_beam_index
    procedure :: get_in_index => parton_expr_get_in_index

<Subevt expr: sub interfaces>+≡
    module subroutine parton_expr_get_beam_index (expr, i_beam)
        class(parton_expr_t), intent(in) :: expr
        integer, dimension(:), intent(out) :: i_beam
    end subroutine parton_expr_get_beam_index
    module subroutine parton_expr_get_in_index (expr, i_in)
        class(parton_expr_t), intent(in) :: expr
        integer, dimension(:), intent(out) :: i_in
    end subroutine parton_expr_get_in_index

<Subevt expr: procedures>+≡
    module subroutine parton_expr_get_beam_index (expr, i_beam)
        class(parton_expr_t), intent(in) :: expr
        integer, dimension(:), intent(out) :: i_beam
        i_beam = expr%i_beam
    end subroutine parton_expr_get_beam_index

    module subroutine parton_expr_get_in_index (expr, i_in)
        class(parton_expr_t), intent(in) :: expr
        integer, dimension(:), intent(out) :: i_in
        i_in = expr%i_in
    end subroutine parton_expr_get_in_index

```

30.1.5 Implementation for full events

This implementation contains the expressions that we can evaluate for the full event. It also contains data that pertain to the event, suitable for communication with external event formats. These data simultaneously serve as pointer targets for the variable lists hidden in the expressions (eval trees).

Squared matrix element and weight values: when reading events from file, the `ref` value is the number in the file, while the `prc` value is the number that we calculate from the momenta in the file, possibly with different parameters. When generating events the first time, or if we do not recalculate, the numbers should coincide. Furthermore, the array of `alt` values is copied from an array of alternative event records. These values should represent calculated values.

```

<Subvt expr: public>+≡
    public :: event_expr_t

<Subvt expr: types>+≡
    type, extends (subvt_expr_t) :: event_expr_t
        logical :: has_reweight = .false.
        logical :: has_analysis = .false.
        class(expr_t), allocatable :: reweight
        class(expr_t), allocatable :: analysis
        logical :: has_id = .false.
        type(string_t) :: id
        logical :: has_num_id = .false.
        integer :: num_id = 0
        logical :: has_index = .false.
        integer :: index = 0
        logical :: has_sqme_ref = .false.
        real(default) :: sqme_ref = 0
        logical :: has_sqme_prc = .false.
        real(default) :: sqme_prc = 0
        logical :: has_weight_ref = .false.
        real(default) :: weight_ref = 0
        logical :: has_weight_prc = .false.
        real(default) :: weight_prc = 0
        logical :: has_excess_prc = .false.
        real(default) :: excess_prc = 0
        integer :: n_alt = 0
        logical :: has_sqme_alt = .false.
        real(default), dimension(:), allocatable :: sqme_alt
        logical :: has_weight_alt = .false.
        real(default), dimension(:), allocatable :: weight_alt
    contains
        <Subvt expr: event expr: TBP>
    end type event_expr_t

```

Finalizer for the expressions.

```

<Subvt expr: event expr: TBP>≡
    procedure :: final => event_expr_final

<Subvt expr: sub interfaces>+≡
    module subroutine event_expr_final (object)
        class(event_expr_t), intent(inout) :: object
    end subroutine event_expr_final

<Subvt expr: procedures>+≡
    module subroutine event_expr_final (object)
        class(event_expr_t), intent(inout) :: object
        call object%base_final ()
        if (object%has_reweight) then

```

```

        call object%reweight%final ()
    end if
    if (object%has_analysis) then
        call object%analysis%final ()
    end if
end subroutine event_expr_final

```

Output: continue writing the active expressions, after the common selection expression.

Note: the `prefix` argument is declared in the `write` method of the `subevt_t` base type. Here, it is unused.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: write => event_expr_write

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_write (object, unit, prefix, pacified)
        class(event_expr_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(*), intent(in), optional :: prefix
        logical, intent(in), optional :: pacified
    end subroutine event_expr_write

<Subevt expr: procedures>+≡
    module subroutine event_expr_write (object, unit, prefix, pacified)
        class(event_expr_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(*), intent(in), optional :: prefix
        logical, intent(in), optional :: pacified
        integer :: u
        u = given_output_unit (unit)
        call object%base_write (u, pacified = pacified)
        if (object%subevt_filled) then
            if (object%has_reweight) then
                call write_separator (u)
                write (u, "(1x,A)") "Reweighting expression:"
                call write_separator (u)
                call object%reweight%write (u)
            end if
            if (object%has_analysis) then
                call write_separator (u)
                write (u, "(1x,A)") "Analysis expression:"
                call write_separator (u)
                call object%analysis%write (u)
            end if
        end if
    end subroutine event_expr_write

```

Initializer. This is required only for the `sqme_alt` and `weight_alt` arrays.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: init => event_expr_init

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_init (expr, n_alt)
        class(event_expr_t), intent(out) :: expr

```

```

        integer, intent(in), optional :: n_alt
    end subroutine event_expr_init
<Subevt expr: procedures>+≡
    module subroutine event_expr_init (expr, n_alt)
        class(event_expr_t), intent(out) :: expr
        integer, intent(in), optional :: n_alt
        if (present (n_alt)) then
            expr%n_alt = n_alt
            allocate (expr%sqme_alt (n_alt), source = 0._default)
            allocate (expr%weight_alt (n_alt), source = 0._default)
        end if
    end subroutine event_expr_init

```

Define variables. We have the variables of the base type plus specific variables for full events. There is the event index.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: setup_vars => event_expr_setup_vars
<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_setup_vars (expr, sqrts)
        class(event_expr_t), intent(inout), target :: expr
        real(default), intent(in) :: sqrts
    end subroutine event_expr_setup_vars
<Subevt expr: procedures>+≡
    module subroutine event_expr_setup_vars (expr, sqrts)
        class(event_expr_t), intent(inout), target :: expr
        real(default), intent(in) :: sqrts
        call expr%base_setup_vars (sqrts)
        call expr%var_list%append_string_ptr (var_str ("process_id"), &
            expr%id, is_known = expr%has_id, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_int_ptr (var_str ("process_num_id"), &
            expr%num_id, is_known = expr%has_num_id, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_real_ptr (var_str ("sqme"), &
            expr%sqme_prc, is_known = expr%has_sqme_prc, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_real_ptr (var_str ("sqme_ref"), &
            expr%sqme_ref, is_known = expr%has_sqme_ref, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_int_ptr (var_str ("event_index"), &
            expr%index, is_known = expr%has_index, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_real_ptr (var_str ("event_weight"), &
            expr%weight_prc, is_known = expr%has_weight_prc, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_real_ptr (var_str ("event_weight_ref"), &
            expr%weight_ref, is_known = expr%has_weight_ref, &
            locked = .true., verbose = .false., intrinsic = .true.)
        call expr%var_list%append_real_ptr (var_str ("event_excess"), &
            expr%excess_prc, is_known = expr%has_excess_prc, &
            locked = .true., verbose = .false., intrinsic = .true.)
    end subroutine event_expr_setup_vars

```

Compile the analysis expression. If the pointer is disassociated, there is no expression.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: setup_analysis => event_expr_setup_analysis

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_setup_analysis (expr, ef_analysis)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_analysis
    end subroutine event_expr_setup_analysis

<Subevt expr: procedures>+≡
    module subroutine event_expr_setup_analysis (expr, ef_analysis)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_analysis
        call ef_analysis%build (expr%analysis)
        if (allocated (expr%analysis)) then
            call expr%setup_var_self ()
            call expr%analysis%setup_lexpr (expr%var_list)
            expr%has_analysis = .true.
        end if
    end subroutine event_expr_setup_analysis

```

Compile the reweight expression.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: setup_reweight => event_expr_setup_reweight

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_setup_reweight (expr, ef_reweight)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_reweight
    end subroutine event_expr_setup_reweight

<Subevt expr: procedures>+≡
    module subroutine event_expr_setup_reweight (expr, ef_reweight)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_reweight
        call ef_reweight%build (expr%reweight)
        if (allocated (expr%reweight)) then
            call expr%setup_var_self ()
            call expr%reweight%setup_expr (expr%var_list)
            expr%has_reweight = .true.
        end if
    end subroutine event_expr_setup_reweight

```

Store the string or numeric process ID. This should be done during initialization.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: set_process_id => event_expr_set_process_id
    procedure :: set_process_num_id => event_expr_set_process_num_id

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_set_process_id (expr, id)
        class(event_expr_t), intent(inout) :: expr
        type(string_t), intent(in) :: id
    end subroutine event_expr_set_process_id

```

```

module subroutine event_expr_set_process_num_id (expr, num_id)
  class(event_expr_t), intent(inout) :: expr
  integer, intent(in) :: num_id
end subroutine event_expr_set_process_num_id

<Subevt expr: procedures>+≡
module subroutine event_expr_set_process_id (expr, id)
  class(event_expr_t), intent(inout) :: expr
  type(string_t), intent(in) :: id
  expr%id = id
  expr%has_id = .true.
end subroutine event_expr_set_process_id

module subroutine event_expr_set_process_num_id (expr, num_id)
  class(event_expr_t), intent(inout) :: expr
  integer, intent(in) :: num_id
  expr%num_id = num_id
  expr%has_num_id = .true.
end subroutine event_expr_set_process_num_id

Reset / set the data that pertain to a particular event. The event index is reset
unless explicitly told to keep it.

<Subevt expr: event expr: TBP>+≡
  procedure :: reset_contents => event_expr_reset_contents
  procedure :: set => event_expr_set

<Subevt expr: sub interfaces>+≡
  module subroutine event_expr_reset_contents (expr)
    class(event_expr_t), intent(inout) :: expr
  end subroutine event_expr_reset_contents
  module subroutine event_expr_set (expr, &
    weight_ref, weight_prc, weight_alt, &
    excess_prc, &
    sqme_ref, sqme_prc, sqme_alt)
    class(event_expr_t), intent(inout) :: expr
    real(default), intent(in), optional :: weight_ref, weight_prc
    real(default), intent(in), optional :: excess_prc
    real(default), intent(in), optional :: sqme_ref, sqme_prc
    real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
  end subroutine event_expr_set

<Subevt expr: procedures>+≡
  module subroutine event_expr_reset_contents (expr)
    class(event_expr_t), intent(inout) :: expr
    call expr%base_reset_contents ()
    expr%has_sqme_ref = .false.
    expr%has_sqme_prc = .false.
    expr%has_sqme_alt = .false.
    expr%has_weight_ref = .false.
    expr%has_weight_prc = .false.
    expr%has_weight_alt = .false.
    expr%has_excess_prc = .false.
  end subroutine event_expr_reset_contents

  module subroutine event_expr_set (expr, &

```

```

        weight_ref, weight_prc, weight_alt, &
        excess_prc, &
        sqme_ref, sqme_prc, sqme_alt)
class(event_expr_t), intent(inout) :: expr
real(default), intent(in), optional :: weight_ref, weight_prc
real(default), intent(in), optional :: excess_prc
real(default), intent(in), optional :: sqme_ref, sqme_prc
real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
if (present (sqme_ref)) then
    expr%has_sqme_ref = .true.
    expr%sqme_ref = sqme_ref
end if
if (present (sqme_prc)) then
    expr%has_sqme_prc = .true.
    expr%sqme_prc = sqme_prc
end if
if (present (sqme_alt)) then
    expr%has_sqme_alt = .true.
    expr%sqme_alt = sqme_alt
end if
if (present (weight_ref)) then
    expr%has_weight_ref = .true.
    expr%weight_ref = weight_ref
end if
if (present (weight_prc)) then
    expr%has_weight_prc = .true.
    expr%weight_prc = weight_prc
end if
if (present (weight_alt)) then
    expr%has_weight_alt = .true.
    expr%weight_alt = weight_alt
end if
if (present (excess_prc)) then
    expr%has_excess_prc = .true.
    expr%excess_prc = excess_prc
end if
end subroutine event_expr_set

```

Access the subevent index.

<Subevt expr: event expr: TBP>+≡

```

procedure :: has_event_index => event_expr_has_event_index
procedure :: get_event_index => event_expr_get_event_index

```

<Subevt expr: sub interfaces>+≡

```

module function event_expr_has_event_index (expr) result (flag)
    class(event_expr_t), intent(in) :: expr
    logical :: flag
end function event_expr_has_event_index
module function event_expr_get_event_index (expr) result (index)
    class(event_expr_t), intent(in) :: expr
    integer :: index
end function event_expr_get_event_index

```

<Subevt expr: procedures>+≡

```

module function event_expr_has_event_index (expr) result (flag)

```

```

class(event_expr_t), intent(in) :: expr
logical :: flag
flag = expr%has_index
end function event_expr_has_event_index

module function event_expr_get_event_index (expr) result (index)
class(event_expr_t), intent(in) :: expr
integer :: index
if (expr%has_index) then
index = expr%index
else
index = 0
end if
end function event_expr_get_event_index

```

Set/increment the subevent index. Initialize it if necessary.

```

<Subevt expr: event expr: TBP>+≡
procedure :: set_event_index => event_expr_set_event_index
procedure :: reset_event_index => event_expr_reset_event_index
procedure :: increment_event_index => event_expr_increment_event_index

<Subevt expr: sub interfaces>+≡
module subroutine event_expr_set_event_index (expr, index)
class(event_expr_t), intent(inout) :: expr
integer, intent(in) :: index
end subroutine event_expr_set_event_index
module subroutine event_expr_reset_event_index (expr)
class(event_expr_t), intent(inout) :: expr
end subroutine event_expr_reset_event_index
module subroutine event_expr_increment_event_index (expr, offset)
class(event_expr_t), intent(inout) :: expr
integer, intent(in), optional :: offset
end subroutine event_expr_increment_event_index

<Subevt expr: procedures>+≡
module subroutine event_expr_set_event_index (expr, index)
class(event_expr_t), intent(inout) :: expr
integer, intent(in) :: index
expr%index = index
expr%has_index = .true.
end subroutine event_expr_set_event_index

module subroutine event_expr_reset_event_index (expr)
class(event_expr_t), intent(inout) :: expr
expr%has_index = .false.
end subroutine event_expr_reset_event_index

module subroutine event_expr_increment_event_index (expr, offset)
class(event_expr_t), intent(inout) :: expr
integer, intent(in), optional :: offset
if (expr%has_index) then
expr%index = expr%index + 1
else if (present (offset)) then
call expr%set_event_index (offset + 1)
else

```

```

        call expr%set_event_index (1)
    end if
end subroutine event_expr_increment_event_index

```

Fill the event expression: take the particle data and kinematics from a `particle_set` object.

We allow the particle content to change for each event. Therefore, we set the event variables each time.

Also increment the event index; initialize it if necessary.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: fill_subevt => event_expr_fill_subevt

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_fill_subevt (expr, particle_set)
        class(event_expr_t), intent(inout) :: expr
        type(particle_set_t), intent(in) :: particle_set
    end subroutine event_expr_fill_subevt

<Subevt expr: procedures>+≡
    module subroutine event_expr_fill_subevt (expr, particle_set)
        class(event_expr_t), intent(inout) :: expr
        type(particle_set_t), intent(in) :: particle_set
        call particle_set%to_subevt (expr%subevt_t, expr%colorize_subevt)
        expr%sqrts_hat = expr%get_sqrts_hat ()
        expr%n_in = expr%get_n_in ()
        expr%n_out = expr%get_n_out ()
        expr%n_tot = expr%n_in + expr%n_out
        expr%subevt_filled = .true.
    end subroutine event_expr_fill_subevt

```

Evaluate, if the event passes the selection. For absent expressions we take default values.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: evaluate => event_expr_evaluate

<Subevt expr: sub interfaces>+≡
    module subroutine event_expr_evaluate &
        (expr, passed, reweight, analysis_flag)
        class(event_expr_t), intent(inout) :: expr
        logical, intent(out) :: passed
        real(default), intent(out) :: reweight
        logical, intent(out) :: analysis_flag
    end subroutine event_expr_evaluate

<Subevt expr: procedures>+≡
    module subroutine event_expr_evaluate (expr, passed, reweight, analysis_flag)
        class(event_expr_t), intent(inout) :: expr
        logical, intent(out) :: passed
        real(default), intent(out) :: reweight
        logical, intent(out) :: analysis_flag
        call expr%base_evaluate (passed)
        if (passed) then
            if (expr%has_reweight) then
                call expr%reweight%evaluate ()
            end if
        end if
    end subroutine event_expr_evaluate

```



```

    if (expr%reweight%is_known ()) then
        reweight = expr%reweight%get_real ()
    else
        call msg_error ("Evaluate reweight expression: &
            &result undefined")
        reweight = 0
    end if
else
    reweight = 1
end if
if (expr%has_analysis) then
    call expr%analysis%evaluate ()
    if (expr%analysis%is_known ()) then
        analysis_flag = expr%analysis%get_log ()
    else
        call msg_error ("Evaluate analysis expression: &
            &result undefined")
        analysis_flag = .false.
    end if
else
    analysis_flag = .true.
end if
end if
end subroutine event_expr_evaluate

```

30.2 Parton states

A `parton_state_t` object contains the effective kinematics and dynamics of an elementary partonic interaction, with or without the beam/structure function state included. The type is abstract and has two distinct extensions. The `isolated_state_t` extension describes the isolated elementary interaction where the `int_eff` subobject contains the complex transition amplitude, exclusive in all quantum numbers. The particle content and kinematics describe the effective partonic state. The `connected_state_t` extension contains the partonic `subevt` and the expressions for cuts and scales which use it.

In the isolated state, the effective partonic interaction may either be identical to the hard interaction, in which case it is just a pointer to the latter. Or it may involve a rearrangement of partons, in which case we allocate it explicitly and flag this by `int_is_allocated`.

The `trace` evaluator contains the absolute square of the effective transition amplitude matrix, summed over final states. It is also summed over initial states, depending on the the beam setup allows. The result is used for integration.

The `matrix` evaluator is the counterpart of `trace` which is kept exclusive in all observable quantum numbers. The `flows` evaluator is furthermore exclusive in colors, but neglecting all color interference. The `matrix` and `flows` evaluators are filled only for sampling points that become part of physical events.

Note: It would be natural to make the evaluators allocatable. The extra `has_XXX` flags indicate whether evaluators are active, instead.

This module contains no unit tests. The tests are covered by the `processes` module below.

```

<parton_states.f90>≡
  <File header>
  module parton_states

    <Use kinds>
    use variables
    use expr_base
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use interactions
    use evaluators

    use beams
    use sf_base
    use prc_core
    use subevt_expr

    <Standard module head>

    <Parton states: public>

    <Parton states: types>

    interface
    <Parton states: sub interfaces>
    end interface

  end module parton_states
<parton_states_sub.f90>≡
  <File header>

  submodule (parton_states) parton_states_s

    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use lorentz
    use subevents
    use helicities
    use colors
    use polarizations
    use process_constants

    implicit none

  contains

    <Parton states: procedures>

  end submodule parton_states_s

```

30.2.1 Abstract base type

The common part are the evaluators, one for the trace (summed over all quantum numbers), one for the transition matrix (summed only over unobservable quantum numbers), and one for the flow distribution (transition matrix without interferences, exclusive in color flow).

```

(Parton states: types)≡
  type, abstract :: parton_state_t
    logical :: has_trace = .false.
    logical :: has_matrix = .false.
    logical :: has_flows = .false.
    type(evaluator_t) :: trace
    type(evaluator_t) :: matrix
    type(evaluator_t) :: flows
  contains
    (Parton states: parton state: TBP)
  end type parton_state_t

```

The `isolated_state_t` extension contains the `sf_chain_eff` object and the (hard) effective interaction `int_eff`, separately, both are implemented as a pointer. The evaluators (trace, matrix, flows) apply to the hard interaction only.

If the effective interaction differs from the hard interaction, the pointer is allocated explicitly. Analogously for `sf_chain_eff`.

```

(Parton states: public)≡
  public :: isolated_state_t

(Parton states: types)+≡
  type, extends (parton_state_t) :: isolated_state_t
    logical :: sf_chain_is_allocated = .false.
    type(sf_chain_instance_t), pointer :: sf_chain_eff => null ()
    logical :: int_is_allocated = .false.
    type(interaction_t), pointer :: int_eff => null ()
  contains
    (Parton states: isolated state: TBP)
  end type isolated_state_t

```

The `connected_state_t` extension contains all data that enable the evaluation of observables for the effective connected state. The evaluators connect the (effective) structure-function chain and hard interaction that were kept separate in the `isolated_state_t`.

The `flows_sf` evaluator is an extended copy of the structure-function

The `expr` subobject consists of the `subevt`, a simple event record, expressions for cuts etc. which refer to this record, and a `var_list` which contains event-specific variables, linked to the process variable list. Variables used within the expressions are looked up in `var_list`.

```

(Parton states: public)+≡
  public :: connected_state_t

(Parton states: types)+≡
  type, extends (parton_state_t) :: connected_state_t
    type(state_flv_content_t) :: state_flv

```

```

    logical :: has_flows_sf = .false.
    type(evaluator_t) :: flows_sf
    logical :: has_expr = .false.
    type(parton_expr_t) :: expr
contains
  <Parton states: connected state: TBP>
end type connected_state_t

```

Output: each evaluator is written only when it is active. The `sf_chain` is only written if it is explicitly allocated.

```

<Parton states: parton state: TBP>≡
  procedure :: write => parton_state_write

<Parton states: sub interfaces>≡
  module subroutine parton_state_write (state, unit, testflag)
    class(parton_state_t), intent(in) :: state
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine parton_state_write

<Parton states: procedures>≡
  module subroutine parton_state_write (state, unit, testflag)
    class(parton_state_t), intent(in) :: state
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    select type (state)
    class is (isolated_state_t)
      if (state%sf_chain_is_allocated) then
        call write_separator (u)
        call state%sf_chain_eff%write (u)
      end if
      if (state%int_is_allocated) then
        call write_separator (u)
        write (u, "(1x,A)") &
          "Effective interaction:"
        call write_separator (u)
        call state%int_eff%basic_write (u, testflag = testflag)
      end if
    class is (connected_state_t)
      if (state%has_flows_sf) then
        call write_separator (u)
        write (u, "(1x,A)") &
          "Evaluator (extension of the beam evaluator &
          &with color contractions):"
        call write_separator (u)
        call state%flows_sf%write (u, testflag = testflag)
      end if
    end select
    if (state%has_trace) then
      call write_separator (u)
      write (u, "(1x,A)") &
        "Evaluator (trace of the squared transition matrix):"
      call write_separator (u)
    end if
  end subroutine parton_state_write

```

```

        call state%trace%write (u, testflag = testflag)
    end if
    if (state%has_matrix) then
        call write_separator (u)
        write (u, "(1x,A)" &
            "Evaluator (squared transition matrix):"
        call write_separator (u)
        call state%matrix%write (u, testflag = testflag)
    end if
    if (state%has_flows) then
        call write_separator (u)
        write (u, "(1x,A)" &
            "Evaluator (squared color-flow matrix):"
        call write_separator (u)
        call state%flows%write (u, testflag = testflag)
    end if
    select type (state)
    class is (connected_state_t)
        if (state%has_expr) then
            call write_separator (u)
            call state%expr%write (u)
        end if
    end select
end subroutine parton_state_write

```

Finalize interaction and evaluators, but only if allocated.

(Parton states: parton state: TBP)+≡

```

    procedure :: final => parton_state_final

```

(Parton states: sub interfaces)+≡

```

    module subroutine parton_state_final (state)
        class(parton_state_t), intent(inout) :: state
    end subroutine parton_state_final

```

(Parton states: procedures)+≡

```

    module subroutine parton_state_final (state)
        class(parton_state_t), intent(inout) :: state
        if (state%has_flows) then
            call state%flows%final ()
            state%has_flows = .false.
        end if
        if (state%has_matrix) then
            call state%matrix%final ()
            state%has_matrix = .false.
        end if
        if (state%has_trace) then
            call state%trace%final ()
            state%has_trace = .false.
        end if
        select type (state)
        class is (connected_state_t)
            if (state%has_flows_sf) then
                call state%flows_sf%final ()
                state%has_flows_sf = .false.
            end if

```

```

        call state%expr%final ()
class is (isolated_state_t)
  if (state%int_is_allocated) then
    call state%int_eff%final ()
    deallocate (state%int_eff)
    state%int_is_allocated = .false.
  end if
  if (state%sf_chain_is_allocated) then
    call state%sf_chain_eff%final ()
  end if
end select
end subroutine parton_state_final

```

30.2.2 Common Initialization

Initialize the isolated parton state. In this version, the effective structure-function chain `sf_chain_eff` and the effective interaction `int_eff` both are trivial pointers to the seed structure-function chain and to the hard interaction, respectively.

```

(Parton states: isolated state: TBP)≡
  procedure :: init => isolated_state_init

(Parton states: sub interfaces)+≡
  module subroutine isolated_state_init (state, sf_chain, int)
    class(isolated_state_t), intent(out) :: state
    type(sf_chain_instance_t), intent(in), target :: sf_chain
    type(interaction_t), intent(in), target :: int
  end subroutine isolated_state_init

(Parton states: procedures)+≡
  module subroutine isolated_state_init (state, sf_chain, int)
    class(isolated_state_t), intent(out) :: state
    type(sf_chain_instance_t), intent(in), target :: sf_chain
    type(interaction_t), intent(in), target :: int
    state%sf_chain_eff => sf_chain
    state%int_eff => int
  end subroutine isolated_state_init

```

30.2.3 Evaluator initialization: isolated state

Create an evaluator for the trace of the squared transition matrix. The trace goes over all outgoing quantum numbers. Whether we trace over incoming quantum numbers other than color, depends on the given `qn_mask_in`.

There are two options: explicitly computing the color factor table (`use_cf` false; `nc` defined), or taking the color factor table from the hard matrix element data.

```

(Parton states: isolated state: TBP)+≡
  procedure :: setup_square_trace => isolated_state_setup_square_trace

```

(Parton states: sub interfaces)+≡

```

module subroutine isolated_state_setup_square_trace (state, core, &
  qn_mask_in, col, keep_fs_flavor)
  class(isolated_state_t), intent(inout), target :: state
  class(prc_core_t), intent(in) :: core
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
  integer, intent(in), dimension(:), allocatable :: col
  logical, intent(in) :: keep_fs_flavor
end subroutine isolated_state_setup_square_trace

```

(Parton states: procedures)+≡

```

module subroutine isolated_state_setup_square_trace (state, core, &
  qn_mask_in, col, keep_fs_flavor)
  class(isolated_state_t), intent(inout), target :: state
  class(prc_core_t), intent(in) :: core
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
  !!! Actually need allocatable attribute here for once because col might
  !!! enter the subroutine non-allocated.
  integer, intent(in), dimension(:), allocatable :: col
  logical, intent(in) :: keep_fs_flavor
  type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
  associate (data => core%data)
    allocate (qn_mask (data%n_in + data%n_out))
    qn_mask( : data%n_in) = &
      quantum_numbers_mask (.false., .true., .false.) &
      .or. qn_mask_in
    qn_mask(data%n_in + 1 : ) = &
      quantum_numbers_mask (.not. keep_fs_flavor, .true., .true.)
    if (core%use_color_factors) then
      call state%trace%init_square (state%int_eff, qn_mask, &
        col_flow_index = data%cf_index, &
        col_factor = data%color_factors, &
        col_index_hi = col, &
        nc = core%nc)
    else
      call state%trace%init_square (state%int_eff, qn_mask, nc = core%nc)
    end if
  end associate
  state%has_trace = .true.
end subroutine isolated_state_setup_square_trace

```

Set up an identity-evaluator for the trace. This implies that *me* is considered to be a squared amplitude, as for example for BLHA matrix elements.

(Parton states: isolated state: TBP)+≡

```

procedure :: setup_identity_trace => isolated_state_setup_identity_trace

```

(Parton states: sub interfaces)+≡

```

module subroutine isolated_state_setup_identity_trace (state, core, &
  qn_mask_in, keep_fs_flavors, keep_colors)
  class(isolated_state_t), intent(inout), target :: state
  class(prc_core_t), intent(in) :: core
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
  logical, intent(in), optional :: keep_fs_flavors, keep_colors
end subroutine isolated_state_setup_identity_trace

```

(Parton states: procedures)+≡

```

module subroutine isolated_state_setup_identity_trace (state, core, &
    qn_mask_in, keep_fs_flavors, keep_colors)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
    logical, intent(in), optional :: keep_fs_flavors, keep_colors
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    logical :: fs_flv_flag, col_flag
    fs_flv_flag = .true.; col_flag = .true.
    if (present(keep_fs_flavors)) fs_flv_flag = .not. keep_fs_flavors
    if (present(keep_colors)) col_flag = .not. keep_colors
    associate (data => core%data)
        allocate (qn_mask (data%n_in + data%n_out))
        qn_mask( : data%n_in) = &
            quantum_numbers_mask (.false., col_flag, .false.) .or. qn_mask_in
        qn_mask(data%n_in + 1 : ) = &
            quantum_numbers_mask (fs_flv_flag, col_flag, .true.)
    end associate
    call state%int_eff%set_mask (qn_mask)
    call state%trace%init_identity (state%int_eff)
    state%has_trace = .true.
end subroutine isolated_state_setup_identity_trace

```

Set up the evaluator for the transition matrix, exclusive in helicities where this is requested.

For all unstable final-state particles we keep polarization according to the applicable decay options. If the process is a decay itself, this applies also to the initial state.

For all polarized final-state particles, we keep polarization including off-diagonal entries. We drop helicity completely for unpolarized final-state particles.

For the initial state, if the particle has not been handled yet, we apply the provided `qn_mask_in` which communicates the beam properties.

(Parton states: isolated state: TBP)+≡

```

procedure :: setup_square_matrix => isolated_state_setup_square_matrix

```

(Parton states: sub interfaces)+≡

```

module subroutine isolated_state_setup_square_matrix &
    (state, core, model, qn_mask_in, col)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    class(model_data_t), intent(in), target :: model
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
    integer, dimension(:), intent(in) :: col
end subroutine isolated_state_setup_square_matrix

```

(Parton states: procedures)+≡

```

module subroutine isolated_state_setup_square_matrix &
    (state, core, model, qn_mask_in, col)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    class(model_data_t), intent(in), target :: model
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in

```



```

integer, dimension(:), intent(in) :: col
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
type(flavor_t), dimension(:), allocatable :: flv
integer :: i
logical :: helmask, helmask_hd
associate (data => core%data)
  allocate (qn_mask (data%n_in + data%n_out))
  allocate (flv (data%n_flv))
  do i = 1, data%n_in + data%n_out
    call flv%init (data%flv_state(i,:), model)
    if ((data%n_in == 1 .or. i > data%n_in) &
        .and. any (.not. flv%is_stable ())) then
      helmask = all (flv%decays_isotropically ())
      helmask_hd = all (flv%decays_diagonal ())
      qn_mask(i) = quantum_numbers_mask (.false., .true., helmask, &
        mask_hd = helmask_hd)
    else if (i > data%n_in) then
      helmask = all (.not. flv%is_polarized ())
      qn_mask(i) = quantum_numbers_mask (.false., .true., helmask)
    else
      qn_mask(i) = quantum_numbers_mask (.false., .true., .false.) &
        .or. qn_mask_in(i)
    end if
  end do
  if (core%use_color_factors) then
    call state%matrix%init_square (state%int_eff, qn_mask, &
      col_flow_index = data%cf_index, &
      col_factor = data%color_factors, &
      col_index_hi = col, &
      nc = core%nc)
  else
    call state%matrix%init_square (state%int_eff, &
      qn_mask, &
      nc = core%nc)
  end if
end associate
state%has_matrix = .true.
end subroutine isolated_state_setup_square_matrix

```

This procedure initializes the evaluator that computes the contributions to color flows, neglecting color interference. The incoming-particle mask can be used to sum over incoming flavor.

Helicity handling: see above.

(Parton states: isolated state: TBP)+≡

```

  procedure :: setup_square_flows => isolated_state_setup_square_flows

```

(Parton states: sub interfaces)+≡

```

module subroutine isolated_state_setup_square_flows &
  (state, core, model, qn_mask_in)
  class(isolated_state_t), intent(inout), target :: state
  class(prc_core_t), intent(in) :: core
  class(model_data_t), intent(in), target :: model
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
end subroutine isolated_state_setup_square_flows

```

```

(Parton states: procedures)+≡
module subroutine isolated_state_setup_square_flows &
  (state, core, model, qn_mask_in)
  class(isolated_state_t), intent(inout), target :: state
  class(prc_core_t), intent(in) :: core
  class(model_data_t), intent(in), target :: model
  type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
  type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: i
  logical :: helmask, helmask_hd
  associate (data => core%data)
    allocate (qn_mask (data%n_in + data%n_out))
    allocate (flv (data%n_flv))
    do i = 1, data%n_in + data%n_out
      call flv%init (data%flv_state(i,:), model)
      if ((data%n_in == 1 .or. i > data%n_in) &
        .and. any (.not. flv%is_stable ())) then
        helmask = all (flv%decays_isotropically ())
        helmask_hd = all (flv%decays_diagonal ())
        qn_mask(i) = quantum_numbers_mask (.false., .false., helmask, &
          mask_hd = helmask_hd)
      else if (i > data%n_in) then
        helmask = all (.not. flv%is_polarized ())
        qn_mask(i) = quantum_numbers_mask (.false., .false., helmask)
      else
        qn_mask(i) = quantum_numbers_mask (.false., .false., .false.) &
          .or. qn_mask_in(i)
      end if
    end do
    call state%flows%init_square (state%int_eff, qn_mask, &
      expand_color_flows = .true.)
  end associate
  state%has_flows = .true.
end subroutine isolated_state_setup_square_flows

```

30.2.4 Evaluator initialization: connected state

Set up a trace evaluator as a product of two evaluators (incoming state, effective interaction). In the result, all quantum numbers are summed over.

If the optional `int` interaction is provided, use this for the first factor in the convolution. Otherwise, use the final interaction of the stored `sf_chain`.

The `resonant` flag applies if we want to construct a decay chain. The resonance property can propagate to the final event output.

If an extended structure function is required `requires_extended_sf`, we have to not consider `sub` as a quantum number.

```

(Parton states: connected state: TBP)≡
  procedure :: setup_connected_trace => connected_state_setup_connected_trace

(Parton states: sub interfaces)+≡
  module subroutine connected_state_setup_connected_trace &
    (state, isolated, int, resonant, undo_helicities, &

```

```

        keep_fs_flavors, requires_extended_sf)
class (connected_state_t), intent(inout), target :: state
type (isolated_state_t), intent(in), target :: isolated
type (interaction_t), intent(in), optional, target :: int
logical, intent(in), optional :: resonant
logical, intent(in), optional :: undo_helicities
logical, intent(in), optional :: keep_fs_flavors
logical, intent(in), optional :: requires_extended_sf
end subroutine connected_state_setup_connected_trace

(Parton states: procedures)+≡
module subroutine connected_state_setup_connected_trace &
    (state, isolated, int, resonant, undo_helicities, &
    keep_fs_flavors, requires_extended_sf)
class (connected_state_t), intent(inout), target :: state
type (isolated_state_t), intent(in), target :: isolated
type (interaction_t), intent(in), optional, target :: int
logical, intent(in), optional :: resonant
logical, intent(in), optional :: undo_helicities
logical, intent(in), optional :: keep_fs_flavors
logical, intent(in), optional :: requires_extended_sf
type (quantum_numbers_mask_t) :: mask
type (interaction_t), pointer :: src_int, beam_int
logical :: reduce, fs_flg_flag
if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
    "connected_state_setup_connected_trace")
reduce = .false.; fs_flg_flag = .true.
if (present (undo_helicities)) reduce = undo_helicities
if (present (keep_fs_flavors)) fs_flg_flag = .not. keep_fs_flavors
mask = quantum_numbers_mask (fs_flg_flag, .true., .true.)
if (present (int)) then
    src_int => int
else
    src_int => isolated%sf_chain_eff%get_out_int_ptr ()
end if

if (debug2_active (D_PROCESS_INTEGRATION)) then
    call src_int%basic_write ()
end if

call state%trace%init_product (src_int, isolated%trace, &
    qn_mask_conn = mask, &
    qn_mask_rest = mask, &
    connections_are_resonant = resonant, &
    ignore_sub_for_qn = requires_extended_sf)

if (reduce) then
    beam_int => isolated%sf_chain_eff%get_beam_int_ptr ()
    call undo_qn_hel (beam_int, mask, beam_int%get_n_tot ())
    call undo_qn_hel (src_int, mask, src_int%get_n_tot ())
    call beam_int%set_matrix_element (cmplx (1, 0, default))
    call src_int%set_matrix_element (cmplx (1, 0, default))
end if

state%has_trace = .true.

```

```

contains
  subroutine undo_qn_hel (int_in, mask, n_tot)
    type(interaction_t), intent(inout) :: int_in
    type(quantum_numbers_mask_t), intent(in) :: mask
    integer, intent(in) :: n_tot
    type(quantum_numbers_mask_t), dimension(n_tot) :: mask_in
    mask_in = mask
    call int_in%set_mask (mask_in)
  end subroutine undo_qn_hel
end subroutine connected_state_setup_connected_trace

```

Set up a matrix evaluator as a product of two evaluators (incoming state, effective interaction). In the intermediate state, color and helicity is summed over. In the final state, we keep the quantum numbers which are present in the original evaluators.

(Parton states: connected state: TBP)+≡
 procedure :: setup_connected_matrix => connected_state_setup_connected_matrix

(Parton states: sub interfaces)+≡
 module subroutine connected_state_setup_connected_matrix &
 (state, isolated, int, resonant, qn_filter_conn)
 class(connected_state_t), intent(inout), target :: state
 type(isolated_state_t), intent(in), target :: isolated
 type(interaction_t), intent(in), optional, target :: int
 logical, intent(in), optional :: resonant
 type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
 end subroutine connected_state_setup_connected_matrix

(Parton states: procedures)+≡
 module subroutine connected_state_setup_connected_matrix &
 (state, isolated, int, resonant, qn_filter_conn)
 class(connected_state_t), intent(inout), target :: state
 type(isolated_state_t), intent(in), target :: isolated
 type(interaction_t), intent(in), optional, target :: int
 logical, intent(in), optional :: resonant
 type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
 type(quantum_numbers_mask_t) :: mask
 type(interaction_t), pointer :: src_int
 mask = quantum_numbers_mask (.false., .true., .true.)
 if (present (int)) then
 src_int => int
 else
 src_int => isolated%sf_chain_eff%get_out_int_ptr ()
 end if
 call state%matrix%init_product &
 (src_int, isolated%matrix, mask, &
 qn_filter_conn = qn_filter_conn, &
 connections_are_resonant = resonant)
 state%has_matrix = .true.
 end subroutine connected_state_setup_connected_matrix

Set up a matrix evaluator as a product of two evaluators (incoming state, effective interaction). In the intermediate state, only helicity is summed over. In

the final state, we keep the quantum numbers which are present in the original evaluators.

If the optional `int` interaction is provided, use this for the first factor in the convolution. Otherwise, use the final interaction of the stored `sf_chain`, after creating an intermediate interaction that includes a correlated color state. We assume that for a caller-provided `int`, this is not necessary.

For fixed-order NLO differential distribution, we are interested at the partonic level, no parton showering takes place as this would demand for a proper matching. So, the flows in the `connected_state` are not needed, and the color part will be masked for the interaction coming from the `sf_chain`. The squared matrix elements coming from the OLP provider at the moment do not come with flows anyhow. This needs to be revised once the matching to the shower is completed.

```

(Parton states: connected state: TBP)+≡
  procedure :: setup_connected_flows => connected_state_setup_connected_flows

(Parton states: sub interfaces)+≡
  module subroutine connected_state_setup_connected_flows &
    (state, isolated, int, resonant, qn_filter_conn, mask_color)
    class(connected_state_t), intent(inout), target :: state
    type(isolated_state_t), intent(in), target :: isolated
    type(interaction_t), intent(in), optional, target :: int
    logical, intent(in), optional :: resonant, mask_color
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
  end subroutine connected_state_setup_connected_flows

(Parton states: procedures)+≡
  module subroutine connected_state_setup_connected_flows &
    (state, isolated, int, resonant, qn_filter_conn, mask_color)
    class(connected_state_t), intent(inout), target :: state
    type(isolated_state_t), intent(in), target :: isolated
    type(interaction_t), intent(in), optional, target :: int
    logical, intent(in), optional :: resonant, mask_color
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
    type(quantum_numbers_mask_t) :: mask
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_sf
    type(interaction_t), pointer :: src_int
    logical :: mask_c
    mask_c = .false.
    if (present (mask_color)) mask_c = mask_color
    mask = quantum_numbers_mask (.false., .false., .true.)
    if (present (int)) then
      src_int => int
    else
      src_int => isolated%sf_chain_eff%get_out_int_ptr ()
      call state%flows_sf%init_color_contractions (src_int)
      state%has_flows_sf = .true.
      src_int => state%flows_sf%interaction_t
      if (mask_c) then
        allocate (mask_sf (src_int%get_n_tot ()))
        mask_sf = quantum_numbers_mask (.false., .true., .false.)
        call src_int%reduce_state_matrix (mask_sf, keep_order = .true.)
      end if
    end if
  end if

```

```

    call state%flows%init_product (src_int, isolated%flows, mask, &
        qn_filter_conn = qn_filter_conn, &
        connections_are_resonant = resonant)
    state%has_flows = .true.
end subroutine connected_state_setup_connected_flows

```

Determine and store the flavor content for the connected state. This queries the matrix evaluator component, which should hold the requested flavor information.

```

<Parton states: connected state: TBP>+≡
    procedure :: setup_state_flv => connected_state_setup_state_flv

<Parton states: sub interfaces>+≡
    module subroutine connected_state_setup_state_flv (state, n_out_hard)
        class(connected_state_t), intent(inout), target :: state
        integer, intent(in) :: n_out_hard
    end subroutine connected_state_setup_state_flv

<Parton states: procedures>+≡
    module subroutine connected_state_setup_state_flv (state, n_out_hard)
        class(connected_state_t), intent(inout), target :: state
        integer, intent(in) :: n_out_hard
        call state%matrix%get_flv_content (state%state_flv, n_out_hard)
    end subroutine connected_state_setup_state_flv

```

Return the current flavor state object.

```

<Parton states: connected state: TBP>+≡
    procedure :: get_state_flv => connected_state_get_state_flv

<Parton states: sub interfaces>+≡
    module function connected_state_get_state_flv (state) result (state_flv)
        class(connected_state_t), intent(in) :: state
        type(state_flv_content_t) :: state_flv
    end function connected_state_get_state_flv

<Parton states: procedures>+≡
    module function connected_state_get_state_flv (state) result (state_flv)
        class(connected_state_t), intent(in) :: state
        type(state_flv_content_t) :: state_flv
        state_flv = state%state_flv
    end function connected_state_get_state_flv

```

30.2.5 Cuts and expressions

Set up the `subevt` that corresponds to the connected interaction. The index arrays refer to the interaction.

We assign the particles as follows: the beam particles are the first two (decay process: one) entries in the trace evaluator. The incoming partons are identified by their link to the outgoing partons of the structure-function chain. The outgoing partons are those of the trace evaluator, which include radiated partons during the structure-function chain.

```

<Parton states: connected state: TBP>+≡
    procedure :: setup_subevt => connected_state_setup_subevt

```

```

(Parton states: sub interfaces)+≡
module subroutine connected_state_setup_subevt &
  (state, sf_chain, f_beam, f_in, f_out)
  class(connected_state_t), intent(inout), target :: state
  type(sf_chain_instance_t), intent(in), target :: sf_chain
  type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
end subroutine connected_state_setup_subevt

(Parton states: procedures)+≡
module subroutine connected_state_setup_subevt &
  (state, sf_chain, f_beam, f_in, f_out)
  class(connected_state_t), intent(inout), target :: state
  type(sf_chain_instance_t), intent(in), target :: sf_chain
  type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
  integer :: n_beam, n_in, n_out, n_vir, n_tot, i, j
  integer, dimension(:), allocatable :: i_beam, i_in, i_out
  integer :: sf_out_i
  type(interaction_t), pointer :: sf_int
  sf_int => sf_chain%get_out_int_ptr ()
  n_beam = size (f_beam)
  n_in = size (f_in)
  n_out = size (f_out)
  n_vir = state%trace%get_n_vir ()
  n_tot = state%trace%get_n_tot ()
  allocate (i_beam (n_beam), i_in (n_in), i_out (n_out))
  i_beam = [(i, i = 1, n_beam)]
  do j = 1, n_in
    sf_out_i = sf_chain%get_out_i (j)
    i_in(j) = interaction_find_link &
      (state%trace%interaction_t, sf_int, sf_out_i)
  end do
  i_out = [(i, i = n_vir + 1, n_tot)]
  call state%expr%setup_subevt (state%trace%interaction_t, &
    i_beam, i_in, i_out, f_beam, f_in, f_out)
  state%has_expr = .true.
end subroutine connected_state_setup_subevt

(Parton states: connected state: TBP)+≡
procedure :: renew_flv_content_subevt => &
  connected_state_renew_flv_content_subevt

(Parton states: sub interfaces)+≡
module subroutine connected_state_renew_flv_content_subevt &
  (state, sf_chain, f_beam, f_in, f_out)
  class(connected_state_t), intent(inout), target :: state
  type(sf_chain_instance_t), intent(in), target :: sf_chain
  type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
end subroutine connected_state_renew_flv_content_subevt

(Parton states: procedures)+≡
module subroutine connected_state_renew_flv_content_subevt &
  (state, sf_chain, f_beam, f_in, f_out)
  class(connected_state_t), intent(inout), target :: state
  type(sf_chain_instance_t), intent(in), target :: sf_chain
  type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
  integer :: n_beam, n_in, n_out, n_vir, n_tot, i, j

```

```

integer, dimension(:), allocatable :: i_beam, i_in, i_out
integer :: sf_out_i
type(interaction_t), pointer :: sf_int
sf_int => sf_chain%get_out_int_ptr ()
n_beam = size (f_beam)
n_in = size (f_in)
n_out = size (f_out)
n_vir = state%trace%get_n_vir ()
n_tot = state%trace%get_n_tot ()
allocate (i_beam (n_beam), i_in (n_in), i_out (n_out))
i_beam = [(i, i = 1, n_beam)]
do j = 1, n_in
    sf_out_i = sf_chain%get_out_i (j)
    i_in(j) = interaction_find_link &
        (state%trace%interaction_t, sf_int, sf_out_i)
end do
i_out = [(i, i = n_vir + 1, n_tot)]
call state%expr%renew_flv_content_subvt (state%trace%interaction_t, &
    i_beam, i_in, i_out, f_beam, f_in, f_out)
state%has_expr = .true.
end subroutine connected_state_renew_flv_content_subvt

```

Initialize the variable list specific for this state/term. We insert event variables (`sqrts_hat`) and link the process variable list. The variable list acquires pointers to subobjects of `state`, which must therefore have a `target` attribute.

```

(Parton states: connected state: TBP)+≡
    procedure :: setup_var_list => connected_state_setup_var_list

(Parton states: sub interfaces)+≡
    module subroutine connected_state_setup_var_list &
        (state, process_var_list, beam_data)
        class(connected_state_t), intent(inout), target :: state
        type(var_list_t), intent(in), target :: process_var_list
        type(beam_data_t), intent(in) :: beam_data
    end subroutine connected_state_setup_var_list

(Parton states: procedures)+≡
    module subroutine connected_state_setup_var_list &
        (state, process_var_list, beam_data)
        class(connected_state_t), intent(inout), target :: state
        type(var_list_t), intent(in), target :: process_var_list
        type(beam_data_t), intent(in) :: beam_data
        call state%expr%setup_vars (beam_data%get_sqrts ())
        call state%expr%link_var_list (process_var_list)
    end subroutine connected_state_setup_var_list

```

Allocate the cut expression etc.

```

(Parton states: connected state: TBP)+≡
    procedure :: setup_cuts => connected_state_setup_cuts
    procedure :: setup_scale => connected_state_setup_scale
    procedure :: setup_fac_scale => connected_state_setup_fac_scale
    procedure :: setup_ren_scale => connected_state_setup_ren_scale
    procedure :: setup_weight => connected_state_setup_weight

```



```

(Parton states: sub interfaces) +=
    module subroutine connected_state_setup_cuts (state, ef_cuts)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_cuts
    end subroutine connected_state_setup_cuts
    module subroutine connected_state_setup_scale (state, ef_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_scale
    end subroutine connected_state_setup_scale
    module subroutine connected_state_setup_fac_scale (state, ef_fac_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_fac_scale
    end subroutine connected_state_setup_fac_scale
    module subroutine connected_state_setup_ren_scale (state, ef_ren_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_ren_scale
    end subroutine connected_state_setup_ren_scale
    module subroutine connected_state_setup_weight (state, ef_weight)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_weight
    end subroutine connected_state_setup_weight

(Parton states: procedures) +=
    module subroutine connected_state_setup_cuts (state, ef_cuts)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_cuts
        call state%expr%setup_selection (ef_cuts)
    end subroutine connected_state_setup_cuts

    module subroutine connected_state_setup_scale (state, ef_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_scale
        call state%expr%setup_scale (ef_scale)
    end subroutine connected_state_setup_scale

    module subroutine connected_state_setup_fac_scale (state, ef_fac_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_fac_scale
        call state%expr%setup_fac_scale (ef_fac_scale)
    end subroutine connected_state_setup_fac_scale

    module subroutine connected_state_setup_ren_scale (state, ef_ren_scale)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_ren_scale
        call state%expr%setup_ren_scale (ef_ren_scale)
    end subroutine connected_state_setup_ren_scale

    module subroutine connected_state_setup_weight (state, ef_weight)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_weight
        call state%expr%setup_weight (ef_weight)
    end subroutine connected_state_setup_weight

```

Reset the expression object: invalidate the subevt.

```

<Parton states: connected state: TBP>+≡
  procedure :: reset_expressions => connected_state_reset_expressions
<Parton states: sub interfaces>+≡
  module subroutine connected_state_reset_expressions (state)
    class(connected_state_t), intent(inout) :: state
    end subroutine connected_state_reset_expressions
<Parton states: procedures>+≡
  module subroutine connected_state_reset_expressions (state)
    class(connected_state_t), intent(inout) :: state
    if (state%has_expr) call state%expr%reset_contents ()
    end subroutine connected_state_reset_expressions

```

30.2.6 Evaluation

Transfer momenta to the trace evaluator and fill the `subevt` with this effective kinematics, if applicable.

Note: we may want to apply a boost for the `subevt`.

```

<Parton states: parton state: TBP>+≡
  procedure :: receive_kinematics => parton_state_receive_kinematics
<Parton states: sub interfaces>+≡
  module subroutine parton_state_receive_kinematics (state)
    class(parton_state_t), intent(inout), target :: state
    end subroutine parton_state_receive_kinematics
<Parton states: procedures>+≡
  module subroutine parton_state_receive_kinematics (state)
    class(parton_state_t), intent(inout), target :: state
    if (state%has_trace) then
      call state%trace%receive_momenta ()
      select type (state)
        class is (connected_state_t)
          if (state%has_expr) then
            call state%expr%fill_subevt (state%trace%interaction_t)
          end if
        end select
      end if
    end subroutine parton_state_receive_kinematics

```

Recover kinematics: We assume that the trace evaluator is filled with momenta. Send those momenta back to the sources, then fill the variables and subevent as above.

The incoming momenta of the connected state are not connected to the isolated state but to the beam interaction. Therefore, the incoming momenta within the isolated state do not become defined, yet. Instead, we reconstruct the beam (and ISR) momentum configuration.

```

<Parton states: parton state: TBP>+≡
  procedure :: send_kinematics => parton_state_send_kinematics
<Parton states: sub interfaces>+≡
  module subroutine parton_state_send_kinematics (state)
    class(parton_state_t), intent(inout), target :: state
    end subroutine parton_state_send_kinematics

```

```

(Parton states: procedures)+≡
module subroutine parton_state_send_kinematics (state)
  class(parton_state_t), intent(inout), target :: state
  if (state%has_trace) then
    call state%trace%send_momenta ()
    select type (state)
    class is (connected_state_t)
      call state%expr%fill_subevt (state%trace%interaction_t)
    end select
  end if
end subroutine parton_state_send_kinematics

```

Evaluate the expressions. The routine evaluates first the cut expression. If the event passes, it evaluates the other expressions. Where no expressions are defined, default values are inserted.

```

(Parton states: connected state: TBP)+≡
  procedure :: evaluate_expressions => connected_state_evaluate_expressions

```

```

(Parton states: sub interfaces)+≡
  module subroutine connected_state_evaluate_expressions (state, passed, &
    scale, fac_scale, ren_scale, weight, scale_forced, force_evaluation)
    class(connected_state_t), intent(inout) :: state
    logical, intent(out) :: passed
    real(default), intent(out) :: scale, weight
    real(default), intent(out), allocatable :: fac_scale, ren_scale
    real(default), intent(in), allocatable, optional :: scale_forced
    logical, intent(in), optional :: force_evaluation
  end subroutine connected_state_evaluate_expressions

```

```

(Parton states: procedures)+≡
  module subroutine connected_state_evaluate_expressions (state, passed, &
    scale, fac_scale, ren_scale, weight, scale_forced, force_evaluation)
    class(connected_state_t), intent(inout) :: state
    logical, intent(out) :: passed
    real(default), intent(out) :: scale, weight
    real(default), intent(out), allocatable :: fac_scale, ren_scale
    real(default), intent(in), allocatable, optional :: scale_forced
    logical, intent(in), optional :: force_evaluation
    if (state%has_expr) then
      call state%expr%evaluate (passed, scale, fac_scale, ren_scale, weight, &
        scale_forced, force_evaluation)
    end if
  end subroutine connected_state_evaluate_expressions

```

Evaluate the structure-function chain, if it is allocated explicitly. The argument is the factorization scale.

If the chain is merely a pointer, the chain should already be evaluated at this point.

```

(Parton states: isolated state: TBP)+≡
  procedure :: evaluate_sf_chain => isolated_state_evaluate_sf_chain

```

```

(Parton states: sub interfaces)+≡
  module subroutine isolated_state_evaluate_sf_chain (state, fac_scale)
    class(isolated_state_t), intent(inout) :: state

```

```

        real(default), intent(in) :: fac_scale
    end subroutine isolated_state_evaluate_sf_chain
<Parton states: procedures>+≡
    module subroutine isolated_state_evaluate_sf_chain (state, fac_scale)
        class(isolated_state_t), intent(inout) :: state
        real(default), intent(in) :: fac_scale
        if (state%sf_chain_is_allocated) &
            call state%sf_chain_eff%evaluate (fac_scale)
    end subroutine isolated_state_evaluate_sf_chain

```

Evaluate the trace.

```

<Parton states: parton state: TBP>+≡
    procedure :: evaluate_trace => parton_state_evaluate_trace
<Parton states: sub interfaces>+≡
    module subroutine parton_state_evaluate_trace (state)
        class(parton_state_t), intent(inout) :: state
    end subroutine parton_state_evaluate_trace
<Parton states: procedures>+≡
    module subroutine parton_state_evaluate_trace (state)
        class(parton_state_t), intent(inout) :: state
        if (state%has_trace) call state%trace%evaluate ()
    end subroutine parton_state_evaluate_trace

<Parton states: parton state: TBP>+≡
    procedure :: evaluate_matrix => parton_state_evaluate_matrix
<Parton states: sub interfaces>+≡
    module subroutine parton_state_evaluate_matrix (state)
        class(parton_state_t), intent(inout) :: state
    end subroutine parton_state_evaluate_matrix
<Parton states: procedures>+≡
    module subroutine parton_state_evaluate_matrix (state)
        class(parton_state_t), intent(inout) :: state
        if (state%has_matrix) call state%matrix%evaluate ()
    end subroutine parton_state_evaluate_matrix

```

Evaluate the extra evaluators that we need for physical events.

```

<Parton states: parton state: TBP>+≡
    procedure :: evaluate_event_data => parton_state_evaluate_event_data
<Parton states: sub interfaces>+≡
    module subroutine parton_state_evaluate_event_data (state, only_momenta)
        class(parton_state_t), intent(inout) :: state
        logical, intent(in), optional :: only_momenta
    end subroutine parton_state_evaluate_event_data
<Parton states: procedures>+≡
    module subroutine parton_state_evaluate_event_data (state, only_momenta)
        class(parton_state_t), intent(inout) :: state
        logical, intent(in), optional :: only_momenta
        logical :: only_mom
        only_mom = .false.; if (present (only_momenta)) only_mom = only_momenta
    end subroutine parton_state_evaluate_event_data

```

```

select type (state)
type is (connected_state_t)
  if (state%has_flows_sf) then
    call state%flows_sf%receive_momenta ()
    if (.not. only_mom) call state%flows_sf%evaluate ()
  end if
end select
if (state%has_matrix) then
  call state%matrix%receive_momenta ()
  if (.not. only_mom) call state%matrix%evaluate ()
end if
if (state%has_flows) then
  call state%flows%receive_momenta ()
  if (.not. only_mom) call state%flows%evaluate ()
end if
end subroutine parton_state_evaluate_event_data

```

Normalize the helicity density matrix by its trace, i.e., factor out the trace and put it into an overall normalization factor. The trace and flow evaluators are unchanged.

```

<Parton states: parton state: TBP>+≡
  procedure :: normalize_matrix_by_trace => &
    parton_state_normalize_matrix_by_trace

<Parton states: sub interfaces>+≡
  module subroutine parton_state_normalize_matrix_by_trace (state)
    class(parton_state_t), intent(inout) :: state
  end subroutine parton_state_normalize_matrix_by_trace

<Parton states: procedures>+≡
  module subroutine parton_state_normalize_matrix_by_trace (state)
    class(parton_state_t), intent(inout) :: state
    if (state%has_matrix) call state%matrix%normalize_by_trace ()
  end subroutine parton_state_normalize_matrix_by_trace

```

30.2.7 Accessing the state

Three functions return a pointer to the event-relevant interactions.

```

<Parton states: parton state: TBP>+≡
  procedure :: get_trace_int_ptr => parton_state_get_trace_int_ptr
  procedure :: get_matrix_int_ptr => parton_state_get_matrix_int_ptr
  procedure :: get_flows_int_ptr => parton_state_get_flows_int_ptr

<Parton states: sub interfaces>+≡
  module function parton_state_get_trace_int_ptr (state) result (ptr)
    class(parton_state_t), intent(in), target :: state
    type(interaction_t), pointer :: ptr
  end function parton_state_get_trace_int_ptr
  module function parton_state_get_matrix_int_ptr (state) result (ptr)
    class(parton_state_t), intent(in), target :: state
    type(interaction_t), pointer :: ptr
  end function parton_state_get_matrix_int_ptr
  module function parton_state_get_flows_int_ptr (state) result (ptr)

```

```

        class(parton_state_t), intent(in), target :: state
        type(interaction_t), pointer :: ptr
    end function parton_state_get_flows_int_ptr

    (Parton states: procedures)+≡
    module function parton_state_get_trace_int_ptr (state) result (ptr)
        class(parton_state_t), intent(in), target :: state
        type(interaction_t), pointer :: ptr
        if (state%has_trace) then
            ptr => state%trace%interaction_t
        else
            ptr => null ()
        end if
    end function parton_state_get_trace_int_ptr

    module function parton_state_get_matrix_int_ptr (state) result (ptr)
        class(parton_state_t), intent(in), target :: state
        type(interaction_t), pointer :: ptr
        if (state%has_matrix) then
            ptr => state%matrix%interaction_t
        else
            ptr => null ()
        end if
    end function parton_state_get_matrix_int_ptr

    module function parton_state_get_flows_int_ptr (state) result (ptr)
        class(parton_state_t), intent(in), target :: state
        type(interaction_t), pointer :: ptr
        if (state%has_flows) then
            ptr => state%flows%interaction_t
        else
            ptr => null ()
        end if
    end function parton_state_get_flows_int_ptr

```

Return the indices of the beam particles and the outgoing particles within the trace (and thus, matrix and flows) evaluator, respectively.

```

    (Parton states: connected state: TBP)+≡
    procedure :: get_beam_index => connected_state_get_beam_index
    procedure :: get_in_index => connected_state_get_in_index

    (Parton states: sub interfaces)+≡
    module subroutine connected_state_get_beam_index (state, i_beam)
        class(connected_state_t), intent(in) :: state
        integer, dimension(:), intent(out) :: i_beam
    end subroutine connected_state_get_beam_index
    module subroutine connected_state_get_in_index (state, i_in)
        class(connected_state_t), intent(in) :: state
        integer, dimension(:), intent(out) :: i_in
    end subroutine connected_state_get_in_index

    (Parton states: procedures)+≡
    module subroutine connected_state_get_beam_index (state, i_beam)
        class(connected_state_t), intent(in) :: state
        integer, dimension(:), intent(out) :: i_beam
    end subroutine connected_state_get_beam_index

```

```

        call state%expr%get_beam_index (i_beam)
    end subroutine connected_state_get_beam_index

    module subroutine connected_state_get_in_index (state, i_in)
        class(connected_state_t), intent(in) :: state
        integer, dimension(:), intent(out) :: i_in
        call state%expr%get_in_index (i_in)
    end subroutine connected_state_get_in_index

    <Parton states: public>+≡
        public :: refill_evaluator

    <Parton states: sub interfaces>+≡
        module subroutine refill_evaluator (sqme, qn, flv_index, evaluator)
            complex(default), intent(in), dimension(:) :: sqme
            type(quantum_numbers_t), intent(in), dimension(:, :) :: qn
            integer, intent(in), dimension(:), optional :: flv_index
            type(evaluator_t), intent(inout) :: evaluator
        end subroutine refill_evaluator

    <Parton states: procedures>+≡
        module subroutine refill_evaluator (sqme, qn, flv_index, evaluator)
            complex(default), intent(in), dimension(:) :: sqme
            type(quantum_numbers_t), intent(in), dimension(:, :) :: qn
            integer, intent(in), dimension(:), optional :: flv_index
            type(evaluator_t), intent(inout) :: evaluator
            integer :: i, i_flv
            do i = 1, size (sqme)
                if (present (flv_index)) then
                    i_flv = flv_index(i)
                else
                    i_flv = i
                end if
                call evaluator%add_to_matrix_element (qn(:, i_flv), sqme(i), &
                    match_only_flavor = .true.)
            end do
        end subroutine refill_evaluator

```

Return the number of outgoing (hard) particles for the state.

```

    <Parton states: parton state: TBP>+≡
        procedure :: get_n_out => parton_state_get_n_out

    <Parton states: sub interfaces>+≡
        module function parton_state_get_n_out (state) result (n)
            class(parton_state_t), intent(in), target :: state
            integer :: n
        end function parton_state_get_n_out

    <Parton states: procedures>+≡
        module function parton_state_get_n_out (state) result (n)
            class(parton_state_t), intent(in), target :: state
            integer :: n
            n = state%trace%get_n_out ()
        end function parton_state_get_n_out

```

30.2.8 Unit tests

```
<parton_states_ut.f90>≡  
  <File header>  
  
  module parton_states_ut  
    use unit_tests  
    use parton_states_uti  
  
    <Standard module head>  
  
    <Parton states: public test>  
  
    contains  
  
    <Parton states: test driver>  
  
  end module parton_states_ut  
<parton_states_uti.f90>≡  
  <File header>  
  
  module parton_states_uti  
  
    <Use kinds>  
    <Use strings>  
    use constants, only: zero  
    use numeric_utils  
    use flavors  
    use colors  
    use helicities  
    use quantum_numbers  
    use sf_base, only: sf_chain_instance_t  
    use state_matrices, only: state_matrix_t  
    use prc_template_me, only: prc_template_me_t  
    use interactions, only: interaction_t  
    use models, only: model_t, create_test_model  
    use parton_states  
  
    <Standard module head>  
  
    <Parton states: test declarations>  
  
    contains  
  
    <Parton states: tests>  
  
  end module parton_states_uti  
  
  <Parton states: public test>≡  
    public :: parton_states_test  
  
  <Parton states: test driver>≡  
    subroutine parton_states_test (u, results)  
      integer, intent(in) :: u  
      type(test_results_t), intent(inout) :: results
```



```

    <Parton states: execute tests>
end subroutine parton_states_test

```

Test a simple isolated state

```

<Parton states: execute tests>≡
    call test (parton_states_1, "parton_states_1", &
        "Create a 2 -> 2 isolated state and compute trace", &
        u, results)

<Parton states: test declarations>≡
    public :: parton_states_1

<Parton states: tests>≡
    subroutine parton_states_1 (u)
        integer, intent(in) :: u
        type(state_matrix_t), allocatable :: state
        type(flavor_t), dimension(2) :: flv_in
        type(flavor_t), dimension(2) :: flv_out1, flv_out2
        type(flavor_t), dimension(4) :: flv_tot
        type(helicity_t), dimension(4) :: hel
        type(color_t), dimension(4) :: col
        integer :: h1, h2, h3, h4
        integer :: f
        integer :: i
        type(quantum_numbers_t), dimension(4) :: qn
        type(prc_template_me_t) :: core
        type(sf_chain_instance_t), target :: sf_chain
        type(interaction_t), target :: int
        type(isolated_state_t) :: isolated_state
        integer :: n_states = 0
        integer, dimension(:), allocatable :: col_flow_index
        type(quantum_numbers_mask_t), dimension(2) :: qn_mask
        integer, dimension(8) :: i_allowed_states
        complex(default), dimension(8) :: me
        complex(default) :: me_check_tot, me_check_1, me_check_2, me2
        logical :: tmp1, tmp2
        type(model_t), pointer :: test_model => null ()

        write (u, "(A)") "* Test output: parton_states_1"
        write (u, "(A)") "* Purpose: Test the standard parton states"
        write (u, "(A)")

        call flv_in%init ([11, -11])
        call flv_out1%init ([1, -1])
        call flv_out2%init ([2, -2])

        write (u, "(A)") "* Using incoming flavors: "
        call flavor_write_array (flv_in, u)
        write (u, "(A)") "* Two outgoing flavor structures: "
        call flavor_write_array (flv_out1, u)
        call flavor_write_array (flv_out2, u)

```

```

write (u, "(A)") "* Initialize state matrix"
allocate (state)
call state%init ()

write (u, "(A)") "* Fill state matrix"
call col(3)%init ([1])
call col(4)%init ([-1])
do f = 1, 2
  do h1 = -1, 1, 2
    do h2 = -1, 1, 2
      do h3 = -1, 1, 2
        do h4 = -1, 1, 2
          n_states = n_states + 1
          call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
          if (f == 1) then
            flv_tot = [flv_in, flv_out1]
          else
            flv_tot = [flv_in, flv_out2]
          end if
          call qn%init (flv_tot, col, hel)
          call state%add_state (qn)
        end do
      end do
    end do
  end do
end do

!!! Two flavors, one color flow, 2 x 2 x 2 x 2 helicity configurations
!!! -> 32 states.
write (u, "(A)")
write (u, "(A,I2)") "* Generated number of states: ", n_states

call state%freeze ()

!!! Indices of the helicity configurations which are non-zero
i_allowed_states = [6, 7, 10, 11, 22, 23, 26, 27]
me = [cmplx (-1.89448E-5_default, 9.94456E-7_default, default), &
      cmplx (-8.37887E-2_default, 4.30842E-3_default, default), &
      cmplx (-1.99997E-1_default, -1.01985E-2_default, default), &
      cmplx ( 1.79717E-5_default, 9.27038E-7_default, default), &
      cmplx (-1.74859E-5_default, 8.78819E-7_default, default), &
      cmplx ( 1.67577E-1_default, -8.61683E-3_default, default), &
      cmplx ( 2.41331E-1_default, 1.23306E-2_default, default), &
      cmplx (-3.59435E-5_default, -1.85407E-6_default, default)]
me_check_tot = cmplx (zero, zero, default)
me_check_1 = cmplx (zero, zero, default)
me_check_2 = cmplx (zero, zero, default)
do i = 1, 8
  me2 = me(i) * conjg (me(i))
  me_check_tot = me_check_tot + me2
  if (i < 5) then
    me_check_1 = me_check_1 + me2
  else
    me_check_2 = me_check_2 + me2
  end if
end do

```

```

        end if
        call state%set_matrix_element (i_allowed_states(i), me(i))
    end do

    !!! Do not forget the color factor
    me_check_tot = 3._default * me_check_tot
    me_check_1 = 3._default * me_check_1
    me_check_2 = 3._default * me_check_2
    write (u, "(A)")

    write (u, "(A)") "* Setup interaction"
    call int%basic_init (2, 0, 2, set_relations = .true.)
    call int%set_state_matrix (state)

    core%data%n_in = 2; core%data%n_out = 2
    core%data%n_flv = 2
    allocate (core%data%flv_state (4, 2))
    core%data%flv_state (1, :) = [11, 11]
    core%data%flv_state (2, :) = [-11, -11]
    core%data%flv_state (3, :) = [1, 2]
    core%data%flv_state (4, :) = [-1, -2]
    core%use_color_factors = .false.
    core%nc = 3

    write (u, "(A)") "* Init isolated state"
    call isolated_state%init (sf_chain, int)
    !!! There is only one color flow.
    allocate (col_flow_index (n_states)); col_flow_index = 1
    call qn_mask%init (.false., .false., .true., mask_cg = .false.)
    write (u, "(A)") "* Give a trace to the isolated state"
    call isolated_state%setup_square_trace (core, qn_mask, col_flow_index, .false.)
    call isolated_state%evaluate_trace ()
    write (u, "(A)")
    write (u, "(A)", advance = "no") "* Squared matrix element correct: "
    write (u, "(L1)") nearly_equal (me_check_tot, &
        isolated_state%trace%get_matrix_element (1), rel_smallness = 0.00001_default)

    write (u, "(A)") "* Give a matrix to the isolated state"
    call create_test_model (var_str ("SM"), test_model)
    call isolated_state%setup_square_matrix (core, test_model, qn_mask, col_flow_index)
    call isolated_state%evaluate_matrix ()

    write (u, "(A)") "* Sub-matrixelements correct: "
    tmp1 = nearly_equal (me_check_1, &
        isolated_state%matrix%get_matrix_element (1), rel_smallness = 0.00001_default)
    tmp2 = nearly_equal (me_check_2, &
        isolated_state%matrix%get_matrix_element (2), rel_smallness = 0.00001_default)
    write (u, "(A,L1,A,L1)") "* 1: ", tmp1, ", 2: ", tmp2

    write (u, "(A)") "* Test output end: parton_states_1"
end subroutine parton_states_1

```

30.3 Process component management

This module contains tools for managing and combining process components and matrix-element code and values, acting at a level below the actual process definition.

30.3.1 Abstract base type

The types introduced here are abstract base types.

```
<pcm_base.f90>≡  
  <File header>
```

```
module pcm_base
```

```
  <Use kinds>
```

```
  <Use strings>
```

```
    use os_interface, only: os_data_t
```

```
    use process_libraries, only: process_library_t
```

```
    use prc_core_def
```

```
    use prc_core
```

```
    use variables, only: var_list_t
```

```
    use mappings, only: mapping_defaults_t
```

```
    use phs_base, only: phs_config_t
```

```
    use phs_forests, only: phs_parameters_t
```

```
    use mci_base, only: mci_t
```

```
    use model_data, only: model_data_t
```

```
    use models, only: model_t
```

```
    use blha_config, only: blha_master_t
```

```
    use blha_olp_interfaces, only: blha_template_t
```

```
    use process_config
```

```
    use process_mci, only: process_mci_entry_t
```

```
  <Standard module head>
```

```
  <PCM base: public>
```

```
  <PCM base: parameters>
```

```
  <PCM base: types>
```

```
  <PCM base: interfaces>
```

```
    interface
```

```
  <PCM base: sub interfaces>
```

```
    end interface
```

```
end module pcm_base
```

```
<pcm_base_sub.f90>≡  
  <File header>
```

```

submodule (pcm_base) pcm_base_s

    use io_units
    use diagnostics
    use format_utils, only: write_integer_array
    use format_utils, only: write_separator
    use physics_defs, only: BORN, NLO_REAL

    implicit none

contains

    <PCM base: procedures>

end submodule pcm_base_s

```

30.3.2 Core management

This object holds information about the cores used by the components and allocates the corresponding manager instance.

`i_component` is the index of the process component which this core belongs to. The pointer to the core definition is a convenient help in configuring the core itself.

We allow for a `blha_config` configuration object that covers BLHA cores. The BLHA standard is suitable generic to warrant support outside of specific type extension (i.e., applies to LO and NLO if requested). The BLHA configuration is allocated only if the core requires it.

```

<PCM base: public>≡
    public :: core_entry_t

<PCM base: types>≡
    type :: core_entry_t
        integer :: i_component = 0
        logical :: active = .false.
        class(prc_core_def_t), pointer :: core_def => null ()
        type(blha_template_t), allocatable :: blha_config
        class(prc_core_t), allocatable :: core
    contains
        <PCM base: core entry: TBP>
    end type core_entry_t

<PCM base: core entry: TBP>≡
    procedure :: get_core_ptr => core_entry_get_core_ptr

<PCM base: sub interfaces>≡
    module function core_entry_get_core_ptr (core_entry) result (core)
        class(core_entry_t), intent(in), target :: core_entry
        class(prc_core_t), pointer :: core
    end function core_entry_get_core_ptr

```

```

(PCM base: procedures)≡
  module function core_entry_get_core_ptr (core_entry) result (core)
    class(core_entry_t), intent(in), target :: core_entry
    class(prc_core_t), pointer :: core
    if (allocated (core_entry%core)) then
      core => core_entry%core
    else
      core => null ()
    end if
  end function core_entry_get_core_ptr

```

Configure the core object after allocation with correct type. The `core_def` object pointer and the index `i_component` of the associated process component are already there.

```

(PCM base: core entry: TBP)+≡
  procedure :: configure => core_entry_configure

(PCM base: sub interfaces)+≡
  module subroutine core_entry_configure (core_entry, lib, id)
    class(core_entry_t), intent(inout) :: core_entry
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: id
  end subroutine core_entry_configure

(PCM base: procedures)+≡
  module subroutine core_entry_configure (core_entry, lib, id)
    class(core_entry_t), intent(inout) :: core_entry
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: id
    call core_entry%core%init &
      (core_entry%core_def, lib, id, core_entry%i_component)
  end subroutine core_entry_configure

```

30.3.3 Process component manager

The process-component manager `pcm` is the master component of the `process_t` object. It serves two purposes:

1. It holds configuration data which allow us to centrally manage the components, terms, etc. of the process object.
2. It implements the methods that realize the algorithm for constructing the process object and computing an integral. This algorithm makes use of the data stored within `pcm`.

To this end, the object is abstract and polymorphic. The two extensions that we support, implement (a) default tree-level calculation, optionally including a sum over sub-processes with different particle content, or (b) the FKS-NLO subtraction algorithm for QCD-corrected processes. In both cases, the type extensions may hold suitable further data.

Data included in the base type:

The number of components determines the `component_selected` array.

`i_phs_config` is a lookup table that holds the PHS configuration index for a given component index.

`i_core` is a lookup table that holds the core-entry index for a given component index.

`i_mci` is a lookup table that holds the integrator (MCI) index for a given component index.

```

<PCM base: public>+≡
  public :: pcm_t

<PCM base: types>+≡
  type, abstract :: pcm_t
    logical :: initialized = .false.
    logical :: has_pdfs = .false.
    integer :: n_components = 0
    integer :: n_cores = 0
    integer :: n_mci = 0
    logical, dimension(:), allocatable :: component_selected
    logical, dimension(:), allocatable :: component_active
    integer, dimension(:), allocatable :: i_phs_config
    integer, dimension(:), allocatable :: i_core
    integer, dimension(:), allocatable :: i_mci
    type(blha_template_t) :: blha_defaults
    logical :: uses_blha = .false.
    type(os_data_t) :: os_data
  contains
    <PCM base: pcm: TBP>
  end type pcm_t

```

The factory method. We use the `inout` intent, so calling this again is an error.

```

<PCM base: pcm: TBP>≡
  procedure(pcm_allocate_workspace), deferred :: allocate_workspace

<PCM base: interfaces>≡
  abstract interface
    subroutine pcm_allocate_workspace (pcm, work)
      import
      class(pcm_t), intent(in) :: pcm
      class(pcm_workspace_t), intent(inout), allocatable :: work
    end subroutine pcm_allocate_workspace
  end interface

<PCM base: pcm: TBP>+≡
  procedure(pcm_is_nlo), deferred :: is_nlo

<PCM base: interfaces>+≡
  abstract interface
    function pcm_is_nlo (pcm) result (is_nlo)
      import
      logical :: is_nlo
      class(pcm_t), intent(in) :: pcm
    end function pcm_is_nlo
  end interface

```

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_final), deferred :: final

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_final (pcm)
      import
      class(pcm_t), intent(inout) :: pcm
    end subroutine pcm_final
  end interface

```

30.3.4 Initialization methods

The PCM has the duty to coordinate and configure the process-object components.

Initialize the PCM configuration itself, using environment data.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_init), deferred :: init

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_init (pcm, env, meta)
      import
      class(pcm_t), intent(out) :: pcm
      type(process_environment_t), intent(in) :: env
      type(process_metadata_t), intent(in) :: meta
    end subroutine pcm_init
  end interface

```

Initialize the BLHA configuration block, the component-independent default settings. This is to be called by `pcm_init`. We use the provided variable list.

This block is filled regardless of whether BLHA is actually used, because why not? We use a default value for the scheme (not set in unit tests).

```

<PCM base: pcm: TBP>+≡
  procedure :: set_blha_defaults => pcm_set_blha_defaults

<PCM base: sub interfaces>+≡
  module subroutine pcm_set_blha_defaults (pcm, polarized_beams, var_list)
    class(pcm_t), intent(inout) :: pcm
    type(var_list_t), intent(in) :: var_list
    logical, intent(in) :: polarized_beams
  end subroutine pcm_set_blha_defaults

<PCM base: procedures>+≡
  module subroutine pcm_set_blha_defaults (pcm, polarized_beams, var_list)
    class(pcm_t), intent(inout) :: pcm
    type(var_list_t), intent(in) :: var_list
    logical, intent(in) :: polarized_beams
    logical :: muon_yukawa_off
    real(default) :: top_yukawa
    type(string_t) :: ew_scheme
    muon_yukawa_off = &
      var_list%get_lval (var_str ("?openloops_switch_off_muon_yukawa"))

```



```

top_yukawa = &
    var_list%get_rval (var_str ("blha_top_yukawa"))
ew_scheme = &
    var_list%get_sval (var_str ("blha_ew_scheme"))
if (ew_scheme == "") ew_scheme = "Gmu"
call pcm%blha_defaults%init &
    (polarized_beams, muon_yukawa_off, top_yukawa, ew_scheme)
end subroutine pcm_set_blha_defaults

```

Read the method settings from the variable list and store them in the BLHA master. The details depend on the pcm concrete type.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_set_blha_methods), deferred :: set_blha_methods
<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_set_blha_methods (pcm, blha_master, var_list)
            import
            class(pcm_t), intent(inout) :: pcm
            type(blha_master_t), intent(inout) :: blha_master
            type(var_list_t), intent(in) :: var_list
        end subroutine pcm_set_blha_methods
    end interface

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration. We may inspect either the PCM itself or the array of process cores.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_get_blha_flv_states), deferred :: get_blha_flv_states
<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_get_blha_flv_states (pcm, core_entry, flv_born, flv_real)
            import
            class(pcm_t), intent(in) :: pcm
            type(core_entry_t), dimension(:), intent(in) :: core_entry
            integer, dimension(:,:), allocatable, intent(out) :: flv_born
            integer, dimension(:,:), allocatable, intent(out) :: flv_real
        end subroutine pcm_get_blha_flv_states
    end interface

```

Allocate the right number of process components. The number is also stored in the process meta. Initially, all components are active but none are selected.

```

<PCM base: pcm: TBP>+≡
    procedure :: allocate_components => pcm_allocate_components
<PCM base: sub interfaces>+≡
    module subroutine pcm_allocate_components (pcm, comp, meta)
        class(pcm_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), allocatable, intent(out) :: comp
        type(process_metadata_t), intent(in) :: meta
    end subroutine pcm_allocate_components

```

```

<PCM base: procedures>+≡
module subroutine pcm_allocate_components (pcm, comp, meta)
  class(pcm_t), intent(inout) :: pcm
  type(process_component_t), dimension(:), allocatable, intent(out) :: comp
  type(process_metadata_t), intent(in) :: meta
  pcm%n_components = meta%n_components
  allocate (comp (pcm%n_components))
  allocate (pcm%component_selected (pcm%n_components), source = .false.)
  allocate (pcm%component_active (pcm%n_components), source = .true.)
end subroutine pcm_allocate_components

```

Each process component belongs to a category/type, which we identify by a universal integer constant. The categories can be taken from the process definition. For easy lookup, we store the categories in an array.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_categorize_components), deferred :: categorize_components

<PCM base: interfaces>+≡
abstract interface
  subroutine pcm_categorize_components (pcm, config)
    import
    class(pcm_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
  end subroutine pcm_categorize_components
end interface

```

Allocate the right number and type(s) of process-core objects, i.e., the interface object between the process and matrix-element code.

Within the `pcm` block, also associate cores with components and store relevant configuration data, including the `i_core` lookup table.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_allocate_cores), deferred :: allocate_cores

<PCM base: interfaces>+≡
abstract interface
  subroutine pcm_allocate_cores (pcm, config, core_entry)
    import
    class(pcm_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
    type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
  end subroutine pcm_allocate_cores
end interface

```

Generate and interface external code for a single core, if this is required.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_prepare_any_external_code), deferred :: &
    prepare_any_external_code

<PCM base: interfaces>+≡
abstract interface
  subroutine pcm_prepare_any_external_code &
    (pcm, core_entry, i_core, libname, model, var_list)
  import

```

```

class(pcm_t), intent(in) :: pcm
type(core_entry_t), intent(inout) :: core_entry
integer, intent(in) :: i_core
type(string_t), intent(in) :: libname
type(model_data_t), intent(in), target :: model
type(var_list_t), intent(in) :: var_list
end subroutine pcm_prepare_any_external_code
end interface

```

Prepare the BLHA configuration for a core object that requires it. This does not affect the core object, which may not yet be allocated.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_setup_blha), deferred :: setup_blha
<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_setup_blha (pcm, core_entry)
      import
      class(pcm_t), intent(in) :: pcm
      type(core_entry_t), intent(inout) :: core_entry
    end subroutine pcm_setup_blha
  end interface

```

Configure the BLHA interface for a core object that requires it. This is separate from the previous method, assuming that the pcm has to allocate the actual cores and acquire some data in-between.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_prepare_blha_core), deferred :: prepare_blha_core
<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_prepare_blha_core (pcm, core_entry, model)
      import
      class(pcm_t), intent(in) :: pcm
      type(core_entry_t), intent(inout) :: core_entry
      class(model_data_t), intent(in), target :: model
    end subroutine pcm_prepare_blha_core
  end interface

```

Allocate and configure the MCI (multi-channel integrator) records and their relation to process components, appropriate for the algorithm implemented by pcm.

Create a mci_t template: the procedure `dispatch_mci` is called as a factory method for allocating the mci_t object with a specific concrete type. The call may depend on the concrete pcm type.

```

<PCM base: public>+≡
  public :: dispatch_mci_proc
<PCM base: interfaces>+≡
  abstract interface
    subroutine dispatch_mci_proc (mci, var_list, process_id, is_nlo)
      import
      class(mci_t), allocatable, intent(out) :: mci

```

```

        type(var_list_t), intent(in) :: var_list
        type(string_t), intent(in) :: process_id
        logical, intent(in), optional :: is_nlo
    end subroutine dispatch_mci_proc
end interface

<PCM base: pcm: TBP>+≡
    procedure(pcm_setup_mci), deferred :: setup_mci
    procedure(pcm_call_dispatch_mci), deferred :: call_dispatch_mci
<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_setup_mci (pcm, mci_entry)
            import
            class(pcm_t), intent(inout) :: pcm
            type(process_mci_entry_t), &
                dimension(:), allocatable, intent(out) :: mci_entry
        end subroutine pcm_setup_mci
    end interface

    abstract interface
        subroutine pcm_call_dispatch_mci (pcm, &
            dispatch_mci, var_list, process_id, mci_template)
            import
            class(pcm_t), intent(inout) :: pcm
            procedure(dispatch_mci_proc) :: dispatch_mci
            type(var_list_t), intent(in) :: var_list
            type(string_t), intent(in) :: process_id
            class(mci_t), intent(out), allocatable :: mci_template
        end subroutine pcm_call_dispatch_mci
    end interface

```

Proceed with PCM configuration based on the core and component configuration data. Base version is empty.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_complete_setup), deferred :: complete_setup
<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_complete_setup (pcm, core_entry, component, model)
            import
            class(pcm_t), intent(inout) :: pcm
            type(core_entry_t), dimension(:), intent(in) :: core_entry
            type(process_component_t), dimension(:), intent(inout) :: component
            type(model_t), intent(in), target :: model
        end subroutine pcm_complete_setup
    end interface

```

Retrieve information

Return the core index that belongs to a particular component.

```

<PCM base: pcm: TBP>+≡
    procedure :: get_i_core => pcm_get_i_core

```

```

<PCM base: sub interfaces>+≡
    module function pcm_get_i_core (pcm, i_component) result (i_core)
        class(pcm_t), intent(in) :: pcm
        integer, intent(in) :: i_component
        integer :: i_core
    end function pcm_get_i_core

<PCM base: procedures>+≡
    module function pcm_get_i_core (pcm, i_component) result (i_core)
        class(pcm_t), intent(in) :: pcm
        integer, intent(in) :: i_component
        integer :: i_core
        if (allocated (pcm%i_core)) then
            i_core = pcm%i_core(i_component)
        else
            i_core = 0
        end if
    end function pcm_get_i_core

```

Phase-space configuration

Allocate and initialize the right number and type(s) of phase-space configuration entries. The `i_phs_config` lookup table must be set accordingly.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_init_phs_config), deferred :: init_phs_config

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_init_phs_config &
            (pcm, phs_entry, meta, env, phs_par, mapping_defs)
        import
        class(pcm_t), intent(inout) :: pcm
        type(process_phs_config_t), &
            dimension(:), allocatable, intent(out) :: phs_entry
        type(process_metadata_t), intent(in) :: meta
        type(process_environment_t), intent(in) :: env
        type(mapping_defaults_t), intent(in) :: mapping_defs
        type(phs_parameters_t), intent(in) :: phs_par
    end subroutine pcm_init_phs_config
    end interface

```

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index `i` and the `active` flag.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_init_component), deferred :: init_component

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_init_component &
            (pcm, component, i, active, phs_config, env, meta, config)
        import
        class(pcm_t), intent(in) :: pcm

```

```

        type(process_component_t), intent(out) :: component
        integer, intent(in) :: i
        logical, intent(in) :: active
        class(phs_config_t), allocatable, intent(in) :: phs_config
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        type(process_config_data_t), intent(in) :: config
    end subroutine pcm_init_component
end interface

```

Record components in the process meta data if they have turned out to be inactive.

```

⟨PCM base: pcm: TBP⟩+=
    procedure :: record_inactive_components => pcm_record_inactive_components

⟨PCM base: sub interfaces⟩+=
    module subroutine pcm_record_inactive_components (pcm, component, meta)
        class(pcm_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_metadata_t), intent(inout) :: meta
    end subroutine pcm_record_inactive_components

⟨PCM base: procedures⟩+=
    module subroutine pcm_record_inactive_components (pcm, component, meta)
        class(pcm_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_metadata_t), intent(inout) :: meta
        integer :: i
        pcm%component_active = component%active
        do i = 1, pcm%n_components
            if (.not. component(i)%active) call meta%deactivate_component (i)
        end do
    end subroutine pcm_record_inactive_components

```

30.3.5 Manager workspace

This object deals with the actual (squared) matrix element values. It holds any central data that are generated and/or used when calculating a particular phase-space point.

Since phase-space points are associated with an integrator, we expect the instances of this type to correspond to MCI instances.

```

⟨PCM base: public⟩+=
    public :: pcm_workspace_t

⟨PCM base: types⟩+=
    type, abstract :: pcm_workspace_t
    !   class(pcm_t), pointer :: config => null ()
    logical :: bad_point = .false.
contains
    ⟨PCM base: pcm instance: TBP⟩
end type pcm_workspace_t

```

```

<PCM base: pcm instance: TBP>≡
    procedure(pcm_work_final), deferred :: final

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_work_final (pcm_work)
            import
            class(pcm_workspace_t), intent(inout) :: pcm_work
        end subroutine pcm_work_final
    end interface

<PCM base: pcm instance: TBP>+≡
    procedure(pcm_work_is_nlo), deferred :: is_nlo

<PCM base: interfaces>+≡
    abstract interface
        function pcm_work_is_nlo (pcm_work) result (is_nlo)
            import
            logical :: is_nlo
            class(pcm_workspace_t), intent(inout) :: pcm_work
        end function pcm_work_is_nlo
    end interface

<XXX PCM base: pcm instance: TBP>≡
    procedure :: link_config => pcm_work_link_config

<XXX PCM base: procedures>≡
    subroutine pcm_work_link_config (pcm_work, config)
        class(pcm_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in), target :: config
        pcm_work%config => config
    end subroutine pcm_work_link_config

<PCM base: pcm instance: TBP>+≡
    procedure :: is_valid => pcm_work_is_valid

<PCM base: sub interfaces>+≡
    module function pcm_work_is_valid (pcm_work) result (valid)
        logical :: valid
        class(pcm_workspace_t), intent(in) :: pcm_work
    end function pcm_work_is_valid

<PCM base: procedures>+≡
    module function pcm_work_is_valid (pcm_work) result (valid)
        logical :: valid
        class(pcm_workspace_t), intent(in) :: pcm_work
        valid = .not. pcm_work%bad_point
    end function pcm_work_is_valid

<PCM base: pcm instance: TBP>+≡
    procedure :: set_bad_point => pcm_work_set_bad_point

```

```

⟨PCM base: sub interfaces⟩+≡
    pure module subroutine pcm_work_set_bad_point (pcm_work, bad_point)
        class(pcm_workspace_t), intent(inout) :: pcm_work
        logical, intent(in) :: bad_point
    end subroutine pcm_work_set_bad_point

⟨PCM base: procedures⟩+≡
    pure module subroutine pcm_work_set_bad_point (pcm_work, bad_point)
        class(pcm_workspace_t), intent(inout) :: pcm_work
        logical, intent(in) :: bad_point
        pcm_work%bad_point = pcm_work%bad_point .or. bad_point
    end subroutine pcm_work_set_bad_point

```

30.4 The process object

```

⟨process.f90⟩≡
    ⟨File header⟩

    module process

        ⟨Use kinds⟩
        ⟨Use strings⟩
        ⟨Use debug⟩
        use diagnostics
        use lorentz
        use rng_base
        use dispatch_rng, only: dispatch_rng_factory
        use dispatch_rng, only: update_rng_seed_in_var_list
        use os_interface
        use sm_qcd
        use mci_base
        use flavors
        use model_data
        use models
        use process_libraries
        use process_constants
        use variables
        use beam_structures
        use beams
        use pdg_arrays
        use expr_base
        use sf_base
        use sf_mappings
        use resonances, only: resonance_history_t, resonance_history_set_t

        use prc_test_core, only: test_t
        use prc_core_def, only: prc_core_def_t
        use prc_core, only: prc_core_t, helicity_selection_t
        use phs_base

        use parton_states, only: connected_state_t
        use pcm_base
    end module process

```



```

    use pcm
    use process_counter
    use process_config
    use process_mci

    <Standard module head>

    <Process: public>

    <Process: types>

    <Process: interfaces>

    interface
    <Process: sub interfaces>
    end interface

contains

    <Process: main procedures>

end module process
<process_sub.f90>≡
    <File header>

submodule (process) process_s

    use io_units
    use format_utils, only: write_separator
    use constants
    use numeric_utils
    use cputime
    use md5
    use integration_results
    use physics_defs
    use interactions
    use particles
    use dispatch_phase_space, only: dispatch_phs
    use prc_external, only: prc_external_t
    use prc_recola, only: prc_recola_t
    use blha_olp_interfaces, only: prc_blha_t, blha_template_t
    use prc_threshold, only: prc_threshold_t
    use phs_fks, only: phs_fks_config_t
    use mappings, only: mapping_defaults_t
    use phs_forests, only: phs_parameters_t
    use phs_wood, only: phs_wood_config_t
    use blha_config, only: blha_master_t

    implicit none

contains

    <Process: procedures>

```

```
end submodule process_s
```

30.4.1 Process status

Store counter and status information in a process object.

```
(Process: types)≡
  type :: process_status_t
  private
  end type process_status_t
```

30.4.2 Process status

Store integration results in a process object.

```
(Process: types)+≡
  type :: process_results_t
  private
  end type process_results_t
```

30.4.3 The process type

NOTE: The description below represents the intended structure after refactoring and disentangling the FKS-NLO vs. LO algorithm dependencies.

A **process** object is the internal representation of integration-run methods and data, as they are controlled by the user via a Sindarin script. The process object provides access to matrix elements (the actual “process” definitions that the user has provided before), it defines the separation into individually integrable components, and it manages phase-space construction, the actual integration over phase space, and the accumulation of results.

As a workspace for individual sampling calls, we introduce an associated **process_instance** object type elsewhere. The **process** object contains data that either define the configuration or accumulate results from a complete integration pass.

After successful phase-space integration, subsequent event generation is not actually represented by the **process** object. However, any event generation refers to an existing **process** object which represents a specific integration pass, and it uses a fresh **process_instance** workspace for calculations.

The process object consists of several subobjects with their specific purposes. The corresponding types are defined below. (Technically, the subobject type definitions have to come before the process type definition, but with NOWEB magic we reverse this order here.)

The **meta** object describes the process globally. All contents become fixed when the object is initialized. Similarly, the **env** component captures the (Sindarin) environment at the point where the process object is initialized.

The **config** object holds physical and technical configuration data that are collected and derived from the environment during process initialization, and which are common to all process components.

The `pcm` object (process-component manager) is polymorphic. This is an object which holds data which represent the process-object structure and breakdown, and it contains the methods that implement the algorithm of managing this structure, accumulating partial results, and finally collecting the pieces. Depending on the generic process type, the contents of `pcm` do vary. In particular, there is some base-type data content and a simple (default) extension which is designed for traditional O'MEGA matrix elements and tree-level integration, possibly with several sub-processes to sum over. The second extension is designed for the FKS phase-space and subtraction algorithm for NLO QCD, which interfaces external one-loop providers.

The `component` subobjects are, first of all, interfaces to the original process-component definitions that have been provided by the user, which the program has already taken to produce matrix-element code and interfaces. The management of those components is deferred by `pcm`, which contains the information that defines the role of each component. In particular, in the default (LO) version, process components correspond to distinct particle combinations which have been included in the original process definition. In the FKS-NLO version, the breakdown of a NLO process into Born, real, virtual, etc. components determines the setup.

The `phs_config` subobjects hold data that allow and implement the construction of phase-space configurations. The type `process_phs_config_t` is a wrapper type around the concrete polymorphic `phs_config_t` object type, which manages phase-space construction, including some bookkeeping required for setting up multi-channel integration. In the LO case, we expect a separate entry for each independent sub-process. For the FKS-NLO algorithm, we expect several entries: a default-type entry which implements the underlying Born phase space, and additional entries which enable the construction of various real-radiation and subtraction kinematics configurations.

A `core_entry` is the interface to existing matrix-element and interaction code. Depending on the process and its components, there may be various distinct matrix elements to compute.

The `mci_entry` objects configure distinct MC input parameter sets and their associated (multi-channel) integrators.

The `rng_factory` object is a single objects which constructs individual random-number generators for various tasks, in a uniform and well-defined way.

The `beam_config` object describes the incoming particles, either the decay mother or the scattering beams. It also contains the spectrum- and structure-function setup, which has to interact with the phase-space and integrator facilities.

The `term` subobjects break down the process in its smallest parts which appear in the calculation. For LO processes, the correspondence between terms and components is one-to-one. The FKS-NLO algorithm requires not just separation of Born, real, and virtual components but also subtraction terms, and a decomposition of the real phase space into singular regions. The general idea is that the integration results of distinct sets of terms are summed over to provide the results of individual components. This is also controlled by the `pcm` subobject.

The `process_status` object is a bookkeeping device that allows us to query the status of an ongoing calculation.

The `process_results` object collects the integration results for external use,

including integration history information.

```

<Process: public>≡
    public :: process_t
<Process: types>+≡
    type :: process_t
    private
    type(process_metadata_t) :: &
        meta
    type(process_environment_t) :: &
        env
    type(process_config_data_t) :: &
        config
    class(pcm_t), allocatable :: &
        pcm
    type(process_component_t), dimension(:), allocatable :: &
        component
    type(process_phs_config_t), dimension(:), allocatable :: &
        phs_entry
    type(core_entry_t), dimension(:), allocatable :: &
        core_entry
    type(process_mci_entry_t), dimension(:), allocatable :: &
        mci_entry
    class(rng_factory_t), allocatable :: &
        rng_factory
    type(process_beam_config_t) :: &
        beam_config
    type(process_term_t), dimension(:), allocatable :: &
        term
    type(process_status_t) :: &
        status
    type(process_results_t) :: &
        result
    contains
    <Process: process: TBP>
end type process_t

```

30.4.4 Process pointer

Wrapper type for storing pointers to process objects in arrays.

```

<Process: public>+≡
    public :: process_ptr_t
<Process: types>+≡
    type :: process_ptr_t
    type(process_t), pointer :: p => null ()
end type process_ptr_t

```

30.4.5 Output

This procedure is an important debugging and inspection tool; it is not used during normal operation. The process object is written to a file (identified by

unit, which may also be standard output). Optional flags determine whether we show everything or just the interesting parts.

The shorthand as a traditional TBP.

```

<Process: process: TBP>≡
    procedure :: write => process_write

<Process: sub interfaces>≡
    module subroutine process_write (process, screen, unit, &
        show_os_data, show_var_list, show_rng, show_expressions, pacify)
        class(process_t), intent(in) :: process
        logical, intent(in) :: screen
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_os_data
        logical, intent(in), optional :: show_var_list
        logical, intent(in), optional :: show_rng
        logical, intent(in), optional :: show_expressions
        logical, intent(in), optional :: pacify
    end subroutine process_write

<Process: procedures>≡
    module subroutine process_write (process, screen, unit, &
        show_os_data, show_var_list, show_rng, show_expressions, pacify)
        class(process_t), intent(in) :: process
        logical, intent(in) :: screen
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_os_data
        logical, intent(in), optional :: show_var_list
        logical, intent(in), optional :: show_rng
        logical, intent(in), optional :: show_expressions
        logical, intent(in), optional :: pacify
        integer :: u, iostat
        character(0) :: iomsg
        integer, dimension(:), allocatable :: v_list
        u = given_output_unit (unit)
        allocate (v_list (0))
        call set_flag (v_list, F_SHOW_OS_DATA, show_os_data)
        call set_flag (v_list, F_SHOW_VAR_LIST, show_var_list)
        call set_flag (v_list, F_SHOW_RNG, show_rng)
        call set_flag (v_list, F_SHOW_EXPRESSIONS, show_expressions)
        call set_flag (v_list, F_PACIFY, pacify)
        if (screen) then
            call process%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
        else
            call process%write_formatted (u, "DT", v_list, iostat, iomsg)
        end if
    end subroutine process_write

```

Standard DTIO procedure with binding.

For the particular application, the screen format is triggered by the LISTDIRECTED option for the iotype format editor string. The other options activate when the particular parameter value is found in v_list.

NOTE: The DTIO generic binding is supported by gfortran since 7.0.

TODO wk 2018: The default could be to show everything, and we should have separate switches for all major parts. Currently, there are only a few.

```

(Process: process: TBP)+≡
    ! generic :: write (formatted) => write_formatted
    procedure :: write_formatted => process_write_formatted

(Process: sub interfaces)+≡
    module subroutine process_write_formatted (dtv, unit, iotype, &
        v_list, iostat, iomsg)
        class(process_t), intent(in) :: dtv
        integer, intent(in) :: unit
        character(*), intent(in) :: iotype
        integer, dimension(:), intent(in) :: v_list
        integer, intent(out) :: iostat
        character(*), intent(inout) :: iomsg
    end subroutine process_write_formatted

(Process: procedures)+≡
    module subroutine process_write_formatted (dtv, unit, iotype, &
        v_list, iostat, iomsg)
        class(process_t), intent(in) :: dtv
        integer, intent(in) :: unit
        character(*), intent(in) :: iotype
        integer, dimension(:), intent(in) :: v_list
        integer, intent(out) :: iostat
        character(*), intent(inout) :: iomsg
        integer :: u
        logical :: screen
        logical :: var_list
        logical :: rng_factory
        logical :: expressions
        logical :: counters
        logical :: os_data
        logical :: model
        logical :: pacify
        integer :: i
        u = unit
        select case (iotype)
        case ("LISTDIRECTED")
            screen = .true.
        case default
            screen = .false.
        end select
        var_list = flagged(v_list, F_SHOW_VAR_LIST)
        rng_factory = flagged(v_list, F_SHOW_RNG, .true.)
        expressions = flagged(v_list, F_SHOW_EXPRESSIONS)
        counters = .true.
        os_data = flagged(v_list, F_SHOW_OS_DATA)
        model = .false.
        pacify = flagged(v_list, F_PACIFY)
        associate (process => dtv)
            if (screen) then
                write (msg_buffer, "(A)") repeat("-", 72)
                call msg_message ()
            else
                call write_separator (u, 2)
            end if
        end associate
    end subroutine process_write_formatted

```

```

call process%meta%write (u, screen)
if (var_list) then
    call process%env%write (u, show_var_list=var_list, &
        show_model=.false., show_lib=.false., &
        show_os_data=os_data)
else if (.not. screen) then
    write (u, "(1x,A)") "Variable list: [not shown]"
end if
if (process%meta%type == PRC_UNKNOWN) then
    call write_separator (u, 2)
    return
else if (screen) then
    return
end if
call write_separator (u)
call process%config%write (u, counters, model, expressions)
if (rng_factory) then
    if (allocated (process%rng_factory)) then
        call write_separator (u)
        call process%rng_factory%write (u)
    end if
end if
call write_separator (u, 2)
if (allocated (process%component)) then
    write (u, "(1x,A)") "Process component configuration:"
    do i = 1, size (process%component)
        call write_separator (u)
        call process%component(i)%write (u)
    end do
else
    write (u, "(1x,A)") "Process component configuration: [undefined]"
end if
call write_separator (u, 2)
if (allocated (process%term)) then
    write (u, "(1x,A)") "Process term configuration:"
    do i = 1, size (process%term)
        call write_separator (u)
        call process%term(i)%write (u)
    end do
else
    write (u, "(1x,A)") "Process term configuration: [undefined]"
end if
call write_separator (u, 2)
call process%beam_config%write (u)
call write_separator (u, 2)
if (allocated (process%mci_entry)) then
    write (u, "(1x,A)") "Multi-channel integrator configurations:"
    do i = 1, size (process%mci_entry)
        call write_separator (u)
        write (u, "(1x,A,I0,A)") "MCI #", i, ":"
        call process%mci_entry(i)%write (u, pacify)
    end do
end if
call write_separator (u, 2)

```

```

end associate
iostat = 0
iomsg = ""
end subroutine process_write_formatted

<Process: process: TBP>+≡
  procedure :: write_meta => process_write_meta

<Process: sub interfaces>+≡
  module subroutine process_write_meta (process, unit, testflag)
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine process_write_meta

<Process: procedures>+≡
  module subroutine process_write_meta (process, unit, testflag)
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u, i
    u = given_output_unit (unit)
    select case (process%meta%type)
    case (PRC_UNKNOWN)
      write (u, "(1x,A)") "Process instance [undefined]"
      return
    case (PRC_DECAY)
      write (u, "(1x,A)", advance="no") "Process instance [decay]:"
    case (PRC_SCATTERING)
      write (u, "(1x,A)", advance="no") "Process instance [scattering]:"
    case default
      call msg_bug ("process_instance_write: undefined process type")
    end select
    write (u, "(1x,A,A,A)") "' ", char (process%meta%id), "' "
    write (u, "(3x,A,A,A)") "Run ID = ' ", char (process%meta%run_id), "' "
    if (allocated (process%meta%component_id)) then
      write (u, "(3x,A)") "Process components:"
      do i = 1, size (process%meta%component_id)
        if (process%pcm%component_selected(i)) then
          write (u, "(3x,'*')", advance="no")
        else
          write (u, "(4x)", advance="no")
        end if
      end do
      write (u, "(1x,I0,9A)") i, ": ' ", &
        char (process%meta%component_id (i)), "' : ", &
        char (process%meta%component_description (i))
    end do
  end if
end subroutine process_write_meta

```

Screen output. Write a short account of the process configuration and the current results. The verbose version lists the components, the short version just the results.

<Process: process: TBP>+≡


```

procedure :: show => process_show

(Process: sub interfaces)+≡
  module subroutine process_show (object, unit, verbose)
    class(process_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine process_show

(Process: procedures)+≡
  module subroutine process_show (object, unit, verbose)
    class(process_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    logical :: verb
    real(default) :: err_percent
    u = given_output_unit (unit)
    verb = .true.; if (present (verbose)) verb = verbose
    if (verb) then
      call object%meta%show (u, object%config%model%get_name ())
      select case (object%meta%type)
        case (PRC_DECAY)
          write (u, "(2x,A)", advance="no") "Computed width ="
        case (PRC_SCATTERING)
          write (u, "(2x,A)", advance="no") "Computed cross section ="
        case default; return
      end select
    else
      if (object%meta%run_id /= "") then
        write (u, "('Run',1x,A,':',1x)", advance="no") &
          char (object%meta%run_id)
      end if
      write (u, "(A)", advance="no") char (object%meta%id)
      select case (object%meta%num_id)
        case (0)
          write (u, "(::~)")
        case default
          write (u, "(1x,'(,I0,~)',':~)") object%meta%num_id
      end select
      write (u, "(2x)", advance="no")
    end if
    if (object%has_integral_tot ()) then
      write (u, "(ES14.7,1x,'+-',ES9.2)", advance="no") &
        object%get_integral_tot (), object%get_error_tot ()
      select case (object%meta%type)
        case (PRC_DECAY)
          write (u, "(1x,A)", advance="no") "GeV"
        case (PRC_SCATTERING)
          write (u, "(1x,A)", advance="no") "fb "
        case default
          write (u, "(1x,A)", advance="no") " "
      end select
      if (object%get_integral_tot () /= 0) then
        err_percent = abs (100 &

```

```

        * object%get_error_tot () / object%get_integral_tot ()
    else
        err_percent = 0
    end if
    if (err_percent == 0) then
        write (u, "(1x,'(,F4.0,4x,')')") err_percent
    else if (err_percent < 0.1) then
        write (u, "(1x,'(,F7.3,1x,')')") err_percent
    else if (err_percent < 1) then
        write (u, "(1x,'(,F6.2,2x,')')") err_percent
    else if (err_percent < 10) then
        write (u, "(1x,'(,F5.1,3x,')')") err_percent
    else
        write (u, "(1x,'(,F4.0,4x,')')") err_percent
    end if
else
    write (u, "(A)") "[integral undefined]"
end if
end subroutine process_show

```

Finalizer. Explicitly iterate over all subobjects that may contain allocated pointers.

TODO wk 2018 (workaround): The finalizer for the `config_data` component is not called. The reason is that this deletes model data local to the process, but these could be referenced by pointers (flavor objects) from some persistent event record. Obviously, such side effects should be avoided, but this requires refactoring the event-handling procedures.

```

(Process: process: TBP)+≡
    procedure :: final => process_final

(Process: sub interfaces)+≡
    module subroutine process_final (process)
        class(process_t), intent(inout) :: process
    end subroutine process_final

(Process: procedures)+≡
    module subroutine process_final (process)
        class(process_t), intent(inout) :: process
        integer :: i
        call process%env%final ()
        if (allocated (process%component)) then
            do i = 1, size (process%component)
                call process%component(i)%final ()
            end do
        end if
        if (allocated (process%term)) then
            do i = 1, size (process%term)
                call process%term(i)%final ()
            end do
        end if
        call process%beam_config%final ()
        if (allocated (process%mci_entry)) then
            do i = 1, size (process%mci_entry)
                call process%mci_entry(i)%final ()
            end do
        end if
    end subroutine process_final

```

```

        end do
    end if
    if (allocated (process%pcm)) then
        call process%pcm%final ()
        deallocate (process%pcm)
    end if
end subroutine process_final

```

Process setup

Initialize a process. We need a process library `lib` and the process identifier `proc_id` (string). We will fetch the current run ID from the variable list `var_list`.

We collect all important data from the environment and store them in the appropriate places. OS data, model, and variable list are copied into `env` (true snapshot), also the process library (pointer only).

The `meta` subobject is initialized with process ID and attributes taken from the process library.

We initialize the `config` subobject with all data that are relevant for this run, using the settings from `env`. These data determine the MD5 sum for this run, which allows us to identify the setup and possibly skips in a later re-run.

We also allocate and initialize the embedded RNG factory. We take the seed from the `var_list`, and we should return the `var_list` to the caller with a new seed.

Finally, we allocate the process component manager `pcm`, which implements the chosen algorithm for process integration. The first task of the manager is to allocate the component array and to determine the component categories (e.g., Born/Virtual etc.).

TODO wk 2018: The `pcm` dispatcher should be provided by the caller, if we eventually want to eliminate dependencies on concrete `pcm_t` extensions.

Gfortran 7/8/9 bug, has to remain in the main module:

```

<Process: process: TBP>+≡
    procedure :: init => process_init

<Process: main procedures>≡
    subroutine process_init &
        (process, proc_id, lib, os_data, model, var_list, beam_structure)
        class(process_t), intent(out) :: process
        type(string_t), intent(in) :: proc_id
        type(process_library_t), intent(in), target :: lib
        type(os_data_t), intent(in) :: os_data
        class(model_t), intent(in), target :: model
        type(var_list_t), intent(inout), target, optional :: var_list
        type(beam_structure_t), intent(in), optional :: beam_structure
        integer :: next_rng_seed
        if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_init")
        associate &
            (meta => process%meta, env => process%env, config => process%config)
            call env%init &
                (model, lib, os_data, var_list, beam_structure)
            call meta%init &

```

```

        (proc_id, lib, env%get_var_list_ptr ())
    call config%init &
        (meta, env)
    call dispatch_rng_factory &
        (process%rng_factory, env%get_var_list_ptr (), next_rng_seed)
    call update_rng_seed_in_var_list (var_list, next_rng_seed)
    call dispatch_pcm &
        (process%pcm, config%process_def%is_nlo ())
    associate (pcm => process%pcm)
        call pcm%init (env, meta)
        call pcm%allocate_components (process%component, meta)
        call pcm%categorize_components (config)
    end associate
end associate
end subroutine process_init

```

30.4.6 Process component manager

The `pcm` (read: process-component manager) takes the responsibility of steering the actual algorithm of configuration and integration. Depending on the concrete type, different algorithms can be implemented.

The first version of this supports just two implementations: leading-order (tree-level) integration and event generation, and NLO (QCD/FKS subtraction). We thus can start with a single logical for steering the dispatcher.

TODO wk 2018: Eventually, we may eliminate all references to the extensions of `pcm_t` from this module and therefore move this outside the module as well. Gfortran 7/8/9 bug, has to be in the main module:

```

<Process: main procedures>+≡
subroutine dispatch_pcm (pcm, is_nlo)
    class(pcm_t), allocatable, intent(out) :: pcm
    logical, intent(in) :: is_nlo
    if (.not. is_nlo) then
        allocate (pcm_default_t :: pcm)
    else
        allocate (pcm_nlo_t :: pcm)
    end if
end subroutine dispatch_pcm

```

This step is performed after phase-space and core objects are done: collect all missing information and prepare the process component manager for the appropriate integration algorithm.

```

<Process: process: TBP>+≡
    procedure :: complete_pcm_setup => process_complete_pcm_setup

<Process: sub interfaces>+≡
    module subroutine process_complete_pcm_setup (process)
        class(process_t), intent(inout) :: process
    end subroutine process_complete_pcm_setup

<Process: procedures>+≡
    module subroutine process_complete_pcm_setup (process)
        class(process_t), intent(inout) :: process

```

```

    call process%pcm%complete_setup &
      (process%core_entry, process%component, process%env%get_model_ptr ())
  end subroutine process_complete_pcm_setup

```

30.4.7 Core management

Allocate cores (interface objects to matrix-element code).

The `dispatch_core` procedure is taken as an argument, so we do not depend on the implementation, and thus on the specific core types.

The `helicity_selection` object collects data that the matrix-element code needs for configuring the appropriate behavior.

After the cores have been allocated, and assuming the phs initial configuration has been done before, we proceed with computing the pcm internal data.

```

<Process: process: TBP>+≡
  procedure :: setup_cores => process_setup_cores

<Process: sub interfaces>+≡
  module subroutine process_setup_cores (process, dispatch_core, &
    helicity_selection, use_color_factors, has_beam_pol)
    class(process_t), intent(inout) :: process
    procedure(dispatch_core_proc) :: dispatch_core
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
  end subroutine process_setup_cores

<Process: procedures>+≡
  module subroutine process_setup_cores (process, dispatch_core, &
    helicity_selection, use_color_factors, has_beam_pol)
    class(process_t), intent(inout) :: process
    procedure(dispatch_core_proc) :: dispatch_core
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
    integer :: i
    associate (pcm => process%pcm)
      call pcm%allocate_cores (process%config, process%core_entry)
      do i = 1, size (process%core_entry)
        call dispatch_core (process%core_entry(i)%core, &
          process%core_entry(i)%core_def, &
          process%config%model, &
          helicity_selection, &
          process%config%qcd, &
          use_color_factors, &
          has_beam_pol)
        call process%core_entry(i)%configure &
          (process%env%get_lib_ptr (), process%meta%id)
        if (process%core_entry(i)%core%uses_blha ()) then
          call pcm%setup_blha (process%core_entry(i))
        end if
      end do
    end associate
  end subroutine process_setup_cores

```

```

(Process: interfaces)≡
  abstract interface
    subroutine dispatch_core_proc (core, core_def, model, &
      helicity_selection, qcd, use_color_factors, has_beam_pol)
    import
    class(prc_core_t), allocatable, intent(inout) :: core
    class(prc_core_def_t), intent(in) :: core_def
    class(model_data_t), intent(in), target, optional :: model
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    type(qcd_t), intent(in), optional :: qcd
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
  end subroutine dispatch_core_proc
end interface

```

Use the pcm to initialize the BLHA interface for each core which requires it.

```

(Process: process: TBP)+≡
  procedure :: prepare_blha_cores => process_prepare_blha_cores

(Process: sub interfaces)+≡
  module subroutine process_prepare_blha_cores (process)
    class(process_t), intent(inout), target :: process
  end subroutine process_prepare_blha_cores

(Process: procedures)+≡
  module subroutine process_prepare_blha_cores (process)
    class(process_t), intent(inout), target :: process
    integer :: i
    associate (pcm => process%pcm)
      do i = 1, size (process%core_entry)
        associate (core_entry => process%core_entry(i))
          if (core_entry%core%uses_blha ()) then
            pcm%uses_blha = .true.
            call pcm%prepare_blha_core (core_entry, process%config%model)
          end if
        end associate
      end do
    end associate
  end subroutine process_prepare_blha_cores

```

Create the BLHA interface data, using PCM for specific data, and write the BLHA contract file(s).

We take various configuration data and copy them to the `blha_master` record, which then creates and writes the contracts.

For assigning the QCD/EW coupling powers, we inspect the first process component only. The other parameters are taken as-is from the process environment variables.

```

(Process: process: TBP)+≡
  procedure :: create_blha_interface => process_create_blha_interface

(Process: sub interfaces)+≡
  module subroutine process_create_blha_interface (process)

```

```

        class(process_t), intent(inout) :: process
    end subroutine process_create_blha_interface

    (Process: procedures)+≡
    module subroutine process_create_blha_interface (process)
        class(process_t), intent(inout) :: process
        integer :: alpha_power, alphas_power
        integer :: openloops_phs_tolerance, openloops_stability_log
        logical :: use_cms
        type(string_t) :: ew_scheme, correction_type
        type(string_t) :: openloops_extra_cmd, openloops_allowed_libs
        type(blha_master_t) :: blha_master
        integer, dimension(:,,:), allocatable :: flv_born, flv_real
        if (process%pcm%uses_blha) then
            call collect_configuration_parameters (process%get_var_list_ptr ())
            call process%component(1)%config%get_coupling_powers &
                (alpha_power, alphas_power)
            associate (pcm => process%pcm)
                call pcm%set_blha_methods (blha_master, process%get_var_list_ptr ())
                call blha_master%set_ew_scheme (ew_scheme)
                call blha_master%allocate_config_files ()
                call blha_master%set_correction_type (correction_type)
                call blha_master%setup_additional_features ( &
                    openloops_phs_tolerance, &
                    use_cms, &
                    openloops_stability_log, &
                    extra_cmd = openloops_extra_cmd, &
                    allowed_libs = openloops_allowed_libs, &
                    beam_structure = process%env%get_beam_structure ())
                call pcm%get_blha_flv_states (process%core_entry, flv_born, flv_real)
                call blha_master%set_photon_characteristics (flv_born, process%config%n_in)
                call blha_master%generate (process%meta%id, &
                    process%config%model, process%config%n_in, &
                    alpha_power, alphas_power, &
                    flv_born, flv_real)
                call blha_master%write_olp (process%meta%id)
            end associate
        end if
    contains
        subroutine collect_configuration_parameters (var_list)
            type(var_list_t), intent(in) :: var_list
            openloops_phs_tolerance = &
                var_list%get_ival (var_str ("openloops_phs_tolerance"))
            openloops_stability_log = &
                var_list%get_ival (var_str ("openloops_stability_log"))
            use_cms = &
                var_list%get_lval (var_str ("?openloops_use_cms"))
            ew_scheme = &
                var_list%get_sval (var_str ("$blha_ew_scheme"))
            correction_type = &
                var_list%get_sval (var_str ("$nlo_correction_type"))
            openloops_extra_cmd = &
                var_list%get_sval (var_str ("$openloops_extra_cmd"))
            openloops_allowed_libs = &
                var_list%get_sval (var_str ("$openloops_allowed_libs"))

```

```

    end subroutine collect_configuration_parameters
end subroutine process_create_blha_interface

```

Initialize the process components, one by one. We require templates for the mci (integrator) and phs_config (phase-space) configuration data.

The `active` flag is set if the component has an associated matrix element, so we can compute it. The case of no core is a unit-test case.

The specifics depend on the algorithm and are delegated to the pcm process-component manager.

The optional `phs_config` overrides a pre-generated config array (for unit test).

```

(Process: process: TBP)+≡
  procedure :: init_components => process_init_components

(Process: sub interfaces)+≡
  module subroutine process_init_components (process, phs_config)
    class(process_t), intent(inout), target :: process
    class(phs_config_t), allocatable, intent(in), optional :: phs_config
  end subroutine process_init_components

(Process: procedures)+≡
  module subroutine process_init_components (process, phs_config)
    class(process_t), intent(inout), target :: process
    class(phs_config_t), allocatable, intent(in), optional :: phs_config
    integer :: i, i_core
    class(prc_core_t), pointer :: core
    logical :: active
    associate (pcm => process%pcm)
      do i = 1, pcm%n_components
        i_core = pcm%get_i_core(i)
        if (i_core > 0) then
          core => process%get_core_ptr (i_core)
          active = core%has_matrix_element ()
        else
          active = .true.
        end if
      end select type (pcm => process%pcm)
      type is (pcm_nlo_t)
        if (pcm%use_real_partition .and. .not. pcm%use_real_singular) then
          if (pcm%component_type(i) == COMP_REAL_SING) then
            active = .false.
          end if
        end if
      end select
    end select
    if (present (phs_config)) then
      call pcm%init_component (process%component(i), &
        i, &
        active, &
        phs_config, &
        process%env, process%meta, process%config)
    else
      call pcm%init_component (process%component(i), &
        i, &
        active, &

```



```

        process%phs_entry(pcm%i_phs_config(i))%phs_config, &
        process%env, process%meta, process%config)
    end if
end do
end associate
end subroutine process_init_components

```

If process components have turned out to be inactive, this has to be recorded in the `meta` block. Delegate to the `pcm`.

```

(Process: process: TBP)+≡
    procedure :: record_inactive_components => process_record_inactive_components

(Process: sub interfaces)+≡
    module subroutine process_record_inactive_components (process)
        class(process_t), intent(inout) :: process
    end subroutine process_record_inactive_components

(Process: procedures)+≡
    module subroutine process_record_inactive_components (process)
        class(process_t), intent(inout) :: process
        associate (pcm => process%pcm)
            call pcm%record_inactive_components (process%component, process%meta)
        end associate
    end subroutine process_record_inactive_components

```

Determine the process terms for each process component.

```

(Process: process: TBP)+≡
    procedure :: setup_terms => process_setup_terms

(Process: sub interfaces)+≡
    module subroutine process_setup_terms (process, with_beams)
        class(process_t), intent(inout), target :: process
        logical, intent(in), optional :: with_beams
    end subroutine process_setup_terms

(Process: procedures)+≡
    module subroutine process_setup_terms (process, with_beams)
        class(process_t), intent(inout), target :: process
        logical, intent(in), optional :: with_beams
        class(model_data_t), pointer :: model
        integer :: i, j, k, i_term
        integer, dimension(:), allocatable :: n_entry
        integer :: n_components, n_tot
        integer :: i_sub
        type(string_t) :: subtraction_method
        class(prc_core_t), pointer :: core => null ()
        logical :: setup_subtraction_component, singular_real
        logical :: requires_spin_correlations
        integer :: nlo_type_to_fetch, n_emitters
        i_sub = 0
        model => process%config%model
        n_components = process%meta%n_components
        allocate (n_entry (n_components), source = 0)
        do i = 1, n_components
            associate (component => process%component(i))

```

```

        if (component%active) then
            n_entry(i) = 1
            if (component%get_nlo_type () == NLO_REAL) then
                select type (pcm => process%pcm)
                    type is (pcm_nlo_t)
                        if (pcm%component_type(i) /= COMP_REAL_FIN) &
                            n_entry(i) = n_entry(i) + pcm%region_data%get_n_phs ()
                        end select
                    end select
                end if
            end if
        end associate
    end do
    n_tot = sum (n_entry)
    allocate (process%term (n_tot))
    k = 0
    if (process%is_nlo_calculation ()) then
        i_sub = process%component(1)%config%get_associated_subtraction ()
        subtraction_method = process%component(i_sub)%config%get_me_method ()
        if (debug_on) call msg_debug2 &
            (D_PROCESS_INTEGRATION, "process_setup_terms: ", subtraction_method)
    end if

    do i = 1, n_components
        associate (component => process%component(i))
            if (.not. component%active) cycle
            allocate (component%i_term (n_entry(i)))
            do j = 1, n_entry(i)
                select type (pcm => process%pcm)
                    type is (pcm_nlo_t)
                        singular_real = component%get_nlo_type () == NLO_REAL &
                            .and. pcm%component_type(i) /= COMP_REAL_FIN
                        class default
                            singular_real = .false.
                        end select
                        setup_subtraction_component = singular_real .and. j == n_entry(i)
                        i_term = k + j
                        component%i_term(j) = i_term
                        if (singular_real) then
                            process%term(i_term)%i_sub = k + n_entry(i)
                        else
                            process%term(i_term)%i_sub = 0
                        end if
                        if (setup_subtraction_component) then
                            select type (pcm => process%pcm)
                                class is (pcm_nlo_t)
                                    process%term(i_term)%i_core = pcm%i_core(pcm%i_sub)
                                end select
                            else
                                process%term(i_term)%i_core = process%pcm%get_i_core(i)
                            end if
                        end if

                        if (process%term(i_term)%i_core == 0) then
                            call msg_bug ("Process '" // char (process%get_id ()) &
                                // "': core not found!")
                        end if
                    end do
                end do
            end associate
        end do
    end do

```

```

end if
core => process%get_core_term (i_term)
if (i_sub > 0) then
  select type (pcm => process%pcm)
  type is (pcm_nlo_t)
    requires_spin_correlations = &
      pcm%region_data%requires_spin_correlations ()
    n_emitters = pcm%region_data%get_n_emitters_sc ()
  class default
    requires_spin_correlations = .false.
    n_emitters = 0
  end select
if (requires_spin_correlations) then
  call process%term(i_term)%init ( &
    i_term, i, j, core, model, &
    nlo_type = component%config%get_nlo_type (), &
    use_beam_pol = with_beams, &
    subtraction_method = subtraction_method, &
    has_pdf = process%pcm%has_pdf, &
    n_emitters = n_emitters)
else
  call process%term(i_term)%init ( &
    i_term, i, j, core, model, &
    nlo_type = component%config%get_nlo_type (), &
    use_beam_pol = with_beams, &
    subtraction_method = subtraction_method, &
    has_pdf = process%pcm%has_pdf)
end if
else
  call process%term(i_term)%init ( &
    i_term, i, j, core, model, &
    nlo_type = component%config%get_nlo_type (), &
    use_beam_pol = with_beams, &
    has_pdf = process%pcm%has_pdf)
end if
end do
end associate
k = k + n_entry(i)
end do
process%config%n_terms = n_tot
end subroutine process_setup_terms

```

Initialize the beam setup. This is the trivial version where the incoming state of the matrix element coincides with the initial state of the process. For a scattering process, we need the c.m. energy, all other variables are set to their default values (no polarization, lab frame and c.m. frame coincide, etc.)

We assume that all components consistently describe a scattering process, i.e., two incoming particles.

Note: The current layout of the `beam_data_t` record requires that the flavor for each beam is unique. For processes with multiple flavors in the initial state, one has to set up beams explicitly. This restriction could be removed by extending the code in the `beams` module.

(Process: process: TBP)+≡

```

    procedure :: setup_beams_sqrts => process_setup_beams_sqrts
  (Process: sub interfaces)+≡
    module subroutine process_setup_beams_sqrts &
      (process, sqrts, beam_structure, i_core)
      class(process_t), intent(inout) :: process
      real(default), intent(in) :: sqrts
      type(beam_structure_t), intent(in), optional :: beam_structure
      integer, intent(in), optional :: i_core
    end subroutine process_setup_beams_sqrts

  (Process: procedures)+≡
    module subroutine process_setup_beams_sqrts &
      (process, sqrts, beam_structure, i_core)
      class(process_t), intent(inout) :: process
      real(default), intent(in) :: sqrts
      type(beam_structure_t), intent(in), optional :: beam_structure
      integer, intent(in), optional :: i_core
      type(pdg_array_t), dimension(:,,:), allocatable :: pdg_in
      integer, dimension(2) :: pdg_scattering
      type(flavor_t), dimension(2) :: flv_in
      integer :: i, i0, ic
      allocate (pdg_in (2, process%meta%n_components))
      i0 = 0
      do i = 1, process%meta%n_components
        if (process%component(i)%active) then
          if (present (i_core)) then
            ic = i_core
          else
            ic = process%pcm%get_i_core (i)
          end if
          associate (core => process%core_entry(ic)%core)
            pdg_in(:,i) = core%data%get_pdg_in ()
          end associate
          if (i0 == 0) i0 = i
        end if
      end do
      do i = 1, process%meta%n_components
        if (.not. process%component(i)%active) then
          pdg_in(:,i) = pdg_in(:,i0)
        end if
      end do
      if (all (pdg_in%get_length () == 1) .and. &
        all (pdg_in(1,:) == pdg_in(1,i0)) .and. &
        all (pdg_in(2,:) == pdg_in(2,i0))) then
        pdg_scattering(:) = pdg_in(:,i0)%get (1)
        call flv_in%init (pdg_scattering, process%config%model)
        call process%beam_config%init_scattering (flv_in, sqrts, beam_structure)
      else
        call msg_fatal ("Setting up process '" // char (process%meta%id) // "':", &
          [var_str (" -----"), &
            var_str ("Inconsistent initial state. This happens if either "), &
            var_str ("several processes with non-matching initial states "), &
            var_str ("have been added, or for a single process with an "), &
            var_str ("initial state flavor sum. In that case, please set beams "), &

```

```

        var_str ("explicitly [singling out a flavor / structure function.]"))
    end if
end subroutine process_setup_beams_sqrts

```

This is the version that applies to decay processes. The energy is the particle mass, hence no extra argument.

```

(Process: process: TBP)+≡
    procedure :: setup_beams_decay => process_setup_beams_decay
(Process: sub interfaces)+≡
    module subroutine process_setup_beams_decay &
        (process, rest_frame, beam_structure, i_core)
        class(process_t), intent(inout), target :: process
        logical, intent(in), optional :: rest_frame
        type(beam_structure_t), intent(in), optional :: beam_structure
        integer, intent(in), optional :: i_core
    end subroutine process_setup_beams_decay
(Process: procedures)+≡
    module subroutine process_setup_beams_decay &
        (process, rest_frame, beam_structure, i_core)
        class(process_t), intent(inout), target :: process
        logical, intent(in), optional :: rest_frame
        type(beam_structure_t), intent(in), optional :: beam_structure
        integer, intent(in), optional :: i_core
        type(pdg_array_t), dimension(:,,:), allocatable :: pdg_in
        integer, dimension(1) :: pdg_decay
        type(flavor_t), dimension(1) :: flv_in
        integer :: i, i0, ic
        allocate (pdg_in (1, process%meta%n_components))
        i0 = 0
        do i = 1, process%meta%n_components
            if (process%component(i)%active) then
                if (present (i_core)) then
                    ic = i_core
                else
                    ic = process%pcm%get_i_core (i)
                end if
                associate (core => process%core_entry(ic)%core)
                    pdg_in(:,i) = core%data%get_pdg_in ()
                end associate
                if (i0 == 0) i0 = i
            end if
        end do
        do i = 1, process%meta%n_components
            if (.not. process%component(i)%active) then
                pdg_in(:,i) = pdg_in(:,i0)
            end if
        end do
        if (all (pdg_in%get_length () == 1) &
            .and. all (pdg_in(1,:) == pdg_in(1,i0))) then
            pdg_decay(:) = pdg_in(:,i0)%get (1)
            call flv_in%init (pdg_decay, process%config%model)
            call process%beam_config%init_decay (flv_in, rest_frame, beam_structure)
        else

```

```

        call msg_fatal ("Setting up decay '" &
            // char (process%meta%id) // "' : decaying particle not unique")
    end if
end subroutine process_setup_beams_decay

```

We have to make sure that the masses of the various flavors in a given position in the particle string coincide.

```

(Process: process: TBP)+≡
    procedure :: check_masses => process_check_masses

(Process: sub interfaces)+≡
    module subroutine process_check_masses (process)
        class(process_t), intent(in) :: process
    end subroutine process_check_masses

(Process: procedures)+≡
    module subroutine process_check_masses (process)
        class(process_t), intent(in) :: process
        type(flavor_t), dimension(:), allocatable :: flv
        real(default), dimension(:), allocatable :: mass
        integer :: i, j
        integer :: i_component
        class(prc_core_t), pointer :: core
        do i = 1, process%get_n_terms ()
            i_component = process%term(i)%i_component
            if (.not. process%component(i_component)%active) cycle
            core => process%get_core_term (i)
            associate (data => core%data)
                allocate (flv (data%n_flv), mass (data%n_flv))
                do j = 1, data%n_in + data%n_out
                    call flv%init (data%flv_state(j,:), process%config%model)
                    mass = flv%get_mass ()
                    if (any (.not. nearly_equal(mass, mass(1)))) then
                        call msg_fatal ("Process '" // char (process%meta%id) // "' : " &
                            // "mass values in flavor combination do not coincide. ")
                    end if
                end do
                deallocate (flv, mass)
            end associate
        end do
    end subroutine process_check_masses

```

Set up index mapping for `region_data` for singular regions equivalent w.r.t. their amplitudes. Has to be called after `region_data` AND the `core` are fully set up. For processes with structure function, subprocesses which lead to the same amplitude for the hard interaction can differ if structure functions are applied. In this case we remap flavor structures to themselves if the equivalent hard interaction flavor structure has no identical initial state.

```

(Process: process: TBP)+≡
    procedure :: optimize_nlo_singular_regions => &
        process_optimize_nlo_singular_regions

(Process: sub interfaces)+≡
    module subroutine process_optimize_nlo_singular_regions (process)

```

```

        class(process_t), intent(inout) :: process
    end subroutine process_optimize_nlo_singular_regions

(Process: procedures)+≡
module subroutine process_optimize_nlo_singular_regions (process)
    class(process_t), intent(inout) :: process
    class(prc_core_t), pointer :: core, core_sub
    integer, dimension(:), allocatable :: eqv_flv_index_born
    integer, dimension(:), allocatable :: eqv_flv_index_real
    integer, dimension(:,:), allocatable :: flv_born, flv_real
    integer :: i_flv, i_flv2, n_in, i
    integer :: i_component, i_core, i_core_sub
    logical :: fetched_born, fetched_real
    logical :: optimize
    fetched_born = .false.; fetched_real = .false.
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
        optimize = pcm%settings%reuse_amplitudes_fks
        if (optimize) then
            do i_component = 1, pcm%n_components
                i_core = pcm%get_i_core(i_component)
                core => process%get_core_ptr (i_core)
                if (.not. core%data_known) cycle
                associate (data => core%data)
                    if (pcm%nlo_type_core(i_core) == NLO_REAL .and. &
                        .not. pcm%component_type(i_component) == COMP_SUB) then
                        if (allocated (core%data%eqv_flv_index)) then
                            eqv_flv_index_real = core%get_equivalent_flv_index ()
                            fetched_real = .true.
                        end if
                        i_core_sub = pcm%get_i_core (pcm%i_sub)
                        core_sub => process%get_core_ptr (i_core_sub)
                        if (allocated (core_sub%data%eqv_flv_index)) then
                            eqv_flv_index_born = core_sub%get_equivalent_flv_index ()
                            fetched_born = .true.
                        end if
                        if (fetched_born .and. fetched_real) exit
                    end if
                end associate
            end do
            if (.not. fetched_born .or. .not. fetched_real) then
                call msg_warning('Failed to fetch flavor equivalence indices. &
                    &Disabling singular region optimization')
                optimize = .false.
                eqv_flv_index_born = [(i, i = 1, pcm%region_data%n_flv_born)]
                eqv_flv_index_real = [(i, i = 1, pcm%region_data%n_flv_real)]
            end if
            if (optimize .and. pcm%has_pdfs) then
                flv_born = pcm%region_data%get_flv_states_born ()
                flv_real = pcm%region_data%get_flv_states_real ()
                n_in = pcm%region_data%n_in
                do i_flv = 1, size (eqv_flv_index_born)
                    do i_flv2 = 1, i_flv
                        if (any (flv_born(1:n_in, eqv_flv_index_born(i_flv)) /= &
                            flv_born(1:n_in, i_flv))) then

```

```

        eqv_flv_index_born(i_flv) = i_flv
        exit
    end if
end do
end do
do i_flv = 1, size (eqv_flv_index_real)
    do i_flv2 = 1, i_flv
        if (any (flv_real(1:n_in, eqv_flv_index_real(i_flv)) /= &
            flv_real(1:n_in, i_flv))) then
            eqv_flv_index_real(i_flv) = i_flv
            exit
        end if
    end do
end do
end if
else
    eqv_flv_index_born = [(i, i = 1, pcm%region_data%n_flv_born)]
    eqv_flv_index_real = [(i, i = 1, pcm%region_data%n_flv_real)]
end if
pcm%region_data%eqv_flv_index_born = eqv_flv_index_born
pcm%region_data%eqv_flv_index_real = eqv_flv_index_real
call pcm%region_data%find_eqv_regions (optimize)
end select
end subroutine process_optimize_nlo_singular_regions

```

For some structure functions we need to get the list of initial state flavors. This is a two-dimensional array. The first index is the beam index, the second index is the component index. Each array element is itself a PDG array object, which consists of the list of incoming PDG values for this beam and component.

```

(Process: process: TBP)+≡
    procedure :: get_pdg_in => process_get_pdg_in

(Process: sub interfaces)+≡
    module subroutine process_get_pdg_in (process, pdg_in)
        class(process_t), intent(in), target :: process
        type(pdg_array_t), dimension(:, :), allocatable, intent(out) :: pdg_in
    end subroutine process_get_pdg_in

(Process: procedures)+≡
    module subroutine process_get_pdg_in (process, pdg_in)
        class(process_t), intent(in), target :: process
        type(pdg_array_t), dimension(:, :), allocatable, intent(out) :: pdg_in
        integer :: i, i_core
        allocate (pdg_in (process%config%n_in, process%meta%n_components))
        do i = 1, process%meta%n_components
            if (process%component(i)%active) then
                i_core = process%pcm%get_i_core (i)
                associate (core => process%core_entry(i_core)%core)
                    pdg_in(:, i) = core%data%get_pdg_in ()
                end associate
            end if
        end do
    end subroutine process_get_pdg_in

```


The phase-space configuration object, in case we need it separately.

```

(Process: process: TBP)+≡
    procedure :: get_phs_config => process_get_phs_config

(Process: sub interfaces)+≡
    module function process_get_phs_config &
        (process, i_component) result (phs_config)
        class(phs_config_t), pointer :: phs_config
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_component
    end function process_get_phs_config

(Process: procedures)+≡
    module function process_get_phs_config &
        (process, i_component) result (phs_config)
        class(phs_config_t), pointer :: phs_config
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_component
        if (allocated (process%component)) then
            if (process%component(i_component)%active) then
                phs_config => process%component(i_component)%phs_config
            else
                phs_config => null ()
            end if
        else
            phs_config => null ()
        end if
    end function process_get_phs_config

```

The resonance history set can be extracted from the phase-space configuration. However, this is only possible if the default phase-space method (wood) has been chosen. If `include_trivial` is set, we include the resonance history with no resonances in the set.

```

(Process: process: TBP)+≡
    procedure :: extract_resonance_history_set &
        => process_extract_resonance_history_set

(Process: sub interfaces)+≡
    module subroutine process_extract_resonance_history_set &
        (process, res_set, include_trivial, i_component)
        class(process_t), intent(in), target :: process
        type(resonance_history_set_t), intent(out) :: res_set
        logical, intent(in), optional :: include_trivial
        integer, intent(in), optional :: i_component
    end subroutine process_extract_resonance_history_set

(Process: procedures)+≡
    module subroutine process_extract_resonance_history_set &
        (process, res_set, include_trivial, i_component)
        class(process_t), intent(in), target :: process
        type(resonance_history_set_t), intent(out) :: res_set
        logical, intent(in), optional :: include_trivial
        integer, intent(in), optional :: i_component
        integer :: i
        i = 1; if (present (i_component)) i = i_component

```

```

if (process%component(i)%active) then
  select type (phs_config => process%get_phs_config (i))
  class is (phs_wood_config_t)
    call phs_config%extract_resonance_history_set &
      (res_set, include_trivial)
  class default
    call msg_error ("process '" // char (process%get_id ()) &
      // "' : extract resonance histories: phase-space method must be &
      &'wood'. No resonances can be determined.")
  end select
end if
end subroutine process_extract_resonance_history_set

```

Initialize from a complete beam setup. If the beam setup does not apply directly to the process, choose a fallback option as a straight scattering or decay process.

```

(Process: process: TBP)+≡
  procedure :: setup_beams_beam_structure => process_setup_beams_beam_structure

(Process: sub interfaces)+≡
  module subroutine process_setup_beams_beam_structure &
    (process, beam_structure, sqrts, decay_rest_frame)
    class(process_t), intent(inout) :: process
    type(beam_structure_t), intent(in) :: beam_structure
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: decay_rest_frame
  end subroutine process_setup_beams_beam_structure

(Process: procedures)+≡
  module subroutine process_setup_beams_beam_structure &
    (process, beam_structure, sqrts, decay_rest_frame)
    class(process_t), intent(inout) :: process
    type(beam_structure_t), intent(in) :: beam_structure
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: decay_rest_frame
    integer :: n_in
    logical :: applies
    n_in = process%get_n_in ()
    call beam_structure%check_against_n_in (process%get_n_in (), applies)
    if (applies) then
      call process%beam_config%init_beam_structure &
        (beam_structure, sqrts, process%get_model_ptr (), decay_rest_frame)
    else if (n_in == 2) then
      call process%setup_beams_sqrts (sqrts, beam_structure)
    else
      call process%setup_beams_decay (decay_rest_frame, beam_structure)
    end if
  end subroutine process_setup_beams_beam_structure

```

Notify the user about beam setup.

```

(Process: process: TBP)+≡
  procedure :: beams_startup_message => process_beams_startup_message

(Process: sub interfaces)+≡
  module subroutine process_beams_startup_message &

```

```

        (process, unit, beam_structure)
        class(process_t), intent(in) :: process
        integer, intent(in), optional :: unit
        type(beam_structure_t), intent(in), optional :: beam_structure
    end subroutine process_beams_startup_message

<Process: procedures>+≡
    module subroutine process_beams_startup_message &
        (process, unit, beam_structure)
        class(process_t), intent(in) :: process
        integer, intent(in), optional :: unit
        type(beam_structure_t), intent(in), optional :: beam_structure
        call process%beam_config%startup_message (unit, beam_structure)
    end subroutine process_beams_startup_message

```

Initialize phase-space configuration by reading out the environment variables. We return the rebuild flags and store parameters in the blocks `phs_par` and `mapping_defs`.

The phase-space configuration object(s) are allocated by `pcm`.

```

<Process: process: TBP>+≡
    procedure :: init_phs_config => process_init_phs_config

<Process: sub interfaces>+≡
    module subroutine process_init_phs_config (process)
        class(process_t), intent(inout) :: process
    end subroutine process_init_phs_config

<Process: procedures>+≡
    module subroutine process_init_phs_config (process)
        class(process_t), intent(inout) :: process

        type(var_list_t), pointer :: var_list
        type(phs_parameters_t) :: phs_par
        type(mapping_defaults_t) :: mapping_defs

        var_list => process%env%get_var_list_ptr ()

        phs_par%m_threshold_s = &
            var_list%get_rval (var_str ("phs_threshold_s"))
        phs_par%m_threshold_t = &
            var_list%get_rval (var_str ("phs_threshold_t"))
        phs_par%off_shell = &
            var_list%get_ival (var_str ("phs_off_shell"))
        phs_par%keep_nonresonant = &
            var_list%get_lval (var_str ("?phs_keep_nonresonant"))
        phs_par%t_channel = &
            var_list%get_ival (var_str ("phs_t_channel"))

        mapping_defs%energy_scale = &
            var_list%get_rval (var_str ("phs_e_scale"))
        mapping_defs%invariant_mass_scale = &
            var_list%get_rval (var_str ("phs_m_scale"))
        mapping_defs%momentum_transfer_scale = &
            var_list%get_rval (var_str ("phs_q_scale"))
        mapping_defs%step_mapping = &

```

```

        var_list%get_lval (var_str ("?phs_step_mapping"))
mapping_defs%step_mapping_exp = &
        var_list%get_lval (var_str ("?phs_step_mapping_exp"))
mapping_defs%enable_s_mapping = &
        var_list%get_lval (var_str ("?phs_s_mapping"))

associate (pcm => process%pcm)
    call pcm%init_phs_config (process%phs_entry, &
        process%meta, process%env, phs_par, mapping_defs)
end associate

end subroutine process_init_phs_config

```

We complete the kinematics configuration after the beam setup, but before we configure the chain of structure functions. The reason is that we need the total energy `sqrts` for the kinematics, but the structure-function setup requires the number of channels, which depends on the kinematics configuration. For instance, the kinematics module may return the need for parameterizing an s-channel resonance.

```

(Process: process: TBP)+≡
    procedure :: configure_phs => process_configure_phs

(Process: sub interfaces)+≡
    module subroutine process_configure_phs (process, rebuild, &
        ignore_mismatch, combined_integration, subdir)
        class(process_t), intent(inout) :: process
        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        logical, intent(in), optional :: combined_integration
        type(string_t), intent(in), optional :: subdir
    end subroutine process_configure_phs

(Process: procedures)+≡
    module subroutine process_configure_phs (process, rebuild, &
        ignore_mismatch, combined_integration, subdir)
        class(process_t), intent(inout) :: process
        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        logical, intent(in), optional :: combined_integration
        type(string_t), intent(in), optional :: subdir
        real(default) :: sqrts
        integer :: i, i_born, nlo_type
        class(phs_config_t), pointer :: phs_config_born
        sqrts = process%get_sqrts ()
        do i = 1, process%meta%n_components
            associate (component => process%component(i))
                if (component%active) then
                    select type (pcm => process%pcm)
                    type is (pcm_default_t)
                        call component%configure_phs (sqrts, process%beam_config, &
                            rebuild, ignore_mismatch, subdir)
                    class is (pcm_nlo_t)
                        nlo_type = component%config%get_nlo_type ()
                        select case (nlo_type)

```

```

        case (BORN, NLO_VIRTUAL, NLO_SUBTRACTION)
            call component%configure_phs (sqrt, process%beam_config, &
                rebuild, ignore_mismatch, subdir)
            call check_and_extend_phs (component)
        case (NLO_REAL, NLO_MISMATCH, NLO_DGLAP)
            i_born = component%config%get_associated_born ()
            if (pcm%component_type(i) /= COMP_REAL_FIN) &
                call check_and_extend_phs (component)
            call process%component(i_born)%get_phs_config &
                (phs_config_born)
            select type (config => component%phs_config)
            type is (phs_fks_config_t)
                select type (phs_config_born)
                type is (phs_wood_config_t)
                    config%md5sum_born_config = &
                        phs_config_born%md5sum_phs_config
                    call config%set_born_config (phs_config_born)
                    call config%set_mode (component%config%get_nlo_type ())
                end select
            end select
            call component%configure_phs (sqrt, &
                process%beam_config, rebuild, ignore_mismatch, subdir)
        end select
    class default
        call msg_bug ("process_configure_phs: unsupported PCM type")
    end select
end if
end associate
end do
contains
    subroutine check_and_extend_phs (component)
        type(process_component_t), intent(inout) :: component
        if (combined_integration) then
            select type (phs_config => component%phs_config)
            class is (phs_wood_config_t)
                phs_config%is_combined_integration = .true.
                call phs_config%increase_n_par ()
            end select
        end if
    end subroutine check_and_extend_phs
end subroutine process_configure_phs

```

(Process: process: TBP)+≡
 procedure :: print_phs_startup_message => process_print_phs_startup_message

(Process: sub interfaces)+≡
 module subroutine process_print_phs_startup_message (process)
 class(process_t), intent(in) :: process
 end subroutine process_print_phs_startup_message

(Process: procedures)+≡
 module subroutine process_print_phs_startup_message (process)
 class(process_t), intent(in) :: process
 integer :: i_component
 do i_component = 1, process%meta%n_components

```

        associate (component => process%component(i_component))
            if (component%active) then
                call component%phs_config%startup_message ()
            end if
        end associate
    end do
end subroutine process_print_phs_startup_message

```

Insert the structure-function configuration data. First allocate the storage, then insert data one by one. The third procedure declares a mapping (of the MC input parameters) for a specific channel and structure-function combination.

We take the number of channels from the corresponding entry in the `config_data` section.

Otherwise, these are simple wrapper routines. The extra level in the call tree may allow for simple addressing of multiple concurrent beam configurations, not implemented currently.

If we do not want structure functions, we simply do not call those procedures.

```

(Process: process: TBP)+≡
    procedure :: init_sf_chain => process_init_sf_chain
    generic :: set_sf_channel => set_sf_channel_single
    procedure :: set_sf_channel_single => process_set_sf_channel
    generic :: set_sf_channel => set_sf_channel_array
    procedure :: set_sf_channel_array => process_set_sf_channel_array

(Process: sub interfaces)+≡
    module subroutine process_init_sf_chain (process, sf_config, sf_trace_file)
        class(process_t), intent(inout) :: process
        type(sf_config_t), dimension(:), intent(in) :: sf_config
        type(string_t), intent(in), optional :: sf_trace_file
    end subroutine process_init_sf_chain
    module subroutine process_set_sf_channel (process, c, sf_channel)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: c
        type(sf_channel_t), intent(in) :: sf_channel
    end subroutine process_set_sf_channel
    module subroutine process_set_sf_channel_array (process, sf_channel)
        class(process_t), intent(inout) :: process
        type(sf_channel_t), dimension(:), intent(in) :: sf_channel
    end subroutine process_set_sf_channel_array

(Process: procedures)+≡
    module subroutine process_init_sf_chain (process, sf_config, sf_trace_file)
        class(process_t), intent(inout) :: process
        type(sf_config_t), dimension(:), intent(in) :: sf_config
        type(string_t), intent(in), optional :: sf_trace_file
        type(string_t) :: file
        if (present (sf_trace_file)) then
            if (sf_trace_file /= "") then
                file = sf_trace_file
            else
                file = process%get_id () // "_sftrace.dat"
            end if
        end if
        call process%beam_config%init_sf_chain (sf_config, file)
    else

```

```

        call process%beam_config%init_sf_chain (sf_config)
    end if
end subroutine process_init_sf_chain

module subroutine process_set_sf_channel (process, c, sf_channel)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: c
    type(sf_channel_t), intent(in) :: sf_channel
    call process%beam_config%set_sf_channel (c, sf_channel)
end subroutine process_set_sf_channel

module subroutine process_set_sf_channel_array (process, sf_channel)
    class(process_t), intent(inout) :: process
    type(sf_channel_t), dimension(:), intent(in) :: sf_channel
    integer :: c
    call process%beam_config%allocate_sf_channels (size (sf_channel))
    do c = 1, size (sf_channel)
        call process%beam_config%set_sf_channel (c, sf_channel(c))
    end do
end subroutine process_set_sf_channel_array

```

Notify about the structure-function setup.

```

(Process: process: TBP)+≡
    procedure :: sf_startup_message => process_sf_startup_message

(Process: sub interfaces)+≡
    module subroutine process_sf_startup_message (process, sf_string, unit)
        class(process_t), intent(in) :: process
        type(string_t), intent(in) :: sf_string
        integer, intent(in), optional :: unit
    end subroutine process_sf_startup_message

(Process: procedures)+≡
    module subroutine process_sf_startup_message (process, sf_string, unit)
        class(process_t), intent(in) :: process
        type(string_t), intent(in) :: sf_string
        integer, intent(in), optional :: unit
        call process%beam_config%sf_startup_message (sf_string, unit)
    end subroutine process_sf_startup_message

```

As soon as both the kinematics configuration and the structure-function setup are complete, we match parameterizations (channels) for both. The matching entries are (re)set in the component phase-space configuration, while the structure-function configuration is left intact.

```

(Process: process: TBP)+≡
    procedure :: collect_channels => process_collect_channels

(Process: sub interfaces)+≡
    module subroutine process_collect_channels (process, coll)
        class(process_t), intent(inout) :: process
        type(phs_channel_collection_t), intent(inout) :: coll
    end subroutine process_collect_channels

```

```

(Process: procedures)+≡
module subroutine process_collect_channels (process, coll)
  class(process_t), intent(inout) :: process
  type(phs_channel_collection_t), intent(inout) :: coll
  integer :: i
  do i = 1, process%meta%n_components
    associate (component => process%component(i))
      if (component%active) &
        call component%collect_channels (coll)
    end associate
  end do
end subroutine process_collect_channels

```

Independently, we should be able to check if any component does not contain phase-space parameters. Such a process can only be integrated if there are structure functions.

```

(Process: process: TBP)+≡
  procedure :: contains_trivial_component => process_contains_trivial_component

```

```

(Process: sub interfaces)+≡
  module function process_contains_trivial_component (process) result (flag)
    class(process_t), intent(in) :: process
    logical :: flag
  end function process_contains_trivial_component

```

```

(Process: procedures)+≡
module function process_contains_trivial_component (process) result (flag)
  class(process_t), intent(in) :: process
  logical :: flag
  integer :: i
  flag = .true.
  do i = 1, process%meta%n_components
    associate (component => process%component(i))
      if (component%active) then
        if (component%get_n_phs_par () == 0) return
      end if
    end associate
  end do
  flag = .false.
end function process_contains_trivial_component

```

```

(Process: process: TBP)+≡
  procedure :: get_master_component => process_get_master_component

```

```

(Process: sub interfaces)+≡
  module function process_get_master_component &
    (process, i_mci) result (i_component)
    integer :: i_component
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
  end function process_get_master_component

```

```

(Process: procedures)+≡
  module function process_get_master_component &
    (process, i_mci) result (i_component)

```



```

integer :: i_component
class(process_t), intent(in) :: process
integer, intent(in) :: i_mci
integer :: i
i_component = 0
do i = 1, size (process%component)
  if (process%component(i)%i_mci == i_mci) then
    i_component = i
    return
  end if
end do
end function process_get_master_component

```

Determine the MC parameter set structure and the MCI configuration for each process component. We need data from the structure-function and phase-space setup, so those should be complete before this is called. We also make a random-number generator instance for each MCI group.

```

(Process: process: TBP)+≡
  procedure :: setup_mci => process_setup_mci

(Process: sub interfaces)+≡
  module subroutine process_setup_mci (process, dispatch_mci)
    class(process_t), intent(inout) :: process
    procedure(dispatch_mci_proc) :: dispatch_mci
  end subroutine process_setup_mci

(Process: procedures)+≡
  module subroutine process_setup_mci (process, dispatch_mci)
    class(process_t), intent(inout) :: process
    procedure(dispatch_mci_proc) :: dispatch_mci
    class(mci_t), allocatable :: mci_template
    integer :: i, i_mci
    if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_setup_mci")
    associate (pcm => process%pcm)
      call pcm%call_dispatch_mci (dispatch_mci, &
        process%get_var_list_ptr (), process%meta%id, mci_template)
      call pcm%setup_mci (process%mci_entry)
      process%config%n_mci = pcm%n_mci
      process%component(:)%i_mci = pcm%i_mci(:)
      do i = 1, pcm%n_components
        i_mci = process%pcm%i_mci(i)
        if (i_mci > 0) then
          associate (component => process%component(i), &
            mci_entry => process%mci_entry(i_mci))
            call mci_entry%configure (mci_template, &
              process%meta%type, &
              i_mci, i, component, process%beam_config%n_sfpar, &
              process%rng_factory)
            call mci_entry%set_parameters (process%get_var_list_ptr ())
          end associate
        end if
      end do
    end associate
  end subroutine process_setup_mci

```

Set cuts. This is a parse node, namely the right-hand side of the `cut` assignment. When creating an instance, we compile this into an evaluation tree. The parse node may be null.

```

(Process: process: TBP)+≡
    procedure :: set_cuts => process_set_cuts

(Process: sub interfaces)+≡
    module subroutine process_set_cuts (process, ef_cuts)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_cuts
    end subroutine process_set_cuts

(Process: procedures)+≡
    module subroutine process_set_cuts (process, ef_cuts)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_cuts
        allocate (process%config%ef_cuts, source = ef_cuts)
    end subroutine process_set_cuts

```

Analogously for the other expressions.

```

(Process: process: TBP)+≡
    procedure :: set_scale => process_set_scale
    procedure :: set_fac_scale => process_set_fac_scale
    procedure :: set_ren_scale => process_set_ren_scale
    procedure :: set_weight => process_set_weight

(Process: sub interfaces)+≡
    module subroutine process_set_scale (process, ef_scale)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_scale
    end subroutine process_set_scale
    module subroutine process_set_weight (process, ef_weight)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_weight
    end subroutine process_set_weight
    module subroutine process_set_fac_scale (process, ef_fac_scale)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_fac_scale
    end subroutine process_set_fac_scale
    module subroutine process_set_ren_scale (process, ef_ren_scale)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_ren_scale
    end subroutine process_set_ren_scale

(Process: procedures)+≡
    module subroutine process_set_scale (process, ef_scale)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_scale
        allocate (process%config%ef_scale, source = ef_scale)
    end subroutine process_set_scale

    module subroutine process_set_fac_scale (process, ef_fac_scale)
        class(process_t), intent(inout) :: process
        class(expr_factory_t), intent(in) :: ef_fac_scale
        allocate (process%config%ef_fac_scale, source = ef_fac_scale)
    end subroutine process_set_fac_scale

```

```

end subroutine process_set_fac_scale

module subroutine process_set_ren_scale (process, ef_ren_scale)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_ren_scale
  allocate (process%config%ef_ren_scale, source = ef_ren_scale)
end subroutine process_set_ren_scale

module subroutine process_set_weight (process, ef_weight)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_weight
  allocate (process%config%ef_weight, source = ef_weight)
end subroutine process_set_weight

```

MD5 sum

The MD5 sum of the process object should reflect the state completely, including integration results. It is used for checking the integrity of event files. This global checksum includes checksums for the various parts. In particular, the MCI object receives a checksum that includes the configuration of all configuration parts relevant for an individual integration. This checksum is used for checking the integrity of integration grids.

We do not need MD5 sums for the process terms, since these are generated from the component definitions.

```

(Process: process: TBP)+≡
  procedure :: compute_md5sum => process_compute_md5sum

(Process: sub interfaces)+≡
  module subroutine process_compute_md5sum (process)
    class(process_t), intent(inout) :: process
  end subroutine process_compute_md5sum

(Process: procedures)+≡
  module subroutine process_compute_md5sum (process)
    class(process_t), intent(inout) :: process
    integer :: i
    call process%config%compute_md5sum ()
    do i = 1, process%config%n_components
      associate (component => process%component(i))
        if (component%active) then
          call component%compute_md5sum ()
        end if
      end associate
    end do
    call process%beam_config%compute_md5sum ()
    do i = 1, process%config%n_mci
      call process%mci_entry(i)%compute_md5sum &
        (process%config, process%component, process%beam_config)
    end do
  end subroutine process_compute_md5sum

(Process: process: TBP)+≡
  procedure :: sampler_test => process_sampler_test

```

```

(Process: sub interfaces)+≡
    module subroutine process_sampler_test (process, sampler, n_calls, i_mci)
        class(process_t), intent(inout) :: process
        class(mci_sampler_t), intent(inout) :: sampler
        integer, intent(in) :: n_calls, i_mci
    end subroutine process_sampler_test

(Process: procedures)+≡
    module subroutine process_sampler_test (process, sampler, n_calls, i_mci)
        class(process_t), intent(inout) :: process
        class(mci_sampler_t), intent(inout) :: sampler
        integer, intent(in) :: n_calls, i_mci
        call process%mci_entry(i_mci)%sampler_test (sampler, n_calls)
    end subroutine process_sampler_test

```

The finalizer should be called after all integration passes have been completed. It will, for instance, write a summary of the integration results.

`integrate_dummy` does a “dummy” integration in the sense that nothing is done but just empty integration results appended.

```

(Process: process: TBP)+≡
    procedure :: final_integration => process_final_integration
    procedure :: integrate_dummy => process_integrate_dummy

(Process: sub interfaces)+≡
    module subroutine process_final_integration (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
    end subroutine process_final_integration
    module subroutine process_integrate_dummy (process)
        class(process_t), intent(inout) :: process
    end subroutine process_integrate_dummy

(Process: procedures)+≡
    module subroutine process_final_integration (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        call process%mci_entry(i_mci)%final_integration ()
    end subroutine process_final_integration

    module subroutine process_integrate_dummy (process)
        class(process_t), intent(inout) :: process
        type(integration_results_t) :: results
        integer :: u_log
        u_log = logfile_unit ()
        call results%init (process%meta%type)
        call results%display_init (screen = .true., unit = u_log)
        call results%new_pass ()
        call results%record (1, 0, 0._default, 0._default, 0._default)
        call results%display_final ()
    end subroutine process_integrate_dummy

```

```

(Process: process: TBP)+≡
    procedure :: integrate => process_integrate

```

<Process: sub interfaces>+≡

```

module subroutine process_integrate (process, i_mci, mci_work, &
    mci_sampler, n_it, n_calls, adapt_grids, adapt_weights, final, &
    pacify, nlo_type)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(mci_work_t), intent(inout) :: mci_work
    class(mci_sampler_t), intent(inout) :: mci_sampler
    integer, intent(in) :: n_it, n_calls
    logical, intent(in), optional :: adapt_grids, adapt_weights
    logical, intent(in), optional :: final
    logical, intent(in), optional :: pacify
    integer, intent(in), optional :: nlo_type
end subroutine process_integrate

```

<Process: procedures>+≡

```

module subroutine process_integrate (process, i_mci, mci_work, &
    mci_sampler, n_it, n_calls, adapt_grids, adapt_weights, final, &
    pacify, nlo_type)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(mci_work_t), intent(inout) :: mci_work
    class(mci_sampler_t), intent(inout) :: mci_sampler
    integer, intent(in) :: n_it, n_calls
    logical, intent(in), optional :: adapt_grids, adapt_weights
    logical, intent(in), optional :: final
    logical, intent(in), optional :: pacify
    integer, intent(in), optional :: nlo_type
    associate (mci_entry => process%mci_entry(i_mci))
        call mci_entry%integrate (mci_work%mci, mci_sampler, n_it, n_calls, &
            adapt_grids, adapt_weights, final, pacify, &
            nlo_type = nlo_type)
        call mci_entry%results%display_pass (pacify)
    end associate
end subroutine process_integrate

```

<Process: process: TBP>+≡

```

procedure :: generate_weighted_event => process_generate_weighted_event

```

<Process: sub interfaces>+≡

```

module subroutine process_generate_weighted_event (process, i_mci, &
    mci_work, mci_sampler, keep_failed_events)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(mci_work_t), intent(inout) :: mci_work
    class(mci_sampler_t), intent(inout) :: mci_sampler
    logical, intent(in) :: keep_failed_events
end subroutine process_generate_weighted_event

```

<Process: procedures>+≡

```

module subroutine process_generate_weighted_event (process, i_mci, &
    mci_work, mci_sampler, keep_failed_events)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(mci_work_t), intent(inout) :: mci_work

```

```

class(mci_sampler_t), intent(inout) :: mci_sampler
logical, intent(in) :: keep_failed_events
associate (mci_entry => process%mci_entry(i_mci))
    call mci_entry%generate_weighted_event (mci_work%mci, &
        mci_sampler, keep_failed_events)
end associate
end subroutine process_generate_weighted_event

```

```

(Process: process: TBP)+≡
    procedure :: generate_unweighted_event => process_generate_unweighted_event

```

```

(Process: sub interfaces)+≡
    module subroutine process_generate_unweighted_event (process, i_mci, &
        mci_work, mci_sampler)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(mci_work_t), intent(inout) :: mci_work
        class(mci_sampler_t), intent(inout) :: mci_sampler
    end subroutine process_generate_unweighted_event

```

```

(Process: procedures)+≡
    module subroutine process_generate_unweighted_event (process, i_mci, &
        mci_work, mci_sampler)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(mci_work_t), intent(inout) :: mci_work
        class(mci_sampler_t), intent(inout) :: mci_sampler
        associate (mci_entry => process%mci_entry(i_mci))
            call mci_entry%generate_unweighted_event &
                (mci_work%mci, mci_sampler)
        end associate
    end subroutine process_generate_unweighted_event

```

Display the final results for the sum of all components. This is useful, obviously, only if there is more than one component and not if a combined integration of all components together has been performed.

```

(Process: process: TBP)+≡
    procedure :: display_summed_results => process_display_summed_results

```

```

(Process: sub interfaces)+≡
    module subroutine process_display_summed_results (process, pacify)
        class(process_t), intent(inout) :: process
        logical, intent(in) :: pacify
    end subroutine process_display_summed_results

```

```

(Process: procedures)+≡
    module subroutine process_display_summed_results (process, pacify)
        class(process_t), intent(inout) :: process
        logical, intent(in) :: pacify
        type(integration_results_t) :: results
        integer :: u_log
        u_log = logfile_unit ()
        call results%init (process%meta%type)
        call results%display_init (screen = .true., unit = u_log)
        call results%new_pass ()
    end subroutine process_display_summed_results

```

```

call results%record (1, 0, &
  process%get_integral (), &
  process%get_error (), &
  process%get_efficiency (), suppress = pacify)
select type (pcm => process%pcm)
class is (pcm_nlo_t)
  !!! Check that Born integral is there
  if (.not. pcm%settings%combined_integration .and. &
    process%component_can_be_integrated (1)) then
    call results%record_correction (process%get_correction (), &
      process%get_correction_error ())
  end if
end select
call results%display_final ()
end subroutine process_display_summed_results

```

Run LaTeX/Metapost to generate a ps/pdf file for the integration history. We (re)write the driver file – just in case it has been missed before – then we compile it.

```

(Process: process: TBP)+≡
  procedure :: display_integration_history => &
    process_display_integration_history

(Process: sub interfaces)+≡
  module subroutine process_display_integration_history &
    (process, i_mci, filename, os_data, eff_reset)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(string_t), intent(in) :: filename
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: eff_reset
  end subroutine process_display_integration_history

(Process: procedures)+≡
  module subroutine process_display_integration_history &
    (process, i_mci, filename, os_data, eff_reset)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(string_t), intent(in) :: filename
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: eff_reset
    call integration_results_write_driver &
      (process%mci_entry(i_mci)%results, filename, eff_reset)
    call integration_results_compile_driver &
      (process%mci_entry(i_mci)%results, filename, os_data)
  end subroutine process_display_integration_history

```

Write a complete logfile (with hardcoded name based on the process ID). We do not write internal data.

```

(Process: process: TBP)+≡
  procedure :: write_logfile => process_write_logfile

(Process: sub interfaces)+≡
  module subroutine process_write_logfile (process, i_mci, filename)

```

```

        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(string_t), intent(in) :: filename
    end subroutine process_write_logfile

    (Process: procedures)+≡
    module subroutine process_write_logfile (process, i_mci, filename)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(string_t), intent(in) :: filename
        type(time_t) :: time
        integer :: unit, u
        unit = free_unit ()
        open (unit = unit, file = char (filename), action = "write", &
            status = "replace")
        u = given_output_unit (unit)
        write (u, "(A)") repeat ("#", 79)
        call process%meta%write (u, .false.)
        write (u, "(A)") repeat ("#", 79)
        write (u, "(3x,A,ES17.10)") "Integral    = ", &
            process%mci_entry(i_mci)%get_integral ()
        write (u, "(3x,A,ES17.10)") "Error        = ", &
            process%mci_entry(i_mci)%get_error ()
        write (u, "(3x,A,ES17.10)") "Accuracy     = ", &
            process%mci_entry(i_mci)%get_accuracy ()
        write (u, "(3x,A,ES17.10)") "Chi2          = ", &
            process%mci_entry(i_mci)%get_chi2 ()
        write (u, "(3x,A,ES17.10)") "Efficiency = ", &
            process%mci_entry(i_mci)%get_efficiency ()
        call process%mci_entry(i_mci)%get_time (time, 10000)
        if (time%is_known ()) then
            write (u, "(3x,A,1x,A)") "T(10k evt) = ", char (time%to_string_dhms ())
        else
            write (u, "(3x,A)") "T(10k evt) = [undefined]"
        end if
        call process%mci_entry(i_mci)%results%write (u)
        write (u, "(A)") repeat ("#", 79)
        call process%mci_entry(i_mci)%results%write_chain_weights (u)
        write (u, "(A)") repeat ("#", 79)
        call process%mci_entry(i_mci)%counter%write (u)
        write (u, "(A)") repeat ("#", 79)
        call process%mci_entry(i_mci)%mci%write_log_entry (u)
        write (u, "(A)") repeat ("#", 79)
        call process%beam_config%data%write (u)
        write (u, "(A)") repeat ("#", 79)
        if (allocated (process%config%ef_cuts)) then
            write (u, "(3x,A)") "Cut expression:"
            call process%config%ef_cuts%write (u)
        else
            write (u, "(3x,A)") "No cuts used."
        end if
        call write_separator (u)
        if (allocated (process%config%ef_scale)) then
            write (u, "(3x,A)") "Scale expression:"
            call process%config%ef_scale%write (u)
        end if
    end module process_write_logfile

```



```

else
  write (u, "(3x,A)") "No scale expression was given."
end if
call write_separator (u)
if (allocated (process%config%ef_fac_scale)) then
  write (u, "(3x,A)") "Factorization scale expression:"
  call process%config%ef_fac_scale%write (u)
else
  write (u, "(3x,A)") "No factorization scale expression was given."
end if
call write_separator (u)
if (allocated (process%config%ef_ren_scale)) then
  write (u, "(3x,A)") "Renormalization scale expression:"
  call process%config%ef_ren_scale%write (u)
else
  write (u, "(3x,A)") "No renormalization scale expression was given."
end if
call write_separator (u)
if (allocated (process%config%ef_weight)) then
  call write_separator (u)
  write (u, "(3x,A)") "Weight expression:"
  call process%config%ef_weight%write (u)
else
  write (u, "(3x,A)") "No weight expression was given."
end if
write (u, "(A)") repeat ("#", 79)
write (u, "(1x,A)") "Summary of quantum-number states:"
write (u, "(1x,A)") " + sign: allowed and contributing"
write (u, "(1x,A)") " no + : switched off at runtime"
call process%write_state_summary (u)
write (u, "(A)") repeat ("#", 79)
call process%env%write (u, show_var_list=.true., &
  show_model=.false., show_lib=.false., show_os_data=.false.)
write (u, "(A)") repeat ("#", 79)
close (u)
end subroutine process_write_logfile

```

Display the quantum-number combinations of the process components, and their current status (allowed or switched off).

```

(Process: process: TBP)+≡
  procedure :: write_state_summary => process_write_state_summary

(Process: sub interfaces)+≡
  module subroutine process_write_state_summary (process, unit)
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: unit
  end subroutine process_write_state_summary

(Process: procedures)+≡
  module subroutine process_write_state_summary (process, unit)
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: unit
    integer :: i, i_component, u
    u = given_output_unit (unit)
    do i = 1, size (process%term)

```

```

        call write_separator (u)
        i_component = process%term(i)%i_component
        if (i_component /= 0) then
            call process%term(i)%write_state_summary &
                (process%get_core_term(i), unit)
        end if
    end do
end subroutine process_write_state_summary

```

Prepare event generation for the specified MCI entry. This implies, in particular, checking the phase-space file.

```

(Process: process: TBP)+≡
    procedure :: prepare_simulation => process_prepare_simulation

(Process: sub interfaces)+≡
    module subroutine process_prepare_simulation (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
    end subroutine process_prepare_simulation

(Process: procedures)+≡
    module subroutine process_prepare_simulation (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        call process%mci_entry(i_mci)%prepare_simulation ()
    end subroutine process_prepare_simulation

```

Retrieve process data

Tell whether integral (and error) are known.

```

(Process: process: TBP)+≡
    generic :: has_integral => has_integral_tot, has_integral_mci
    procedure :: has_integral_tot => process_has_integral_tot
    procedure :: has_integral_mci => process_has_integral_mci

(Process: sub interfaces)+≡
    module function process_has_integral_tot (process) result (flag)
        logical :: flag
        class(process_t), intent(in) :: process
    end function process_has_integral_tot
    module function process_has_integral_mci (process, i_mci) result (flag)
        logical :: flag
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
    end function process_has_integral_mci

(Process: procedures)+≡
    module function process_has_integral_mci (process, i_mci) result (flag)
        logical :: flag
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        if (allocated (process%mci_entry)) then
            flag = process%mci_entry(i_mci)%has_integral ()
        else

```

```

        flag = .false.
    end if
end function process_has_integral_mci

module function process_has_integral_tot (process) result (flag)
    logical :: flag
    class(process_t), intent(in) :: process
    integer :: i, j, i_component
    if (allocated (process%mci_entry)) then
        flag = .true.
        do i = 1, size (process%mci_entry)
            do j = 1, size (process%mci_entry(i)%i_component)
                i_component = process%mci_entry(i)%i_component(j)
                if (process%component_can_be_integrated (i_component)) &
                    flag = flag .and. process%mci_entry(i)%has_integral ()
            end do
        end do
    else
        flag = .false.
    end if
end function process_has_integral_tot

```

Return the current integral and error obtained by the integrator i_mci.

(Process: process: TBP)+≡

```

generic :: get_integral => get_integral_tot, get_integral_mci
generic :: get_error => get_error_tot, get_error_mci
generic :: get_efficiency => get_efficiency_tot, get_efficiency_mci
procedure :: get_integral_tot => process_get_integral_tot
procedure :: get_integral_mci => process_get_integral_mci
procedure :: get_error_tot => process_get_error_tot
procedure :: get_error_mci => process_get_error_mci
procedure :: get_efficiency_tot => process_get_efficiency_tot
procedure :: get_efficiency_mci => process_get_efficiency_mci

```

(Process: sub interfaces)+≡

```

module function process_get_integral_mci (process, i_mci) result (integral)
    real(default) :: integral
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
end function process_get_integral_mci
module function process_get_error_mci (process, i_mci) result (error)
    real(default) :: error
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
end function process_get_error_mci
module function process_get_efficiency_mci &
    (process, i_mci) result (efficiency)
    real(default) :: efficiency
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
end function process_get_efficiency_mci
module function process_get_integral_tot (process) result (integral)
    real(default) :: integral
    class(process_t), intent(in) :: process

```

```

end function process_get_integral_tot
module function process_get_error_tot (process) result (error)
  real(default) :: variance
  class(process_t), intent(in) :: process
  real(default) :: error
end function process_get_error_tot
module function process_get_efficiency_tot (process) result (efficiency)
  real(default) :: efficiency
  class(process_t), intent(in) :: process
end function process_get_efficiency_tot

(Process: procedures) +=
module function process_get_integral_mci (process, i_mci) result (integral)
  real(default) :: integral
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_mci
  integral = process%mci_entry(i_mci)%get_integral ()
end function process_get_integral_mci

module function process_get_error_mci (process, i_mci) result (error)
  real(default) :: error
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_mci
  error = process%mci_entry(i_mci)%get_error ()
end function process_get_error_mci

module function process_get_efficiency_mci &
  (process, i_mci) result (efficiency)
  real(default) :: efficiency
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_mci
  efficiency = process%mci_entry(i_mci)%get_efficiency ()
end function process_get_efficiency_mci

module function process_get_integral_tot (process) result (integral)
  real(default) :: integral
  class(process_t), intent(in) :: process
  integer :: i, j, i_component
  integral = zero
  if (allocated (process%mci_entry)) then
    do i = 1, size (process%mci_entry)
      do j = 1, size (process%mci_entry(i)%i_component)
        i_component = process%mci_entry(i)%i_component(j)
        if (process%component_can_be_integrated(i_component)) &
          integral = integral + process%mci_entry(i)%get_integral ()
      end do
    end do
  end if
end function process_get_integral_tot

module function process_get_error_tot (process) result (error)
  real(default) :: variance
  class(process_t), intent(in) :: process
  real(default) :: error
  integer :: i, j, i_component

```

```

variance = zero
if (allocated (process%mci_entry)) then
  do i = 1, size (process%mci_entry)
    do j = 1, size (process%mci_entry(i)%i_component)
      i_component = process%mci_entry(i)%i_component(j)
      if (process%component_can_be_integrated(i_component)) &
        variance = variance + process%mci_entry(i)%get_error () ** 2
    end do
  end do
end if
error = sqrt (variance)
end function process_get_error_tot

module function process_get_efficiency_tot (process) result (efficiency)
  real(default) :: efficiency
  class(process_t), intent(in) :: process
  real(default) :: den, eff, int
  integer :: i, j, i_component
  den = zero
  if (allocated (process%mci_entry)) then
    do i = 1, size (process%mci_entry)
      do j = 1, size (process%mci_entry(i)%i_component)
        i_component = process%mci_entry(i)%i_component(j)
        if (process%component_can_be_integrated(i_component)) then
          int = process%get_integral (i)
          if (int > 0) then
            eff = process%mci_entry(i)%get_efficiency ()
            if (eff > 0) then
              den = den + int / eff
            else
              efficiency = 0
              return
            end if
          end if
        end if
      end do
    end do
  end if
  if (den > 0) then
    efficiency = process%get_integral () / den
  else
    efficiency = 0
  end if
end function process_get_efficiency_tot

```

Let us call the ratio of the NLO and the LO result $\iota = I_{NLO}/I_{LO}$. Then usual error propagation gives

$$\sigma_{\iota}^2 = \left(\frac{\partial \iota}{\partial I_{LO}} \right)^2 \sigma_{I_{LO}}^2 + \left(\frac{\partial \iota}{\partial I_{NLO}} \right)^2 \sigma_{I_{NLO}}^2 = \frac{I_{NLO}^2 \sigma_{I_{LO}}^2}{I_{LO}^4} + \frac{\sigma_{I_{NLO}}^2}{I_{LO}^2}.$$

$\langle Process: TBP \rangle \equiv$

```

procedure :: get_correction => process_get_correction
procedure :: get_correction_error => process_get_correction_error

```

```

(Process: sub interfaces)+≡
    module function process_get_correction (process) result (ratio)
        real(default) :: ratio
        class(process_t), intent(in) :: process
    end function process_get_correction
    module function process_get_correction_error (process) result (error)
        real(default) :: error
        class(process_t), intent(in) :: process
    end function process_get_correction_error

(Process: procedures)+≡
    module function process_get_correction (process) result (ratio)
        real(default) :: ratio
        class(process_t), intent(in) :: process
        integer :: i_mci, i_component
        real(default) :: int_born, int_nlo
        int_nlo = zero
        int_born = process%mci_entry(1)%get_integral ()
        i_mci = 2
        do i_component = 2, size (process%component)
            if (process%component_can_be_integrated (i_component)) then
                int_nlo = int_nlo + process%mci_entry(i_mci)%get_integral ()
                i_mci = i_mci + 1
            end if
        end do
        ratio = int_nlo / int_born * 100
    end function process_get_correction

    module function process_get_correction_error (process) result (error)
        real(default) :: error
        class(process_t), intent(in) :: process
        real(default) :: int_born, sum_int_nlo
        real(default) :: err_born, err2
        integer :: i_mci, i_component
        sum_int_nlo = zero; err2 = zero
        int_born = process%mci_entry(1)%get_integral ()
        err_born = process%mci_entry(1)%get_error ()
        i_mci = 2
        do i_component = 2, size (process%component)
            if (process%component_can_be_integrated (i_component)) then
                sum_int_nlo = sum_int_nlo + process%mci_entry(i_mci)%get_integral ()
                err2 = err2 + process%mci_entry(i_mci)%get_error()**2
                i_mci = i_mci + 1
            end if
        end do
        error = sqrt (err2 / int_born**2 + sum_int_nlo**2 * err_born**2 / int_born**4) * 100
    end function process_get_correction_error

```

This routine asks beam_config for the frame.

```

(Process: process: TBP)+≡
    procedure :: lab_is_cm => process_lab_is_cm

(Process: sub interfaces)+≡
    pure module function process_lab_is_cm (process) result (lab_is_cm)
        logical :: lab_is_cm
    end function process_lab_is_cm

```

```

        class(process_t), intent(in) :: process
    end function process_lab_is_cm

<Process: procedures>+≡
    pure module function process_lab_is_cm (process) result (lab_is_cm)
        logical :: lab_is_cm
        class(process_t), intent(in) :: process
        lab_is_cm = process%beam_config%lab_is_cm
    end function process_lab_is_cm

<Process: process: TBP>+≡
    procedure :: get_component_ptr => process_get_component_ptr

<Process: sub interfaces>+≡
    module function process_get_component_ptr (process, i) result (component)
        type(process_component_t), pointer :: component
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i
    end function process_get_component_ptr

<Process: procedures>+≡
    module function process_get_component_ptr (process, i) result (component)
        type(process_component_t), pointer :: component
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i
        component => process%component(i)
    end function process_get_component_ptr

<Process: process: TBP>+≡
    procedure :: get_qcd => process_get_qcd

<Process: sub interfaces>+≡
    module function process_get_qcd (process) result (qcd)
        type(qcd_t) :: qcd
        class(process_t), intent(in) :: process
    end function process_get_qcd

<Process: procedures>+≡
    module function process_get_qcd (process) result (qcd)
        type(qcd_t) :: qcd
        class(process_t), intent(in) :: process
        qcd = process%config%get_qcd ()
    end function process_get_qcd

<Process: process: TBP>+≡
    generic :: get_component_type => get_component_type_single
    procedure :: get_component_type_single => process_get_component_type_single

<Process: sub interfaces>+≡
    elemental module function process_get_component_type_single &
        (process, i_component) result (comp_type)
        integer :: comp_type
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_component_type_single

```

```

(Process: procedures)+≡
    elemental module function process_get_component_type_single &
        (process, i_component) result (comp_type)
        integer :: comp_type
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        comp_type = process%component(i_component)%component_type
    end function process_get_component_type_single

(Process: process: TBP)+≡
    generic :: get_component_type => get_component_type_all
    procedure :: get_component_type_all => process_get_component_type_all

(Process: sub interfaces)+≡
    module function process_get_component_type_all &
        (process) result (comp_type)
        integer, dimension(:), allocatable :: comp_type
        class(process_t), intent(in) :: process
    end function process_get_component_type_all

(Process: procedures)+≡
    module function process_get_component_type_all &
        (process) result (comp_type)
        integer, dimension(:), allocatable :: comp_type
        class(process_t), intent(in) :: process
        allocate (comp_type (size (process%component)))
        comp_type = process%component%component_type
    end function process_get_component_type_all

(Process: process: TBP)+≡
    procedure :: get_component_i_terms => process_get_component_i_terms

(Process: sub interfaces)+≡
    module function process_get_component_i_terms &
        (process, i_component) result (i_term)
        integer, dimension(:), allocatable :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_component_i_terms

(Process: procedures)+≡
    module function process_get_component_i_terms &
        (process, i_component) result (i_term)
        integer, dimension(:), allocatable :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        allocate (i_term (size (process%component(i_component)%i_term)))
        i_term = process%component(i_component)%i_term
    end function process_get_component_i_terms

(Process: process: TBP)+≡
    procedure :: get_n_allowed_born => process_get_n_allowed_born

```



```

(Process: sub interfaces)+≡
    module function process_get_n_allowed_born (process, i_born) result (n_born)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_born
        integer :: n_born
    end function process_get_n_allowed_born

```

```

(Process: procedures)+≡
    module function process_get_n_allowed_born (process, i_born) result (n_born)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_born
        integer :: n_born
        n_born = process%term(i_born)%n_allowed
    end function process_get_n_allowed_born

```

Workaround getter. Would be better to remove this.

```

(Process: process: TBP)+≡
    procedure :: get_pcm_ptr => process_get_pcm_ptr

```

```

(Process: sub interfaces)+≡
    module function process_get_pcm_ptr (process) result (pcm)
        class(pcm_t), pointer :: pcm
        class(process_t), intent(in), target :: process
    end function process_get_pcm_ptr

```

```

(Process: procedures)+≡
    module function process_get_pcm_ptr (process) result (pcm)
        class(pcm_t), pointer :: pcm
        class(process_t), intent(in), target :: process
        pcm => process%pcm
    end function process_get_pcm_ptr

```

```

(Process: process: TBP)+≡
    generic :: component_can_be_integrated => component_can_be_integrated_single
    generic :: component_can_be_integrated => component_can_be_integrated_all
    procedure :: component_can_be_integrated_single => &
        process_component_can_be_integrated_single

```

```

(Process: sub interfaces)+≡
    module function process_component_can_be_integrated_single &
        (process, i_component) result (active)
        logical :: active
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_component_can_be_integrated_single

```

```

(Process: procedures)+≡
    module function process_component_can_be_integrated_single &
        (process, i_component) result (active)
        logical :: active
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        logical :: combined_integration
        select type (pcm => process%pcm)
        type is (pcm_nlo_t)
            combined_integration = pcm%settings%combined_integration

```

```

class default
    combined_integration = .false.
end select
associate (component => process%component(i_component))
    active = component%can_be_integrated ()
    if (combined_integration) &
        active = active .and. component%component_type <= COMP_MASTER
    end associate
end function process_component_can_be_integrated_single

(Process: process: TBP)+≡
    procedure :: component_can_be_integrated_all => &
        process_component_can_be_integrated_all

(Process: sub interfaces)+≡
    module function process_component_can_be_integrated_all &
        (process) result (val)
        logical, dimension(:), allocatable :: val
        class(process_t), intent(in) :: process
    end function process_component_can_be_integrated_all

(Process: procedures)+≡
    module function process_component_can_be_integrated_all (process) result (val)
        logical, dimension(:), allocatable :: val
        class(process_t), intent(in) :: process
        integer :: i
        allocate (val (size (process%component)))
        do i = 1, size (process%component)
            val(i) = process%component_can_be_integrated (i)
        end do
    end function process_component_can_be_integrated_all

(Process: process: TBP)+≡
    procedure :: reset_selected_cores => process_reset_selected_cores

(Process: sub interfaces)+≡
    pure module subroutine process_reset_selected_cores (process)
        class(process_t), intent(inout) :: process
    end subroutine process_reset_selected_cores

(Process: procedures)+≡
    pure module subroutine process_reset_selected_cores (process)
        class(process_t), intent(inout) :: process
        process%pcm%component_selected = .false.
    end subroutine process_reset_selected_cores

(Process: process: TBP)+≡
    procedure :: select_components => process_select_components

(Process: sub interfaces)+≡
    pure module subroutine process_select_components (process, indices)
        class(process_t), intent(inout) :: process
        integer, dimension(:), intent(in) :: indices
    end subroutine process_select_components

```

```

<Process: procedures>+≡
  pure module subroutine process_select_components (process, indices)
    class(process_t), intent(inout) :: process
    integer, dimension(:), intent(in) :: indices
    associate (pcm => process%pcm)
      pcm%component_selected(indices) = .true.
    end associate
  end subroutine process_select_components

<Process: process: TBP>+≡
  procedure :: component_is_selected => process_component_is_selected

<Process: sub interfaces>+≡
  pure module function process_component_is_selected &
    (process, index) result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: index
  end function process_component_is_selected

<Process: procedures>+≡
  pure module function process_component_is_selected &
    (process, index) result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: index
    associate (pcm => process%pcm)
      val = pcm%component_selected(index)
    end associate
  end function process_component_is_selected

<Process: process: TBP>+≡
  procedure :: get_coupling_powers => process_get_coupling_powers

<Process: sub interfaces>+≡
  pure module subroutine process_get_coupling_powers &
    (process, alpha_power, alphas_power)
    class(process_t), intent(in) :: process
    integer, intent(out) :: alpha_power, alphas_power
  end subroutine process_get_coupling_powers

<Process: procedures>+≡
  pure module subroutine process_get_coupling_powers &
    (process, alpha_power, alphas_power)
    class(process_t), intent(in) :: process
    integer, intent(out) :: alpha_power, alphas_power
    call process%component(1)%config%get_coupling_powers &
      (alpha_power, alphas_power)
  end subroutine process_get_coupling_powers

<Process: process: TBP>+≡
  procedure :: get_real_component => process_get_real_component

```

```

(Process: sub interfaces)+≡
    module function process_get_real_component (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
    end function process_get_real_component

(Process: procedures)+≡
    module function process_get_real_component (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer :: i_component
        type(process_component_def_t), pointer :: config => null ()
        i_real = 0
        do i_component = 1, size (process%component)
            config => process%get_component_def_ptr (i_component)
            if (config%get_nlo_type () == NLO_REAL) then
                i_real = i_component
                exit
            end if
        end do
    end function process_get_real_component

(Process: process: TBP)+≡
    procedure :: extract_active_component_mci => &
        process_extract_active_component_mci

(Process: sub interfaces)+≡
    module function process_extract_active_component_mci &
        (process) result (i_active)
        integer :: i_active
        class(process_t), intent(in) :: process
    end function process_extract_active_component_mci

(Process: procedures)+≡
    module function process_extract_active_component_mci &
        (process) result (i_active)
        integer :: i_active
        class(process_t), intent(in) :: process
        integer :: i_mci, j, i_component, n_active
        call count_n_active ()
        if (n_active /= 1) i_active = 0
    contains
        subroutine count_n_active ()
            n_active = 0
            do i_mci = 1, size (process%mci_entry)
                associate (mci_entry => process%mci_entry(i_mci))
                    do j = 1, size (mci_entry%i_component)
                        i_component = mci_entry%i_component(j)
                        associate (component => process%component (i_component))
                            if (component%can_be_integrated ()) then
                                i_active = i_mci
                                n_active = n_active + 1
                            end if
                        end associate
                    end do
                end associate
            end do
        end subroutine count_n_active
    end module

```

```

        end associate
    end do
    end subroutine count_n_active
end function process_extract_active_component_mci

```

```

<Process: process: TBP>+≡
    procedure :: uses_real_partition => process_uses_real_partition

<Process: sub interfaces>+≡
    module function process_uses_real_partition (process) result (val)
        logical :: val
        class(process_t), intent(in) :: process
    end function process_uses_real_partition

<Process: procedures>+≡
    module function process_uses_real_partition (process) result (val)
        logical :: val
        class(process_t), intent(in) :: process
        val = any (process%mci_entry%real_partition_type /= REAL_FULL)
    end function process_uses_real_partition

```

Return the MD5 sums that summarize the process component definitions. These values should be independent of parameters, beam details, expressions, etc. They can be used for checking the integrity of a process when reusing an old event file.

```

<Process: process: TBP>+≡
    procedure :: get_md5sum_prc => process_get_md5sum_prc

<Process: sub interfaces>+≡
    module function process_get_md5sum_prc &
        (process, i_component) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_md5sum_prc

<Process: procedures>+≡
    module function process_get_md5sum_prc (process, i_component) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        if (process%component(i_component)%active) then
            md5sum = process%component(i_component)%config%get_md5sum ()
        else
            md5sum = ""
        end if
    end function process_get_md5sum_prc

```

Return the MD5 sums that summarize the state of the MCI integrators. These values should encode all process data, integration and phase space configuration, etc., and the integration results. They can thus be used for checking the integrity of an event-generation setup when reusing an old event file.

```

<Process: process: TBP>+≡
    procedure :: get_md5sum_mci => process_get_md5sum_mci

```

```

(Process: sub interfaces)+≡
    module function process_get_md5sum_mci (process, i_mci) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
    end function process_get_md5sum_mci

```

```

(Process: procedures)+≡
    module function process_get_md5sum_mci (process, i_mci) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        md5sum = process%mci_entry(i_mci)%get_md5sum ()
    end function process_get_md5sum_mci

```

Return the MD5 sum of the process configuration. This should encode the process setup, data, and expressions, but no integration results.

```

(Process: process: TBP)+≡
    procedure :: get_md5sum_cfg => process_get_md5sum_cfg

```

```

(Process: sub interfaces)+≡
    module function process_get_md5sum_cfg (process) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
    end function process_get_md5sum_cfg

```

```

(Process: procedures)+≡
    module function process_get_md5sum_cfg (process) result (md5sum)
        character(32) :: md5sum
        class(process_t), intent(in) :: process
        md5sum = process%config%md5sum
    end function process_get_md5sum_cfg

```

```

(Process: process: TBP)+≡
    procedure :: get_n_cores => process_get_n_cores

```

```

(Process: sub interfaces)+≡
    module function process_get_n_cores (process) result (n)
        integer :: n
        class(process_t), intent(in) :: process
    end function process_get_n_cores

```

```

(Process: procedures)+≡
    module function process_get_n_cores (process) result (n)
        integer :: n
        class(process_t), intent(in) :: process
        n = process%pcm%n_cores
    end function process_get_n_cores

```

```

(Process: process: TBP)+≡
    procedure :: get_base_i_term => process_get_base_i_term

```

```

(Process: sub interfaces)+≡
    module function process_get_base_i_term &
        (process, i_component) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_base_i_term

(Process: procedures)+≡
    module function process_get_base_i_term (process, i_component) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        i_term = process%component(i_component)%i_term(1)
    end function process_get_base_i_term

(Process: process: TBP)+≡
    procedure :: get_core_term => process_get_core_term

(Process: sub interfaces)+≡
    module function process_get_core_term (process, i_term) result (core)
        class(prc_core_t), pointer :: core
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_term
    end function process_get_core_term

(Process: procedures)+≡
    module function process_get_core_term (process, i_term) result (core)
        class(prc_core_t), pointer :: core
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_term
        integer :: i_core
        i_core = process%term(i_term)%i_core
        core => process%core_entry(i_core)%get_core_ptr ()
    end function process_get_core_term

(Process: process: TBP)+≡
    procedure :: get_core_ptr => process_get_core_ptr

(Process: sub interfaces)+≡
    module function process_get_core_ptr (process, i_core) result (core)
        class(prc_core_t), pointer :: core
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_core
    end function process_get_core_ptr

(Process: procedures)+≡
    module function process_get_core_ptr (process, i_core) result (core)
        class(prc_core_t), pointer :: core
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_core
        if (allocated (process%core_entry)) then
            core => process%core_entry(i_core)%get_core_ptr ()
        else
            core => null ()
        end if
    end function

```

```

end function process_get_core_ptr

<Process: process: TBP>+≡
  procedure :: get_term_ptr => process_get_term_ptr

<Process: sub interfaces>+≡
  module function process_get_term_ptr (process, i) result (term)
    type(process_term_t), pointer :: term
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i
  end function process_get_term_ptr

<Process: procedures>+≡
  module function process_get_term_ptr (process, i) result (term)
    type(process_term_t), pointer :: term
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i
    term => process%term(i)
  end function process_get_term_ptr

<Process: process: TBP>+≡
  procedure :: get_i_term => process_get_i_term

<Process: sub interfaces>+≡
  module function process_get_i_term (process, i_core) result (i_term)
    integer :: i_term
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_core
  end function process_get_i_term

<Process: procedures>+≡
  module function process_get_i_term (process, i_core) result (i_term)
    integer :: i_term
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_core
    do i_term = 1, process%get_n_terms ()
      if (process%term(i_term)%i_core == i_core) return
    end do
    i_term = -1
  end function process_get_i_term

<Process: process: TBP>+≡
  procedure :: get_i_core => process_get_i_core

<Process: sub interfaces>+≡
  module function process_get_i_core (process, i_term) result (i_core)
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_term
    integer :: i_core
  end function process_get_i_core

<Process: procedures>+≡
  module function process_get_i_core (process, i_term) result (i_core)
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_term
    integer :: i_core

```



```

        i_core = process%term(i_term)%i_core
    end function process_get_i_core

    <Process: process: TBP>+=
        procedure :: set_i_mci_work => process_set_i_mci_work

    <Process: sub interfaces>+=
        module subroutine process_set_i_mci_work (process, i_mci)
            class(process_t), intent(inout) :: process
            integer, intent(in) :: i_mci
        end subroutine process_set_i_mci_work

    <Process: procedures>+=
        module subroutine process_set_i_mci_work (process, i_mci)
            class(process_t), intent(inout) :: process
            integer, intent(in) :: i_mci
            process%mci_entry(i_mci)%i_mci = i_mci
        end subroutine process_set_i_mci_work

    <Process: process: TBP>+=
        procedure :: get_i_mci_work => process_get_i_mci_work

    <Process: sub interfaces>+=
        pure module function process_get_i_mci_work &
            (process, i_mci) result (i_mci_work)
            integer :: i_mci_work
            class(process_t), intent(in) :: process
            integer, intent(in) :: i_mci
        end function process_get_i_mci_work

    <Process: procedures>+=
        pure module function process_get_i_mci_work &
            (process, i_mci) result (i_mci_work)
            integer :: i_mci_work
            class(process_t), intent(in) :: process
            integer, intent(in) :: i_mci
            i_mci_work = process%mci_entry(i_mci)%i_mci
        end function process_get_i_mci_work

    <Process: process: TBP>+=
        procedure :: get_i_sub => process_get_i_sub

    <Process: sub interfaces>+=
        elemental module function process_get_i_sub (process, i_term) result (i_sub)
            integer :: i_sub
            class(process_t), intent(in) :: process
            integer, intent(in) :: i_term
        end function process_get_i_sub

    <Process: procedures>+=
        elemental module function process_get_i_sub (process, i_term) result (i_sub)
            integer :: i_sub
            class(process_t), intent(in) :: process
            integer, intent(in) :: i_term
            i_sub = process%term(i_term)%i_sub
        end function process_get_i_sub

```

```

(Process: process: TBP)+≡
    procedure :: get_i_term_virtual => process_get_i_term_virtual

(Process: sub interfaces)+≡
    elemental module function process_get_i_term_virtual &
        (process) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
    end function process_get_i_term_virtual

(Process: procedures)+≡
    elemental module function process_get_i_term_virtual (process) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer :: i_component
        i_term = 0
        do i_component = 1, size (process%component)
            if (process%component(i_component)%get_nlo_type () == NLO_VIRTUAL) &
                i_term = process%component(i_component)%i_term(1)
        end do
    end function process_get_i_term_virtual

(Process: process: TBP)+≡
    generic :: component_is_active => component_is_active_single
    procedure :: component_is_active_single => process_component_is_active_single

(Process: sub interfaces)+≡
    elemental module function process_component_is_active_single &
        (process, i_comp) result (val)
        logical :: val
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_comp
    end function process_component_is_active_single

(Process: procedures)+≡
    elemental module function process_component_is_active_single &
        (process, i_comp) result (val)
        logical :: val
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_comp
        val = process%component(i_comp)%is_active ()
    end function process_component_is_active_single

(Process: process: TBP)+≡
    generic :: component_is_active => component_is_active_all
    procedure :: component_is_active_all => process_component_is_active_all

(Process: sub interfaces)+≡
    pure module function process_component_is_active_all (process) result (val)
        logical, dimension(:), allocatable :: val
        class(process_t), intent(in) :: process
    end function process_component_is_active_all

(Process: procedures)+≡
    pure module function process_component_is_active_all (process) result (val)
        logical, dimension(:), allocatable :: val

```

```

class(process_t), intent(in) :: process
allocate (val (size (process%component)))
val = process%component%is_active ()
end function process_component_is_active_all

```

30.4.8 Default iterations

If the user does not specify the passes and iterations for integration, we should be able to give reasonable defaults. These depend on the process, therefore we implement the following procedures as methods of the process object. The algorithm is not very sophisticated yet, it may be improved by looking at the process in more detail.

We investigate only the first process component, assuming that it characterizes the complexity of the process reasonable well.

The number of passes is limited to two: one for adaption, one for integration.

```

(Process: process: TBP)+≡
  procedure :: get_n_pass_default => process_get_n_pass_default
  procedure :: adapt_grids_default => process_adapt_grids_default
  procedure :: adapt_weights_default => process_adapt_weights_default

(Process: sub interfaces)+≡
  module function process_get_n_pass_default (process) result (n_pass)
    class(process_t), intent(in) :: process
    integer :: n_pass
  end function process_get_n_pass_default
  module function process_adapt_grids_default (process, pass) result (flag)
    class(process_t), intent(in) :: process
    integer, intent(in) :: pass
    logical :: flag
  end function process_adapt_grids_default
  module function process_adapt_weights_default (process, pass) result (flag)
    class(process_t), intent(in) :: process
    integer, intent(in) :: pass
    logical :: flag
  end function process_adapt_weights_default

(Process: procedures)+≡
  module function process_get_n_pass_default (process) result (n_pass)
    class(process_t), intent(in) :: process
    integer :: n_pass
    integer :: n_eff
    type(process_component_def_t), pointer :: config
    config => process%component(1)%config
    n_eff = config%get_n_tot () - 2
    select case (n_eff)
    case (1)
      n_pass = 1
    case default
      n_pass = 2
    end select
  end function process_get_n_pass_default

  module function process_adapt_grids_default (process, pass) result (flag)

```

```

class(process_t), intent(in) :: process
integer, intent(in) :: pass
logical :: flag
integer :: n_eff
type(process_component_def_t), pointer :: config
config => process%component(1)%config
n_eff = config%get_n_tot () - 2
select case (n_eff)
case (1)
    flag = .false.
case default
    select case (pass)
    case (1); flag = .true.
    case (2); flag = .false.
    case default
        call msg_bug ("adapt grids default: impossible pass index")
    end select
end select
end function process_adapt_grids_default

module function process_adapt_weights_default (process, pass) result (flag)
class(process_t), intent(in) :: process
integer, intent(in) :: pass
logical :: flag
integer :: n_eff
type(process_component_def_t), pointer :: config
config => process%component(1)%config
n_eff = config%get_n_tot () - 2
select case (n_eff)
case (1)
    flag = .false.
case default
    select case (pass)
    case (1); flag = .true.
    case (2); flag = .false.
    case default
        call msg_bug ("adapt weights default: impossible pass index")
    end select
end select
end function process_adapt_weights_default

```

The number of iterations and calls per iteration depends on the number of outgoing particles.

```

(Process: process: TBP)+≡
    procedure :: get_n_it_default => process_get_n_it_default
    procedure :: get_n_calls_default => process_get_n_calls_default

(Process: sub interfaces)+≡
    module function process_get_n_it_default (process, pass) result (n_it)
        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_it
    end function process_get_n_it_default
    module function process_get_n_calls_default (process, pass) result (n_calls)

```

```

        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_calls
    end function process_get_n_calls_default

    (Process: procedures)+≡
    module function process_get_n_it_default (process, pass) result (n_it)
        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_it
        integer :: n_eff
        type(process_component_def_t), pointer :: config
        config => process%component(1)%config
        n_eff = config%get_n_tot () - 2
        select case (pass)
        case (1)
            select case (n_eff)
            case (1); n_it = 1
            case (2); n_it = 3
            case (3); n_it = 5
            case (4:5); n_it = 10
            case (6); n_it = 15
            case (7:); n_it = 20
            end select
        case (2)
            select case (n_eff)
            case (:3); n_it = 3
            case (4:); n_it = 5
            end select
        end select
    end function process_get_n_it_default

    module function process_get_n_calls_default (process, pass) result (n_calls)
        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_calls
        integer :: n_eff
        type(process_component_def_t), pointer :: config
        config => process%component(1)%config
        n_eff = config%get_n_tot () - 2
        select case (pass)
        case (1)
            select case (n_eff)
            case (1); n_calls = 100
            case (2); n_calls = 1000
            case (3); n_calls = 5000
            case (4); n_calls = 10000
            case (5); n_calls = 20000
            case (6:); n_calls = 50000
            end select
        case (2)
            select case (n_eff)
            case (:3); n_calls = 10000
            case (4); n_calls = 20000
            case (5); n_calls = 50000

```

```

        case (6);    n_calls = 100000
        case (7:);  n_calls = 200000
        end select
    end select
end function process_get_n_calls_default

```

30.4.9 Constant process data

Manually set the Run ID (unit test only).

```

(Process: process: TBP)+≡
    procedure :: set_run_id => process_set_run_id

(Process: sub interfaces)+≡
    module subroutine process_set_run_id (process, run_id)
        class(process_t), intent(inout) :: process
        type(string_t), intent(in) :: run_id
    end subroutine process_set_run_id

(Process: procedures)+≡
    module subroutine process_set_run_id (process, run_id)
        class(process_t), intent(inout) :: process
        type(string_t), intent(in) :: run_id
        process%meta%run_id = run_id
    end subroutine process_set_run_id

```

The following methods return basic process data that stay constant after initialization.

The process and IDs.

```

(Process: process: TBP)+≡
    procedure :: get_id => process_get_id
    procedure :: get_num_id => process_get_num_id
    procedure :: get_run_id => process_get_run_id
    procedure :: get_library_name => process_get_library_name

(Process: sub interfaces)+≡
    module function process_get_id (process) result (id)
        class(process_t), intent(in) :: process
        type(string_t) :: id
    end function process_get_id
    module function process_get_num_id (process) result (id)
        class(process_t), intent(in) :: process
        integer :: id
    end function process_get_num_id
    module function process_get_run_id (process) result (id)
        class(process_t), intent(in) :: process
        type(string_t) :: id
    end function process_get_run_id
    module function process_get_library_name (process) result (id)
        class(process_t), intent(in) :: process
        type(string_t) :: id
    end function process_get_library_name

```

```

<Process: procedures>+≡
  module function process_get_id (process) result (id)
    class(process_t), intent(in) :: process
    type(string_t) :: id
    id = process%meta%id
  end function process_get_id

  module function process_get_num_id (process) result (id)
    class(process_t), intent(in) :: process
    integer :: id
    id = process%meta%num_id
  end function process_get_num_id

  module function process_get_run_id (process) result (id)
    class(process_t), intent(in) :: process
    type(string_t) :: id
    id = process%meta%run_id
  end function process_get_run_id

  module function process_get_library_name (process) result (id)
    class(process_t), intent(in) :: process
    type(string_t) :: id
    id = process%meta%lib_name
  end function process_get_library_name

```

The number of incoming particles.

```

<Process: process: TBP>+≡
  procedure :: get_n_in => process_get_n_in

<Process: sub interfaces>+≡
  module function process_get_n_in (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
  end function process_get_n_in

<Process: procedures>+≡
  module function process_get_n_in (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%config%n_in
  end function process_get_n_in

```

The number of MCI data sets.

```

<Process: process: TBP>+≡
  procedure :: get_n_mci => process_get_n_mci

<Process: sub interfaces>+≡
  module function process_get_n_mci (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
  end function process_get_n_mci

<Process: procedures>+≡
  module function process_get_n_mci (process) result (n)
    class(process_t), intent(in) :: process

```

```

integer :: n
n = process%config%n_mci
end function process_get_n_mci

```

The number of process components, total.

```

(Process: process: TBP)+≡
  procedure :: get_n_components => process_get_n_components

(Process: sub interfaces)+≡
  module function process_get_n_components (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
  end function process_get_n_components

(Process: procedures)+≡
  module function process_get_n_components (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%meta%n_components
  end function process_get_n_components

```

The number of process terms, total.

```

(Process: process: TBP)+≡
  procedure :: get_n_terms => process_get_n_terms

(Process: sub interfaces)+≡
  module function process_get_n_terms (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
  end function process_get_n_terms

(Process: procedures)+≡
  module function process_get_n_terms (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%config%n_terms
  end function process_get_n_terms

```

Return the indices of the components that belong to a specific MCI entry.

```

(Process: process: TBP)+≡
  procedure :: get_i_component => process_get_i_component

(Process: sub interfaces)+≡
  module subroutine process_get_i_component (process, i_mci, i_component)
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
    integer, dimension(:), intent(out), allocatable :: i_component
  end subroutine process_get_i_component

(Process: procedures)+≡
  module subroutine process_get_i_component (process, i_mci, i_component)
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
    integer, dimension(:), intent(out), allocatable :: i_component
    associate (mci_entry => process%mci_entry(i_mci))

```



```

        allocate (i_component (size (mci_entry%i_component)))
        i_component = mci_entry%i_component
    end associate
end subroutine process_get_i_component

```

Return the ID of a specific component.

```

(Process: process: TBP)+≡
    procedure :: get_component_id => process_get_component_id

(Process: sub interfaces)+≡
    module function process_get_component_id (process, i_component) result (id)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        type(string_t) :: id
    end function process_get_component_id

(Process: procedures)+≡
    module function process_get_component_id (process, i_component) result (id)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        type(string_t) :: id
        id = process%meta%component_id(i_component)
    end function process_get_component_id

```

Return a pointer to the definition of a specific component.

```

(Process: process: TBP)+≡
    procedure :: get_component_def_ptr => process_get_component_def_ptr

(Process: sub interfaces)+≡
    module function process_get_component_def_ptr &
        (process, i_component) result (ptr)
        type(process_component_def_t), pointer :: ptr
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_component_def_ptr

(Process: procedures)+≡
    module function process_get_component_def_ptr &
        (process, i_component) result (ptr)
        type(process_component_def_t), pointer :: ptr
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        ptr => process%config%process_def%get_component_def_ptr (i_component)
    end function process_get_component_def_ptr

```

These procedures extract and restore (by transferring the allocation) the process core. This is useful for changing process parameters from outside this module.

```

(Process: process: TBP)+≡
    procedure :: extract_core => process_extract_core
    procedure :: restore_core => process_restore_core

(Process: sub interfaces)+≡
    module subroutine process_extract_core (process, i_term, core)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_term

```

```

        class(prc_core_t), intent(inout), allocatable :: core
    end subroutine process_extract_core
    module subroutine process_restore_core (process, i_term, core)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_term
        class(prc_core_t), intent(inout), allocatable :: core
    end subroutine process_restore_core
<Process: procedures>+≡
    module subroutine process_extract_core (process, i_term, core)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_term
        class(prc_core_t), intent(inout), allocatable :: core
        integer :: i_core
        i_core = process%term(i_term)%i_core
        call move_alloc (from = process%core_entry(i_core)%core, to = core)
    end subroutine process_extract_core

    module subroutine process_restore_core (process, i_term, core)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_term
        class(prc_core_t), intent(inout), allocatable :: core
        integer :: i_core
        i_core = process%term(i_term)%i_core
        call move_alloc (from = core, to = process%core_entry(i_core)%core)
    end subroutine process_restore_core

```

The block of process constants.

```

<Process: process: TBP>+≡
    procedure :: get_constants => process_get_constants
<Process: sub interfaces>+≡
    module function process_get_constants (process, i_core) result (data)
        type(process_constants_t) :: data
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_core
    end function process_get_constants
<Process: procedures>+≡
    module function process_get_constants (process, i_core) result (data)
        type(process_constants_t) :: data
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_core
        data = process%core_entry(i_core)%core%data
    end function process_get_constants

<Process: process: TBP>+≡
    procedure :: get_config => process_get_config
<Process: sub interfaces>+≡
    module function process_get_config (process) result (config)
        type(process_config_data_t) :: config
        class(process_t), intent(in) :: process
    end function process_get_config

```

```

(Process: procedures)+≡
  module function process_get_config (process) result (config)
    type(process_config_data_t) :: config
    class(process_t), intent(in) :: process
    config = process%config
  end function process_get_config

```

Construct an MD5 sum for the constant data, including the NLO type.

For the NLO type NLO_MISMATCH, we pretend that this was NLO_SUBTRACTION instead.

TODO wk 2018: should not depend explicitly on NLO data.

```

(Process: process: TBP)+≡
  procedure :: get_md5sum_constants => process_get_md5sum_constants

(Process: sub interfaces)+≡
  module function process_get_md5sum_constants (process, i_component, &
    type_string, nlo_type) result (this_md5sum)
    character(32) :: this_md5sum
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    type(string_t), intent(in) :: type_string
    integer, intent(in) :: nlo_type
  end function process_get_md5sum_constants

(Process: procedures)+≡
  module function process_get_md5sum_constants (process, i_component, &
    type_string, nlo_type) result (this_md5sum)
    character(32) :: this_md5sum
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    type(string_t), intent(in) :: type_string
    integer, intent(in) :: nlo_type
    type(process_constants_t) :: data
    integer :: unit
    call process%env%fill_process_constants (process%meta%id, i_component, data)
    unit = data%fill_unit_for_md5sum (.false.)
    write (unit, '(A)') char(type_string)
    select case (nlo_type)
    case (NLO_MISMATCH)
      write (unit, '(IO)') NLO_SUBTRACTION
    case default
      write (unit, '(IO)') nlo_type
    end select
    rewind (unit)
    this_md5sum = md5sum (unit)
    close (unit)
  end function process_get_md5sum_constants

```

Return the set of outgoing flavors that are associated with a particular term.

We deduce this from the effective interaction.

```

(Process: process: TBP)+≡
  procedure :: get_term_flv_out => process_get_term_flv_out

```

```

(Process: sub interfaces)+≡
  module subroutine process_get_term_flv_out (process, i_term, flv)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_term
    type(flavor_t), dimension(:,,:), allocatable, intent(out) :: flv
  end subroutine process_get_term_flv_out

```

```

(Process: procedures)+≡
  module subroutine process_get_term_flv_out (process, i_term, flv)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_term
    type(flavor_t), dimension(:,,:), allocatable, intent(out) :: flv
    type(interaction_t), pointer :: int
    int => process%term(i_term)%int_eff
    if (.not. associated (int)) int => process%term(i_term)%int
    call int%get_flv_out (flv)
  end subroutine process_get_term_flv_out

```

Return true if there is any unstable particle in any of the process terms. We decide this based on the provided model instance, not the one that is stored in the process object.

```

(Process: process: TBP)+≡
  procedure :: contains_unstable => process_contains_unstable

```

```

(Process: sub interfaces)+≡
  module function process_contains_unstable (process, model) result (flag)
    class(process_t), intent(in) :: process
    class(model_data_t), intent(in), target :: model
    logical :: flag
  end function process_contains_unstable

```

```

(Process: procedures)+≡
  module function process_contains_unstable (process, model) result (flag)
    class(process_t), intent(in) :: process
    class(model_data_t), intent(in), target :: model
    logical :: flag
    integer :: i_term
    type(flavor_t), dimension(:,,:), allocatable :: flv
    flag = .false.
    do i_term = 1, process%get_n_terms ()
      call process%get_term_flv_out (i_term, flv)
      call flv%set_model (model)
      flag = .not. all (flv%is_stable ())
      deallocate (flv)
    end do
    if (flag) return
  end function process_contains_unstable

```

The nominal process energy.

```

(Process: process: TBP)+≡
  procedure :: get_sqrts => process_get_sqrts

```

```

(Process: sub interfaces)+≡
  module function process_get_sqrts (process) result (sqrts)
    class(process_t), intent(in) :: process

```

```

        real(default) :: sqrts
    end function process_get_sqrts

(Process: procedures)+≡
module function process_get_sqrts (process) result (sqrts)
    class(process_t), intent(in) :: process
    real(default) :: sqrts
    sqrts = process%beam_config%data%get_sqrts ()
end function process_get_sqrts

```

The lab-frame beam energy/energies..

```

(Process: process: TBP)+≡
    procedure :: get_energy => process_get_energy

(Process: sub interfaces)+≡
    module function process_get_energy (process) result (e)
        class(process_t), intent(in) :: process
        real(default), dimension(:), allocatable :: e
    end function process_get_energy

(Process: procedures)+≡
module function process_get_energy (process) result (e)
    class(process_t), intent(in) :: process
    real(default), dimension(:), allocatable :: e
    e = process%beam_config%data%get_energy ()
end function process_get_energy

```

The beam polarization in case of simple degrees.

```

(Process: process: TBP)+≡
    procedure :: get_polarization => process_get_polarization

(Process: sub interfaces)+≡
    module function process_get_polarization (process) result (pol)
        class(process_t), intent(in) :: process
        real(default), dimension(process%beam_config%data%n) :: pol
    end function process_get_polarization

(Process: procedures)+≡
module function process_get_polarization (process) result (pol)
    class(process_t), intent(in) :: process
    real(default), dimension(process%beam_config%data%n) :: pol
    pol = process%beam_config%data%get_polarization ()
end function process_get_polarization

```

```

(Process: process: TBP)+≡
    procedure :: get_meta => process_get_meta

(Process: sub interfaces)+≡
    module function process_get_meta (process) result (meta)
        type(process_metadata_t) :: meta
        class(process_t), intent(in) :: process
    end function process_get_meta

```

```

(Process: procedures)+≡
  module function process_get_meta (process) result (meta)
    type(process_metadata_t) :: meta
    class(process_t), intent(in) :: process
    meta = process%meta
  end function process_get_meta

(Process: process: TBP)+≡
  procedure :: has_matrix_element => process_has_matrix_element

(Process: sub interfaces)+≡
  module function process_has_matrix_element &
    (process, i, is_term_index) result (active)
    logical :: active
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: i
    logical, intent(in), optional :: is_term_index
  end function process_has_matrix_element

(Process: procedures)+≡
  module function process_has_matrix_element &
    (process, i, is_term_index) result (active)
    logical :: active
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: i
    logical, intent(in), optional :: is_term_index
    integer :: i_component
    logical :: is_term
    is_term = .false.
    if (present (i)) then
      if (present (is_term_index)) is_term = is_term_index
      if (is_term) then
        i_component = process%term(i)%i_component
      else
        i_component = i
      end if
      active = process%component(i_component)%active
    else
      active = any (process%component%active)
    end if
  end function process_has_matrix_element

```

Pointer to the beam data object.

```

(Process: process: TBP)+≡
  procedure :: get_beam_data_ptr => process_get_beam_data_ptr

(Process: sub interfaces)+≡
  module function process_get_beam_data_ptr (process) result (beam_data)
    class(process_t), intent(in), target :: process
    type(beam_data_t), pointer :: beam_data
  end function process_get_beam_data_ptr

(Process: procedures)+≡
  module function process_get_beam_data_ptr (process) result (beam_data)
    class(process_t), intent(in), target :: process

```

```

        type(beam_data_t), pointer :: beam_data
        beam_data => process%beam_config%data
    end function process_get_beam_data_ptr

    <Process: process: TBP>+≡
        procedure :: get_beam_config => process_get_beam_config

    <Process: sub interfaces>+≡
        module function process_get_beam_config (process) result (beam_config)
            type(process_beam_config_t) :: beam_config
            class(process_t), intent(in) :: process
        end function process_get_beam_config

    <Process: procedures>+≡
        module function process_get_beam_config (process) result (beam_config)
            type(process_beam_config_t) :: beam_config
            class(process_t), intent(in) :: process
            beam_config = process%beam_config
        end function process_get_beam_config

    <Process: process: TBP>+≡
        procedure :: get_beam_config_ptr => process_get_beam_config_ptr

    <Process: sub interfaces>+≡
        module function process_get_beam_config_ptr (process) result (beam_config)
            type(process_beam_config_t), pointer :: beam_config
            class(process_t), intent(in), target :: process
        end function process_get_beam_config_ptr

    <Process: procedures>+≡
        module function process_get_beam_config_ptr (process) result (beam_config)
            type(process_beam_config_t), pointer :: beam_config
            class(process_t), intent(in), target :: process
            beam_config => process%beam_config
        end function process_get_beam_config_ptr

    Get the PDF set currently in use, if any.

    <Process: process: TBP>+≡
        procedure :: get_pdf_set => process_get_pdf_set

    <Process: sub interfaces>+≡
        module function process_get_pdf_set (process) result (pdf_set)
            class(process_t), intent(in) :: process
            integer :: pdf_set
        end function process_get_pdf_set

    <Process: procedures>+≡
        module function process_get_pdf_set (process) result (pdf_set)
            class(process_t), intent(in) :: process
            integer :: pdf_set
            pdf_set = process%beam_config%get_pdf_set ()
        end function process_get_pdf_set

    <Process: process: TBP>+≡
        procedure :: pcm_contains_pdfs => process_pcm_contains_pdfs

```

```

(Process: sub interfaces)+≡
    module function process_pcm_contains_pdfs (process) result (has_pdfs)
        logical :: has_pdfs
        class(process_t), intent(in) :: process
    end function process_pcm_contains_pdfs

```

```

(Process: procedures)+≡
    module function process_pcm_contains_pdfs (process) result (has_pdfs)
        logical :: has_pdfs
        class(process_t), intent(in) :: process
        has_pdfs = process%pcm%has_pdfs
    end function process_pcm_contains_pdfs

```

Get the beam spectrum file currently in use, if any.

```

(Process: process: TBP)+≡
    procedure :: get_beam_file => process_get_beam_file

(Process: sub interfaces)+≡
    module function process_get_beam_file (process) result (file)
        class(process_t), intent(in) :: process
        type(string_t) :: file
    end function process_get_beam_file

(Process: procedures)+≡
    module function process_get_beam_file (process) result (file)
        class(process_t), intent(in) :: process
        type(string_t) :: file
        file = process%beam_config%get_beam_file ()
    end function process_get_beam_file

```

Pointer to the process variable list.

```

(Process: process: TBP)+≡
    procedure :: get_var_list_ptr => process_get_var_list_ptr

(Process: sub interfaces)+≡
    module function process_get_var_list_ptr (process) result (ptr)
        class(process_t), intent(in), target :: process
        type(var_list_t), pointer :: ptr
    end function process_get_var_list_ptr

(Process: procedures)+≡
    module function process_get_var_list_ptr (process) result (ptr)
        class(process_t), intent(in), target :: process
        type(var_list_t), pointer :: ptr
        ptr => process%env%get_var_list_ptr ()
    end function process_get_var_list_ptr

```

Pointer to the common model.

```

(Process: process: TBP)+≡
    procedure :: get_model_ptr => process_get_model_ptr

(Process: sub interfaces)+≡
    module function process_get_model_ptr (process) result (ptr)
        class(process_t), intent(in) :: process
        class(model_data_t), pointer :: ptr
    end function process_get_model_ptr

```



```

(Process: procedures)+≡
  module function process_get_model_ptr (process) result (ptr)
    class(process_t), intent(in) :: process
    class(model_data_t), pointer :: ptr
    ptr => process%config%model
  end function process_get_model_ptr

```

Use the embedded RNG factory to spawn a new random-number generator instance. (This modifies the state of the factory.)

```

(Process: process: TBP)+≡
  procedure :: make_rng => process_make_rng

(Process: sub interfaces)+≡
  module subroutine process_make_rng (process, rng)
    class(process_t), intent(inout) :: process
    class(rng_t), intent(out), allocatable :: rng
  end subroutine process_make_rng

(Process: procedures)+≡
  module subroutine process_make_rng (process, rng)
    class(process_t), intent(inout) :: process
    class(rng_t), intent(out), allocatable :: rng
    if (allocated (process%rng_factory)) then
      call process%rng_factory%make (rng)
    else
      call msg_bug ("Process: make rng: factory not allocated")
    end if
  end subroutine process_make_rng

```

30.4.10 Compute an amplitude

Each process variant should allow for computing an amplitude value directly, without generating a process instance.

The process component is selected by the index *i*. The term within the process component is selected by *j*. The momentum combination is transferred as the array *p*. The function sets the specific quantum state via the indices of a flavor *f*, helicity *h*, and color *c* combination. Each index refers to the list of flavor, helicity, and color states, respectively, as stored in the process data.

Optionally, we may set factorization and renormalization scale. If unset, the partonic c.m. energy is inserted.

The function checks arguments for validity. For invalid arguments (quantum states), we return zero.

```

(Process: process: TBP)+≡
  procedure :: compute_amplitude => process_compute_amplitude

(Process: sub interfaces)+≡
  module function process_compute_amplitude (process, i_core, i, j, p, &
    f, h, c, fac_scale, ren_scale, alpha_qcd_forced) result (amp)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_core
    integer, intent(in) :: i, j
    type(vector4_t), dimension(:), intent(in) :: p

```

```

integer, intent(in) :: f, h, c
real(default), intent(in), optional :: fac_scale, ren_scale
real(default), intent(in), allocatable, optional :: alpha_qcd_forced
complex(default) :: amp
end function process_compute_amplitude

<Process: procedures>+≡
module function process_compute_amplitude (process, i_core, i, j, p, &
    f, h, c, fac_scale, ren_scale, alpha_qcd_forced) result (amp)
class(process_t), intent(in), target :: process
integer, intent(in) :: i_core
integer, intent(in) :: i, j
type(vector4_t), dimension(:), intent(in) :: p
integer, intent(in) :: f, h, c
real(default), intent(in), optional :: fac_scale, ren_scale
real(default), intent(in), allocatable, optional :: alpha_qcd_forced
real(default) :: fscale, rscale
real(default), allocatable :: aqcd_forced
complex(default) :: amp
class(prc_core_t), pointer :: core
amp = 0
if (0 < i .and. i <= process%meta%n_components) then
    if (process%component(i)%active) then
        associate (core => process%core_entry(i_core)%core)
            associate (data => core%data)
                if (size(p) == data%n_in + data%n_out &
                    .and. 0 < f .and. f <= data%n_flv &
                    .and. 0 < h .and. h <= data%n_hel &
                    .and. 0 < c .and. c <= data%n_col) then
                    if (present (fac_scale)) then
                        fscale = fac_scale
                    else
                        fscale = sum (p(data%n_in+1:)) ** 1
                    end if
                    if (present (ren_scale)) then
                        rscale = ren_scale
                    else
                        rscale = fscale
                    end if
                    if (present (alpha_qcd_forced)) then
                        if (allocated (alpha_qcd_forced)) &
                            allocate (aqcd_forced, source = alpha_qcd_forced)
                        end if
                        amp = core%compute_amplitude (j, p, f, h, c, &
                            fscale, rscale, aqcd_forced)
                    end if
                end associate
            end associate
        end associate
    else
        amp = 0
    end if
end if
end function process_compute_amplitude

```

Sanity check for the process library. We abort the program if it has changed after process initialization.

```

(Process: process: TBP)+≡
    procedure :: check_library_sanity => process_check_library_sanity

(Process: sub interfaces)+≡
    module subroutine process_check_library_sanity (process)
        class(process_t), intent(in) :: process
    end subroutine process_check_library_sanity

(Process: procedures)+≡
    module subroutine process_check_library_sanity (process)
        class(process_t), intent(in) :: process
        call process%env%check_lib_sanity (process%meta)
    end subroutine process_check_library_sanity

```

Reset the association to a process library.

```

(Process: process: TBP)+≡
    procedure :: reset_library_ptr => process_reset_library_ptr

(Process: sub interfaces)+≡
    module subroutine process_reset_library_ptr (process)
        class(process_t), intent(inout) :: process
    end subroutine process_reset_library_ptr

(Process: procedures)+≡
    module subroutine process_reset_library_ptr (process)
        class(process_t), intent(inout) :: process
        call process%env%reset_lib_ptr ()
    end subroutine process_reset_library_ptr

(Process: process: TBP)+≡
    procedure :: set_counter_mci_entry => process_set_counter_mci_entry

(Process: sub interfaces)+≡
    module subroutine process_set_counter_mci_entry (process, i_mci, counter)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(process_counter_t), intent(in) :: counter
    end subroutine process_set_counter_mci_entry

(Process: procedures)+≡
    module subroutine process_set_counter_mci_entry (process, i_mci, counter)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(process_counter_t), intent(in) :: counter
        process%mci_entry(i_mci)%counter = counter
    end subroutine process_set_counter_mci_entry

```

This is for suppression of numerical noise in the integration results stored in the `process_mci_entry` type. As the error and efficiency enter the MD5 sum, we recompute it.

```

(Process: process: TBP)+≡
    procedure :: pacify => process_pacify

```

```

(Process: sub interfaces)+≡
    module subroutine process_pacify (process, efficiency_reset, error_reset)
        class(process_t), intent(inout) :: process
        logical, intent(in), optional :: efficiency_reset, error_reset
    end subroutine process_pacify

(Process: procedures)+≡
    module subroutine process_pacify (process, efficiency_reset, error_reset)
        class(process_t), intent(inout) :: process
        logical, intent(in), optional :: efficiency_reset, error_reset
        logical :: eff_reset, err_reset
        integer :: i
        eff_reset = .false.
        err_reset = .false.
        if (present (efficiency_reset)) eff_reset = efficiency_reset
        if (present (error_reset)) err_reset = error_reset
        if (allocated (process%mci_entry)) then
            do i = 1, size (process%mci_entry)
                call process%mci_entry(i)%results%pacify (efficiency_reset)
                if (allocated (process%mci_entry(i)%mci)) then
                    associate (mci => process%mci_entry(i)%mci)
                        if (process%mci_entry(i)%mci%error_known &
                            .and. err_reset) &
                            mci%error = 0
                        if (process%mci_entry(i)%mci%efficiency_known &
                            .and. eff_reset) &
                            mci%efficiency = 1
                        call mci%pacify (efficiency_reset, error_reset)
                        call mci%compute_md5sum ()
                    end associate
                end if
            end do
        end if
    end subroutine process_pacify

```

The following methods are used only in the unit tests; the access process internals directly that would otherwise be hidden.

```

(Process: process: TBP)+≡
    procedure :: test_allocate_sf_channels
    procedure :: test_set_component_sf_channel
    procedure :: test_get_mci_ptr

(Process: sub interfaces)+≡
    module subroutine test_allocate_sf_channels (process, n)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: n
    end subroutine test_allocate_sf_channels
    module subroutine test_set_component_sf_channel (process, c)
        class(process_t), intent(inout) :: process
        integer, dimension(:), intent(in) :: c
    end subroutine test_set_component_sf_channel
    module subroutine test_get_mci_ptr (process, mci)
        class(process_t), intent(in), target :: process
        class(mci_t), intent(out), pointer :: mci
    end subroutine test_get_mci_ptr

```

```

(Process: procedures)+≡
module subroutine test_allocate_sf_channels (process, n)
  class(process_t), intent(inout) :: process
  integer, intent(in) :: n
  call process%beam_config%allocate_sf_channels (n)
end subroutine test_allocate_sf_channels

module subroutine test_set_component_sf_channel (process, c)
  class(process_t), intent(inout) :: process
  integer, dimension(:), intent(in) :: c
  call process%component(1)%phs_config%set_sf_channel (c)
end subroutine test_set_component_sf_channel

module subroutine test_get_mci_ptr (process, mci)
  class(process_t), intent(in), target :: process
  class(mci_t), intent(out), pointer :: mci
  mci => process%mci_entry(1)%mci
end subroutine test_get_mci_ptr

(Process: process: TBP)+≡
procedure :: init_mci_work => process_init_mci_work

(Process: sub interfaces)+≡
module subroutine process_init_mci_work (process, mci_work, i)
  class(process_t), intent(in), target :: process
  type(mci_work_t), intent(out) :: mci_work
  integer, intent(in) :: i
end subroutine process_init_mci_work

(Process: procedures)+≡
module subroutine process_init_mci_work (process, mci_work, i)
  class(process_t), intent(in), target :: process
  type(mci_work_t), intent(out) :: mci_work
  integer, intent(in) :: i
  call mci_work%init (process%mci_entry(i))
end subroutine process_init_mci_work

```

Prepare the process core with type `test_me`, or otherwise the externally provided `type_string` version. The toy dispatchers as a procedure argument come handy, knowing that we need to support only the `test_me` and `template` matrix-element types. Gfortran 7/8/9 bug, has to remain in the main module:

```

(Process: process: TBP)+≡
procedure :: setup_test_cores => process_setup_test_cores

(Process: main procedures)+≡
subroutine dispatch_test_me_core (core, core_def, model, &
  helicity_selection, qcd, use_color_factors, has_beam_pol)
  use prc_test_core, only: test_t
  class(prc_core_t), allocatable, intent(inout) :: core
  class(prc_core_def_t), intent(in) :: core_def
  class(model_data_t), intent(in), target, optional :: model
  type(helicity_selection_t), intent(in), optional :: helicity_selection
  type(qcd_t), intent(in), optional :: qcd
  logical, intent(in), optional :: use_color_factors

```

```

        logical, intent(in), optional :: has_beam_pol
        allocate (test_t :: core)
    end subroutine dispatch_test_me_core

subroutine dispatch_template_core (core, core_def, model, &
    helicity_selection, qcd, use_color_factors, has_beam_pol)
    use prc_template_me, only: prc_template_me_t
    class(prc_core_t), allocatable, intent(inout) :: core
    class(prc_core_def_t), intent(in) :: core_def
    class(model_data_t), intent(in), target, optional :: model
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    type(qcd_t), intent(in), optional :: qcd
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
    allocate (prc_template_me_t :: core)
    select type (core)
    type is (prc_template_me_t)
        call core%set_parameters (model)
    end select
end subroutine dispatch_template_core

subroutine process_setup_test_cores (process, type_string)
    class(process_t), intent(inout) :: process
    class(prc_core_t), allocatable :: core
    type(string_t), intent(in), optional :: type_string
    if (present (type_string)) then
        select case (char (type_string))
        case ("template")
            call process%setup_cores (dispatch_template_core)
        case ("test_me")
            call process%setup_cores (dispatch_test_me_core)
        case default
            call msg_bug ("process setup test cores: unsupported type string")
        end select
    else
        call process%setup_cores (dispatch_test_me_core)
    end if
end subroutine process_setup_test_cores

<Process: process: TBP>+≡
    procedure :: get_connected_states => process_get_connected_states

<Process: sub interfaces>+≡
    module function process_get_connected_states (process, i_component, &
        connected_terms) result (connected)
        type(connected_state_t), dimension(:), allocatable :: connected
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        type(connected_state_t), dimension(:), intent(in) :: connected_terms
    end function process_get_connected_states

<Process: procedures>+≡
    module function process_get_connected_states (process, i_component, &
        connected_terms) result (connected)
        type(connected_state_t), dimension(:), allocatable :: connected

```

```

class(process_t), intent(in) :: process
integer, intent(in) :: i_component
type(connected_state_t), dimension(:), intent(in) :: connected_terms
integer :: i, i_conn
integer :: n_conn
n_conn = 0
do i = 1, process%get_n_terms ()
  if (process%term(i)%i_component == i_component) then
    n_conn = n_conn + 1
  end if
end do
allocate (connected (n_conn))
i_conn = 1
do i = 1, process%get_n_terms ()
  if (process%term(i)%i_component == i_component) then
    connected (i_conn) = connected_terms(i)
    i_conn = i_conn + 1
  end if
end do
end function process_get_connected_states

```

30.4.11 NLO specifics

These subroutines (and the NLO specific properties they work on) could potentially be moved to `pcm_nlo_t` and used more generically in `process_t` with an appropriate interface in `pcm_t`

TODO wk 2018: This is used only by event initialization, which deals with an incomplete process object.

```

(Process: process: TBP)+≡
  procedure :: init_nlo_settings => process_init_nlo_settings

(Process: sub interfaces)+≡
  module subroutine process_init_nlo_settings (process, var_list)
    class(process_t), intent(inout) :: process
    type(var_list_t), intent(in), target :: var_list
  end subroutine process_init_nlo_settings

(Process: procedures)+≡
  module subroutine process_init_nlo_settings (process, var_list)
    class(process_t), intent(inout) :: process
    type(var_list_t), intent(in), target :: var_list
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
      call pcm%init_nlo_settings (var_list)
      if (debug_active (D_SUBTRACTION) .or. debug_active (D_VIRTUAL)) &
        call pcm%settings%write ()
    class default
      call msg_fatal ("Attempt to set nlo_settings with a non-NLO pcm!")
    end select
  end subroutine process_init_nlo_settings

```

```

(Process: process: TBP)+≡
    generic :: get_nlo_type_component => get_nlo_type_component_single
    procedure :: get_nlo_type_component_single => &
        process_get_nlo_type_component_single

(Process: sub interfaces)+≡
    elemental module function process_get_nlo_type_component_single &
        (process, i_component) result (val)
        integer :: val
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_nlo_type_component_single

(Process: procedures)+≡
    elemental module function process_get_nlo_type_component_single &
        (process, i_component) result (val)
        integer :: val
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        val = process%component(i_component)%get_nlo_type ()
    end function process_get_nlo_type_component_single

(Process: process: TBP)+≡
    generic :: get_nlo_type_component => get_nlo_type_component_all
    procedure :: get_nlo_type_component_all => process_get_nlo_type_component_all

(Process: sub interfaces)+≡
    pure module function process_get_nlo_type_component_all &
        (process) result (val)
        integer, dimension(:), allocatable :: val
        class(process_t), intent(in) :: process
    end function process_get_nlo_type_component_all

(Process: procedures)+≡
    pure module function process_get_nlo_type_component_all (process) result (val)
        integer, dimension(:), allocatable :: val
        class(process_t), intent(in) :: process
        allocate (val (size (process%component)))
        val = process%component%get_nlo_type ()
    end function process_get_nlo_type_component_all

(Process: process: TBP)+≡
    procedure :: is_nlo_calculation => process_is_nlo_calculation

(Process: sub interfaces)+≡
    module function process_is_nlo_calculation (process) result (nlo)
        logical :: nlo
        class(process_t), intent(in) :: process
    end function process_is_nlo_calculation

(Process: procedures)+≡
    module function process_is_nlo_calculation (process) result (nlo)
        logical :: nlo
        class(process_t), intent(in) :: process
        select type (pcm => process%pcm)
        type is (pcm_nlo_t)

```



```

        nlo = .true.
    class default
        nlo = .false.
    end select
end function process_is_nlo_calculation

<Process: process: TBP>+≡
    procedure :: get_negative_sf => process_get_negative_sf

<Process: sub interfaces>+≡
    module function process_get_negative_sf (process) result (neg_sf)
        logical :: neg_sf
        class(process_t), intent(in) :: process
    end function process_get_negative_sf

<Process: procedures>+≡
    module function process_get_negative_sf (process) result (neg_sf)
        logical :: neg_sf
        class(process_t), intent(in) :: process
        neg_sf = process%config%process_def%get_negative_sf ()
    end function process_get_negative_sf

<Process: process: TBP>+≡
    procedure :: is_combined_nlo_integration &
        => process_is_combined_nlo_integration

<Process: sub interfaces>+≡
    module function process_is_combined_nlo_integration &
        (process) result (combined)
        logical :: combined
        class(process_t), intent(in) :: process
    end function process_is_combined_nlo_integration

<Process: procedures>+≡
    module function process_is_combined_nlo_integration &
        (process) result (combined)
        logical :: combined
        class(process_t), intent(in) :: process
        select type (pcm => process%pcm)
        type is (pcm_nlo_t)
            combined = pcm%settings%combined_integration
        class default
            combined = .false.
        end select
    end function process_is_combined_nlo_integration

<Process: process: TBP>+≡
    procedure :: component_is_real_finite => process_component_is_real_finite

<Process: sub interfaces>+≡
    pure module function process_component_is_real_finite &
        (process, i_component) result (val)
        logical :: val
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_component_is_real_finite

```

```

(Process: procedures)+≡
  pure module function process_component_is_real_finite &
    (process, i_component) result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    val = process%component(i_component)%component_type == COMP_REAL_FIN
  end function process_component_is_real_finite

```

Return nlo data of a process component

```

(Process: process: TBP)+≡
  procedure :: get_component_nlo_type => process_get_component_nlo_type

(Process: sub interfaces)+≡
  elemental module function process_get_component_nlo_type &
    (process, i_component) result (nlo_type)
    integer :: nlo_type
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
  end function process_get_component_nlo_type

(Process: procedures)+≡
  elemental module function process_get_component_nlo_type &
    (process, i_component) result (nlo_type)
    integer :: nlo_type
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    nlo_type = process%component(i_component)%config%get_nlo_type ()
  end function process_get_component_nlo_type

```

Return a pointer to the core that belongs to a component.

```

(Process: process: TBP)+≡
  procedure :: get_component_core_ptr => process_get_component_core_ptr

(Process: sub interfaces)+≡
  module function process_get_component_core_ptr &
    (process, i_component) result (core)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_component
    class(prc_core_t), pointer :: core
  end function process_get_component_core_ptr

(Process: procedures)+≡
  module function process_get_component_core_ptr &
    (process, i_component) result (core)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_component
    class(prc_core_t), pointer :: core
    integer :: i_core
    i_core = process%pcm%get_i_core(i_component)
    core => process%core_entry(i_core)%core
  end function process_get_component_core_ptr

```

```

<Process: process: TBP>+=
    procedure :: get_component_associated_born &
        => process_get_component_associated_born

<Process: sub interfaces>+=
    module function process_get_component_associated_born &
        (process, i_component) result (i_born)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        integer :: i_born
    end function process_get_component_associated_born

<Process: procedures>+=
    module function process_get_component_associated_born &
        (process, i_component) result (i_born)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        integer :: i_born
        i_born = process%component(i_component)%config%get_associated_born ()
    end function process_get_component_associated_born

<Process: process: TBP>+=
    procedure :: get_first_real_component => process_get_first_real_component

<Process: sub interfaces>+=
    module function process_get_first_real_component (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
    end function process_get_first_real_component

<Process: procedures>+=
    module function process_get_first_real_component (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        i_real = process%component(1)%config%get_associated_real ()
    end function process_get_first_real_component

<Process: process: TBP>+=
    procedure :: get_first_real_term => process_get_first_real_term

<Process: sub interfaces>+=
    module function process_get_first_real_term (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer :: i_component, i_term
    end function process_get_first_real_term

<Process: procedures>+=
    module function process_get_first_real_term (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer :: i_component, i_term
        i_component = process%component(1)%config%get_associated_real ()
        i_real = 0
        do i_term = 1, size (process%term)
            if (process%term(i_term)%i_component == i_component) then

```

```

        i_real = i_term
        exit
    end if
end do
    if (i_real == 0) call msg_fatal ("Did not find associated real term!")
end function process_get_first_real_term

(Process: process: TBP)+≡
    procedure :: get_associated_real_fin => process_get_associated_real_fin
(Process: sub interfaces)+≡
    elemental module function process_get_associated_real_fin &
        (process, i_component) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
    end function process_get_associated_real_fin
(Process: procedures)+≡
    elemental module function process_get_associated_real_fin &
        (process, i_component) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        i_real = process%component(i_component)%config%get_associated_real_fin ()
    end function process_get_associated_real_fin

(Process: process: TBP)+≡
    procedure :: select_i_term => process_select_i_term
(Process: sub interfaces)+≡
    pure module function process_select_i_term (process, i_mci) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
    end function process_select_i_term
(Process: procedures)+≡
    pure module function process_select_i_term (process, i_mci) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        integer :: i_component, i_sub
        i_component = process%mc_entry(i_mci)%i_component(1)
        i_term = process%component(i_component)%i_term(1)
        i_sub = process%term(i_term)%i_sub
        if (i_sub > 0) &
            i_term = process%term(i_sub)%i_term_global
    end function process_select_i_term

```

Would be better to do this at the level of the writer of the core but one has to bring NLO information there.

```

(Process: process: TBP)+≡
    procedure :: prepare_any_external_code &
        => process_prepare_any_external_code

```

```

<Process: sub interfaces>+=
    module subroutine process_prepare_any_external_code (process)
        class(process_t), intent(inout), target :: process
        end subroutine process_prepare_any_external_code

<Process: procedures>+=
    module subroutine process_prepare_any_external_code (process)
        class(process_t), intent(inout), target :: process
        integer :: i
        if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
            "process_prepare_external_code")
        associate (pcm => process%pcm)
            do i = 1, pcm%n_cores
                call pcm%prepare_any_external_code ( &
                    process%core_entry(i), i, &
                    process%get_library_name (), &
                    process%config%model, &
                    process%env%get_var_list_ptr ())
            end do
        end associate
    end subroutine process_prepare_any_external_code

```

30.5 Process config

```

<process_config.f90>=
<File header>

module process_config

<Use kinds>
<Use strings>
    use os_interface
    use sf_base
    use sf_mappings
    use mappings, only: mapping_defaults_t
    use phs_forests, only: phs_parameters_t
    use sm_qcd
    use integration_results
    use flavors
    use interactions
    use model_data
    use models
    use process_libraries
    use process_constants
    use prc_core
    use beams
    use mci_base
    use beam_structures
    use dispatch_beams, only: dispatch_qcd
    use phs_base
    use expr_base
    use variables

```

```

    <Standard module head>

    <Process config: public>

    <Process config: parameters>

    <Process config: types>

    interface
    <Process config: sub interfaces>
    end interface

contains

    <Process config: main procedures>

end module process_config

<process_config_sub.f90>≡
    <File header>

    submodule (process_config) process_config_s

        use format_utils, only: write_separator
        use io_units
        use diagnostics
        use md5
        use physics_defs
        use helicities
        use colors
        use quantum_numbers
        use state_matrices
        use prc_external
        use prc_openloops, only: prc_openloops_t
        use prc_threshold, only: prc_threshold_t
        use blha_olp_interfaces, only: prc_blha_t

        implicit none

contains

    <Process config: procedures>

end submodule process_config_s

```

Identifiers for the NLO setup.

```

<Process config: parameters>≡
    integer, parameter, public :: COMP_DEFAULT = 0
    integer, parameter, public :: COMP_REAL_FIN = 1
    integer, parameter, public :: COMP_MASTER = 2
    integer, parameter, public :: COMP_VIRT = 3
    integer, parameter, public :: COMP_REAL = 4
    integer, parameter, public :: COMP_REAL_SING = 5

```

```

integer, parameter, public :: COMP_MISMATCH = 6
integer, parameter, public :: COMP_PDF = 7
integer, parameter, public :: COMP_SUB = 8
integer, parameter, public :: COMP_RESUM = 9

```

30.5.1 Output selection flags

We declare a number of identifiers for write methods, so they only displays selected parts. The identifiers can be supplied to the `vlist` array argument of the standard F2008 derived-type writer call.

```

(Process config: parameters)+≡
  integer, parameter, public :: F_PACIFY = 1
  integer, parameter, public :: F_SHOW_VAR_LIST = 11
  integer, parameter, public :: F_SHOW_EXPRESSIONS = 12
  integer, parameter, public :: F_SHOW_LIB = 13
  integer, parameter, public :: F_SHOW_MODEL = 14
  integer, parameter, public :: F_SHOW_QCD = 15
  integer, parameter, public :: F_SHOW_OS_DATA = 16
  integer, parameter, public :: F_SHOW_RNG = 17
  integer, parameter, public :: F_SHOW_BEAMS = 18

```

This is a simple function that returns true if a flag value is present in `v_list`, but not its negative. If neither is present, it returns default.

```

(Process config: public)≡
  public :: flagged

(Process config: sub interfaces)≡
  module function flagged (v_list, id, def) result (flag)
    logical :: flag
    integer, dimension(:), intent(in) :: v_list
    integer, intent(in) :: id
    logical, intent(in), optional :: def
  end function flagged

(Process config: procedures)≡
  module function flagged (v_list, id, def) result (flag)
    logical :: flag
    integer, dimension(:), intent(in) :: v_list
    integer, intent(in) :: id
    logical, intent(in), optional :: def
    logical :: default_result
    default_result = .false.; if (present (def)) default_result = def
    if (default_result) then
      flag = all (v_list /= -id)
    else
      flag = all (v_list /= -id) .and. any (v_list == id)
    end if
  end function flagged

```

Related: if flag is set (unset), append value (its negative) to the `v_list`, respectively. `v_list` must be allocated.

```

(Process config: public)+≡
  public :: set_flag

```

```

<Process config: sub interfaces>+≡
    module subroutine set_flag (v_list, value, flag)
        integer, dimension(:), intent(inout), allocatable :: v_list
        integer, intent(in) :: value
        logical, intent(in), optional :: flag
    end subroutine set_flag
<Process config: procedures>+≡
    module subroutine set_flag (v_list, value, flag)
        integer, dimension(:), intent(inout), allocatable :: v_list
        integer, intent(in) :: value
        logical, intent(in), optional :: flag
        if (present (flag)) then
            if (flag) then
                v_list = [v_list, value]
            else
                v_list = [v_list, -value]
            end if
        end if
    end subroutine set_flag

```

30.5.2 Generic configuration data

This information concerns physical and technical properties of the process. It is fixed upon initialization, using data from the process specification and the variable list.

The number **n_in** is the number of incoming beam particles, simultaneously the number of incoming partons, 1 for a decay and 2 for a scattering process. (The number of outgoing partons may depend on the process component.)

The number **n_components** is the number of components that constitute the current process.

The number **n_terms** is the number of distinct contributions to the scattering matrix that constitute the current process. Each component may generate several terms.

The number **n_mci** is the number of independent MC integration configurations that this process uses. Distinct process components that share a MCI configuration may be combined pointwise. (Nevertheless, a given MC variable set may correspond to several “nearby” kinematical configurations.) This is also the number of distinct sampling-function results that this process can generate. Process components that use distinct variable sets are added only once after an integration pass has completed.

The **model** pointer identifies the physics model and its parameters. This is a pointer to an external object.

Various **parse_node_t** objects are taken from the SINDARIN input. They encode expressions for evaluating cuts and scales. The workspaces for evaluating those expressions are set up in the **effective_state** subobjects. Note that these are really pointers, so the actual nodes are not stored inside the process object.

The **md5sum** is taken and used to verify the process configuration when re-reading data from file.

```

<Process config: public>+≡

```



```

public :: process_config_data_t
<Process config: types>≡
type :: process_config_data_t
  class(process_def_t), pointer :: process_def => null ()
  integer :: n_in = 0
  integer :: n_components = 0
  integer :: n_terms = 0
  integer :: n_mci = 0
  type(string_t) :: model_name
  class(model_data_t), pointer :: model => null ()
  type(qcd_t) :: qcd
  class(expr_factory_t), allocatable :: ef_cuts
  class(expr_factory_t), allocatable :: ef_scale
  class(expr_factory_t), allocatable :: ef_fac_scale
  class(expr_factory_t), allocatable :: ef_ren_scale
  class(expr_factory_t), allocatable :: ef_weight
  character(32) :: md5sum = ""
contains
  <Process config: process config data: TBP>
end type process_config_data_t

```

Here, we may compress the expressions for cuts etc.

```

<Process config: process config data: TBP>≡
  procedure :: write => process_config_data_write

<Process config: sub interfaces>+≡
  module subroutine process_config_data_write &
    (config, u, counters, model, expressions)
    class(process_config_data_t), intent(in) :: config
    integer, intent(in) :: u
    logical, intent(in) :: counters
    logical, intent(in) :: model
    logical, intent(in) :: expressions
  end subroutine process_config_data_write

<Process config: procedures>+≡
  module subroutine process_config_data_write &
    (config, u, counters, model, expressions)
    class(process_config_data_t), intent(in) :: config
    integer, intent(in) :: u
    logical, intent(in) :: counters
    logical, intent(in) :: model
    logical, intent(in) :: expressions
    write (u, "(1x,A)") "Configuration data:"
    if (counters) then
      write (u, "(3x,A,I0)") "Number of incoming particles = ", &
        config%n_in
      write (u, "(3x,A,I0)") "Number of process components = ", &
        config%n_components
      write (u, "(3x,A,I0)") "Number of process terms      = ", &
        config%n_terms
      write (u, "(3x,A,I0)") "Number of MCI configurations = ", &
        config%n_mci
    end if

```

```

if (associated (config%model)) then
  write (u, "(3x,A,A)") "Model = ", char (config%model_name)
  if (model) then
    call write_separator (u)
    call config%model%write (u)
    call write_separator (u)
  end if
else
  write (u, "(3x,A,A,A)") "Model = ", char (config%model_name), &
    " [not associated]"
end if
call config%qcd%write (u, show_md5sum = .false.)
call write_separator (u)
if (expressions) then
  if (allocated (config%ef_cuts)) then
    call write_separator (u)
    write (u, "(3x,A)") "Cut expression:"
    call config%ef_cuts%write (u)
  end if
  if (allocated (config%ef_scale)) then
    call write_separator (u)
    write (u, "(3x,A)") "Scale expression:"
    call config%ef_scale%write (u)
  end if
  if (allocated (config%ef_fac_scale)) then
    call write_separator (u)
    write (u, "(3x,A)") "Factorization scale expression:"
    call config%ef_fac_scale%write (u)
  end if
  if (allocated (config%ef_ren_scale)) then
    call write_separator (u)
    write (u, "(3x,A)") "Renormalization scale expression:"
    call config%ef_ren_scale%write (u)
  end if
  if (allocated (config%ef_weight)) then
    call write_separator (u)
    write (u, "(3x,A)") "Weight expression:"
    call config%ef_weight%write (u)
  end if
else
  call write_separator (u)
  write (u, "(3x,A)") "Expressions (cut, scales, weight): [not shown]"
end if
if (config%md5sum /= "") then
  call write_separator (u)
  write (u, "(3x,A,A,A)") "MD5 sum (config) = ', config%md5sum, '"
end if
end subroutine process_config_data_write

```

Initialize. We use information from the process metadata and from the process library, given the process ID. We also store the currently active OS data set.

The model pointer references the model data within the `env` record. That should be an instance of the global model.

We initialize the QCD object, unless the environment information is unavailable (unit tests).

The RNG factory object is imported by moving the allocation. Gfortran 7/8/9 bug: has to remain in the main module:

```

(Process config: process config data: TBP)+≡
  procedure :: init => process_config_data_init

(Process config: main procedures)≡
  subroutine process_config_data_init (config, meta, env)
    class(process_config_data_t), intent(out) :: config
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    config%process_def => env%lib%get_process_def_ptr (meta%id)
    config%n_in = config%process_def%get_n_in ()
    config%n_components = size (meta%component_id)
    config%model => env%get_model_ptr ()
    config%model_name = config%model%get_name ()
    if (env%got_var_list ()) then
      call dispatch_qcd &
        (config%qcd, env%get_var_list_ptr (), env%get_os_data ())
    end if
  end subroutine process_config_data_init

```

Return a copy of the QCD data block.

```

(Process config: process config data: TBP)+≡
  procedure :: get_qcd => process_config_data_get_qcd

(Process config: sub interfaces)+≡
  module function process_config_data_get_qcd (config) result (qcd)
    class(process_config_data_t), intent(in) :: config
    type(qcd_t) :: qcd
  end function process_config_data_get_qcd

(Process config: procedures)+≡
  module function process_config_data_get_qcd (config) result (qcd)
    class(process_config_data_t), intent(in) :: config
    type(qcd_t) :: qcd
    qcd = config%qcd
  end function process_config_data_get_qcd

```

Compute the MD5 sum of the configuration data. This encodes, in particular, the model and the expressions for cut, scales, weight, etc. It should not contain the IDs and number of components, etc., since the MD5 sum should be useful for integrating individual components.

This is done only once. If the MD5 sum is nonempty, the calculation is skipped.

```

(Process config: process config data: TBP)+≡
  procedure :: compute_md5sum => process_config_data_compute_md5sum

(Process config: sub interfaces)+≡
  module subroutine process_config_data_compute_md5sum (config)
    class(process_config_data_t), intent(inout) :: config
  end subroutine process_config_data_compute_md5sum

```

```

<Process config: procedures>+≡
  module subroutine process_config_data_compute_md5sum (config)
    class(process_config_data_t), intent(inout) :: config
    integer :: u
    if (config%md5sum == "") then
      u = free_unit ()
      open (u, status = "scratch", action = "readwrite")
      call config%write (u, counters = .false., &
        model = .true., expressions = .true.)
      rewind (u)
      config%md5sum = md5sum (u)
      close (u)
    end if
  end subroutine process_config_data_compute_md5sum

<Process config: process config data: TBP>+≡
  procedure :: get_md5sum => process_config_data_get_md5sum

<Process config: sub interfaces>+≡
  pure module function process_config_data_get_md5sum (config) result (md5)
    character(32) :: md5
    class(process_config_data_t), intent(in) :: config
  end function process_config_data_get_md5sum

<Process config: procedures>+≡
  pure module function process_config_data_get_md5sum (config) result (md5)
    character(32) :: md5
    class(process_config_data_t), intent(in) :: config
    md5 = config%md5sum
  end function process_config_data_get_md5sum

```

30.5.3 Environment

This record stores a snapshot of the process environment at the point where the process object is created.

Model and variable list are implemented as pointer, so they always have the **target** attribute.

For unit-testing purposes, setting the var list is optional. If not set, the pointer is null.

```

<Process config: public>+≡
  public :: process_environment_t

<Process config: types>+≡
  type :: process_environment_t
  private
    type(model_t), pointer :: model => null ()
    type(var_list_t), pointer :: var_list => null ()
    logical :: var_list_is_set = .false.
    type(process_library_t), pointer :: lib => null ()
    type(beam_structure_t) :: beam_structure
    type(os_data_t) :: os_data
  contains
    <Process config: process environment: TBP>

```

```
end type process_environment_t
```

Model and local var list are snapshots and need a finalizer.

```
<Process config: process environment: TBP>≡
  procedure :: final => process_environment_final

<Process config: sub interfaces>+≡
  module subroutine process_environment_final (env)
    class(process_environment_t), intent(inout) :: env
  end subroutine process_environment_final

<Process config: procedures>+≡
  module subroutine process_environment_final (env)
    class(process_environment_t), intent(inout) :: env
    if (associated (env%model)) then
      call env%model%final ()
      deallocate (env%model)
    end if
    if (associated (env%var_list)) then
      call env%var_list%final (follow_link=.true.)
      deallocate (env%var_list)
    end if
  end subroutine process_environment_final
```

Output, DTIO compatible.

```
<Process config: process environment: TBP>+≡
  procedure :: write => process_environment_write
  procedure :: write_formatted => process_environment_write_formatted
  ! generic :: write (formatted) => write_formatted

<Process config: sub interfaces>+≡
  module subroutine process_environment_write (env, unit, &
    show_var_list, show_model, show_lib, show_beams, show_os_data)
    class(process_environment_t), intent(in) :: env
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_var_list
    logical, intent(in), optional :: show_model
    logical, intent(in), optional :: show_lib
    logical, intent(in), optional :: show_beams
    logical, intent(in), optional :: show_os_data
  end subroutine process_environment_write

<Process config: procedures>+≡
  module subroutine process_environment_write (env, unit, &
    show_var_list, show_model, show_lib, show_beams, show_os_data)
    class(process_environment_t), intent(in) :: env
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_var_list
    logical, intent(in), optional :: show_model
    logical, intent(in), optional :: show_lib
    logical, intent(in), optional :: show_beams
    logical, intent(in), optional :: show_os_data
    integer :: u, iostat
    integer, dimension(:), allocatable :: v_list
    character(0) :: iomsg
```

```

u = given_output_unit (unit)
allocate (v_list (0))
call set_flag (v_list, F_SHOW_VAR_LIST, show_var_list)
call set_flag (v_list, F_SHOW_MODEL, show_model)
call set_flag (v_list, F_SHOW_LIB, show_lib)
call set_flag (v_list, F_SHOW_BEAMS, show_beams)
call set_flag (v_list, F_SHOW_OS_DATA, show_os_data)
call env%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
end subroutine process_environment_write

```

DTIO standard write.

(Process config: sub interfaces)+≡

```

module subroutine process_environment_write_formatted &
  (dtv, unit, iotype, v_list, iostat, iomsg)
class(process_environment_t), intent(in) :: dtv
integer, intent(in) :: unit
character(*), intent(in) :: iotype
integer, dimension(:), intent(in) :: v_list
integer, intent(out) :: iostat
character(*), intent(inout) :: iomsg
end subroutine process_environment_write_formatted

```

(Process config: procedures)+≡

```

module subroutine process_environment_write_formatted &
  (dtv, unit, iotype, v_list, iostat, iomsg)
class(process_environment_t), intent(in) :: dtv
integer, intent(in) :: unit
character(*), intent(in) :: iotype
integer, dimension(:), intent(in) :: v_list
integer, intent(out) :: iostat
character(*), intent(inout) :: iomsg
associate (env => dtv)
  if (flagged (v_list, F_SHOW_VAR_LIST, .true.)) then
    write (unit, "(1x,A)") "Variable list:"
    if (associated (env%var_list)) then
      call write_separator (unit)
      call env%var_list%write (unit)
    else
      write (unit, "(3x,A)") "[not allocated]"
    end if
    call write_separator (unit)
  end if
  if (flagged (v_list, F_SHOW_MODEL, .true.)) then
    write (unit, "(1x,A)") "Model:"
    if (associated (env%model)) then
      call write_separator (unit)
      call env%model%write (unit)
    else
      write (unit, "(3x,A)") "[not allocated]"
    end if
    call write_separator (unit)
  end if
  if (flagged (v_list, F_SHOW_LIB, .true.)) then
    write (unit, "(1x,A)") "Process library:"

```

```

        if (associated (env%lib)) then
            call write_separator (unit)
            call env%lib%write (unit)
        else
            write (unit, "(3x,A)") "[not allocated]"
        end if
    end if
    if (flagged (v_list, F_SHOW_BEAMS, .true.)) then
        call write_separator (unit)
        call env%beam_structure%write (unit)
    end if
    if (flagged (v_list, F_SHOW_OS_DATA, .true.)) then
        write (unit, "(1x,A)") "Operating-system data:"
        call write_separator (unit)
        call env%os_data%write (unit)
    end if
end associate
iostat = 0
end subroutine process_environment_write_formatted

```

Initialize: Make a snapshot of the provided model. Make a link to the current process library.

Also make a snapshot of the variable list, if provided. If none is provided, there is an empty variable list nevertheless, so a pointer lookup does not return null.

If no beam structure is provided, the beam-structure member is empty and will yield a number of zero beams when queried.

<Process config: process environment: TBP>+≡

```

    procedure :: init => process_environment_init

```

<Process config: sub interfaces>+≡

```

    module subroutine process_environment_init &
        (env, model, lib, os_data, var_list, beam_structure)
    class(process_environment_t), intent(out) :: env
    type(model_t), intent(in), target :: model
    type(process_library_t), intent(in), target :: lib
    type(os_data_t), intent(in) :: os_data
    type(var_list_t), intent(in), target, optional :: var_list
    type(beam_structure_t), intent(in), optional :: beam_structure
    end subroutine process_environment_init

```

<Process config: procedures>+≡

```

    module subroutine process_environment_init &
        (env, model, lib, os_data, var_list, beam_structure)
    class(process_environment_t), intent(out) :: env
    type(model_t), intent(in), target :: model
    type(process_library_t), intent(in), target :: lib
    type(os_data_t), intent(in) :: os_data
    type(var_list_t), intent(in), target, optional :: var_list
    type(beam_structure_t), intent(in), optional :: beam_structure
    allocate (env%model)
    call env%model%init_instance (model)
    env%lib => lib
    env%os_data = os_data

```

```

allocate (env%var_list)
if (present (var_list)) then
  call env%var_list%init_snapshot (var_list, follow_link=.true.)
  env%var_list_is_set = .true.
end if
if (present (beam_structure)) then
  env%beam_structure = beam_structure
end if
end subroutine process_environment_init

```

Indicate whether a variable list has been provided upon initialization.

```

(Process config: process environment: TBP)+≡
  procedure :: got_var_list => process_environment_got_var_list

(Process config: sub interfaces)+≡
  module function process_environment_got_var_list (env) result (flag)
    class(process_environment_t), intent(in) :: env
    logical :: flag
  end function process_environment_got_var_list

(Process config: procedures)+≡
  module function process_environment_got_var_list (env) result (flag)
    class(process_environment_t), intent(in) :: env
    logical :: flag
    flag = env%var_list_is_set
  end function process_environment_got_var_list

```

Return a pointer to the variable list.

```

(Process config: process environment: TBP)+≡
  procedure :: get_var_list_ptr => process_environment_get_var_list_ptr

(Process config: sub interfaces)+≡
  module function process_environment_get_var_list_ptr (env) result (var_list)
    class(process_environment_t), intent(in) :: env
    type(var_list_t), pointer :: var_list
  end function process_environment_get_var_list_ptr

(Process config: procedures)+≡
  module function process_environment_get_var_list_ptr (env) result (var_list)
    class(process_environment_t), intent(in) :: env
    type(var_list_t), pointer :: var_list
    var_list => env%var_list
  end function process_environment_get_var_list_ptr

```

Return a pointer to the model, if it exists.

```

(Process config: process environment: TBP)+≡
  procedure :: get_model_ptr => process_environment_get_model_ptr

(Process config: sub interfaces)+≡
  module function process_environment_get_model_ptr (env) result (model)
    class(process_environment_t), intent(in) :: env
    type(model_t), pointer :: model
  end function process_environment_get_model_ptr

```



```

(Process config: procedures)+≡
  module function process_environment_get_model_ptr (env) result (model)
    class(process_environment_t), intent(in) :: env
    type(model_t), pointer :: model
    model => env%model
  end function process_environment_get_model_ptr

```

Return the process library pointer.

```

(Process config: process environment: TBP)+≡
  procedure :: get_lib_ptr => process_environment_get_lib_ptr

(Process config: sub interfaces)+≡
  module function process_environment_get_lib_ptr (env) result (lib)
    class(process_environment_t), intent(inout) :: env
    type(process_library_t), pointer :: lib
  end function process_environment_get_lib_ptr

(Process config: procedures)+≡
  module function process_environment_get_lib_ptr (env) result (lib)
    class(process_environment_t), intent(inout) :: env
    type(process_library_t), pointer :: lib
    lib => env%lib
  end function process_environment_get_lib_ptr

```

Clear the process library pointer, in case the library is deleted.

```

(Process config: process environment: TBP)+≡
  procedure :: reset_lib_ptr => process_environment_reset_lib_ptr

(Process config: sub interfaces)+≡
  module subroutine process_environment_reset_lib_ptr (env)
    class(process_environment_t), intent(inout) :: env
  end subroutine process_environment_reset_lib_ptr

(Process config: procedures)+≡
  module subroutine process_environment_reset_lib_ptr (env)
    class(process_environment_t), intent(inout) :: env
    env%lib => null ()
  end subroutine process_environment_reset_lib_ptr

```

Check whether the process library has changed, in case the library is recompiled, etc.

```

(Process config: process environment: TBP)+≡
  procedure :: check_lib_sanity => process_environment_check_lib_sanity

(Process config: sub interfaces)+≡
  module subroutine process_environment_check_lib_sanity (env, meta)
    class(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
  end subroutine process_environment_check_lib_sanity

(Process config: procedures)+≡
  module subroutine process_environment_check_lib_sanity (env, meta)
    class(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
    if (associated (env%lib)) then

```

```

        if (env%lib%get_update_counter () /= meta%lib_update_counter) then
            call msg_fatal ("Process '" // char (meta%id) &
                // "': library has been recompiled after integration")
        end if
    end if
end if
end subroutine process_environment_check_lib_sanity

```

Fill the data block using the appropriate process-library access entry.

```

(Process config: process environment: TBP)+≡
    procedure :: fill_process_constants => &
        process_environment_fill_process_constants

(Process config: sub interfaces)+≡
    module subroutine process_environment_fill_process_constants &
        (env, id, i_component, data)
        class(process_environment_t), intent(in) :: env
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
    end subroutine process_environment_fill_process_constants

(Process config: procedures)+≡
    module subroutine process_environment_fill_process_constants &
        (env, id, i_component, data)
        class(process_environment_t), intent(in) :: env
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
        call env%lib%fill_constants (id, i_component, data)
    end subroutine process_environment_fill_process_constants

```

Return the entire beam structure.

```

(Process config: process environment: TBP)+≡
    procedure :: get_beam_structure => process_environment_get_beam_structure

(Process config: sub interfaces)+≡
    module function process_environment_get_beam_structure &
        (env) result (beam_structure)
        class(process_environment_t), intent(in) :: env
        type(beam_structure_t) :: beam_structure
    end function process_environment_get_beam_structure

(Process config: procedures)+≡
    module function process_environment_get_beam_structure &
        (env) result (beam_structure)
        class(process_environment_t), intent(in) :: env
        type(beam_structure_t) :: beam_structure
        beam_structure = env%beam_structure
    end function process_environment_get_beam_structure

```

Check the beam structure for PDFs.

```

(Process config: process environment: TBP)+≡
    procedure :: has_pdfs => process_environment_has_pdfs

```

```

<Process config: sub interfaces>+≡
    module function process_environment_has_pdfs (env) result (flag)
        class(process_environment_t), intent(in) :: env
        logical :: flag
    end function process_environment_has_pdfs

```

```

<Process config: procedures>+≡
    module function process_environment_has_pdfs (env) result (flag)
        class(process_environment_t), intent(in) :: env
        logical :: flag
        flag = env%beam_structure%has_pdf ()
    end function process_environment_has_pdfs

```

Check the beam structure for polarized beams.

```

<Process config: process environment: TBP>+≡
    procedure :: has_polarized_beams => process_environment_has_polarized_beams

<Process config: sub interfaces>+≡
    module function process_environment_has_polarized_beams (env) result (flag)
        class(process_environment_t), intent(in) :: env
        logical :: flag
    end function process_environment_has_polarized_beams

<Process config: procedures>+≡
    module function process_environment_has_polarized_beams (env) result (flag)
        class(process_environment_t), intent(in) :: env
        logical :: flag
        flag = env%beam_structure%has_polarized_beams ()
    end function process_environment_has_polarized_beams

```

Return a copy of the OS data block.

```

<Process config: process environment: TBP>+≡
    procedure :: get_os_data => process_environment_get_os_data

<Process config: sub interfaces>+≡
    module function process_environment_get_os_data (env) result (os_data)
        class(process_environment_t), intent(in) :: env
        type(os_data_t) :: os_data
    end function process_environment_get_os_data

<Process config: procedures>+≡
    module function process_environment_get_os_data (env) result (os_data)
        class(process_environment_t), intent(in) :: env
        type(os_data_t) :: os_data
        os_data = env%os_data
    end function process_environment_get_os_data

```

30.5.4 Metadata

This information describes the process. It is fixed upon initialization.

The id string is the name of the process object, as given by the user. The matrix element generator will use this string for naming Fortran procedures and types, so it should qualify as a Fortran name.

The `num_id` is meaningful if nonzero. It is used for communication with external programs or file standards which do not support string IDs.

The `run_id` string distinguishes among several runs for the same process. It identifies process instances with respect to adapted integration grids and similar run-specific data. The run ID is kept when copying processes for creating instances, however, so it does not distinguish event samples.

The `lib_name` identifies the process library where the process definition and the process driver are located.

The `lib_index` is the index of entry in the process library that corresponds to the current process.

The `component_id` array identifies the individual process components.

The `component_description` is an array of human-readable strings that characterize the process components, for instance `a, b => c, d`.

The `active` mask array marks those components which are active. The others are skipped.

```

(Process config: public)+≡
    public :: process_metadata_t

(Process config: types)+≡
    type :: process_metadata_t
        integer :: type = PRC_UNKNOWN
        type(string_t) :: id
        integer :: num_id = 0
        type(string_t) :: run_id
        type(string_t), allocatable :: lib_name
        integer :: lib_update_counter = 0
        integer :: lib_index = 0
        integer :: n_components = 0
        type(string_t), dimension(:), allocatable :: component_id
        type(string_t), dimension(:), allocatable :: component_description
        logical, dimension(:), allocatable :: active
    contains
        (Process config: process metadata: TBP)
    end type process_metadata_t

```

Output: ID and run ID. We write the variable list only upon request.

```

(Process config: process metadata: TBP)≡
    procedure :: write => process_metadata_write

(Process config: sub interfaces)+≡
    module subroutine process_metadata_write (meta, u, screen)
        class(process_metadata_t), intent(in) :: meta
        integer, intent(in) :: u
        logical, intent(in) :: screen
    end subroutine process_metadata_write

(Process config: procedures)+≡
    module subroutine process_metadata_write (meta, u, screen)
        class(process_metadata_t), intent(in) :: meta
        integer, intent(in) :: u
        logical, intent(in) :: screen
        integer :: i
        select case (meta%type)
        case (PRC_UNKNOWN)

```

```

        if (screen) then
            write (msg_buffer, "(A)") "Process [undefined]"
        else
            write (u, "(1x,A)") "Process [undefined]"
        end if
    return
case (PRC_DECAY)
    if (screen) then
        write (msg_buffer, "(A,1x,A,A,A)") "Process [decay]:", &
            "'", char (meta%id), "'"
    else
        write (u, "(1x,A)", advance="no") "Process [decay]:"
    end if
case (PRC_SCATTERING)
    if (screen) then
        write (msg_buffer, "(A,1x,A,A,A)") "Process [scattering]:", &
            "'", char (meta%id), "'"
    else
        write (u, "(1x,A)", advance="no") "Process [scattering]:"
    end if
case default
    call msg_bug ("process_write: undefined process type")
end select
if (screen) then
    call msg_message ()
else
    write (u, "(1x,A,A,A)") "'", char (meta%id), "'"
end if
if (meta%num_id /= 0) then
    if (screen) then
        write (msg_buffer, "(2x,A,I0)") "ID (num)      = ", meta%num_id
        call msg_message ()
    else
        write (u, "(3x,A,I0)") "ID (num)      = ", meta%num_id
    end if
end if
if (screen) then
    if (meta%run_id /= "") then
        write (msg_buffer, "(2x,A,A,A)") "Run ID      = '", &
            char (meta%run_id), "'"
        call msg_message ()
    end if
else
    write (u, "(3x,A,A,A)") "Run ID      = '", char (meta%run_id), "'"
end if
if (allocated (meta%lib_name)) then
    if (screen) then
        write (msg_buffer, "(2x,A,A,A)") "Library name = '", &
            char (meta%lib_name), "'"
        call msg_message ()
    else
        write (u, "(3x,A,A,A)") "Library name = '", &
            char (meta%lib_name), "'"
    end if
end if

```

```

else
  if (screen) then
    write (msg_buffer, "(2x,A)") "Library name = [not associated]"
    call msg_message ()
  else
    write (u, "(3x,A)") "Library name = [not associated]"
  end if
end if
if (screen) then
  write (msg_buffer, "(2x,A,I0)") "Process index = ", meta%lib_index
  call msg_message ()
else
  write (u, "(3x,A,I0)") "Process index = ", meta%lib_index
end if
if (allocated (meta%component_id)) then
  if (screen) then
    if (any (meta%active)) then
      write (msg_buffer, "(2x,A)") "Process components:"
    else
      write (msg_buffer, "(2x,A)") "Process components: [none]"
    end if
    call msg_message ()
  else
    write (u, "(3x,A)") "Process components:"
  end if
  do i = 1, size (meta%component_id)
    if (.not. meta%active(i)) cycle
    if (screen) then
      write (msg_buffer, "(4x,I0,9A)") i, ": ', &
        char (meta%component_id (i)), "' : ", &
        char (meta%component_description (i))
      call msg_message ()
    else
      write (u, "(5x,I0,9A)") i, ": ', &
        char (meta%component_id (i)), "' : ", &
        char (meta%component_description (i))
    end if
  end do
end if
if (screen) then
  write (msg_buffer, "(A)") repeat ("-", 72)
  call msg_message ()
else
  call write_separator (u)
end if
end subroutine process_metadata_write

```

Short output: list components.

(Process config: process metadata: TBP)+≡

procedure :: show => process_metadata_show

(Process config: sub interfaces)+≡

```

module subroutine process_metadata_show (meta, u, model_name)
  class(process_metadata_t), intent(in) :: meta

```

```

        integer, intent(in) :: u
        type(string_t), intent(in) :: model_name
    end subroutine process_metadata_show

<Process config: procedures>+≡
module subroutine process_metadata_show (meta, u, model_name)
    class(process_metadata_t), intent(in) :: meta
    integer, intent(in) :: u
    type(string_t), intent(in) :: model_name
    integer :: i
    select case (meta%type)
    case (PRC_UNKNOWN)
        write (u, "(A)") "Process: [undefined]"
        return
    case default
        write (u, "(A)", advance="no") "Process:"
    end select
    write (u, "(1x,A)", advance="no") char (meta%id)
    select case (meta%num_id)
    case (0)
    case default
        write (u, "(1x,'(,I0,')')", advance="no") meta%num_id
    end select
    select case (char (model_name))
    case ("")
    case default
        write (u, "(1x,'[,A,']')", advance="no") char (model_name)
    end select
    write (u, *)
    if (allocated (meta%component_id)) then
        do i = 1, size (meta%component_id)
            if (meta%active(i)) then
                write (u, "(2x,I0,':',1x,A)") i, &
                    char (meta%component_description (i))
            end if
        end do
    end if
end subroutine process_metadata_show

```

Initialize. Find process ID and run ID.

Also find the process ID in the process library and retrieve some metadata from there.

```

<Process config: process metadata: TBP>+≡
    procedure :: init => process_metadata_init

<Process config: sub interfaces>+≡
module subroutine process_metadata_init (meta, id, lib, var_list)
    class(process_metadata_t), intent(out) :: meta
    type(string_t), intent(in) :: id
    type(process_library_t), intent(in), target :: lib
    type(var_list_t), intent(in) :: var_list
end subroutine process_metadata_init

<Process config: procedures>+≡
module subroutine process_metadata_init (meta, id, lib, var_list)

```

```

class(process_metadata_t), intent(out) :: meta
type(string_t), intent(in) :: id
type(process_library_t), intent(in), target :: lib
type(var_list_t), intent(in) :: var_list
select case (lib%get_n_in (id))
case (1); meta%type = PRC_DECAY
case (2); meta%type = PRC_SCATTERING
case default
    call msg_bug ("Process '" // char (id) // "': impossible n_in")
end select
meta%id = id
meta%run_id = var_list%get_sval (var_str ("$_run_id"))
allocate (meta%lib_name)
meta%lib_name = lib%get_name ()
meta%lib_update_counter = lib%get_update_counter ()
if (lib%contains (id)) then
    meta%lib_index = lib%get_entry_index (id)
    meta%num_id = lib%get_num_id (id)
    call lib%get_component_list (id, meta%component_id)
    meta%n_components = size (meta%component_id)
    call lib%get_component_description_list &
        (id, meta%component_description)
    allocate (meta%active (meta%n_components), source = .true.)
else
    call msg_fatal ("Process library does not contain process '" &
        // char (id) // "'")
end if
if (.not. lib%is_active ()) then
    call msg_bug ("Process init: inactive library not handled yet")
end if
end subroutine process_metadata_init

```

Mark a component as inactive.

```

<Process config: process metadata: TBP>+≡
    procedure :: deactivate_component => process_metadata_deactivate_component

<Process config: sub interfaces>+≡
    module subroutine process_metadata_deactivate_component (meta, i)
        class(process_metadata_t), intent(inout) :: meta
        integer, intent(in) :: i
        end subroutine process_metadata_deactivate_component

<Process config: procedures>+≡
    module subroutine process_metadata_deactivate_component (meta, i)
        class(process_metadata_t), intent(inout) :: meta
        integer, intent(in) :: i
        call msg_message ("Process component '" &
            // char (meta%component_id(i)) // "': matrix element vanishes")
        meta%active(i) = .false.
    end subroutine process_metadata_deactivate_component

```


30.5.5 Phase-space configuration

A process can have a number of independent phase-space configuration entries, depending on the process definition and evaluation algorithm. Each entry holds various configuration-parameter data and the actual `phs_config_t` record, which can vary in concrete type.

```

(Process config: public)+≡
    public :: process_phs_config_t

(Process config: types)+≡
    type :: process_phs_config_t
        type(phs_parameters_t) :: phs_par
        type(mapping_defaults_t) :: mapping_defs
        class(phs_config_t), allocatable :: phs_config
    contains
        (Process config: process phs config: TBP)
    end type process_phs_config_t

```

Output, DTIO compatible.

```

(Process config: process phs config: TBP)≡
    procedure :: write => process_phs_config_write
    procedure :: write_formatted => process_phs_config_write_formatted
    ! generic :: write (formatted) => write_formatted

(Process config: sub interfaces)+≡
    module subroutine process_phs_config_write (phs_config, unit)
        class(process_phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
    end subroutine process_phs_config_write

(Process config: procedures)+≡
    module subroutine process_phs_config_write (phs_config, unit)
        class(process_phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        integer :: u, iostat
        integer, dimension(:), allocatable :: v_list
        character(0) :: iomsg
        u = given_output_unit (unit)
        allocate (v_list (0))
        call phs_config%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
    end subroutine process_phs_config_write

```

DTIO standard write.

```

(Process config: sub interfaces)+≡
    module subroutine process_phs_config_write_formatted &
        (dtv, unit, iotype, v_list, iostat, iomsg)
        class(process_phs_config_t), intent(in) :: dtv
        integer, intent(in) :: unit
        character(*), intent(in) :: iotype
        integer, dimension(:), intent(in) :: v_list
        integer, intent(out) :: iostat
        character(*), intent(inout) :: iomsg
    end subroutine process_phs_config_write_formatted

```

```

<Process config: procedures>+≡
  module subroutine process_phs_config_write_formatted &
    (dtv, unit, iotype, v_list, iostat, iomsg)
    class(process_phs_config_t), intent(in) :: dtv
    integer, intent(in) :: unit
    character(*), intent(in) :: iotype
    integer, dimension(:), intent(in) :: v_list
    integer, intent(out) :: iostat
    character(*), intent(inout) :: iomsg
    associate (phs_config => dtv)
      write (unit, "(1x, A)") "Phase-space configuration entry:"
      call phs_config%phs_par%write (unit)
      call phs_config%mapping_defs%write (unit)
    end associate
    iostat = 0
  end subroutine process_phs_config_write_formatted

```

30.5.6 Beam configuration

The object `data` holds all details about the initial beam configuration. The allocatable array `sf` holds the structure-function configuration blocks. There are `n_strfun` entries in the structure-function chain (not counting the initial beam object). We maintain `n_channel` independent parameterizations of this chain. If this is greater than zero, we need a multi-channel sampling algorithm, where for each point one channel is selected to generate kinematics.

The number of parameters that are required for generating a structure-function chain is `n_sfpar`.

The flag `azimuthal_dependence` tells whether the process setup is symmetric about the beam axis in the c.m. system. This implies that there is no transversal beam polarization. The flag `lab_is_cm` is obvious.

```

<Process config: public>+≡
  public :: process_beam_config_t

<Process config: types>+≡
  type :: process_beam_config_t
    type(beam_data_t) :: data
    integer :: n_strfun = 0
    integer :: n_channel = 1
    integer :: n_sfpar = 0
    type(sf_config_t), dimension(:), allocatable :: sf
    type(sf_channel_t), dimension(:), allocatable :: sf_channel
    logical :: azimuthal_dependence = .false.
    logical :: lab_is_cm = .true.
    character(32) :: md5sum = ""
    logical :: sf_trace = .false.
    type(string_t) :: sf_trace_file
  contains
    <Process config: process beam config: TBP>
  end type process_beam_config_t

```

Here we write beam data only if they are actually used.

The `verbose` flag is passed to the beam-data writer.

```

<Process config: process beam config: TBP>≡
  procedure :: write => process_beam_config_write

<Process config: sub interfaces>+≡
  module subroutine process_beam_config_write (object, unit, verbose)
    class(process_beam_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
  end subroutine process_beam_config_write

<Process config: procedures>+≡
  module subroutine process_beam_config_write (object, unit, verbose)
    class(process_beam_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i, c
    u = given_output_unit (unit)
    call object%data%write (u, verbose = verbose)
    if (object%data%initialized) then
      write (u, "(3x,A,L1)") "Azimuthal dependence      = ", &
        object%azimuthal_dependence
      write (u, "(3x,A,L1)") "Lab frame is c.m. frame = ", &
        object%lab_is_cm
      if (object%md5sum /= "") then
        write (u, "(3x,A,A,A)") "MD5 sum (beams/strf) = '", &
          object%md5sum, "'"
      end if
      if (allocated (object%sf)) then
        do i = 1, size (object%sf)
          call object%sf(i)%write (u)
        end do
        if (any_sf_channel_has_mapping (object%sf_channel)) then
          write (u, "(1x,A,L1)") "Structure-function mappings per channel:"
          do c = 1, object%n_channel
            write (u, "(3x,I0,':')", advance="no") c
            call object%sf_channel(c)%write (u)
          end do
        end if
      end if
    end if
  end subroutine process_beam_config_write

```

The beam data have a finalizer. We assume that there is none for the structure-function data.

```

<Process config: process beam config: TBP>+≡
  procedure :: final => process_beam_config_final

<Process config: sub interfaces>+≡
  module subroutine process_beam_config_final (object)
    class(process_beam_config_t), intent(inout) :: object
  end subroutine process_beam_config_final

```

```

(Process config: procedures)+≡
module subroutine process_beam_config_final (object)
  class(process_beam_config_t), intent(inout) :: object
  call object%data%final ()
end subroutine process_beam_config_final

```

Initialize the beam setup with a given beam structure object.

```

(Process config: process beam config: TBP)+≡
procedure :: init_beam_structure => process_beam_config_init_beam_structure

```

```

(Process config: sub interfaces)+≡
module subroutine process_beam_config_init_beam_structure &
  (beam_config, beam_structure, sqrts, model, decay_rest_frame)
  class(process_beam_config_t), intent(out) :: beam_config
  type(beam_structure_t), intent(in) :: beam_structure
  logical, intent(in), optional :: decay_rest_frame
  real(default), intent(in) :: sqrts
  class(model_data_t), intent(in), target :: model
end subroutine process_beam_config_init_beam_structure

```

```

(Process config: procedures)+≡
module subroutine process_beam_config_init_beam_structure &
  (beam_config, beam_structure, sqrts, model, decay_rest_frame)
  class(process_beam_config_t), intent(out) :: beam_config
  type(beam_structure_t), intent(in) :: beam_structure
  logical, intent(in), optional :: decay_rest_frame
  real(default), intent(in) :: sqrts
  class(model_data_t), intent(in), target :: model
  call beam_config%data%init_structure (beam_structure, &
    sqrts, model, decay_rest_frame)
  beam_config%lab_is_cm = beam_config%data%lab_is_cm
end subroutine process_beam_config_init_beam_structure

```

Initialize the beam setup for a scattering process with specified flavor combination, other properties taken from the beam structure object (if any).

```

(Process config: process beam config: TBP)+≡
procedure :: init_scattering => process_beam_config_init_scattering

```

```

(Process config: sub interfaces)+≡
module subroutine process_beam_config_init_scattering &
  (beam_config, flv_in, sqrts, beam_structure)
  class(process_beam_config_t), intent(out) :: beam_config
  type(flavor_t), dimension(2), intent(in) :: flv_in
  real(default), intent(in) :: sqrts
  type(beam_structure_t), intent(in), optional :: beam_structure
end subroutine process_beam_config_init_scattering

```

```

(Process config: procedures)+≡
module subroutine process_beam_config_init_scattering &
  (beam_config, flv_in, sqrts, beam_structure)
  class(process_beam_config_t), intent(out) :: beam_config
  type(flavor_t), dimension(2), intent(in) :: flv_in
  real(default), intent(in) :: sqrts
  type(beam_structure_t), intent(in), optional :: beam_structure
  if (present (beam_structure)) then

```

```

        if (beam_structure%polarized ()) then
            call beam_config%data%init_sqrts (sqrts, flv_in, &
                beam_structure%get_smatrix (), beam_structure%get_pol_f ())
        else
            call beam_config%data%init_sqrts (sqrts, flv_in)
        end if
    else
        call beam_config%data%init_sqrts (sqrts, flv_in)
    end if
end subroutine process_beam_config_init_scattering

```

Initialize the beam setup for a decay process with specified flavor, other properties taken from the beam structure object (if present).

For a cascade decay, we set `rest_frame` to false, indicating a event-wise varying momentum. The beam data itself are initialized for the particle at rest.

```

(Process config: process beam config: TBP)+≡
    procedure :: init_decay => process_beam_config_init_decay

(Process config: sub interfaces)+≡
    module subroutine process_beam_config_init_decay &
        (beam_config, flv_in, rest_frame, beam_structure)
        class(process_beam_config_t), intent(out) :: beam_config
        type(flavor_t), dimension(1), intent(in) :: flv_in
        logical, intent(in), optional :: rest_frame
        type(beam_structure_t), intent(in), optional :: beam_structure
    end subroutine process_beam_config_init_decay

(Process config: procedures)+≡
    module subroutine process_beam_config_init_decay &
        (beam_config, flv_in, rest_frame, beam_structure)
        class(process_beam_config_t), intent(out) :: beam_config
        type(flavor_t), dimension(1), intent(in) :: flv_in
        logical, intent(in), optional :: rest_frame
        type(beam_structure_t), intent(in), optional :: beam_structure
        if (present (beam_structure)) then
            if (beam_structure%polarized ()) then
                call beam_config%data%init_decay (flv_in, &
                    beam_structure%get_smatrix (), beam_structure%get_pol_f (), &
                    rest_frame = rest_frame)
            else
                call beam_config%data%init_decay (flv_in, rest_frame = rest_frame)
            end if
        else
            call beam_config%data%init_decay (flv_in, &
                rest_frame = rest_frame)
        end if
        beam_config%lab_is_cm = beam_config%data%lab_is_cm
    end subroutine process_beam_config_init_decay

```

Print an informative message.

```

(Process config: process beam config: TBP)+≡
    procedure :: startup_message => process_beam_config_startup_message

```

```

(Process config: sub interfaces)+≡
    module subroutine process_beam_config_startup_message &
        (beam_config, unit, beam_structure)
        class(process_beam_config_t), intent(in) :: beam_config
        integer, intent(in), optional :: unit
        type(beam_structure_t), intent(in), optional :: beam_structure
    end subroutine process_beam_config_startup_message

(Process config: procedures)+≡
    module subroutine process_beam_config_startup_message &
        (beam_config, unit, beam_structure)
        class(process_beam_config_t), intent(in) :: beam_config
        integer, intent(in), optional :: unit
        type(beam_structure_t), intent(in), optional :: beam_structure
        integer :: u
        u = free_unit ()
        open (u, status="scratch", action="readwrite")
        if (present (beam_structure)) then
            call beam_structure%write (u)
        end if
        call beam_config%data%write (u)
        rewind (u)
        do
            read (u, "(1x,A)", end=1) msg_buffer
            call msg_message ()
        end do
1    continue
        close (u)
    end subroutine process_beam_config_startup_message

```

Allocate the structure-function array.

```

(Process config: process beam config: TBP)+≡
    procedure :: init_sf_chain => process_beam_config_init_sf_chain

(Process config: sub interfaces)+≡
    module subroutine process_beam_config_init_sf_chain &
        (beam_config, sf_config, sf_trace_file)
        class(process_beam_config_t), intent(inout) :: beam_config
        type(sf_config_t), dimension(:), intent(in) :: sf_config
        type(string_t), intent(in), optional :: sf_trace_file
    end subroutine process_beam_config_init_sf_chain

(Process config: procedures)+≡
    module subroutine process_beam_config_init_sf_chain &
        (beam_config, sf_config, sf_trace_file)
        class(process_beam_config_t), intent(inout) :: beam_config
        type(sf_config_t), dimension(:), intent(in) :: sf_config
        type(string_t), intent(in), optional :: sf_trace_file
        integer :: i
        beam_config%n_strfun = size (sf_config)
        allocate (beam_config%sf (beam_config%n_strfun))
        do i = 1, beam_config%n_strfun
            associate (sf => sf_config(i))
                call beam_config%sf(i)%init (sf%i, sf%data)
                if (.not. sf%data%is_generator ()) then

```

```

        beam_config%n_sfpar = beam_config%n_sfpar + sf%data%get_n_par ()
    end if
end associate
end do
if (present (sf_trace_file)) then
    beam_config%sf_trace = .true.
    beam_config%sf_trace_file = sf_trace_file
end if
end subroutine process_beam_config_init_sf_chain

```

Allocate the structure-function mapping channel array, given the requested number of channels.

```

(Process config: process beam config: TBP)+≡
    procedure :: allocate_sf_channels => process_beam_config_allocate_sf_channels

(Process config: sub interfaces)+≡
    module subroutine process_beam_config_allocate_sf_channels &
        (beam_config, n_channel)
        class(process_beam_config_t), intent(inout) :: beam_config
        integer, intent(in) :: n_channel
    end subroutine process_beam_config_allocate_sf_channels

(Process config: procedures)+≡
    module subroutine process_beam_config_allocate_sf_channels &
        (beam_config, n_channel)
        class(process_beam_config_t), intent(inout) :: beam_config
        integer, intent(in) :: n_channel
        beam_config%n_channel = n_channel
        call allocate_sf_channels (beam_config%sf_channel, &
            n_channel = n_channel, &
            n_strfun = beam_config%n_strfun)
    end subroutine process_beam_config_allocate_sf_channels

```

Set a structure-function mapping channel for an array of structure-function entries, for a single channel. (The default is no mapping.)

```

(Process config: process beam config: TBP)+≡
    procedure :: set_sf_channel => process_beam_config_set_sf_channel

(Process config: sub interfaces)+≡
    module subroutine process_beam_config_set_sf_channel &
        (beam_config, c, sf_channel)
        class(process_beam_config_t), intent(inout) :: beam_config
        integer, intent(in) :: c
        type(sf_channel_t), intent(in) :: sf_channel
    end subroutine process_beam_config_set_sf_channel

(Process config: procedures)+≡
    module subroutine process_beam_config_set_sf_channel &
        (beam_config, c, sf_channel)
        class(process_beam_config_t), intent(inout) :: beam_config
        integer, intent(in) :: c
        type(sf_channel_t), intent(in) :: sf_channel
        beam_config%sf_channel(c) = sf_channel
    end subroutine process_beam_config_set_sf_channel

```

Print an informative startup message.

```

(Process config: process beam config: TBP)+≡
  procedure :: sf_startup_message => process_beam_config_sf_startup_message

(Process config: sub interfaces)+≡
  module subroutine process_beam_config_sf_startup_message &
    (beam_config, sf_string, unit)
    class(process_beam_config_t), intent(in) :: beam_config
    type(string_t), intent(in) :: sf_string
    integer, intent(in), optional :: unit
  end subroutine process_beam_config_sf_startup_message

(Process config: procedures)+≡
  module subroutine process_beam_config_sf_startup_message &
    (beam_config, sf_string, unit)
    class(process_beam_config_t), intent(in) :: beam_config
    type(string_t), intent(in) :: sf_string
    integer, intent(in), optional :: unit
    if (beam_config%n_strfun > 0) then
      call msg_message ("Beam structure: " // char (sf_string), unit = unit)
      write (msg_buffer, "(A,3(1x,I0,1x,A))") &
        "Beam structure:", &
        beam_config%n_channel, "channels,", &
        beam_config%n_sfpar, "dimensions"
      call msg_message (unit = unit)
      if (beam_config%sf_trace) then
        call msg_message ("Beam structure: tracing &
          &values in '" // char (beam_config%sf_trace_file) // "'")
      end if
    end if
  end subroutine process_beam_config_sf_startup_message

```

Return the PDF set currently in use, if any. This should be unique, so we scan the structure functions until we get a nonzero number.

(This implies that if the PDF set is not unique (e.g., proton and photon structure used together), this does not work correctly.)

```

(Process config: process beam config: TBP)+≡
  procedure :: get_pdf_set => process_beam_config_get_pdf_set

(Process config: sub interfaces)+≡
  module function process_beam_config_get_pdf_set &
    (beam_config) result (pdf_set)
    class(process_beam_config_t), intent(in) :: beam_config
    integer :: pdf_set
  end function process_beam_config_get_pdf_set

(Process config: procedures)+≡
  module function process_beam_config_get_pdf_set (beam_config) result (pdf_set)
    class(process_beam_config_t), intent(in) :: beam_config
    integer :: pdf_set
    integer :: i
    pdf_set = 0
    if (allocated (beam_config%sf)) then
      do i = 1, size (beam_config%sf)
        pdf_set = beam_config%sf(i)%get_pdf_set ()
      end do
    end if
  end function process_beam_config_get_pdf_set

```



```

        if (pdf_set /= 0) return
    end do
end if
end function process_beam_config_get_pdf_set

```

Return the beam file.

```

<Process config: process beam config: TBP>+≡
    procedure :: get_beam_file => process_beam_config_get_beam_file

<Process config: sub interfaces>+≡
    module function process_beam_config_get_beam_file &
        (beam_config) result (file)
        class(process_beam_config_t), intent(in) :: beam_config
        type(string_t) :: file
    end function process_beam_config_get_beam_file

<Process config: procedures>+≡
    module function process_beam_config_get_beam_file (beam_config) result (file)
        class(process_beam_config_t), intent(in) :: beam_config
        type(string_t) :: file
        integer :: i
        file = ""
        if (allocated (beam_config%sf)) then
            do i = 1, size (beam_config%sf)
                file = beam_config%sf(i)%get_beam_file ()
                if (file /= "") return
            end do
        end if
    end function process_beam_config_get_beam_file

```

Compute the MD5 sum for the complete beam setup. We rely on the default output of `write` to contain all relevant data.

This is done only once, when the MD5 sum is still empty.

```

<Process config: process beam config: TBP>+≡
    procedure :: compute_md5sum => process_beam_config_compute_md5sum

<Process config: sub interfaces>+≡
    module subroutine process_beam_config_compute_md5sum (beam_config)
        class(process_beam_config_t), intent(inout) :: beam_config
    end subroutine process_beam_config_compute_md5sum

<Process config: procedures>+≡
    module subroutine process_beam_config_compute_md5sum (beam_config)
        class(process_beam_config_t), intent(inout) :: beam_config
        integer :: u
        if (beam_config%md5sum == "") then
            u = free_unit ()
            open (u, status = "scratch", action = "readwrite")
            call beam_config%write (u, verbose=.true.)
            rewind (u)
            beam_config%md5sum = md5sum (u)
            close (u)
        end if
    end subroutine process_beam_config_compute_md5sum

```

```

<Process config: process beam config: TBP>+≡
    procedure :: get_md5sum => process_beam_config_get_md5sum

<Process config: sub interfaces>+≡
    pure module function process_beam_config_get_md5sum &
        (beam_config) result (md5)
        character(32) :: md5
        class(process_beam_config_t), intent(in) :: beam_config
    end function process_beam_config_get_md5sum

<Process config: procedures>+≡
    pure module function process_beam_config_get_md5sum (beam_config) result (md5)
        character(32) :: md5
        class(process_beam_config_t), intent(in) :: beam_config
        md5 = beam_config%md5sum
    end function process_beam_config_get_md5sum

<Process config: process beam config: TBP>+≡
    procedure :: has_structure_function => &
        process_beam_config_has_structure_function

<Process config: sub interfaces>+≡
    pure module function process_beam_config_has_structure_function &
        (beam_config) result (has_sf)
        logical :: has_sf
        class(process_beam_config_t), intent(in) :: beam_config
    end function process_beam_config_has_structure_function

<Process config: procedures>+≡
    pure module function process_beam_config_has_structure_function &
        (beam_config) result (has_sf)
        logical :: has_sf
        class(process_beam_config_t), intent(in) :: beam_config
        has_sf = beam_config%n_strfun > 0
    end function process_beam_config_has_structure_function

```

30.5.7 Process components

A process component is an individual contribution to a process (scattering or decay) which needs not be physical. The sum over all components should be physical.

The `index` identifies this component within its parent process.

The actual process component is stored in the `core` subobject. We use a polymorphic subobject instead of an extension of `process_component_t`, because the individual entries in the array of process components can have different types. In short, `process_component_t` is a wrapper for the actual process variants.

If the `active` flag is false, we should skip this component. This happens if the associated process has vanishing matrix element.

The index array `i_term` points to the individual terms generated by this component. The indices refer to the parent process.

The index `i_mci` is the index of the MC integrator and parameter set which are associated to this process component.

```

<Process config: public>+≡
    public :: process_component_t

<Process config: types>+≡
    type :: process_component_t
        type(process_component_def_t), pointer :: config => null ()
        integer :: index = 0
        logical :: active = .false.
        integer, dimension(:), allocatable :: i_term
        integer :: i_mci = 0
        class(phs_config_t), allocatable :: phs_config
        character(32) :: md5sum_phs = ""
        integer :: component_type = COMP_DEFAULT
    contains
        <Process config: process component: TBP>
    end type process_component_t

```

Finalizer. The MCI template may (potentially) need a finalizer. The process configuration finalizer may include closing an open scratch file.

```

<Process config: process component: TBP>≡
    procedure :: final => process_component_final

<Process config: sub interfaces>+≡
    module subroutine process_component_final (object)
        class(process_component_t), intent(inout) :: object
    end subroutine process_component_final

<Process config: procedures>+≡
    module subroutine process_component_final (object)
        class(process_component_t), intent(inout) :: object
        if (allocated (object%phs_config)) then
            call object%phs_config%final ()
        end if
    end subroutine process_component_final

```

The meaning of `verbose` depends on the process variant.

```

<Process config: process component: TBP>+≡
    procedure :: write => process_component_write

<Process config: sub interfaces>+≡
    module subroutine process_component_write (object, unit)
        class(process_component_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_component_write

<Process config: procedures>+≡
    module subroutine process_component_write (object, unit)
        class(process_component_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%config)) then
            write (u, "(1x,A,I0)") "Component #", object%index

```

```

        call object%config%write (u)
        if (object%md5sum_phs /= "") then
            write (u, "(3x,A,A,A)") "MD5 sum (phs)          = ', &
                object%md5sum_phs, "'
        end if
    else
        write (u, "(1x,A)") "Process component: [not allocated]"
    end if
    if (.not. object%active) then
        write (u, "(1x,A)") "[Inactive]"
        return
    end if
    write (u, "(1x,A)") "Referenced data:"
    if (allocated (object%i_term)) then
        write (u, "(3x,A,999(1x,I0))") "Terms              =", &
            object%i_term
    else
        write (u, "(3x,A)") "Terms                      = [undefined]"
    end if
    if (object%i_mci /= 0) then
        write (u, "(3x,A,I0)") "MC dataset              = ", object%i_mci
    else
        write (u, "(3x,A)") "MC dataset                  = [undefined]"
    end if
    if (allocated (object%phs_config)) then
        call object%phs_config%write (u)
    end if
end subroutine process_component_write

```

Initialize the component.

```

<Process config: process component: TBP>+≡
    procedure :: init => process_component_init

<Process config: sub interfaces>+≡
    module subroutine process_component_init (component, &
        i_component, env, meta, config, &
        active, &
        phs_config_template)
        class(process_component_t), intent(out) :: component
        integer, intent(in) :: i_component
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        type(process_config_data_t), intent(in) :: config
        logical, intent(in) :: active
        class(phs_config_t), intent(in), allocatable :: phs_config_template
    end subroutine process_component_init

<Process config: procedures>+≡
    module subroutine process_component_init (component, &
        i_component, env, meta, config, &
        active, &
        phs_config_template)
        class(process_component_t), intent(out) :: component
        integer, intent(in) :: i_component
        type(process_environment_t), intent(in) :: env

```

```

type(process_metadata_t), intent(in) :: meta
type(process_config_data_t), intent(in) :: config
logical, intent(in) :: active
class(phs_config_t), intent(in), allocatable :: phs_config_template

type(process_constants_t) :: data

component%index = i_component
component%config => &
    config%process_def%get_component_def_ptr (i_component)

component%active = active
if (component%active) then
    allocate (component%phs_config, source = phs_config_template)
    call env%fill_process_constants (meta%id, i_component, data)
    call component%phs_config%init (data, config%model)
end if
end subroutine process_component_init

```

```

<Process config: process component: TBP>+≡
    procedure :: is_active => process_component_is_active

<Process config: sub interfaces>+≡
    elemental module function process_component_is_active &
        (component) result (active)
        logical :: active
        class(process_component_t), intent(in) :: component
    end function process_component_is_active

<Process config: procedures>+≡
    elemental module function process_component_is_active &
        (component) result (active)
        logical :: active
        class(process_component_t), intent(in) :: component
        active = component%active
    end function process_component_is_active

```

Finalize the phase-space configuration.

```

<Process config: process component: TBP>+≡
    procedure :: configure_phs => process_component_configure_phs

<Process config: sub interfaces>+≡
    module subroutine process_component_configure_phs &
        (component, sqrts, beam_config, rebuild, &
         ignore_mismatch, subdir)
        class(process_component_t), intent(inout) :: component
        real(default), intent(in) :: sqrts
        type(process_beam_config_t), intent(in) :: beam_config
        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        type(string_t), intent(in), optional :: subdir
    end subroutine process_component_configure_phs

```

```

(Process config: procedures)+≡
  module subroutine process_component_configure_phs &
    (component, sqrts, beam_config, rebuild, &
     ignore_mismatch, subdir)
    class(process_component_t), intent(inout) :: component
    real(default), intent(in) :: sqrts
    type(process_beam_config_t), intent(in) :: beam_config
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    type(string_t), intent(in), optional :: subdir
    logical :: no_strfun
    integer :: nlo_type
    no_strfun = beam_config%n_strfun == 0
    nlo_type = component%config%get_nlo_type ()
    call component%phs_config%configure (sqrts, &
     azimuthal_dependence = beam_config%azimuthal_dependence, &
     sqrts_fixed = no_strfun, &
     lab_is_cm = beam_config%lab_is_cm .and. no_strfun, &
     rebuild = rebuild, ignore_mismatch = ignore_mismatch, &
     nlo_type = nlo_type, &
     subdir = subdir)
  end subroutine process_component_configure_phs

```

The process component possesses two MD5 sums: the checksum of the component definition, which should be available when the component is initialized, and the phase-space MD5 sum, which is available after configuration.

```

(Process config: process component: TBP)+≡
  procedure :: compute_md5sum => process_component_compute_md5sum

(Process config: sub interfaces)+≡
  module subroutine process_component_compute_md5sum (component)
    class(process_component_t), intent(inout) :: component
  end subroutine process_component_compute_md5sum

(Process config: procedures)+≡
  module subroutine process_component_compute_md5sum (component)
    class(process_component_t), intent(inout) :: component
    component%md5sum_phs = component%phs_config%get_md5sum ()
  end subroutine process_component_compute_md5sum

```

Match phase-space channels with structure-function channels, where applicable.

This calls a method of the `phs_config` phase-space implementation.

```

(Process config: process component: TBP)+≡
  procedure :: collect_channels => process_component_collect_channels

(Process config: sub interfaces)+≡
  module subroutine process_component_collect_channels (component, coll)
    class(process_component_t), intent(inout) :: component
    type(phs_channel_collection_t), intent(inout) :: coll
  end subroutine process_component_collect_channels

(Process config: procedures)+≡
  module subroutine process_component_collect_channels (component, coll)
    class(process_component_t), intent(inout) :: component
    type(phs_channel_collection_t), intent(inout) :: coll

```

```

    call component%phs_config%collect_channels (coll)
end subroutine process_component_collect_channels

```

```

(Process config: process component: TBP)+≡
  procedure :: get_config => process_component_get_config

(Process config: sub interfaces)+≡
  module function process_component_get_config (component) &
    result (config)
    type(process_component_def_t) :: config
    class(process_component_t), intent(in) :: component
  end function process_component_get_config

(Process config: procedures)+≡
  module function process_component_get_config (component) &
    result (config)
    type(process_component_def_t) :: config
    class(process_component_t), intent(in) :: component
    config = component%config
  end function process_component_get_config

```

```

(Process config: process component: TBP)+≡
  procedure :: get_md5sum => process_component_get_md5sum

(Process config: sub interfaces)+≡
  pure module function process_component_get_md5sum (component) result (md5)
    type(string_t) :: md5
    class(process_component_t), intent(in) :: component
  end function process_component_get_md5sum

(Process config: procedures)+≡
  pure module function process_component_get_md5sum (component) result (md5)
    type(string_t) :: md5
    class(process_component_t), intent(in) :: component
    md5 = component%config%get_md5sum () // component%md5sum_phs
  end function process_component_get_md5sum

```

Return the number of phase-space parameters.

```

(Process config: process component: TBP)+≡
  procedure :: get_n_phs_par => process_component_get_n_phs_par

(Process config: sub interfaces)+≡
  module function process_component_get_n_phs_par (component) result (n_par)
    class(process_component_t), intent(in) :: component
    integer :: n_par
  end function process_component_get_n_phs_par

(Process config: procedures)+≡
  module function process_component_get_n_phs_par (component) result (n_par)
    class(process_component_t), intent(in) :: component
    integer :: n_par
    n_par = component%phs_config%get_n_par ()
  end function process_component_get_n_phs_par

```

```

(Process config: process component: TBP)+≡
    procedure :: get_phs_config => process_component_get_phs_config

(Process config: sub interfaces)+≡
    module subroutine process_component_get_phs_config (component, phs_config)
        class(process_component_t), intent(in), target :: component
        class(phs_config_t), intent(out), pointer :: phs_config
    end subroutine process_component_get_phs_config

(Process config: procedures)+≡
    module subroutine process_component_get_phs_config (component, phs_config)
        class(process_component_t), intent(in), target :: component
        class(phs_config_t), intent(out), pointer :: phs_config
        phs_config => component%phs_config
    end subroutine process_component_get_phs_config

(Process config: process component: TBP)+≡
    procedure :: get_nlo_type => process_component_get_nlo_type

(Process config: sub interfaces)+≡
    elemental module function process_component_get_nlo_type &
        (component) result (nlo_type)
        integer :: nlo_type
        class(process_component_t), intent(in) :: component
    end function process_component_get_nlo_type

(Process config: procedures)+≡
    elemental module function process_component_get_nlo_type &
        (component) result (nlo_type)
        integer :: nlo_type
        class(process_component_t), intent(in) :: component
        nlo_type = component%config%get_nlo_type ()
    end function process_component_get_nlo_type

(Process config: process component: TBP)+≡
    procedure :: needs_mci_entry => process_component_needs_mci_entry

(Process config: sub interfaces)+≡
    module function process_component_needs_mci_entry &
        (component, combined_integration) result (value)
        logical :: value
        class(process_component_t), intent(in) :: component
        logical, intent(in), optional :: combined_integration
    end function process_component_needs_mci_entry

(Process config: procedures)+≡
    module function process_component_needs_mci_entry &
        (component, combined_integration) result (value)
        logical :: value
        class(process_component_t), intent(in) :: component
        logical, intent(in), optional :: combined_integration
        value = component%active
        if (present (combined_integration)) then
            if (combined_integration) &
                value = value .and. component%component_type <= COMP_MASTER
        end if
    end function

```



```

end function process_component_needs_mci_entry

<Process config: process component: TBP>+≡
  procedure :: can_be_integrated => process_component_can_be_integrated

<Process config: sub interfaces>+≡
  elemental module function process_component_can_be_integrated &
    (component) result (active)
    logical :: active
    class(process_component_t), intent(in) :: component
  end function process_component_can_be_integrated

<Process config: procedures>+≡
  elemental module function process_component_can_be_integrated &
    (component) result (active)
    logical :: active
    class(process_component_t), intent(in) :: component
    active = component%config%can_be_integrated ()
  end function process_component_can_be_integrated

```

30.5.8 Process terms

For straightforward tree-level calculations, each process component corresponds to a unique elementary interaction. However, in the case of NLO calculations with subtraction terms, a process component may split into several separate contributions to the scattering, which are qualified by interactions with distinct kinematics and particle content. We represent their configuration as `process_term_t` objects, the actual instances will be introduced below as `term_instance_t`. In any case, the process term contains an elementary interaction with a definite quantum-number and momentum content.

The index `i_term_global` identifies the term relative to the process.

The index `i_component` identifies the process component which generates this term, relative to the parent process.

The index `i_term` identifies the term relative to the process component (not the process).

The `data` subobject holds all process constants.

The number of allowed flavor/helicity/color combinations is stored as `n_allowed`. This is the total number of independent entries in the density matrix. For each combination, the index of the flavor, helicity, and color state is stored in the arrays `flv`, `hel`, and `col`, respectively.

The flag `rearrange` is true if we need to rearrange the particles of the hard interaction, to obtain the effective parton state.

The interaction `int` holds the quantum state for the (resolved) hard interaction, the parent-child relations of the particles, and their momenta. The momenta are not filled yet; this is postponed to copies of `int` which go into the process instances.

If recombination is in effect, we should allocate `int_eff` to describe the rearranged partonic state.

This type is public only for use in a unit test.

```

<Process config: public>+≡
  public :: process_term_t

```

```

(Process config: types)+≡
  type :: process_term_t
    integer :: i_term_global = 0
    integer :: i_component = 0
    integer :: i_term = 0
    integer :: i_sub = 0
    integer :: i_core = 0
    integer :: n_allowed = 0
    type(process_constants_t) :: data
    real(default) :: alpha_s = 0
    integer, dimension(:), allocatable :: flv, hel, col
    integer :: n_sub, n_sub_color, n_sub_spin
    type(interaction_t) :: int
    type(interaction_t), pointer :: int_eff => null ()
  contains
    (Process config: process term: TBP)
  end type process_term_t

```

For the output, we skip the process constants and the tables of allowed quantum numbers. Those can also be read off from the interaction object.

```

(Process config: process term: TBP)≡
  procedure :: write => process_term_write

(Process config: sub interfaces)+≡
  module subroutine process_term_write (term, unit)
    class(process_term_t), intent(in) :: term
    integer, intent(in), optional :: unit
  end subroutine process_term_write

(Process config: procedures)+≡
  module subroutine process_term_write (term, unit)
    class(process_term_t), intent(in) :: term
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,I0)") "Term #", term%i_term_global
    write (u, "(3x,A,I0)") "Process component index      = ", &
      term%i_component
    write (u, "(3x,A,I0)") "Term index w.r.t. component = ", &
      term%i_term
    call write_separator (u)
    write (u, "(1x,A)") "Hard interaction:"
    call write_separator (u)
    call term%int%basic_write (u)
  end subroutine process_term_write

```

Write an account of all quantum number states and their current status.

```

(Process config: process term: TBP)+≡
  procedure :: write_state_summary => process_term_write_state_summary

(Process config: sub interfaces)+≡
  module subroutine process_term_write_state_summary (term, core, unit)
    class(process_term_t), intent(in) :: term
    class(prc_core_t), intent(in) :: core

```

```

        integer, intent(in), optional :: unit
    end subroutine process_term_write_state_summary

<Process config: procedures>+≡
module subroutine process_term_write_state_summary (term, core, unit)
    class(process_term_t), intent(in) :: term
    class(prc_core_t), intent(in) :: core
    integer, intent(in), optional :: unit
    integer :: u, i, f, h, c
    type(state_iterator_t) :: it
    character :: sgn
    u = given_output_unit (unit)
    write (u, "(1x,A,I0)") "Term #", term%i_term_global
    call it%init (term%int%get_state_matrix_ptr ())
    do while (it%is_valid ())
        i = it%get_me_index ()
        f = term%flv(i)
        h = term%hel(i)
        if (allocated (term%col)) then
            c = term%col(i)
        else
            c = 1
        end if
        if (core%is_allowed (term%i_term, f, h, c)) then
            sgn = "+"
        else
            sgn = " "
        end if
        write (u, "(1x,A1,1x,I0,2x)", advance="no") sgn, i
        call quantum_numbers_write (it%get_quantum_numbers (), u)
        write (u, *)
        call it%advance ()
    end do
end subroutine process_term_write_state_summary

```

Finalizer: the `int` and potentially `int_eff` components have a finalizer that we must call.

```

<Process config: process term: TBP>+≡
    procedure :: final => process_term_final

<Process config: sub interfaces>+≡
    module subroutine process_term_final (term)
        class(process_term_t), intent(inout) :: term
    end subroutine process_term_final

<Process config: procedures>+≡
module subroutine process_term_final (term)
    class(process_term_t), intent(inout) :: term
    call term%int%final ()
end subroutine process_term_final

```

Initialize the term. We copy the process constants from the `core` object and set up the `int` hard interaction accordingly.

The `alpha_s` value is useful for writing external event records. This is the constant value which may be overridden by an event-specific running value. If the model does not contain the strong coupling, the value is zero.

The `rearrange` part is commented out; this or something equivalent could become relevant for NLO algorithms.

```

(Process config: process term: TBP)+≡
  procedure :: init => process_term_init

(Process config: sub interfaces)+≡
  module subroutine process_term_init &
    (term, i_term_global, i_component, i_term, core, model, &
     nlo_type, use_beam_pol, subtraction_method, &
     has_pdfs, n_emitters)
    class(process_term_t), intent(inout), target :: term
    integer, intent(in) :: i_term_global
    integer, intent(in) :: i_component
    integer, intent(in) :: i_term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: use_beam_pol
    type(string_t), intent(in), optional :: subtraction_method
    logical, intent(in), optional :: has_pdfs
    integer, intent(in), optional :: n_emitters
  end subroutine process_term_init

(Process config: procedures)+≡
  module subroutine process_term_init &
    (term, i_term_global, i_component, i_term, core, model, &
     nlo_type, use_beam_pol, subtraction_method, &
     has_pdfs, n_emitters)
    class(process_term_t), intent(inout), target :: term
    integer, intent(in) :: i_term_global
    integer, intent(in) :: i_component
    integer, intent(in) :: i_term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: use_beam_pol
    type(string_t), intent(in), optional :: subtraction_method
    logical, intent(in), optional :: has_pdfs
    integer, intent(in), optional :: n_emitters
    class(modelpar_data_t), pointer :: alpha_s_ptr
    logical :: use_internal_color
    term%i_term_global = i_term_global
    term%i_component = i_component
    term%i_term = i_term
    call core%get_constants (term%data, i_term)
    alpha_s_ptr => model%get_par_data_ptr (var_str ("alphas"))
    if (associated (alpha_s_ptr)) then
      term%alpha_s = alpha_s_ptr%get_real ()
    else
      term%alpha_s = -1
    end if
    use_internal_color = .false.
  end module

```

```

if (present (subtraction_method)) &
  use_internal_color = (char (subtraction_method) == 'omega') &
  .or. (char (subtraction_method) == 'threshold')
call term%setup_interaction (core, model, nlo_type = nlo_type, &
  pol_beams = use_beam_pol, use_internal_color = use_internal_color, &
  has_pdfs = has_pdfs, n_emitters = n_emitters)
end subroutine process_term_init

```

We fetch the process constants which determine the quantum numbers and use those to create the interaction. The interaction contains incoming and outgoing particles, no virtuals. The incoming particles are parents of the outgoing ones.

Keeping previous WHIZARD conventions, we invert the color assignment (but not flavor or helicity) for the incoming particles. When the color-flow square matrix is evaluated, this inversion is done again, so in the color-flow sequence we get the color assignments of the matrix element.

Why are these four subtraction entries for structure-function aware interactions? Taking the soft or collinear limit of the real-emission matrix element, the behavior of the parton energy fractions has to be taken into account. In the pure real case, x_{\oplus} and x_{\ominus} are given by

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}}.$$

In the soft limit, $\xi \rightarrow 0$, this yields $x_{\oplus} = \bar{x}_{\oplus}$ and $x_{\ominus} = \bar{x}_{\ominus}$. In the collinear limit, $y \rightarrow 1$, it is $x_{\oplus} = \bar{x}_{\oplus}/(1-\xi)$ and $x_{\ominus} = \bar{x}_{\ominus}$. Likewise, in the anti-collinear limit $y \rightarrow -1$, the inverse relation holds. We therefore have to distinguish four cases with the PDF assignments $f(x_{\oplus}) \cdot f(x_{\ominus})$, $f(\bar{x}_{\oplus}) \cdot f(\bar{x}_{\ominus})$, $f(\bar{x}_{\oplus}/(1-\xi)) \cdot f(\bar{x}_{\ominus})$ and $f(\bar{x}_{\oplus}) \cdot f(\bar{x}_{\ominus}/(1-\xi))$.

The `n_emitters` optional argument is provided by the caller if this term requires spin-correlated matrix elements, and thus involves additional subtractions.

```

(Process config: process term: TBP)+≡
  procedure :: setup_interaction => process_term_setup_interaction

(Process config: sub interfaces)+≡
  module subroutine process_term_setup_interaction (term, core, model, &
    nlo_type, pol_beams, has_pdfs, use_internal_color, n_emitters)
    class(process_term_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model
    logical, intent(in), optional :: pol_beams
    logical, intent(in), optional :: has_pdfs
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: use_internal_color
    integer, intent(in), optional :: n_emitters
  end subroutine process_term_setup_interaction

(Process config: procedures)+≡
  module subroutine process_term_setup_interaction (term, core, model, &
    nlo_type, pol_beams, has_pdfs, use_internal_color, n_emitters)
    class(process_term_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model

```

```

logical, intent(in), optional :: pol_beams
logical, intent(in), optional :: has_pdfs
integer, intent(in), optional :: nlo_type
logical, intent(in), optional :: use_internal_color
integer, intent(in), optional :: n_emitters
integer :: n, n_tot
type(flavor_t), dimension(:), allocatable :: flv
type(color_t), dimension(:), allocatable :: col
type(helicity_t), dimension(:), allocatable :: hel
type(quantum_numbers_t), dimension(:), allocatable :: qn
logical :: is_pol, use_color
integer :: nlo_t, n_sub
is_pol = .false.; if (present (pol_beams)) is_pol = pol_beams
nlo_t = BORN; if (present (nlo_type)) nlo_t = nlo_type
n_tot = term%data%n_in + term%data%n_out
call count_number_of_states ()
term%n_allowed = n
call compute_n_sub (n_emitters, has_pdfs)
call fill_quantum_numbers ()
call term%int%basic_init &
      (term%data%n_in, 0, term%data%n_out, set_relations = .true.)
select type (core)
class is (prc_blha_t)
  call setup_states_blha_olp ()
type is (prc_threshold_t)
  call setup_states_threshold ()
class is (prc_external_t)
  call setup_states_other_prc_external ()
class default
  call setup_states_omega ()
end select
call term%int%freeze ()
contains
subroutine count_number_of_states ()
  integer :: f, h, c
  n = 0
  select type (core)
  class is (prc_external_t)
    do f = 1, term%data%n_flv
      do h = 1, term%data%n_hel
        do c = 1, term%data%n_col
          n = n + 1
        end do
      end do
    end do
  class default !!! Omega and all test cores
    do f = 1, term%data%n_flv
      do h = 1, term%data%n_hel
        do c = 1, term%data%n_col
          if (core%is_allowed (term%i_term, f, h, c)) n = n + 1
        end do
      end do
    end do
  end select
end subroutine

```

```

end subroutine count_number_of_states

subroutine compute_n_sub (n_emitters, has_pdfs)
  integer, intent(in), optional :: n_emitters
  logical, intent(in), optional :: has_pdfs
  logical :: can_have_sub
  integer :: n_sub_color, n_sub_spin
  use_color = .false.; if (present (use_internal_color)) &
    use_color = use_internal_color
  can_have_sub = nlo_t == NLO_VIRTUAL .or. &
    (nlo_t == NLO_REAL .and. term%i_term_global == term%i_sub) .or. &
    nlo_t == NLO_MISMATCH .or. nlo_t == NLO_DGLAP
  n_sub_color = 0; n_sub_spin = 0
  if (can_have_sub) then
    if (.not. use_color) n_sub_color = n_tot * (n_tot - 1) / 2
    if (nlo_t == NLO_REAL) then
      if (present (n_emitters)) then
        n_sub_spin = 6 * n_emitters
      end if
    end if
  end if
  n_sub = n_sub_color + n_sub_spin
  !!! For the virtual subtraction we also need the finite virtual contribution
  !!! corresponding to the  $\epsilon^0$ -pole
  if (nlo_t == NLO_VIRTUAL) n_sub = n_sub + 1
  if (present (has_pdfs)) then
    if (has_pdfs &
      .and. ((nlo_t == NLO_REAL .and. can_have_sub) &
        .or. nlo_t == NLO_DGLAP)) then
      !!! necessary dummy, needs refactoring,
      !!! c.f. [[term_instance_evaluate_interaction_external_tree]]
      n_sub = n_sub + n_beams_rescaled
    end if
  end if
  term%n_sub = n_sub
  term%n_sub_color = n_sub_color
  term%n_sub_spin = n_sub_spin
end subroutine compute_n_sub

subroutine fill_quantum_numbers ()
  integer :: nn
  logical :: can_have_sub
  select type (core)
  class is (prc_external_t)
    can_have_sub = nlo_t == NLO_VIRTUAL .or. &
      (nlo_t == NLO_REAL .and. term%i_term_global == term%i_sub) .or. &
      nlo_t == NLO_MISMATCH .or. nlo_t == NLO_DGLAP
    if (can_have_sub) then
      nn = (n_sub + 1) * n
    else
      nn = n
    end if
  class default
    nn = n
  end select
end subroutine fill_quantum_numbers

```

```

end select
allocate (term%flv (nn), term%col (nn), term%hel (nn))
allocate (flv (n_tot), col (n_tot), hel (n_tot))
allocate (qn (n_tot))
end subroutine fill_quantum_numbers

subroutine setup_states_blha_olp ()
integer :: s, f, c, h, i
i = 0
associate (data => term%data)
do s = 0, n_sub
do f = 1, data%n_flv
do h = 1, data%n_hel
do c = 1, data%n_col
i = i + 1
term%flv(i) = f
term%hel(i) = h
!!! Dummy-initialization of color
term%col(i) = c
call flv%init (data%flv_state (:,f), model)
call color_init_from_array (col, &
data%col_state(:,c), data%ghost_flag(:,c))
call col(1:data%n_in)%invert ()
if (is_pol) then
select type (core)
type is (prc_openloops_t)
call hel%init (data%hel_state (:,h))
call qn%init (flv, hel, col, s)
class default
call msg_fatal ("Polarized beams only supported by OpenLoops")
end select
else
call qn%init (flv, col, s)
end if
call qn%tag_hard_process ()
call term%int%add_state (qn)
end do
end do
end do
end do
end associate
end subroutine setup_states_blha_olp

subroutine setup_states_threshold ()
integer :: s, f, c, h, i
i = 0
n_sub = 0; if (nlo_t == NLO_VIRTUAL) n_sub = 1
associate (data => term%data)
do s = 0, n_sub
do f = 1, term%data%n_flv
do h = 1, data%n_hel
do c = 1, data%n_col
i = i + 1
term%flv(i) = f

```



```

        term%hel(i) = h
        !!! Dummy-initialization of color
        term%col(i) = 1
        call flv%init (term%data%flv_state (:,f), model)
        if (is_pol) then
            call hel%init (data%hel_state (:,h))
            call qn%init (flv, hel, s)
        else
            call qn%init (flv, s)
        end if
        call qn%tag_hard_process ()
        call term%int%add_state (qn)
    end do
end do
end do
end do
end associate
end subroutine setup_states_threshold

subroutine setup_states_other_prc_external ()
    integer :: s, f, i, c, h
    if (is_pol) &
        call msg_fatal ("Polarized beams only supported by OpenLoops")
    i = 0
    !!! n_sub = 0; if (nlo_t == NLO_VIRTUAL) n_sub = 1
    associate (data => term%data)
        do s = 0, n_sub
            do f = 1, data%n_flv
                do h = 1, data%n_hel
                    do c = 1, data%n_col
                        i = i + 1
                        term%flv(i) = f
                        term%hel(i) = h
                        !!! Dummy-initialization of color
                        term%col(i) = c
                        call flv%init (data%flv_state (:,f), model)
                        call color_init_from_array (col, &
                            data%col_state(:, :, c), data%ghost_flag(:, c))
                        call col(1:data%n_in)%invert ()
                        call qn%init (flv, col, s)
                        call qn%tag_hard_process ()
                        call term%int%add_state (qn)
                    end do
                end do
            end do
        end do
    end associate
end subroutine setup_states_other_prc_external

subroutine setup_states_omega ()
    integer :: f, h, c, i
    i = 0
    associate (data => term%data)
        do f = 1, data%n_flv

```

```

do h = 1, data%n_hel
do c = 1, data%n_col
  if (core%is_allowed (term%i_term, f, h, c)) then
    i = i + 1
    term%flv(i) = f
    term%hel(i) = h
    term%col(i) = c
    call flv%init (data%flv_state(:,f), model)
    call color_init_from_array (col, &
      data%col_state(:,c), &
      data%ghost_flag(:,c))
    call col(:data%n_in)%invert ()
    call hel%init (data%hel_state(:,h))
    call qn%init (flv, col, hel)
    call qn%tag_hard_process ()
    call term%int%add_state (qn)
  end if
end do
end do
end do
end associate
end subroutine setup_states_omega

end subroutine process_term_setup_interaction

```

<Process config: process term: TBP>+≡

```
procedure :: get_process_constants => process_term_get_process_constants
```

<Process config: sub interfaces>+≡

```

module subroutine process_term_get_process_constants &
  (term, prc_constants)
  class(process_term_t), intent(inout) :: term
  type(process_constants_t), intent(out) :: prc_constants
end subroutine process_term_get_process_constants

```

<Process config: procedures>+≡

```

module subroutine process_term_get_process_constants &
  (term, prc_constants)
  class(process_term_t), intent(inout) :: term
  type(process_constants_t), intent(out) :: prc_constants
  prc_constants = term%data
end subroutine process_term_get_process_constants

```

30.6 Process call statistics

Very simple object for statistics. Could be moved to a more basic chapter.

<process_counter.f90>≡

<File header>

```
module process_counter
```

<Standard module head>

```

    <Process counter: public>

    <Process counter: parameters>

    <Process counter: types>

    interface
    <Process counter: sub interfaces>
    end interface

```

```

end module process_counter

```

This object can record process calls, categorized by evaluation status. It is a part of the `mci_entry` component below.

```

<Process counter: public>≡
    public :: process_counter_t

<Process counter: types>≡
    type :: process_counter_t
        integer :: total = 0
        integer :: failed_kinematics = 0
        integer :: failed_cuts = 0
        integer :: has_passed = 0
        integer :: evaluated = 0
        integer :: complete = 0
    contains
    <Process counter: process counter: TBP>
end type process_counter_t

```

Here are the corresponding numeric codes:

```

<Process counter: parameters>≡
    integer, parameter, public :: STAT_UNDEFINED = 0
    integer, parameter, public :: STAT_INITIAL = 1
    integer, parameter, public :: STAT_ACTIVATED = 2
    integer, parameter, public :: STAT_BEAM_MOMENTA = 3
    integer, parameter, public :: STAT_FAILED_KINEMATICS = 4
    integer, parameter, public :: STAT_SEED_KINEMATICS = 5
    integer, parameter, public :: STAT_HARD_KINEMATICS = 6
    integer, parameter, public :: STAT_EFF_KINEMATICS = 7
    integer, parameter, public :: STAT_FAILED_CUTS = 8
    integer, parameter, public :: STAT_PASSED_CUTS = 9
    integer, parameter, public :: STAT_EVALUATED_TRACE = 10
    integer, parameter, public :: STAT_EVENT_COMPLETE = 11

```

Output.

```

<Process counter: process counter: TBP>≡
    procedure :: write => process_counter_write

<Process counter: sub interfaces>≡
    module subroutine process_counter_write (object, unit)
        class(process_counter_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_counter_write

```

```

<Process counter: procedures>≡
  module subroutine process_counter_write (object, unit)
    class(process_counter_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (object%total > 0) then
      write (u, "(1x,A)") "Call statistics (current run):"
      write (u, "(3x,A,I0)") "total          = ", object%total
      write (u, "(3x,A,I0)") "failed kin. = ", object%failed_kinematics
      write (u, "(3x,A,I0)") "failed cuts = ", object%failed_cuts
      write (u, "(3x,A,I0)") "passed cuts = ", object%has_passed
      write (u, "(3x,A,I0)") "evaluated   = ", object%evaluated
    else
      write (u, "(1x,A)") "Call statistics (current run): [no calls]"
    end if
  end subroutine process_counter_write

```

```

<process_counter_sub.f90>≡
  <File header>

  submodule (process_counter) process_counter_s

    use io_units

    implicit none

  contains

    <Process counter: procedures>

  end submodule process_counter_s

```

Reset. Just enforce default initialization.

```

<Process counter: process counter: TBP>+≡
  procedure :: reset => process_counter_reset

<Process counter: sub interfaces>+≡
  module subroutine process_counter_reset (counter)
    class(process_counter_t), intent(out) :: counter
  end subroutine process_counter_reset

<Process counter: procedures>+≡
  module subroutine process_counter_reset (counter)
    class(process_counter_t), intent(out) :: counter
    counter%total = 0
    counter%failed_kinematics = 0
    counter%failed_cuts = 0
    counter%has_passed = 0
    counter%evaluated = 0
    counter%complete = 0
  end subroutine process_counter_reset

```

We record an event according to the lowest status code greater or equal to the actual status. This is actually done by the process instance; the process object just copies the instance counter.

```

<Process counter: process counter: TBP>+≡
    procedure :: record => process_counter_record

<Process counter: sub interfaces>+≡
    module subroutine process_counter_record (counter, status)
        class(process_counter_t), intent(inout) :: counter
        integer, intent(in) :: status
    end subroutine process_counter_record

<Process counter: procedures>+≡
    module subroutine process_counter_record (counter, status)
        class(process_counter_t), intent(inout) :: counter
        integer, intent(in) :: status
        if (status <= STAT_FAILED_KINEMATICS) then
            counter%failed_kinematics = counter%failed_kinematics + 1
        else if (status <= STAT_FAILED_CUTS) then
            counter%failed_cuts = counter%failed_cuts + 1
        else if (status <= STAT_PASSED_CUTS) then
            counter%has_passed = counter%has_passed + 1
        else
            counter%evaluated = counter%evaluated + 1
        end if
        counter%total = counter%total + 1
    end subroutine process_counter_record

```

30.7 Multi-channel integration

```

<process_mci.f90>≡
    <File header>

    module process_mci

        <Use kinds>
        <Use strings>
        use cputime
        use rng_base
        use mci_base
        use variables
        use integration_results
        use process_libraries
        use phs_base
        use process_counter
        use process_config

        <Standard module head>

        <Process mci: public>

        <Process mci: parameters>

```

```

    <Process mci: types>

    interface
    <Process mci: sub interfaces>
    end interface

    end module process_mci

    <process_mci_sub.f90>≡
    <File header>

    submodule (process_mci) process_mci_s

    <Use debug>
    use io_units
    use diagnostics
    use physics_defs
    use md5

    implicit none

    contains

    <Process mci: procedures>

    end submodule process_mci_s

```

30.7.1 Process MCI entry

The `process_mci_entry_t` block contains, for each process component that is integrated independently, the configuration data for its MC input parameters. Each input parameter set is handled by a `mci_t` integrator.

The MC input parameter set is broken down into the parameters required by the structure-function chain and the parameters required by the phase space of the elementary process.

The MD5 sum collects all information about the associated processes that may affect the integration. It does not contain the MCI object itself or integration results.

MC integration is organized in passes. Each pass may consist of several iterations, and for each iteration there is a number of calls. We store explicitly the values that apply to the current pass. Previous values are archived in the `results` object.

The `counter` receives the counter statistics from the associated process instance, for diagnostics.

The `results` object records results, broken down in passes and iterations.

```

    <Process mci: public>≡
    public :: process_mci_entry_t

    <Process mci: types>≡
    type :: process_mci_entry_t
    integer :: i_mci = 0
    integer, dimension(:), allocatable :: i_component

```

```

integer :: process_type = PRC_UNKNOWN
integer :: n_par = 0
integer :: n_par_sf = 0
integer :: n_par_phs = 0
character(32) :: md5sum = ""
integer :: pass = 0
integer :: n_it = 0
integer :: n_calls = 0
logical :: activate_timer = .false.
real(default) :: error_threshold = 0
class(mci_t), allocatable :: mci
type(process_counter_t) :: counter
type(integration_results_t) :: results
logical :: negative_weights = .false.
logical :: combined_integration = .false.
integer :: real_partition_type = REAL_FULL
contains
  <Process mci: process mci entry: TBP>
end type process_mci_entry_t

```

Finalizer for the mci component.

```

<Process mci: process mci entry: TBP>≡
  procedure :: final => process_mci_entry_final

<Process mci: sub interfaces>≡
  module subroutine process_mci_entry_final (object)
    class(process_mci_entry_t), intent(inout) :: object
  end subroutine process_mci_entry_final

<Process mci: procedures>≡
  module subroutine process_mci_entry_final (object)
    class(process_mci_entry_t), intent(inout) :: object
    if (allocated (object%mci)) call object%mci%final ()
  end subroutine process_mci_entry_final

```

Output. Write pass/iteration information only if set (the pass index is nonzero). Write the MCI block only if it exists (for some self-tests it does not). Write results only if there are any.

```

<Process mci: process mci entry: TBP>+≡
  procedure :: write => process_mci_entry_write

<Process mci: sub interfaces>+≡
  module subroutine process_mci_entry_write (object, unit, pacify)
    class(process_mci_entry_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
  end subroutine process_mci_entry_write

<Process mci: procedures>+≡
  module subroutine process_mci_entry_write (object, unit, pacify)
    class(process_mci_entry_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u
    u = given_output_unit (unit)

```

```

write (u, "(3x,A,I0)") "Associated components = ", object%i_component
write (u, "(3x,A,I0)") "MC input parameters = ", object%n_par
write (u, "(3x,A,I0)") "MC parameters (SF) = ", object%n_par_sf
write (u, "(3x,A,I0)") "MC parameters (PHS) = ", object%n_par_phs
if (object%pass > 0) then
  write (u, "(3x,A,I0)") "Current pass = ", object%pass
  write (u, "(3x,A,I0)") "Number of iterations = ", object%n_it
  write (u, "(3x,A,I0)") "Number of calls = ", object%n_calls
end if
if (object%md5sum /= "") then
  write (u, "(3x,A,A,A)") "MD5 sum (components) = ', object%md5sum, '"
end if
if (allocated (object%mc_i)) then
  call object%mc_i%write (u)
end if
call object%counter%write (u)
if (object%results%exist ()) then
  call object%results%write (u, suppress = pacify)
  call object%results%write_chain_weights (u)
end if
end subroutine process_mci_entry_write

```

Configure the MCI entry. This is intent(inout) since some specific settings may be done before this. The actual `mci_t` object is an instance of the `mci_template` argument, which determines the concrete types.

In a unit-test context, the `mci_template` argument may be unallocated.

We obtain the number of channels and the number of parameters separately for the structure-function chain and for the associated process component. We assume that the phase-space object has already been configured.

We assume that there is only one process component directly associated with an MCI entry.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: configure => process_mci_entry_configure

(Process mci: sub interfaces)+≡
  module subroutine process_mci_entry_configure (mci_entry, mci_template, &
    process_type, i_mci, i_component, component, &
    n_sfpar, rng_factory)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_t), intent(in), allocatable :: mci_template
    integer, intent(in) :: process_type
    integer, intent(in) :: i_mci
    integer, intent(in) :: i_component
    type(process_component_t), intent(in), target :: component
    integer, intent(in) :: n_sfpar
    class(rng_factory_t), intent(inout) :: rng_factory
  end subroutine process_mci_entry_configure

(Process mci: procedures)+≡
  module subroutine process_mci_entry_configure (mci_entry, mci_template, &
    process_type, i_mci, i_component, component, &
    n_sfpar, rng_factory)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_t), intent(in), allocatable :: mci_template

```



```

integer, intent(in) :: process_type
integer, intent(in) :: i_mci
integer, intent(in) :: i_component
type(process_component_t), intent(in), target :: component
integer, intent(in) :: n_sfpar
class(rng_factory_t), intent(inout) :: rng_factory
class(rng_t), allocatable :: rng
associate (phs_config => component%phs_config)
  mci_entry%i_mci = i_mci
  call mci_entry%create_component_list (i_component, component%get_config ())
  mci_entry%n_par_sf = n_sfpar
  mci_entry%n_par_phs = phs_config%get_n_par ()
  mci_entry%n_par = mci_entry%n_par_sf + mci_entry%n_par_phs
  mci_entry%process_type = process_type
  if (allocated (mci_template)) then
    allocate (mci_entry%mci, source = mci_template)
    call mci_entry%mci%record_index (mci_entry%i_mci)
    call mci_entry%mci%set_dimensions &
      (mci_entry%n_par, phs_config%get_n_channel ())
    call mci_entry%mci%declare_flat_dimensions &
      (phs_config%get_flat_dimensions ())
    if (phs_config%provides_equivalences) then
      call mci_entry%mci%declare_equivalences &
        (phs_config%channel, mci_entry%n_par_sf)
    end if
    if (phs_config%provides_chains) then
      call mci_entry%mci%declare_chains (phs_config%chain)
    end if
    call rng_factory%make (rng)
    call mci_entry%mci%import_rng (rng)
  end if
  call mci_entry%results%init (process_type)
end associate
end subroutine process_mci_entry_configure

```

(Process mci: parameters)≡

```

integer, parameter, public :: REAL_FULL = 0
integer, parameter, public :: REAL_SINGULAR = 1
integer, parameter, public :: REAL_FINITE = 2

```

(Process mci: process mci entry: TBP)+≡

```

procedure :: create_component_list => &
  process_mci_entry_create_component_list

```

(Process mci: sub interfaces)+≡

```

module subroutine process_mci_entry_create_component_list (mci_entry, &
  i_component, component_config)
  class (process_mci_entry_t), intent(inout) :: mci_entry
  integer, intent(in) :: i_component
  type(process_component_def_t), intent(in) :: component_config
end subroutine process_mci_entry_create_component_list

```

(Process mci: procedures)+≡

```

module subroutine process_mci_entry_create_component_list (mci_entry, &
  i_component, component_config)

```

```

class (process_mci_entry_t), intent(inout) :: mci_entry
integer, intent(in) :: i_component
type(process_component_def_t), intent(in) :: component_config
integer, dimension(:), allocatable :: i_list
integer :: n
integer, save :: i_rfin_offset = 0
if (debug_on) call msg_debug &
    (D_PROCESS_INTEGRATION, "process_mci_entry_create_component_list")
if (mci_entry%combined_integration) then
    if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
        "mci_entry%real_partition_type", mci_entry%real_partition_type)
    n = get_n_components (mci_entry%real_partition_type)
    allocate (i_list (n))
    select case (mci_entry%real_partition_type)
    case (REAL_FULL)
        i_list = component_config%get_association_list ()
        allocate (mci_entry%i_component (size (i_list)))
        mci_entry%i_component = i_list
    case (REAL_SINGULAR)
        i_list = component_config%get_association_list (ASSOCIATED_REAL_FIN)
        allocate (mci_entry%i_component (size(i_list)))
        mci_entry%i_component = i_list
    case (REAL_FINITE)
        allocate (mci_entry%i_component (1))
        mci_entry%i_component(1) = &
            component_config%get_associated_real_fin () + i_rfin_offset
        i_rfin_offset = i_rfin_offset + 1
    end select
else
    allocate (mci_entry%i_component (1))
    mci_entry%i_component(1) = i_component
end if
contains
function get_n_components (real_partition_type) result (n_components)
integer :: n_components
integer, intent(in) :: real_partition_type
select case (real_partition_type)
case (REAL_FULL)
    n_components = size (component_config%get_association_list ())
case (REAL_SINGULAR)
    n_components = size (component_config%get_association_list &
        (ASSOCIATED_REAL_FIN))
end select
if (debug_on) call msg_debug &
    (D_PROCESS_INTEGRATION, "n_components", n_components)
end function get_n_components
end subroutine process_mci_entry_create_component_list

```

Set some additional parameters.

(Process mci: process mci entry: TBP)+≡

```
procedure :: set_parameters => process_mci_entry_set_parameters
```

(Process mci: sub interfaces)+≡

```
module subroutine process_mci_entry_set_parameters (mci_entry, var_list)
```

```

        class(process_mci_entry_t), intent(inout) :: mci_entry
        type(var_list_t), intent(in) :: var_list
    end subroutine process_mci_entry_set_parameters
<Process mci: procedures>+≡
module subroutine process_mci_entry_set_parameters (mci_entry, var_list)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    type(var_list_t), intent(in) :: var_list
    integer :: integration_results_verbosity
    real(default) :: error_threshold
    integration_results_verbosity = &
        var_list%get_ival (var_str ("integration_results_verbosity"))
    error_threshold = &
        var_list%get_rval (var_str ("error_threshold"))
    mci_entry%activate_timer = &
        var_list%get_lval (var_str ("?integration_timer"))
    call mci_entry%results%set_verbosity (integration_results_verbosity)
    call mci_entry%results%set_error_threshold (error_threshold)
end subroutine process_mci_entry_set_parameters

```

Compute an MD5 sum that summarizes all information that could influence integration results, for the associated process components. We take the process-configuration MD5 sum which represents parameters, cuts, etc., the MD5 sums for the process component definitions and their phase space objects (which should be configured), and the beam configuration MD5 sum. (The QCD setup is included in the process configuration data MD5 sum.)

Done only once, when the MD5 sum is still empty.

```

<Process mci: process mci entry: TBP>+≡
    procedure :: compute_md5sum => process_mci_entry_compute_md5sum
<Process mci: sub interfaces>+≡
    module subroutine process_mci_entry_compute_md5sum (mci_entry, &
        config, component, beam_config)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        type(process_config_data_t), intent(in) :: config
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_beam_config_t), intent(in) :: beam_config
    end subroutine process_mci_entry_compute_md5sum
<Process mci: procedures>+≡
module subroutine process_mci_entry_compute_md5sum (mci_entry, &
    config, component, beam_config)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    type(process_config_data_t), intent(in) :: config
    type(process_component_t), dimension(:), intent(in) :: component
    type(process_beam_config_t), intent(in) :: beam_config
    type(string_t) :: buffer
    integer :: i
    if (mci_entry%md5sum == "") then
        buffer = config%get_md5sum () // beam_config%get_md5sum ()
        do i = 1, size (component)
            if (component(i)%is_active ()) then
                buffer = buffer // component(i)%get_md5sum ()
            end if
        end do
    end if
end do

```

```

        mci_entry%md5sum = md5sum (char (buffer))
    end if
    if (allocated (mci_entry%md5sum)) then
        call mci_entry%md5sum (mci_entry%md5sum)
    end if
end subroutine process_mci_entry_compute_md5sum

```

Test the MCI sampler by calling it a given number of time, discarding the results. The instance should be initialized.

The `mci_entry` is `intent(inout)` because the integrator contains the random-number state.

```

(Process mci: process mci entry: TBP)+≡
    procedure :: sampler_test => process_mci_entry_sampler_test

(Process mci: sub interfaces)+≡
    module subroutine process_mci_entry_sampler_test &
        (mci_entry, mci_sampler, n_calls)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        class(mci_sampler_t), intent(inout), target :: mci_sampler
        integer, intent(in) :: n_calls
    end subroutine process_mci_entry_sampler_test

(Process mci: procedures)+≡
    module subroutine process_mci_entry_sampler_test &
        (mci_entry, mci_sampler, n_calls)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        class(mci_sampler_t), intent(inout), target :: mci_sampler
        integer, intent(in) :: n_calls
        call mci_entry%md5sum (mci_sampler, n_calls)
    end subroutine process_mci_entry_sampler_test

```

Integrate.

The `integrate` method counts as an integration pass; the pass count is increased by one. We transfer the pass parameters (number of iterations and number of calls) to the actual integration routine.

The `mci_entry` is `intent(inout)` because the integrator contains the random-number state.

Note: The results are written to screen and to logfile. This behavior is hardcoded.

```

(Process mci: process mci entry: TBP)+≡
    procedure :: integrate => process_mci_entry_integrate
    procedure :: final_integration => process_mci_entry_final_integration

(Process mci: sub interfaces)+≡
    module subroutine process_mci_entry_integrate (mci_entry, mci_instance, &
        mci_sampler, n_it, n_calls, &
        adapt_grids, adapt_weights, final, pacify, &
        nlo_type)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        class(mci_instance_t), intent(inout) :: mci_instance
        class(mci_sampler_t), intent(inout) :: mci_sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
    end subroutine process_mci_entry_integrate

```

```

        logical, intent(in), optional :: adapt_grids
        logical, intent(in), optional :: adapt_weights
        logical, intent(in), optional :: final, pacify
        integer, intent(in), optional :: nlo_type
    end subroutine process_mci_entry_integrate
    module subroutine process_mci_entry_final_integration (mci_entry)
        class(process_mci_entry_t), intent(inout) :: mci_entry
    end subroutine process_mci_entry_final_integration

```

(Process mci: procedures)+≡

```

    module subroutine process_mci_entry_integrate (mci_entry, mci_instance, &
        mci_sampler, n_it, n_calls, &
        adapt_grids, adapt_weights, final, pacify, &
        nlo_type)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        class(mci_instance_t), intent(inout) :: mci_instance
        class(mci_sampler_t), intent(inout) :: mci_sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        logical, intent(in), optional :: adapt_grids
        logical, intent(in), optional :: adapt_weights
        logical, intent(in), optional :: final, pacify
        integer, intent(in), optional :: nlo_type
        integer :: u_log
        u_log = logfile_unit ()
        mci_entry%pass = mci_entry%pass + 1
        mci_entry%n_it = n_it
        mci_entry%n_calls = n_calls
        if (mci_entry%pass == 1) &
            call mci_entry%pci%startup_message (n_calls = n_calls)
        call mci_entry%pci%set_timer (active = mci_entry%activate_timer)
        call mci_entry%results%display_init (screen = .true., unit = u_log)
        call mci_entry%results%new_pass ()
        if (present (nlo_type)) then
            select case (nlo_type)
            case (NLO_VIRTUAL, NLO_REAL, NLO_MISMATCH, NLO_DGLAP)
                mci_instance%negative_weights = .true.
            end select
        end if
        call mci_entry%pci%add_pass (adapt_grids, adapt_weights, final)
        call mci_entry%pci%start_timer ()
        call mci_entry%pci%integrate (mci_instance, mci_sampler, n_it, &
            n_calls, mci_entry%results, pacify = pacify)
        call mci_entry%pci%stop_timer ()
        if (signal_is_pending ()) return
    end subroutine process_mci_entry_integrate

    module subroutine process_mci_entry_final_integration (mci_entry)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        call mci_entry%results%display_final ()
        call mci_entry%time_message ()
    end subroutine process_mci_entry_final_integration

```

If appropriate, issue an informative message about the expected time for an

event sample.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: get_time => process_mci_entry_get_time
  procedure :: time_message => process_mci_entry_time_message

(Process mci: sub interfaces)+≡
  module subroutine process_mci_entry_get_time (mci_entry, time, sample)
    class(process_mci_entry_t), intent(in) :: mci_entry
    type(time_t), intent(out) :: time
    integer, intent(in) :: sample
  end subroutine process_mci_entry_get_time
  module subroutine process_mci_entry_time_message (mci_entry)
    class(process_mci_entry_t), intent(in) :: mci_entry
  end subroutine process_mci_entry_time_message

(Process mci: procedures)+≡
  module subroutine process_mci_entry_get_time (mci_entry, time, sample)
    class(process_mci_entry_t), intent(in) :: mci_entry
    type(time_t), intent(out) :: time
    integer, intent(in) :: sample
    real(default) :: time_last_pass, efficiency, calls
    time_last_pass = mci_entry%mci%get_time ()
    calls = mci_entry%results%get_n_calls ()
    efficiency = mci_entry%mci%get_efficiency ()
    if (time_last_pass > 0 .and. calls > 0 .and. efficiency > 0) then
      time = nint (time_last_pass / calls / efficiency * sample)
    end if
  end subroutine process_mci_entry_get_time

  module subroutine process_mci_entry_time_message (mci_entry)
    class(process_mci_entry_t), intent(in) :: mci_entry
    type(time_t) :: time
    integer :: sample
    sample = 10000
    call mci_entry%get_time (time, sample)
    if (time%is_known ()) then
      call msg_message ("Time estimate for generating 10000 events: " &
        // char (time%to_string_dhms ()))
    end if
  end subroutine process_mci_entry_time_message

```

Prepare event generation. (For the test integrator, this does nothing. It is relevant for the VAMP integrator.)

```

(Process mci: process mci entry: TBP)+≡
  procedure :: prepare_simulation => process_mci_entry_prepare_simulation

(Process mci: sub interfaces)+≡
  module subroutine process_mci_entry_prepare_simulation (mci_entry)
    class(process_mci_entry_t), intent(inout) :: mci_entry
  end subroutine process_mci_entry_prepare_simulation

(Process mci: procedures)+≡
  module subroutine process_mci_entry_prepare_simulation (mci_entry)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    call mci_entry%mci%prepare_simulation ()

```

```
end subroutine process_mci_entry_prepare_simulation
```

Generate an event. The instance should be initialized, otherwise event generation is directed by the mci integrator subobject. The integrator instance is contained in a `mci_work` subobject of the process instance, which simultaneously serves as the sampler object. (We avoid the anti-aliasing rules if we assume that the sampling itself does not involve the integrator instance contained in the process instance.)

Regarding weighted events, we only take events which are valid, which means that they have valid kinematics and have passed cuts. Therefore, we have a rejection loop. For unweighted events, the unweighting routine should already take care of this.

The `keep_failed` flag determines whether events which failed cuts are nevertheless produced, to be recorded with zero weight. Alternatively, failed events are dropped, and this fact is recorded by the counter `n_dropped`.

```
(Process mci: process mci entry: TBP)+≡
  procedure :: generate_weighted_event => &
    process_mci_entry_generate_weighted_event
  procedure :: generate_unweighted_event => &
    process_mci_entry_generate_unweighted_event

(Process mci: sub interfaces)+≡
  module subroutine process_mci_entry_generate_weighted_event (mci_entry, &
    mci_instance, mci_sampler, keep_failed)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    logical, intent(in) :: keep_failed
  end subroutine process_mci_entry_generate_weighted_event
  module subroutine process_mci_entry_generate_unweighted_event &
    (mci_entry, mci_instance, mci_sampler)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
  end subroutine process_mci_entry_generate_unweighted_event

(Process mci: procedures)+≡
  module subroutine process_mci_entry_generate_weighted_event (mci_entry, &
    mci_instance, mci_sampler, keep_failed)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    logical, intent(in) :: keep_failed
    logical :: generate_new
    generate_new = .true.
    call mci_instance%reset_n_event_dropped ()
    REJECTION: do while (generate_new)
      call mci_entry%mci%generate_weighted_event (mci_instance, mci_sampler)
      if (signal_is_pending ()) return
      if (.not. mci_sampler%is_valid()) then
        if (keep_failed) then
          generate_new = .false.
        else

```

```

        call mci_instance%record_event_dropped ()
        generate_new = .true.
    end if
else
    generate_new = .false.
end if
end do REJECTION
end subroutine process_mci_entry_generate_weighted_event

module subroutine process_mci_entry_generate_unweighted_event &
    (mci_entry, mci_instance, mci_sampler)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    call mci_entry%mci%generate_unweighted_event (mci_instance, mci_sampler)
end subroutine process_mci_entry_generate_unweighted_event

```

Extract results.

```

(Process mci: process mci entry: TBP)+≡
    procedure :: has_integral => process_mci_entry_has_integral
    procedure :: get_integral => process_mci_entry_get_integral
    procedure :: get_error => process_mci_entry_get_error
    procedure :: get_accuracy => process_mci_entry_get_accuracy
    procedure :: get_chi2 => process_mci_entry_get_chi2
    procedure :: get_efficiency => process_mci_entry_get_efficiency

(Process mci: sub interfaces)+≡
    module function process_mci_entry_has_integral (mci_entry) result (flag)
        class(process_mci_entry_t), intent(in) :: mci_entry
        logical :: flag
    end function process_mci_entry_has_integral
    module function process_mci_entry_get_integral (mci_entry) result (integral)
        class(process_mci_entry_t), intent(in) :: mci_entry
        real(default) :: integral
    end function process_mci_entry_get_integral
    module function process_mci_entry_get_error (mci_entry) result (error)
        class(process_mci_entry_t), intent(in) :: mci_entry
        real(default) :: error
    end function process_mci_entry_get_error
    module function process_mci_entry_get_accuracy (mci_entry) result (accuracy)
        class(process_mci_entry_t), intent(in) :: mci_entry
        real(default) :: accuracy
    end function process_mci_entry_get_accuracy
    module function process_mci_entry_get_chi2 (mci_entry) result (chi2)
        class(process_mci_entry_t), intent(in) :: mci_entry
        real(default) :: chi2
    end function process_mci_entry_get_chi2
    module function process_mci_entry_get_efficiency &
        (mci_entry) result (efficiency)
        class(process_mci_entry_t), intent(in) :: mci_entry
        real(default) :: efficiency
    end function process_mci_entry_get_efficiency

(Process mci: procedures)+≡
    module function process_mci_entry_has_integral (mci_entry) result (flag)

```



```

class(process_mci_entry_t), intent(in) :: mci_entry
logical :: flag
flag = mci_entry%results%exist ()
end function process_mci_entry_has_integral

module function process_mci_entry_get_integral (mci_entry) result (integral)
class(process_mci_entry_t), intent(in) :: mci_entry
real(default) :: integral
integral = mci_entry%results%get_integral ()
end function process_mci_entry_get_integral

module function process_mci_entry_get_error (mci_entry) result (error)
class(process_mci_entry_t), intent(in) :: mci_entry
real(default) :: error
error = mci_entry%results%get_error ()
end function process_mci_entry_get_error

module function process_mci_entry_get_accuracy (mci_entry) result (accuracy)
class(process_mci_entry_t), intent(in) :: mci_entry
real(default) :: accuracy
accuracy = mci_entry%results%get_accuracy ()
end function process_mci_entry_get_accuracy

module function process_mci_entry_get_chi2 (mci_entry) result (chi2)
class(process_mci_entry_t), intent(in) :: mci_entry
real(default) :: chi2
chi2 = mci_entry%results%get_chi2 ()
end function process_mci_entry_get_chi2

module function process_mci_entry_get_efficiency &
(mci_entry) result (efficiency)
class(process_mci_entry_t), intent(in) :: mci_entry
real(default) :: efficiency
efficiency = mci_entry%results%get_efficiency ()
end function process_mci_entry_get_efficiency

```

Return the MCI checksum. This may be the one used for configuration, but may also incorporate results, if they change the state of the integrator (adaptation).

(Process mci: process mci entry: TBP)+≡

```
procedure :: get_md5sum => process_mci_entry_get_md5sum
```

(Process mci: sub interfaces)+≡

```

pure module function process_mci_entry_get_md5sum (entry) result (md5sum)
class(process_mci_entry_t), intent(in) :: entry
character(32) :: md5sum
end function process_mci_entry_get_md5sum

```

(Process mci: procedures)+≡

```

pure module function process_mci_entry_get_md5sum (entry) result (md5sum)
class(process_mci_entry_t), intent(in) :: entry
character(32) :: md5sum
md5sum = entry%mci%get_md5sum ()
end function process_mci_entry_get_md5sum

```

30.7.2 MC parameter set and MCI instance

For each process component that is associated with a multi-channel integration (MCI) object, the `mci_work_t` object contains the currently active parameter set. It also holds the implementation of the `mci_instance_t` that the integrator needs for doing its work.

```

(Process mci: public)+≡
    public :: mci_work_t

(Process mci: types)+≡
    type :: mci_work_t
        type(process_mci_entry_t), pointer :: config => null ()
        real(default), dimension(:), allocatable :: x
        class(mci_instance_t), pointer :: mci => null ()
        type(process_counter_t) :: counter
        logical :: keep_failed_events = .false.
        integer :: n_event_dropped = 0
    contains
        (Process mci: mci work: TBP)
    end type mci_work_t

```

First write configuration data, then the current values.

```

(Process mci: mci work: TBP)≡
    procedure :: write => mci_work_write

(Process mci: sub interfaces)+≡
    module subroutine mci_work_write (mci_work, unit, testflag)
        class(mci_work_t), intent(in) :: mci_work
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
    end subroutine mci_work_write

(Process mci: procedures)+≡
    module subroutine mci_work_write (mci_work, unit, testflag)
        class(mci_work_t), intent(in) :: mci_work
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A,I0,A)") "Active MCI instance #", &
            mci_work%config%i_mci, " ="
        write (u, "(2x)", advance="no")
        do i = 1, mci_work%config%n_par
            write (u, "(1x,F7.5)", advance="no") mci_work%x(i)
            if (i == mci_work%config%n_par_sf) &
                write (u, "(1x,'|')", advance="no")
        end do
        write (u, *)
        if (associated (mci_work%mci)) then
            call mci_work%mci%write (u, pacify = testflag)
            call mci_work%counter%write (u)
        end if
    end subroutine mci_work_write

```

The mci component may require finalization.

```

(Process mci: mci work: TBP)+≡
  procedure :: final => mci_work_final

(Process mci: sub interfaces)+≡
  module subroutine mci_work_final (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
  end subroutine mci_work_final

(Process mci: procedures)+≡
  module subroutine mci_work_final (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
    if (associated (mci_work%mci)) then
      call mci_work%mci%final ()
      deallocate (mci_work%mci)
    end if
  end subroutine mci_work_final

```

Initialize with the maximum length that we will need. Contents are not initialized.

The integrator inside the mci_entry object is responsible for allocating and initializing its own instance, which is referred to by a pointer in the mci_work object.

```

(Process mci: mci work: TBP)+≡
  procedure :: init => mci_work_init

(Process mci: sub interfaces)+≡
  module subroutine mci_work_init (mci_work, mci_entry)
    class(mci_work_t), intent(out) :: mci_work
    type(process_mci_entry_t), intent(in), target :: mci_entry
  end subroutine mci_work_init

(Process mci: procedures)+≡
  module subroutine mci_work_init (mci_work, mci_entry)
    class(mci_work_t), intent(out) :: mci_work
    type(process_mci_entry_t), intent(in), target :: mci_entry
    mci_work%config => mci_entry
    allocate (mci_work%x (mci_entry%n_par))
    if (allocated (mci_entry%mci)) then
      call mci_entry%mci%allocate_instance (mci_work%mci)
      call mci_work%mci%init (mci_entry%mci)
    end if
  end subroutine mci_work_init

```

Set parameters explicitly, either all at once, or separately for the structure-function and process parts.

```

(Process mci: mci work: TBP)+≡
  procedure :: set => mci_work_set
  procedure :: set_x_strfun => mci_work_set_x_strfun
  procedure :: set_x_process => mci_work_set_x_process

(Process mci: sub interfaces)+≡
  module subroutine mci_work_set (mci_work, x)
    class(mci_work_t), intent(inout) :: mci_work
    real(default), dimension(:), intent(in) :: x

```

```

end subroutine mci_work_set
module subroutine mci_work_set_x_strfun (mci_work, x)
  class(mci_work_t), intent(inout) :: mci_work
  real(default), dimension(:), intent(in) :: x
end subroutine mci_work_set_x_strfun
module subroutine mci_work_set_x_process (mci_work, x)
  class(mci_work_t), intent(inout) :: mci_work
  real(default), dimension(:), intent(in) :: x
end subroutine mci_work_set_x_process

(Process mci: procedures)+≡
module subroutine mci_work_set (mci_work, x)
  class(mci_work_t), intent(inout) :: mci_work
  real(default), dimension(:), intent(in) :: x
  mci_work%x = x
end subroutine mci_work_set

module subroutine mci_work_set_x_strfun (mci_work, x)
  class(mci_work_t), intent(inout) :: mci_work
  real(default), dimension(:), intent(in) :: x
  mci_work%x(1 : mci_work%config%n_par_sf) = x
end subroutine mci_work_set_x_strfun

module subroutine mci_work_set_x_process (mci_work, x)
  class(mci_work_t), intent(inout) :: mci_work
  real(default), dimension(:), intent(in) :: x
  mci_work%x(mci_work%config%n_par_sf + 1 : mci_work%config%n_par) = x
end subroutine mci_work_set_x_process

```

Return the array of active components, i.e., those that correspond to the currently selected MC parameter set.

```

(Process mci: mci work: TBP)+≡
  procedure :: get_active_components => mci_work_get_active_components

(Process mci: sub interfaces)+≡
  module function mci_work_get_active_components &
    (mci_work) result (i_component)
    class(mci_work_t), intent(in) :: mci_work
    integer, dimension(:), allocatable :: i_component
  end function mci_work_get_active_components

(Process mci: procedures)+≡
  module function mci_work_get_active_components (mci_work) result (i_component)
    class(mci_work_t), intent(in) :: mci_work
    integer, dimension(:), allocatable :: i_component
    allocate (i_component (size (mci_work%config%i_component)))
    i_component = mci_work%config%i_component
  end function mci_work_get_active_components

```

Return the active parameters as a simple array with correct length. Do this separately for the structure-function parameters and the process parameters.

```

(Process mci: mci work: TBP)+≡
  procedure :: get_x_strfun => mci_work_get_x_strfun
  procedure :: get_x_process => mci_work_get_x_process

```

```

(Process mci: sub interfaces)+≡
    pure module function mci_work_get_x_strfun (mci_work) result (x)
        class(mci_work_t), intent(in) :: mci_work
        real(default), dimension(mci_work%config%n_par_sf) :: x
    end function mci_work_get_x_strfun
    pure module function mci_work_get_x_process (mci_work) result (x)
        class(mci_work_t), intent(in) :: mci_work
        real(default), dimension(mci_work%config%n_par_phs) :: x
    end function mci_work_get_x_process

(Process mci: procedures)+≡
    pure module function mci_work_get_x_strfun (mci_work) result (x)
        class(mci_work_t), intent(in) :: mci_work
        real(default), dimension(mci_work%config%n_par_sf) :: x
        x = mci_work%x(1 : mci_work%config%n_par_sf)
    end function mci_work_get_x_strfun

    pure module function mci_work_get_x_process (mci_work) result (x)
        class(mci_work_t), intent(in) :: mci_work
        real(default), dimension(mci_work%config%n_par_phs) :: x
        x = mci_work%x(mci_work%config%n_par_sf + 1 : mci_work%config%n_par)
    end function mci_work_get_x_process

```

Initialize and finalize event generation for the specified MCI entry. This also resets the counter.

```

(Process mci: mci work: TBP)+≡
    procedure :: init_simulation => mci_work_init_simulation
    procedure :: final_simulation => mci_work_final_simulation

(Process mci: sub interfaces)+≡
    module subroutine mci_work_final_simulation (mci_work)
        class(mci_work_t), intent(inout) :: mci_work
    end subroutine mci_work_final_simulation
    module subroutine mci_work_init_simulation &
        (mci_work, safety_factor, keep_failed_events)
        class(mci_work_t), intent(inout) :: mci_work
        real(default), intent(in), optional :: safety_factor
        logical, intent(in), optional :: keep_failed_events
    end subroutine mci_work_init_simulation

(Process mci: procedures)+≡
    module subroutine mci_work_init_simulation &
        (mci_work, safety_factor, keep_failed_events)
        class(mci_work_t), intent(inout) :: mci_work
        real(default), intent(in), optional :: safety_factor
        logical, intent(in), optional :: keep_failed_events
        call mci_work%mci%init_simulation (safety_factor)
        call mci_work%counter%reset ()
        if (present (keep_failed_events)) &
            mci_work%keep_failed_events = keep_failed_events
    end subroutine mci_work_init_simulation

    module subroutine mci_work_final_simulation (mci_work)
        class(mci_work_t), intent(inout) :: mci_work
        call mci_work%mci%final_simulation ()
    end subroutine mci_work_final_simulation

```

```
end subroutine mci_work_final_simulation
```

Counter.

```
<Process mci: mci work: TBP>+≡
  procedure :: reset_counter => mci_work_reset_counter
  procedure :: record_call => mci_work_record_call
  procedure :: get_counter => mci_work_get_counter

<Process mci: sub interfaces>+≡
  module subroutine mci_work_reset_counter (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
  end subroutine mci_work_reset_counter
  module subroutine mci_work_record_call (mci_work, status)
    class(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: status
  end subroutine mci_work_record_call
  pure module function mci_work_get_counter (mci_work) result (counter)
    class(mci_work_t), intent(in) :: mci_work
    type(process_counter_t) :: counter
  end function mci_work_get_counter

<Process mci: procedures>+≡
  module subroutine mci_work_reset_counter (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
    call mci_work%counter%reset ()
  end subroutine mci_work_reset_counter

  module subroutine mci_work_record_call (mci_work, status)
    class(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: status
    call mci_work%counter%record (status)
  end subroutine mci_work_record_call

  pure module function mci_work_get_counter (mci_work) result (counter)
    class(mci_work_t), intent(in) :: mci_work
    type(process_counter_t) :: counter
    counter = mci_work%counter
  end function mci_work_get_counter
```

30.8 Process component manager

```
<pcm.f90>≡
  <File header>

  module pcm

    <Use kinds>
    <Use strings>
    use lorentz
    use model_data, only: model_data_t
    use models, only: model_t
    use quantum_numbers, only: quantum_numbers_t, quantum_numbers_mask_t
```

```

use variables, only: var_list_t
use nlo_data, only: nlo_settings_t
use nlo_data, only: fks_template_t
use nlo_data, only: FKS_DEFAULT, FKS_RESONANCES
use mci_base, only: mci_t
use phs_base, only: phs_config_t
use mappings, only: mapping_defaults_t
use phs_forests, only: phs_parameters_t
use phs_fks, only: isr_kinematics_t, real_kinematics_t
use phs_fks, only: phs_identifier_t
use fks_regions, only: region_data_t
use phs_fks, only: phs_fks_generator_t
use phs_fks, only: dalitz_plot_t
use phs_fks, only: phs_fks_config_t, get_filtered_resonance_histories
use dispatch_phase_space, only: dispatch_phs
use real_subtraction, only: real_subtraction_t, soft_mismatch_t
use real_subtraction, only: INTEGRATION, FIXED_ORDER_EVENTS
use real_subtraction, only: real_partition_t, powheg_damping_simple_t
use real_subtraction, only: real_partition_fixed_order_t
use virtual, only: virtual_t
use dglap_remnant, only: dglap_remnant_t
use blha_config, only: blha_master_t

use pcm_base
use process_config
use process_mci, only: process_mci_entry_t
use process_mci, only: REAL_SINGULAR, REAL_FINITE

<Standard module head>

<PCM: public>

<PCM: types>

    interface
    <PCM: sub interfaces>
    end interface

contains

    <PCM: main procedures>

end module pcm

<pcm_sub.f90>≡
    <File header>

submodule (pcm) pcm_s

    <Use debug>
    use constants, only: zero, two
    use diagnostics
    use phs_points, only: assignment(=)
    use io_units, only: free_unit
    use os_interface

```

```

    use process_constants, only: process_constants_t
    use physics_defs
    use flavors, only: flavor_t
    use interactions, only: interaction_t
    use dispatch_fks, only: dispatch_fks_setup
    use process_libraries, only: process_component_def_t
    use resonances, only: resonance_history_t, resonance_history_set_t
    use prc_threshold, only: threshold_def_t
    use blha_olp_interfaces, only: prc_blha_t

    implicit none

contains

<PCM: procedures>

end submodule pcm_s

```

30.8.1 Default process component manager

This is the configuration object which has the duty of allocating the corresponding instance. The default version is trivial.

```

<PCM: public>≡
    public :: pcm_default_t

<PCM: types>≡
    type, extends (pcm_t) :: pcm_default_t
    contains
    <PCM: pcm default: TBP>
    end type pcm_default_t

Gfortran 7/8/9 bug, has to remain in the main module:

<PCM: pcm default: TBP>≡
    procedure :: allocate_workspace => pcm_default_allocate_workspace

<PCM: main procedures>≡
    subroutine pcm_default_allocate_workspace (pcm, work)
    class(pcm_default_t), intent(in) :: pcm
    class(pcm_workspace_t), intent(inout), allocatable :: work
    allocate (pcm_default_workspace_t :: work)
    end subroutine pcm_default_allocate_workspace

```

Finalizer: apply to core manager.

```

<PCM: pcm default: TBP>+≡
    procedure :: final => pcm_default_final

<PCM: sub interfaces>≡
    module subroutine pcm_default_final (pcm)
    class(pcm_default_t), intent(inout) :: pcm
    end subroutine pcm_default_final

```



```

<PCM: procedures>≡
  module subroutine pcm_default_final (pcm)
    class(pcm_default_t), intent(inout) :: pcm
  end subroutine pcm_default_final

<PCM: pcm default: TBP>+≡
  procedure :: is_nlo => pcm_default_is_nlo
<PCM: sub interfaces>+≡
  module function pcm_default_is_nlo (pcm) result (is_nlo)
    logical :: is_nlo
    class(pcm_default_t), intent(in) :: pcm
  end function pcm_default_is_nlo
<PCM: procedures>+≡
  module function pcm_default_is_nlo (pcm) result (is_nlo)
    logical :: is_nlo
    class(pcm_default_t), intent(in) :: pcm
    is_nlo = .false.
  end function pcm_default_is_nlo

Initialize configuration data, using environment variables.
<PCM: pcm default: TBP>+≡
  procedure :: init => pcm_default_init
<PCM: sub interfaces>+≡
  module subroutine pcm_default_init (pcm, env, meta)
    class(pcm_default_t), intent(out) :: pcm
    type(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
  end subroutine pcm_default_init
<PCM: procedures>+≡
  module subroutine pcm_default_init (pcm, env, meta)
    class(pcm_default_t), intent(out) :: pcm
    type(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
    pcm%has_pdfs = env%has_pdfs ()
    call pcm%set_blha_defaults &
      (env%has_polarized_beams (), env%get_var_list_ptr ())
    pcm%os_data = env%get_os_data ()
  end subroutine pcm_default_init

<PCM: types>+≡
  type, extends (pcm_workspace_t) :: pcm_default_workspace_t
  contains
  <PCM: pcm instance default: TBP>
  end type pcm_default_workspace_t

<PCM: pcm instance default: TBP>≡
  procedure :: final => pcm_default_workspace_final
<PCM: sub interfaces>+≡
  module subroutine pcm_default_workspace_final (pcm_work)
    class(pcm_default_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_default_workspace_final

```

```

<PCM: procedures>+≡
  module subroutine pcm_default_workspace_final (pcm_work)
    class(pcm_default_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_default_workspace_final

<PCM: pcm instance default: TBP>+≡
  procedure :: is_nlo => pcm_default_workspace_is_nlo

<PCM: sub interfaces>+≡
  module function pcm_default_workspace_is_nlo (pcm_work) result (is_nlo)
    logical :: is_nlo
    class(pcm_default_workspace_t), intent(inout) :: pcm_work
  end function pcm_default_workspace_is_nlo

<PCM: procedures>+≡
  module function pcm_default_workspace_is_nlo (pcm_work) result (is_nlo)
    logical :: is_nlo
    class(pcm_default_workspace_t), intent(inout) :: pcm_work
    is_nlo = .false.
  end function pcm_default_workspace_is_nlo

```

30.8.2 Implementations for the default manager

Categorize components. Nothing to do here, all components are of Born type.

```

<PCM: pcm default: TBP>+≡
  procedure :: categorize_components => pcm_default_categorize_components

<PCM: sub interfaces>+≡
  module subroutine pcm_default_categorize_components (pcm, config)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
  end subroutine pcm_default_categorize_components

<PCM: procedures>+≡
  module subroutine pcm_default_categorize_components (pcm, config)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
  end subroutine pcm_default_categorize_components

```

Phase-space configuration

Default setup for tree processes: a single phase-space configuration that is valid for all components.

```

<PCM: pcm default: TBP>+≡
  procedure :: init_phs_config => pcm_default_init_phs_config

<PCM: sub interfaces>+≡
  module subroutine pcm_default_init_phs_config &
    (pcm, phs_entry, meta, env, phs_par, mapping_defs)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_phs_config_t), &
      dimension(:), allocatable, intent(out) :: phs_entry

```

```

        type(process_metadata_t), intent(in) :: meta
        type(process_environment_t), intent(in) :: env
        type(mapping_defaults_t), intent(in) :: mapping_defs
        type(phs_parameters_t), intent(in) :: phs_par
    end subroutine pcm_default_init_phs_config
<PCM: procedures>+≡
    module subroutine pcm_default_init_phs_config &
        (pcm, phs_entry, meta, env, phs_par, mapping_defs)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_phs_config_t), &
        dimension(:), allocatable, intent(out) :: phs_entry
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    type(mapping_defaults_t), intent(in) :: mapping_defs
    type(phs_parameters_t), intent(in) :: phs_par
    allocate (phs_entry (1))
    allocate (pcm%i_phs_config (pcm%n_components), source=1)
    call dispatch_phs (phs_entry(1)%phs_config, &
        env%get_var_list_ptr (), &
        env%get_os_data (), &
        meta%id, &
        mapping_defs, phs_par)
    end subroutine pcm_default_init_phs_config

```

Core management

The default component manager assigns one core per component. We allocate and configure the core objects, using the process-component configuration data.

```

<PCM: pcm default: TBP>+≡
    procedure :: allocate_cores => pcm_default_allocate_cores
<PCM: sub interfaces>+≡
    module subroutine pcm_default_allocate_cores (pcm, config, core_entry)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
    type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
    end subroutine pcm_default_allocate_cores
<PCM: procedures>+≡
    module subroutine pcm_default_allocate_cores (pcm, config, core_entry)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
    type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
    type(process_component_def_t), pointer :: component_def
    integer :: i
    allocate (pcm%i_core (pcm%n_components), source = 0)
    pcm%n_cores = pcm%n_components
    allocate (core_entry (pcm%n_cores))
    do i = 1, pcm%n_cores
        pcm%i_core(i) = i
        core_entry(i)%i_component = i
        component_def => config%process_def%get_component_def_ptr (i)
        core_entry(i)%core_def => component_def%get_core_def_ptr ()
    end do
    end subroutine pcm_default_allocate_cores

```

```

        core_entry(i)%active = component_def%can_be_integrated ()
    end do
end subroutine pcm_default_allocate_cores

```

Extra code is required for certain core types (threshold) or if BLHA uses an external OLP (Born only, this case) for getting its matrix elements.

<PCM: pcm default: TBP>+≡

```

    procedure :: prepare_any_external_code => &
        pcm_default_prepare_any_external_code

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_default_prepare_any_external_code &
        (pcm, core_entry, i_core, libname, model, var_list)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    integer, intent(in) :: i_core
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    type(var_list_t), intent(in) :: var_list
end subroutine pcm_default_prepare_any_external_code

```

<PCM: procedures>+≡

```

    module subroutine pcm_default_prepare_any_external_code &
        (pcm, core_entry, i_core, libname, model, var_list)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    integer, intent(in) :: i_core
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    type(var_list_t), intent(in) :: var_list
    if (core_entry%active) then
        associate (core => core_entry%core)
            if (core%needs_external_code ()) then
                call core%prepare_external_code &
                    (core%data%flv_state, &
                     var_list, pcm%os_data, libname, model, i_core, .false.)
            end if
            call core%set_equivalent_flv_hel_indices ()
        end associate
    end if
end subroutine pcm_default_prepare_any_external_code

```

Allocate and configure the BLHA record for a specific core, assuming that the core type requires it. In the default case, this is a Born configuration.

<PCM: pcm default: TBP>+≡

```

    procedure :: setup_blha => pcm_default_setup_blha

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_default_setup_blha (pcm, core_entry)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
end subroutine pcm_default_setup_blha

```

```

<PCM: procedures>+≡
module subroutine pcm_default_setup_blha (pcm, core_entry)
  class(pcm_default_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  allocate (core_entry%blha_config, source = pcm%blha_defaults)
  call core_entry%blha_config%set_born ()
end subroutine pcm_default_setup_blha

```

Apply the configuration, using pcm data.

```

<PCM: pcm default: TBP>+≡
  procedure :: prepare_blha_core => pcm_default_prepare_blha_core

<PCM: sub interfaces>+≡
  module subroutine pcm_default_prepare_blha_core (pcm, core_entry, model)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    class(model_data_t), intent(in), target :: model
  end subroutine pcm_default_prepare_blha_core

<PCM: procedures>+≡
module subroutine pcm_default_prepare_blha_core (pcm, core_entry, model)
  class(pcm_default_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  class(model_data_t), intent(in), target :: model
  integer :: n_in
  integer :: n_legs
  integer :: n_flv
  integer :: n_hel
  select type (core => core_entry%core)
  class is (prc_blha_t)
    associate (blha_config => core_entry%blha_config)
      n_in = core%data%n_in
      n_legs = core%data%get_n_tot ()
      n_flv = core%data%n_flv
      n_hel = blha_config%get_n_hel (core%data%flv_state (1:n_in,1), model)
      call core%init_blha (blha_config, n_in, n_legs, n_flv, n_hel)
      call core%init_driver (pcm%os_data)
    end associate
  end select
end subroutine pcm_default_prepare_blha_core

```

Read the method settings from the variable list and store them in the BLHA master. This version: no NLO flag.

```

<PCM: pcm default: TBP>+≡
  procedure :: set_blha_methods => pcm_default_set_blha_methods

<PCM: sub interfaces>+≡
  module subroutine pcm_default_set_blha_methods (pcm, blha_master, var_list)
    class(pcm_default_t), intent(inout) :: pcm
    type(blha_master_t), intent(inout) :: blha_master
    type(var_list_t), intent(in) :: var_list
  end subroutine pcm_default_set_blha_methods

```

```

<PCM: procedures>+≡
  module subroutine pcm_default_set_blha_methods (pcm, blha_master, var_list)
    class(pcm_default_t), intent(inout) :: pcm
    type(blha_master_t), intent(inout) :: blha_master
    type(var_list_t), intent(in) :: var_list
    call blha_master%set_methods (.false., var_list)
  end subroutine pcm_default_set_blha_methods

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration.

The default version looks at the first process core only, to get the Born data. (Multiple cores are thus unsupported.) The NLO flavor table is left unallocated.

```

<PCM: pcm default: TBP>+≡
  procedure :: get_blha_flv_states => pcm_default_get_blha_flv_states

<PCM: sub interfaces>+≡
  module subroutine pcm_default_get_blha_flv_states &
    (pcm, core_entry, flv_born, flv_real)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    integer, dimension(:,:), allocatable, intent(out) :: flv_born
    integer, dimension(:,:), allocatable, intent(out) :: flv_real
  end subroutine pcm_default_get_blha_flv_states

```

```

<PCM: procedures>+≡
  module subroutine pcm_default_get_blha_flv_states &
    (pcm, core_entry, flv_born, flv_real)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    integer, dimension(:,:), allocatable, intent(out) :: flv_born
    integer, dimension(:,:), allocatable, intent(out) :: flv_real
    flv_born = core_entry(1)%core%data%flv_state
  end subroutine pcm_default_get_blha_flv_states

```

Allocate and configure the MCI (multi-channel integrator) records. There is one record per active process component. Second procedure: call the MCI dispatcher with default-setup arguments.

```

<PCM: pcm default: TBP>+≡
  procedure :: setup_mci => pcm_default_setup_mci
  procedure :: call_dispatch_mci => pcm_default_call_dispatch_mci

<PCM: sub interfaces>+≡
  module subroutine pcm_default_setup_mci (pcm, mci_entry)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_mci_entry_t), &
      dimension(:), allocatable, intent(out) :: mci_entry
  end subroutine pcm_default_setup_mci
  module subroutine pcm_default_call_dispatch_mci (pcm, &
    dispatch_mci, var_list, process_id, mci_template)
    class(pcm_default_t), intent(inout) :: pcm
    procedure(dispatch_mci_proc) :: dispatch_mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    class(mci_t), allocatable, intent(out) :: mci_template
  end subroutine pcm_default_call_dispatch_mci

```

<PCM: procedures>+≡

```

module subroutine pcm_default_setup_mci (pcm, mci_entry)
  class(pcm_default_t), intent(inout) :: pcm
  type(process_mci_entry_t), &
    dimension(:), allocatable, intent(out) :: mci_entry
  class(mci_t), allocatable :: mci_template
  integer :: i, i_mci
  pcm%n_mci = count (pcm%component_active)
  allocate (pcm%i_mci (pcm%n_components), source = 0)
  i_mci = 0
  do i = 1, pcm%n_components
    if (pcm%component_active(i)) then
      i_mci = i_mci + 1
      pcm%i_mci(i) = i_mci
    end if
  end do
  allocate (mci_entry (pcm%n_mci))
end subroutine pcm_default_setup_mci

module subroutine pcm_default_call_dispatch_mci (pcm, &
  dispatch_mci, var_list, process_id, mci_template)
  class(pcm_default_t), intent(inout) :: pcm
  procedure(dispatch_mci_proc) :: dispatch_mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  class(mci_t), allocatable, intent(out) :: mci_template
  call dispatch_mci (mci_template, var_list, process_id)
end subroutine pcm_default_call_dispatch_mci

```

Nothing left to do for the default algorithm.

<PCM: pcm default: TBP>+≡

```

procedure :: complete_setup => pcm_default_complete_setup

```

<PCM: sub interfaces>+≡

```

module subroutine pcm_default_complete_setup &
  (pcm, core_entry, component, model)
  class(pcm_default_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  type(process_component_t), dimension(:), intent(inout) :: component
  type(model_t), intent(in), target :: model
end subroutine pcm_default_complete_setup

```

<PCM: procedures>+≡

```

module subroutine pcm_default_complete_setup &
  (pcm, core_entry, component, model)
  class(pcm_default_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  type(process_component_t), dimension(:), intent(inout) :: component
  type(model_t), intent(in), target :: model
end subroutine pcm_default_complete_setup

```

Component management

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index `i` and the `active` flag.

In the default mode, all components are marked as master components.

<PCM: pcm default: TBP>+≡

```
procedure :: init_component => pcm_default_init_component
```

<PCM: sub interfaces>+≡

```
module subroutine pcm_default_init_component (pcm, component, i, active, &
      phs_config, env, meta, config)
  class(pcm_default_t), intent(in) :: pcm
  type(process_component_t), intent(out) :: component
  integer, intent(in) :: i
  logical, intent(in) :: active
  class(phs_config_t), allocatable, intent(in) :: phs_config
  type(process_environment_t), intent(in) :: env
  type(process_metadata_t), intent(in) :: meta
  type(process_config_data_t), intent(in) :: config
end subroutine pcm_default_init_component
```

<PCM: procedures>+≡

```
module subroutine pcm_default_init_component (pcm, component, i, active, &
      phs_config, env, meta, config)
  class(pcm_default_t), intent(in) :: pcm
  type(process_component_t), intent(out) :: component
  integer, intent(in) :: i
  logical, intent(in) :: active
  class(phs_config_t), allocatable, intent(in) :: phs_config
  type(process_environment_t), intent(in) :: env
  type(process_metadata_t), intent(in) :: meta
  type(process_config_data_t), intent(in) :: config
  call component%init (i, &
    env, meta, config, &
    active, &
    phs_config)
  component%component_type = COMP_MASTER
end subroutine pcm_default_init_component
```

30.8.3 NLO process component manager

The NLO-aware version of the process-component manager.

This is the configuration object, which has the duty of allocating the corresponding instance. This is the nontrivial NLO version.

<PCM: public>+≡

```
public :: pcm_nlo_t
```

<PCM: types>+≡

```
type, extends (pcm_t) :: pcm_nlo_t
  type(string_t) :: id
  logical :: combined_integration = .false.
  logical :: vis_fks_regions = .false.
  integer, dimension(:), allocatable :: nlo_type
```



```

integer, dimension(:), allocatable :: nlo_type_core
integer, dimension(:), allocatable :: component_type
integer :: i_born = 0
integer :: i_real = 0
integer :: i_sub = 0
type(nlo_settings_t) :: settings
type(region_data_t) :: region_data
logical :: use_real_partition = .false.
logical :: use_real_singular = .false.
real(default) :: real_partition_scale = 0
class(real_partition_t), allocatable :: real_partition
type(dalitz_plot_t) :: dalitz_plot
type(quantum_numbers_t), dimension(:, :), allocatable :: qn_real, qn_born
contains
<PCM: pcm nlo: TBP>
end type pcm_nlo_t

```

Initialize configuration data, using environment variables.

```

<PCM: pcm nlo: TBP>≡
  procedure :: init => pcm_nlo_init

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_init (pcm, env, meta)
    class(pcm_nlo_t), intent(out) :: pcm
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
  end subroutine pcm_nlo_init

<PCM: procedures>+≡
  module subroutine pcm_nlo_init (pcm, env, meta)
    class(pcm_nlo_t), intent(out) :: pcm
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    type(var_list_t), pointer :: var_list
    type(fks_template_t) :: fks_template
    pcm%id = meta%id
    pcm%has_pdfs = env%has_pdfs ()
    var_list => env%get_var_list_ptr ()
    call dispatch_fks_setup (fks_template, var_list)
    call pcm%settings%init (var_list, fks_template)
    pcm%combined_integration = &
      var_list%get_lval (var_str ('?combined_nlo_integration'))
    select case (char (var_list%get_sval (var_str ("$_real_partition_mode"))))
    case ("default", "off")
      pcm%use_real_partition = .false.
      pcm%use_real_singular = .false.
    case ("all", "on", "singular")
      pcm%use_real_partition = .true.
      pcm%use_real_singular = .true.
    case ("finite")
      pcm%use_real_partition = .true.
      pcm%use_real_singular = .false.
    case default
      call msg_fatal ("The real partition mode can only be " // &
        "default, off, all, on, singular or finite.")
    end select
  end subroutine pcm_nlo_init

```

```

end select
pcm%real_partition_scale = &
    var_list%get_rval (var_str ("real_partition_scale"))
pcm%vis_fks_regions = &
    var_list%get_lval (var_str ("?vis_fks_regions"))
call pcm%set_blha_defaults &
    (env%has_polarized_beams (), env%get_var_list_ptr ())
pcm%os_data = env%get_os_data ()
end subroutine pcm_nlo_init

```

Init/rewrite NLO settings without the FKS template.

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: init_nlo_settings => pcm_nlo_init_nlo_settings

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_init_nlo_settings (pcm, var_list)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(var_list_t), intent(in), target :: var_list
    end subroutine pcm_nlo_init_nlo_settings

<PCM: procedures>+≡
    module subroutine pcm_nlo_init_nlo_settings (pcm, var_list)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(var_list_t), intent(in), target :: var_list
        call pcm%settings%init (var_list)
    end subroutine pcm_nlo_init_nlo_settings

```

As appropriate for the NLO/FKS algorithm, the category defined by the process, is called `nlo_type`. We refine this by setting the component category `component_type` separately.

The component types `COMP_MISMATCH`, `COMP_PDF`, `COMP_SUB` are set only if the algorithm uses combined integration. Otherwise, they are set to `COMP_DEFAULT`.

The component type `COMP_REAL` is further distinguished between `COMP_REAL_SING` or `COMP_REAL_FIN`, if the algorithm uses real partitions. The former acts as a reference component for the latter, and we always assume that it is the first real component.

Each component is assigned its own core. Exceptions: the finite-real component gets the same core as the singular-real component. The mismatch component gets the same core as the subtraction component.

TODO wk 2018: this convention for real components can be improved. Check whether all component types should be assigned, not just for combined integration.

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: categorize_components => pcm_nlo_categorize_components

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_categorize_components (pcm, config)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_config_data_t), intent(in) :: config
    end subroutine pcm_nlo_categorize_components

<PCM: procedures>+≡
    module subroutine pcm_nlo_categorize_components (pcm, config)
        class(pcm_nlo_t), intent(inout) :: pcm

```

```

type(process_config_data_t), intent(in) :: config
type(process_component_def_t), pointer :: component_def
integer :: i
allocate (pcm%nlo_type (pcm%n_components), source = COMPONENT_UNDEFINED)
allocate (pcm%component_type (pcm%n_components), source = COMP_DEFAULT)
do i = 1, pcm%n_components
  component_def => config%process_def%get_component_def_ptr (i)
  pcm%nlo_type(i) = component_def%get_nlo_type ()
  if (pcm%combined_integration) then
    select case (pcm%nlo_type(i))
    case (BORN)
      pcm%i_born = i
      pcm%component_type(i) = COMP_MASTER
    case (NLO_REAL)
      pcm%component_type(i) = COMP_REAL
    case (NLO_VIRTUAL)
      pcm%component_type(i) = COMP_VIRT
    case (NLO_MISMATCH)
      pcm%component_type(i) = COMP_MISMATCH
    case (NLO_DGLAP)
      pcm%component_type(i) = COMP_PDF
    case (NLO_SUBTRACTION)
      pcm%component_type(i) = COMP_SUB
      pcm%i_sub = i
    end select
  else
    select case (pcm%nlo_type(i))
    case (BORN)
      pcm%i_born = i
      pcm%component_type(i) = COMP_MASTER
    case (NLO_REAL)
      pcm%component_type(i) = COMP_REAL
    case (NLO_VIRTUAL)
      pcm%component_type(i) = COMP_VIRT
    case (NLO_MISMATCH)
      pcm%component_type(i) = COMP_MISMATCH
    case (NLO_SUBTRACTION)
      pcm%i_sub = i
    end select
  end if
end do
call refine_real_type ( &
  pack ([i, i=1, pcm%n_components]), &
  pcm%component_type==COMP_REAL))
contains
subroutine refine_real_type (i_real)
  integer, dimension(:), intent(in) :: i_real
  pcm%i_real = i_real(1)
  if (pcm%use_real_partition) then
    pcm%component_type (i_real(1)) = COMP_REAL_SING
    pcm%component_type (i_real(2:)) = COMP_REAL_FIN
  end if
end subroutine refine_real_type
end subroutine pcm_nlo_categorize_components

```

Phase-space initial configuration

Setup for the NLO/PHS processes: two phase-space configurations, (1) Born/wood, (2) real correction/FKS. All components use either one of these two configurations.

TODO wk 2018: The `first_real_component` identifier is really ugly. Nothing should rely on the ordering.

```
<PCM: pcm_nlo: TBP>+≡
  procedure :: init_phs_config => pcm_nlo_init_phs_config

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_init_phs_config &
    (pcm, phs_entry, meta, env, phs_par, mapping_defs)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(process_phs_config_t), &
      dimension(:), allocatable, intent(out) :: phs_entry
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    type(mapping_defaults_t), intent(in) :: mapping_defs
    type(phs_parameters_t), intent(in) :: phs_par
  end subroutine pcm_nlo_init_phs_config

<PCM: procedures>+≡
  module subroutine pcm_nlo_init_phs_config &
    (pcm, phs_entry, meta, env, phs_par, mapping_defs)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(process_phs_config_t), &
      dimension(:), allocatable, intent(out) :: phs_entry
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    type(mapping_defaults_t), intent(in) :: mapping_defs
    type(phs_parameters_t), intent(in) :: phs_par
    integer :: i
    logical :: first_real_component
    allocate (phs_entry (2))
    call dispatch_phs (phs_entry(1)%phs_config, &
      env%get_var_list_ptr (), &
      env%get_os_data (), &
      meta%id, &
      mapping_defs, phs_par, &
      var_str ("wood"))
    call dispatch_phs (phs_entry(2)%phs_config, &
      env%get_var_list_ptr (), &
      env%get_os_data (), &
      meta%id, &
      mapping_defs, phs_par, &
      var_str ("fks"))
    allocate (pcm%i_phs_config (pcm%n_components), source=0)
    first_real_component = .true.
    do i = 1, pcm%n_components
      select case (pcm%nlo_type(i))
        case (BORN, NLO_VIRTUAL, NLO_SUBTRACTION)
```

```

        pcm%i_phs_config(i) = 1
    case (NLO_REAL)
        if (pcm%use_real_partition) then
            if (pcm%use_real_singular) then
                if (first_real_component) then
                    pcm%i_phs_config(i) = 2
                    first_real_component = .false.
                else
                    pcm%i_phs_config(i) = 1
                end if
            else
                pcm%i_phs_config(i) = 1
            end if
        else
            pcm%i_phs_config(i) = 2
        end if
    case (NLO_MISMATCH, NLO_DGLAP, GKS)
        pcm%i_phs_config(i) = 2
    end select
end do
end subroutine pcm_nlo_init_phs_config

```

Core management

Allocate the core (matrix-element interface) objects that we will need for evaluation. Every component gets an associated core, except for the real-finite and mismatch components (if any). Those components are associated with their previous corresponding real-singular and subtraction cores, respectively.

After cores are allocated, configure the region-data block that is maintained by the NLO process-component manager.

(PCM: pcm_nlo: TBP)+≡

```

    procedure :: allocate_cores => pcm_nlo_allocate_cores

```

(PCM: sub interfaces)+≡

```

    module subroutine pcm_nlo_allocate_cores (pcm, config, core_entry)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_config_data_t), intent(in) :: config
        type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
    end subroutine pcm_nlo_allocate_cores

```

(PCM: procedures)+≡

```

    module subroutine pcm_nlo_allocate_cores (pcm, config, core_entry)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_config_data_t), intent(in) :: config
        type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
        type(process_component_def_t), pointer :: component_def
        integer :: i, i_core
        allocate (pcm%i_core (pcm%n_components), source = 0)
        pcm%n_cores = pcm%n_components &
            - count (pcm%component_type(:) == COMP_REAL_FIN) &
            - count (pcm%component_type(:) == COMP_MISMATCH)
        allocate (core_entry (pcm%n_cores))
        allocate (pcm%nlo_type_core (pcm%n_cores), source = BORN)
    end subroutine pcm_nlo_allocate_cores

```

```

i_core = 0
do i = 1, pcm%n_components
  select case (pcm%component_type(i))
  case default
    i_core = i_core + 1
    pcm%i_core(i) = i_core
    pcm%nlo_type_core(i_core) = pcm%nlo_type(i)
    core_entry(i_core)%i_component = i
    component_def => config%process_def%get_component_def_ptr (i)
    core_entry(i_core)%core_def => component_def%get_core_def_ptr ()
    select case (pcm%nlo_type(i))
    case default
      core_entry(i)%active = component_def%can_be_integrated ()
    case (NLO_REAL, NLO_SUBTRACTION)
      core_entry(i)%active = .true.
    end select
  case (COMP_REAL_FIN)
    pcm%i_core(i) = pcm%i_core(pcm%i_real)
  case (COMP_MISMATCH)
    pcm%i_core(i) = pcm%i_core(pcm%i_sub)
  end select
end do
end subroutine pcm_nlo_allocate_cores

```

Extra code is required for certain core types (threshold) or if BLHA uses an external OLP for getting its matrix elements. OMega matrix elements, by definition, do not need extra code. NLO-virtual or subtraction matrix elements always need extra code.

More precisely: for the Born and virtual matrix element, the extra code is accessed only if the component is active. The radiation (real) and the subtraction corrections (singular and finite), extra code is accessed in any case.

The flavor state is taken from the `region_data` table in the `pcm` record. We use the Born and real flavor-state tables as appropriate.

(PCM: pcm nlo: TBP)+≡

```

procedure :: prepare_any_external_code => &
  pcm_nlo_prepare_any_external_code

```

(PCM: sub interfaces)+≡

```

module subroutine pcm_nlo_prepare_any_external_code &
  (pcm, core_entry, i_core, libname, model, var_list)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  integer, intent(in) :: i_core
  type(string_t), intent(in) :: libname
  type(model_data_t), intent(in), target :: model
  type(var_list_t), intent(in) :: var_list
end subroutine pcm_nlo_prepare_any_external_code

```

(PCM: procedures)+≡

```

module subroutine pcm_nlo_prepare_any_external_code &
  (pcm, core_entry, i_core, libname, model, var_list)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  integer, intent(in) :: i_core

```

```

type(string_t), intent(in) :: libname
type(model_data_t), intent(in), target :: model
type(var_list_t), intent(in) :: var_list
integer, dimension(:,:), allocatable :: flv_born, flv_real
integer :: i
call pcm%region_data%get_all_flv_states (flv_born, flv_real)
if (core_entry%active) then
  associate (core => core_entry%core)
    if (core%needs_external_code ()) then
      select case (pcm%nlo_type (core_entry%i_component))
      case default
        call core%data%set_flv_state (flv_born)
      case (NLO_REAL)
        call core%data%set_flv_state (flv_real)
      end select
      call core%prepare_external_code &
        (core%data%flv_state, &
         var_list, pcm%os_data, libname, model, i_core, .true.)
    end if
    call core%set_equivalent_flv_hel_indices ()
  end associate
end if
end subroutine pcm_nlo_prepare_any_external_code

```

Allocate and configure the BLHA record for a specific core, assuming that the core type requires it. The configuration depends on the NLO type of the core.

(PCM: pcm nlo: TBP)+≡

```

procedure :: setup_blha => pcm_nlo_setup_blha

```

(PCM: sub interfaces)+≡

```

module subroutine pcm_nlo_setup_blha (pcm, core_entry)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
end subroutine pcm_nlo_setup_blha

```

(PCM: procedures)+≡

```

module subroutine pcm_nlo_setup_blha (pcm, core_entry)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  allocate (core_entry%blha_config, source = pcm%blha_defaults)
  select case (pcm%nlo_type(core_entry%i_component))
  case (BORN)
    call core_entry%blha_config%set_born ()
  case (NLO_REAL)
    call core_entry%blha_config%set_real_trees ()
  case (NLO_VIRTUAL)
    call core_entry%blha_config%set_loop ()
  case (NLO_SUBTRACTION)
    call core_entry%blha_config%set_subtraction ()
    call core_entry%blha_config%set_internal_color_correlations ()
  case (NLO_DGLAP)
    call core_entry%blha_config%set_dglap ()
  end select
end subroutine pcm_nlo_setup_blha

```

After phase-space configuration data and core entries are available, we fill tables and compute the remaining NLO data that will steer the integration and subtraction algorithm.

There are three parts: recognize a threshold-type process core (if it exists), prepare the region-data tables (always), and prepare for real partitioning (if requested).

The real-component phase space acts as the source for resonance-history information, required for the region data.

```

<PCM: pcm_nlo: TBP>+≡
  procedure :: complete_setup => pcm_nlo_complete_setup

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_complete_setup (pcm, core_entry, component, model)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    type(process_component_t), dimension(:), intent(inout) :: component
    type(model_t), intent(in), target :: model
  end subroutine pcm_nlo_complete_setup

<PCM: procedures>+≡
  module subroutine pcm_nlo_complete_setup (pcm, core_entry, component, model)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    type(process_component_t), dimension(:), intent(inout) :: component
    type(model_t), intent(in), target :: model
    integer :: alpha_power, alphas_power
    call pcm%handle_threshold_core (core_entry)
    call component(1)%config%get_coupling_powers (alpha_power, alphas_power)
    call pcm%setup_region_data (core_entry, &
      model, alpha_power, alphas_power, component(pcm%i_real)%phs_config)
    call pcm%setup_real_partition ()
  end subroutine pcm_nlo_complete_setup

```

Apply the BLHA configuration to a core object, using the region data from pcm for determining the particle content.

```

<PCM: pcm_nlo: TBP>+≡
  procedure :: prepare_blha_core => pcm_nlo_prepare_blha_core

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_prepare_blha_core (pcm, core_entry, model)
    class(pcm_nlo_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    class(model_data_t), intent(in), target :: model
  end subroutine pcm_nlo_prepare_blha_core

<PCM: procedures>+≡
  module subroutine pcm_nlo_prepare_blha_core (pcm, core_entry, model)
    class(pcm_nlo_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    class(model_data_t), intent(in), target :: model
    integer :: n_in
    integer :: n_legs
    integer :: n_flv
    integer :: n_hel
    select type (core => core_entry%core)

```



```

class is (prc_blha_t)
  associate (blha_config => core_entry%blha_config)
    n_in = core%data%n_in
    select case (pcm%nlo_type(core_entry%i_component))
    case (NLO_REAL)
      n_legs = pcm%region_data%get_n_legs_real ()
      n_flv = pcm%region_data%get_n_flv_real ()
    case default
      n_legs = pcm%region_data%get_n_legs_born ()
      n_flv = pcm%region_data%get_n_flv_born ()
    end select
    n_hel = blha_config%get_n_hel (core%data%flv_state (1:n_in,1), model)
    call core%init_blha (blha_config, n_in, n_legs, n_flv, n_hel)
    call core%init_driver (pcm%os_data)
  end associate
end select
end subroutine pcm_nlo_prepare_blha_core

```

Read the method settings from the variable list and store them in the BLHA master. This version: NLO flag set.

```

<PCM: pcm nlo: TBP>+≡
  procedure :: set_blha_methods => pcm_nlo_set_blha_methods

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_set_blha_methods (pcm, blha_master, var_list)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(blha_master_t), intent(inout) :: blha_master
    type(var_list_t), intent(in) :: var_list
  end subroutine pcm_nlo_set_blha_methods

<PCM: procedures>+≡
  module subroutine pcm_nlo_set_blha_methods (pcm, blha_master, var_list)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(blha_master_t), intent(inout) :: blha_master
    type(var_list_t), intent(in) :: var_list
    call blha_master%set_methods (.true., var_list)
    call pcm%blha_defaults%set_loop_method (blha_master)
  end subroutine pcm_nlo_set_blha_methods

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration.

The NLO version copies the tables from the region data inside pcm. The core array is not needed.

```

<PCM: pcm nlo: TBP>+≡
  procedure :: get_blha_flv_states => pcm_nlo_get_blha_flv_states

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_get_blha_flv_states &
    (pcm, core_entry, flv_born, flv_real)
    class(pcm_nlo_t), intent(in) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    integer, dimension(:,:), allocatable, intent(out) :: flv_born
    integer, dimension(:,:), allocatable, intent(out) :: flv_real
  end subroutine pcm_nlo_get_blha_flv_states

```

<PCM: procedures>+≡

```

module subroutine pcm_nlo_get_blha_flv_states &
  (pcm, core_entry, flv_born, flv_real)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  integer, dimension(:,:), allocatable, intent(out) :: flv_born
  integer, dimension(:,:), allocatable, intent(out) :: flv_real
  call pcm%region_data%get_all_flv_states (flv_born, flv_real)
end subroutine pcm_nlo_get_blha_flv_states

```

Allocate and configure the MCI (multi-channel integrator) records. The relation depends on the `combined_integration` setting. If we integrate components separately, each component gets its own record, except for the subtraction component. If we do the combination, there is one record for the master (Born) component and a second one for the real-finite component, if present.

Each entry acquires some NLO-specific initialization. Generic configuration follows later.

Second procedure: call the MCI dispatcher with NLO-setup arguments.

<PCM: pcm_nlo: TBP>+≡

```

procedure :: setup_mci => pcm_nlo_setup_mci
procedure :: call_dispatch_mci => pcm_nlo_call_dispatch_mci

```

<PCM: sub interfaces>+≡

```

module subroutine pcm_nlo_setup_mci (pcm, mci_entry)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(process_mci_entry_t), &
    dimension(:), allocatable, intent(out) :: mci_entry
end subroutine pcm_nlo_setup_mci
module subroutine pcm_nlo_call_dispatch_mci (pcm, &
  dispatch_mci, var_list, process_id, mci_template)
  class(pcm_nlo_t), intent(inout) :: pcm
  procedure(dispatch_mci_proc) :: dispatch_mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  class(mci_t), allocatable, intent(out) :: mci_template
end subroutine pcm_nlo_call_dispatch_mci

```

<PCM: procedures>+≡

```

module subroutine pcm_nlo_setup_mci (pcm, mci_entry)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(process_mci_entry_t), &
    dimension(:), allocatable, intent(out) :: mci_entry
  class(mci_t), allocatable :: mci_template
  integer :: i, i_mci
  if (pcm%combined_integration) then
    pcm%n_mci = 1 &
      + count (pcm%component_active(:) &
        & .and. pcm%component_type(:) == COMP_REAL_FIN)
    allocate (pcm%i_mci (pcm%n_components), source = 0)
    do i = 1, pcm%n_components
      if (pcm%component_active(i)) then
        select case (pcm%component_type(i))
        case (COMP_MASTER)
          pcm%i_mci(i) = 1

```

```

        case (COMP_REAL_FIN)
            pcm%i_mci(i) = 2
        end select
    end if
end do
else
    pcm%n_mci = count (pcm%component_active(:) &
        & .and. pcm%nlo_type(:) /= NLO_SUBTRACTION)
    allocate (pcm%i_mci (pcm%n_components), source = 0)
    i_mci = 0
    do i = 1, pcm%n_components
        if (pcm%component_active(i)) then
            select case (pcm%nlo_type(i))
            case default
                i_mci = i_mci + 1
                pcm%i_mci(i) = i_mci
            case (NLO_SUBTRACTION)
            end select
        end if
    end do
end if
allocate (mci_entry (pcm%n_mci))
mci_entry(:)%combined_integration = pcm%combined_integration
if (pcm%use_real_partition) then
    do i = 1, pcm%n_components
        i_mci = pcm%i_mci(i)
        if (i_mci > 0) then
            select case (pcm%component_type(i))
            case (COMP_REAL_FIN)
                mci_entry(i_mci)%real_partition_type = REAL_FINITE
            case default
                mci_entry(i_mci)%real_partition_type = REAL_SINGULAR
            end select
        end if
    end do
end if
end subroutine pcm_nlo_setup_mci

module subroutine pcm_nlo_call_dispatch_mci (pcm, &
    dispatch_mci, var_list, process_id, mci_template)
    class(pcm_nlo_t), intent(inout) :: pcm
    procedure(dispatch_mci_proc) :: dispatch_mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    class(mci_t), allocatable, intent(out) :: mci_template
    call dispatch_mci (mci_template, var_list, process_id, is_nlo = .true.)
end subroutine pcm_nlo_call_dispatch_mci

```

Check for a threshold core and adjust the configuration accordingly, before singular region data are considered.

<PCM: pcm nlo: TBP>+≡

procedure :: handle_threshold_core => pcm_nlo_handle_threshold_core

<PCM: sub interfaces>+≡

```

module subroutine pcm_nlo_handle_threshold_core (pcm, core_entry)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
end subroutine pcm_nlo_handle_threshold_core

```

(PCM: procedures)+≡

```

module subroutine pcm_nlo_handle_threshold_core (pcm, core_entry)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  integer :: i
  do i = 1, size (core_entry)
    select type (core => core_entry(i)%core_def)
      type is (threshold_def_t)
        pcm%settings%factorization_mode = FACTORIZATION_THRESHOLD
        return
      end select
    end do
end subroutine pcm_nlo_handle_threshold_core

```

Configure the singular-region tables based on the process data for the Born and Real (singular) cores, using also the appropriate FKS phase-space configuration object.

In passing, we may create a table of resonance histories that are relevant for the singular-region configuration.

TODO wk 2018: check whether `phs_entry` needs to be `intent(inout)`.

(PCM: pcm nlo: TBP)+≡

```

procedure :: setup_region_data => pcm_nlo_setup_region_data

```

(PCM: sub interfaces)+≡

```

module subroutine pcm_nlo_setup_region_data &
  (pcm, core_entry, model, alpha_power, alphas_power, phs_config)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  type(model_t), intent(in), target :: model
  integer, intent(in) :: alpha_power, alphas_power
  class(phs_config_t), intent(inout), optional :: phs_config
end subroutine pcm_nlo_setup_region_data

```

(PCM: procedures)+≡

```

module subroutine pcm_nlo_setup_region_data &
  (pcm, core_entry, model, alpha_power, alphas_power, phs_config)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(core_entry_t), dimension(:), intent(in) :: core_entry
  type(model_t), intent(in), target :: model
  integer, intent(in) :: alpha_power, alphas_power
  class(phs_config_t), intent(inout), optional :: phs_config
  type(process_constants_t) :: data_born, data_real
  integer, dimension (:,:), allocatable :: flavor_born, flavor_real
  type(resonance_history_t), dimension(:), allocatable :: resonance_histories
  type(var_list_t), pointer :: var_list
  logical :: success
  data_born = core_entry(pcm%i_core(pcm%i_born))%core%data
  data_real = core_entry(pcm%i_core(pcm%i_real))%core%data
  call data_born%get_flv_state (flavor_born)
  call data_real%get_flv_state (flavor_real)

```

```

call pcm%region_data%init &
  (data_born%n_in, model, flavor_born, flavor_real, &
   pcm%settings%nlo_correction_type, alpha_power, alphas_power)
associate (template => pcm%settings%fks_template)
  if (template%mapping_type == FKS_RESONANCES) then
    if (.not. present(phs_config)) then
      call msg_bug("setup_region_data: real phase space required to setup the resonance hist
    end if
    select type (phs_config)
    type is (phs_fks_config_t)
      call get_filtered_resonance_histories (phs_config, &
        data_born%n_in, flavor_born, model, &
        template%excluded_resonances, &
        resonance_histories, success)
    end select
    if (.not. success) template%mapping_type = FKS_DEFAULT
  end if
  call pcm%region_data%setup_fks_mappings (template, data_born%n_in)
!!! Check again, mapping_type might have changed
  if (template%mapping_type == FKS_RESONANCES) then
    call pcm%region_data%set_resonance_mappings (resonance_histories)
    call pcm%region_data%init_resonance_information ()
    pcm%settings%use_resonance_mappings = .true.
  end if
end associate
if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
  call pcm%region_data%set_isr_pseudo_regions ()
  call pcm%region_data%split_up_interference_regions_for_threshold ()
end if
call pcm%region_data%compute_number_of_phase_spaces ()
call pcm%region_data%set_i_phs_to_i_con ()
call pcm%region_data%write_to_file &
  (pcm%id, pcm%vis_fks_regions, pcm%os_data)
if (debug_active (D_SUBTRACTION)) &
  call pcm%region_data%check_consistency (.true.)
end subroutine pcm_nlo_setup_region_data

```

After region data are set up, we allocate and configure the `real_partition` objects, if requested. Gfortran 7/8/9 bug, has to remain in the main module:

```

(PCM: pcm_nlo: TBP)+≡
  procedure :: setup_real_partition => pcm_nlo_setup_real_partition

(PCM: main procedures)+≡
  subroutine pcm_nlo_setup_real_partition (pcm)
    class(pcm_nlo_t), intent(inout) :: pcm
    if (pcm%use_real_partition) then
      if (.not. allocated (pcm%real_partition)) then
        allocate (real_partition_fixed_order_t :: pcm%real_partition)
        select type (partition => pcm%real_partition)
        type is (real_partition_fixed_order_t)
          call pcm%region_data%get_all_ftuples (partition%fks_pairs)
          partition%scale = pcm%real_partition_scale
        end select
      end if
    end if
  end subroutine

```

```

end if
end subroutine pcm_nlo_setup_real_partition

```

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index *i* and the **active** flag. For a subtraction component, the **active** flag is overridden.

In the nlo mode, the component types have been determined before.

TODO wk 2018: the component type need not be stored in the component; we may remove this when everything is controlled by pcm.

(PCM: pcm nlo: TBP)+≡

```

procedure :: init_component => pcm_nlo_init_component

```

(PCM: sub interfaces)+≡

```

module subroutine pcm_nlo_init_component (pcm, component, i, active, &
    phs_config, env, meta, config)
    class(pcm_nlo_t), intent(in) :: pcm
    type(process_component_t), intent(out) :: component
    integer, intent(in) :: i
    logical, intent(in) :: active
    class(phs_config_t), allocatable, intent(in) :: phs_config
    type(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
    type(process_config_data_t), intent(in) :: config
end subroutine pcm_nlo_init_component

```

(PCM: procedures)+≡

```

module subroutine pcm_nlo_init_component (pcm, component, i, active, &
    phs_config, env, meta, config)
    class(pcm_nlo_t), intent(in) :: pcm
    type(process_component_t), intent(out) :: component
    integer, intent(in) :: i
    logical, intent(in) :: active
    class(phs_config_t), allocatable, intent(in) :: phs_config
    type(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
    type(process_config_data_t), intent(in) :: config
    logical :: activate
    select case (pcm%nlo_type(i))
    case default; activate = active
    case (NLO_SUBTRACTION); activate = .false.
    end select
    call component%init (i, &
        env, meta, config, &
        activate, &
        phs_config)
    component%component_type = pcm%component_type(i)
end subroutine pcm_nlo_init_component

```

Override the base method: record the active components in the PCM object, and report inactive components (except for the subtraction component).

(PCM: pcm nlo: TBP)+≡

```

procedure :: record_inactive_components => pcm_nlo_record_inactive_components

```

```

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_record_inactive_components (pcm, component, meta)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_metadata_t), intent(inout) :: meta
    end subroutine pcm_nlo_record_inactive_components

<PCM: procedures>+≡
    module subroutine pcm_nlo_record_inactive_components (pcm, component, meta)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_metadata_t), intent(inout) :: meta
        integer :: i
        pcm%component_active = component%active
        do i = 1, pcm%n_components
            select case (pcm%nlo_type(i))
            case (NLO_SUBTRACTION)
            case default
                if (.not. component(i)%active) call meta%deactivate_component (i)
            end select
        end do
    end subroutine pcm_nlo_record_inactive_components

<PCM: pcm nlo: TBP>+≡
    procedure :: core_is_radiation => pcm_nlo_core_is_radiation

<PCM: sub interfaces>+≡
    module function pcm_nlo_core_is_radiation (pcm, i_core) result (is_rad)
        logical :: is_rad
        class(pcm_nlo_t), intent(in) :: pcm
        integer, intent(in) :: i_core
    end function pcm_nlo_core_is_radiation

<PCM: procedures>+≡
    module function pcm_nlo_core_is_radiation (pcm, i_core) result (is_rad)
        logical :: is_rad
        class(pcm_nlo_t), intent(in) :: pcm
        integer, intent(in) :: i_core
        is_rad = pcm%nlo_type(i_core) == NLO_REAL ! .and. .not. pcm%cm%sub(i_core)
    end function pcm_nlo_core_is_radiation

<PCM: pcm nlo: TBP>+≡
    procedure :: get_n_flv_born => pcm_nlo_get_n_flv_born

<PCM: sub interfaces>+≡
    module function pcm_nlo_get_n_flv_born (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
    end function pcm_nlo_get_n_flv_born

<PCM: procedures>+≡
    module function pcm_nlo_get_n_flv_born (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
        n_flv = pcm_nlo%region_data%n_flv_born
    end function pcm_nlo_get_n_flv_born

```

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: get_n_flv_real => pcm_nlo_get_n_flv_real

<PCM: sub interfaces>+≡
    module function pcm_nlo_get_n_flv_real (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
    end function pcm_nlo_get_n_flv_real

<PCM: procedures>+≡
    module function pcm_nlo_get_n_flv_real (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
        n_flv = pcm_nlo%region_data%n_flv_real
    end function pcm_nlo_get_n_flv_real

<PCM: pcm_nlo: TBP>+≡
    procedure :: get_n_alr => pcm_nlo_get_n_alr

<PCM: sub interfaces>+≡
    module function pcm_nlo_get_n_alr (pcm) result (n_alr)
        integer :: n_alr
        class(pcm_nlo_t), intent(in) :: pcm
    end function pcm_nlo_get_n_alr

<PCM: procedures>+≡
    module function pcm_nlo_get_n_alr (pcm) result (n_alr)
        integer :: n_alr
        class(pcm_nlo_t), intent(in) :: pcm
        n_alr = pcm%region_data%n_regions
    end function pcm_nlo_get_n_alr

<PCM: pcm_nlo: TBP>+≡
    procedure :: get_flv_states => pcm_nlo_get_flv_states

<PCM: sub interfaces>+≡
    module function pcm_nlo_get_flv_states (pcm, born) result (flv)
        integer, dimension(:,:), allocatable :: flv
        class(pcm_nlo_t), intent(in) :: pcm
        logical, intent(in) :: born
    end function pcm_nlo_get_flv_states

<PCM: procedures>+≡
    module function pcm_nlo_get_flv_states (pcm, born) result (flv)
        integer, dimension(:,:), allocatable :: flv
        class(pcm_nlo_t), intent(in) :: pcm
        logical, intent(in) :: born
        if (born) then
            flv = pcm%region_data%get_flv_states_born ()
        else
            flv = pcm%region_data%get_flv_states_real ()
        end if
    end function pcm_nlo_get_flv_states

<PCM: pcm_nlo: TBP>+≡
    procedure :: get_qn => pcm_nlo_get_qn

```



```

<PCM: sub interfaces>+≡
  module function pcm_nlo_get_qn (pcm, born) result (qn)
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    class(pcm_nlo_t), intent(in) :: pcm
    logical, intent(in) :: born
  end function pcm_nlo_get_qn

```

```

<PCM: procedures>+≡
  module function pcm_nlo_get_qn (pcm, born) result (qn)
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    class(pcm_nlo_t), intent(in) :: pcm
    logical, intent(in) :: born
    if (born) then
      qn = pcm%qn_born
    else
      qn = pcm%qn_real
    end if
  end function pcm_nlo_get_qn

```

Check if there are massive emitters. Since the mass-structure of all underlying Born configurations have to be the same (**This does not have to be the case when different components are generated at LO**) , we just use the first one to determine this.

```

<PCM: pcm nlo: TBP>+≡
  procedure :: has_massive_emitter => pcm_nlo_has_massive_emitter

<PCM: sub interfaces>+≡
  module function pcm_nlo_has_massive_emitter (pcm) result (val)
    logical :: val
    class(pcm_nlo_t), intent(in) :: pcm
  end function pcm_nlo_has_massive_emitter

<PCM: procedures>+≡
  module function pcm_nlo_has_massive_emitter (pcm) result (val)
    logical :: val
    class(pcm_nlo_t), intent(in) :: pcm
    integer :: i
    val = .false.
    associate (reg_data => pcm%region_data)
      do i = reg_data%n_in + 1, reg_data%n_legs_born
        if (any (i == reg_data%emitters)) &
          val = val.or. reg_data%flv_born(1)%massive(i)
      end do
    end associate
  end function pcm_nlo_has_massive_emitter

```

Returns an array which specifies if the particle at position i is massive.

```

<PCM: pcm nlo: TBP>+≡
  procedure :: get_mass_info => pcm_nlo_get_mass_info

<PCM: sub interfaces>+≡
  module function pcm_nlo_get_mass_info (pcm, i_flv) result (massive)
    class(pcm_nlo_t), intent(in) :: pcm
    integer, intent(in) :: i_flv
    logical, dimension(:), allocatable :: massive
  end function pcm_nlo_get_mass_info

```

<PCM: procedures>+≡

```

module function pcm_nlo_get_mass_info (pcm, i_flv) result (massive)
  class(pcm_nlo_t), intent(in) :: pcm
  integer, intent(in) :: i_flv
  logical, dimension(:), allocatable :: massive
  allocate (massive (size (pcm%region_data%flv_born(i_flv)%massive)))
  massive = pcm%region_data%flv_born(i_flv)%massive
end function pcm_nlo_get_mass_info

```

Gfortran 7/8/9 bug, has to remain in the main module:

<PCM: pcm_nlo: TBP>+≡

```

procedure :: allocate_workspace => pcm_nlo_allocate_workspace

```

<PCM: main procedures>+≡

```

subroutine pcm_nlo_allocate_workspace (pcm, work)
  class(pcm_nlo_t), intent(in) :: pcm
  class(pcm_workspace_t), intent(inout), allocatable :: work
  allocate (pcm_nlo_workspace_t :: work)
end subroutine pcm_nlo_allocate_workspace

```

<PCM: pcm_nlo: TBP>+≡

```

procedure :: init_qn => pcm_nlo_init_qn

```

<PCM: sub interfaces>+≡

```

module subroutine pcm_nlo_init_qn (pcm, model)
  class(pcm_nlo_t), intent(inout) :: pcm
  class(model_data_t), intent(in) :: model
end subroutine pcm_nlo_init_qn

```

<PCM: procedures>+≡

```

module subroutine pcm_nlo_init_qn (pcm, model)
  class(pcm_nlo_t), intent(inout) :: pcm
  class(model_data_t), intent(in) :: model
  integer, dimension(:,:), allocatable :: flv_states
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: i
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  allocate (flv_states (pcm%region_data%n_legs_born, &
    pcm%region_data%n_flv_born))
  flv_states = pcm%get_flv_states (.true.)
  allocate (pcm%qn_born (size (flv_states, dim = 1), &
    size (flv_states, dim = 2)))
  allocate (flv (size (flv_states, dim = 1)))
  allocate (qn (size (flv_states, dim = 1)))
  do i = 1, pcm%get_n_flv_born ()
    call flv%init (flv_states (:,i), model)
    call qn%init (flv)
    pcm%qn_born(:,i) = qn
  end do
  deallocate (flv); deallocate (qn)
  deallocate (flv_states)
  allocate (flv_states (pcm%region_data%n_legs_real, pcm%region_data%n_flv_real))
  flv_states = pcm%get_flv_states (.false.)
  allocate (pcm%qn_real (size (flv_states, dim = 1), size (flv_states, dim = 2)))

```

```

allocate (flv (size (flv_states, dim = 1)))
allocate (qn (size (flv_states, dim = 1)))
do i = 1, pcm%get_n_flv_real ()
    call flv%init (flv_states (:,i), model)
    call qn%init (flv)
    pcm%qn_real(:,i) = qn
end do
end subroutine pcm_nlo_init_qn

```

Gfortran 7/8/9 bug, has to remain in the main module:

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: allocate_ps_matching => pcm_nlo_allocate_ps_matching

```

```

<PCM: main procedures>+≡
    subroutine pcm_nlo_allocate_ps_matching (pcm)
        class(pcm_nlo_t), intent(inout) :: pcm
        if (.not. allocated (pcm%real_partition)) then
            allocate (powheg_damping_simple_t :: pcm%real_partition)
        end if
    end subroutine pcm_nlo_allocate_ps_matching

```

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: activate_dalitz_plot => pcm_nlo_activate_dalitz_plot

```

```

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_activate_dalitz_plot (pcm, filename)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(string_t), intent(in) :: filename
    end subroutine pcm_nlo_activate_dalitz_plot

```

```

<PCM: procedures>+≡
    module subroutine pcm_nlo_activate_dalitz_plot (pcm, filename)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(string_t), intent(in) :: filename
        call pcm%dalitz_plot%init (free_unit (), filename, .false.)
        call pcm%dalitz_plot%write_header ()
    end subroutine pcm_nlo_activate_dalitz_plot

```

```

<PCM: pcm_nlo: TBP>+≡
    procedure :: register_dalitz_plot => pcm_nlo_register_dalitz_plot

```

```

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_register_dalitz_plot (pcm, emitter, p)
        class(pcm_nlo_t), intent(inout) :: pcm
        integer, intent(in) :: emitter
        type(vector4_t), intent(in), dimension(:) :: p
    end subroutine pcm_nlo_register_dalitz_plot

```

```

<PCM: procedures>+≡
    module subroutine pcm_nlo_register_dalitz_plot (pcm, emitter, p)
        class(pcm_nlo_t), intent(inout) :: pcm
        integer, intent(in) :: emitter
        type(vector4_t), intent(in), dimension(:) :: p
        real(default) :: k0_n, k0_np1
        k0_n = p(emitter)%p(0)

```

```

    k0_np1 = p(size(p))%p(0)
    call pcm%dalitz_plot%register (k0_n, k0_np1)
end subroutine pcm_nlo_register_dalitz_plot

```

<PCM: pcm nlo: TBP>+≡

```

    procedure :: setup_phs_generator => pcm_nlo_setup_phs_generator

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_setup_phs_generator (pcm, pcm_work, generator, &
        sqrts, mode, singular_jacobian)
        class(pcm_nlo_t), intent(in) :: pcm
        type(phs_fks_generator_t), intent(inout) :: generator
        type(pcm_nlo_workspace_t), intent(in), target :: pcm_work
        real(default), intent(in) :: sqrts
        integer, intent(in), optional:: mode
        logical, intent(in), optional :: singular_jacobian
    end subroutine pcm_nlo_setup_phs_generator

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_setup_phs_generator (pcm, pcm_work, generator, &
        sqrts, mode, singular_jacobian)
        class(pcm_nlo_t), intent(in) :: pcm
        type(phs_fks_generator_t), intent(inout) :: generator
        type(pcm_nlo_workspace_t), intent(in), target :: pcm_work
        real(default), intent(in) :: sqrts
        integer, intent(in), optional:: mode
        logical, intent(in), optional :: singular_jacobian
        logical :: yorn
        yorn = .false.; if (present (singular_jacobian)) yorn = singular_jacobian
        call generator%connect_kinematics (pcm_work%isr_kinematics, &
            pcm_work%real_kinematics, pcm%has_massive_emitter ())
        generator%n_in = pcm%region_data%n_in
        call generator%set_sqrts_hat (sqrts)
        call generator%set_emitters (pcm%region_data%emitters)
        call generator%setup_masses (pcm%region_data%n_legs_born)
        generator%is_massive = pcm%get_mass_info (1)
        generator%singular_jacobian = yorn
        if (present (mode)) generator%mode = mode
        call generator%set_xi_and_y_bounds (pcm%settings%fks_template%xi_min, &
            pcm%settings%fks_template%y_max)
    end subroutine pcm_nlo_setup_phs_generator

```

<PCM: pcm nlo: TBP>+≡

```

    procedure :: final => pcm_nlo_final

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_final (pcm)
        class(pcm_nlo_t), intent(inout) :: pcm
    end subroutine pcm_nlo_final

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_final (pcm)
        class(pcm_nlo_t), intent(inout) :: pcm
        if (allocated (pcm%real_partition)) deallocate (pcm%real_partition)
        call pcm%dalitz_plot%final ()
    end subroutine pcm_nlo_final

```

```

end subroutine pcm_nlo_final

<PCM: pcm_nlo: TBP>+≡
  procedure :: is_nlo => pcm_nlo_is_nlo

<PCM: sub interfaces>+≡
  module function pcm_nlo_is_nlo (pcm) result (is_nlo)
    logical :: is_nlo
    class(pcm_nlo_t), intent(in) :: pcm
  end function pcm_nlo_is_nlo

<PCM: procedures>+≡
  module function pcm_nlo_is_nlo (pcm) result (is_nlo)
    logical :: is_nlo
    class(pcm_nlo_t), intent(in) :: pcm
    is_nlo = .true.
  end function pcm_nlo_is_nlo

```

As a first implementation, it acts as a wrapper for the NLO controller object and the squared matrix-element collector.

```

<PCM: public>+≡
  public :: pcm_nlo_workspace_t

<PCM: types>+≡
  type, extends (pcm_workspace_t) :: pcm_nlo_workspace_t
    type(real_kinematics_t), pointer :: real_kinematics => null ()
    type(isr_kinematics_t), pointer :: isr_kinematics => null ()
    type(real_subtraction_t) :: real_sub
    type(virtual_t) :: virtual
    type(soft_mismatch_t) :: soft_mismatch
    type(dglap_remnant_t) :: dglap_remnant
    integer, dimension(:), allocatable :: i_mci_to_real_component
  contains
    <PCM: pcm_instance: TBP>
  end type pcm_nlo_workspace_t

<PCM: pcm_instance: TBP>≡
  procedure :: set_radiation_event => pcm_nlo_workspace_set_radiation_event
  procedure :: set_subtraction_event => pcm_nlo_workspace_set_subtraction_event

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_workspace_set_radiation_event (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_nlo_workspace_set_radiation_event
  module subroutine pcm_nlo_workspace_set_subtraction_event (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_nlo_workspace_set_subtraction_event

<PCM: procedures>+≡
  module subroutine pcm_nlo_workspace_set_radiation_event (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    pcm_work%real_sub%radiation_event = .true.
    pcm_work%real_sub%subtraction_event = .false.
  end subroutine pcm_nlo_workspace_set_radiation_event

```

```

module subroutine pcm_nlo_workspace_set_subtraction_event (pcm_work)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  pcm_work%real_sub%radiation_event = .false.
  pcm_work%real_sub%subtraction_event = .true.
end subroutine pcm_nlo_workspace_set_subtraction_event

<PCM: pcm instance: TBP>+≡
  procedure :: disable_subtraction => pcm_nlo_workspace_disable_subtraction

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_workspace_disable_subtraction (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_nlo_workspace_disable_subtraction

<PCM: procedures>+≡
  module subroutine pcm_nlo_workspace_disable_subtraction (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    pcm_work%real_sub%subtraction_deactivated = .true.
  end subroutine pcm_nlo_workspace_disable_subtraction

<PCM: pcm instance: TBP>+≡
  procedure :: init_config => pcm_nlo_workspace_init_config

<PCM: sub interfaces>+≡
  module subroutine pcm_nlo_workspace_init_config (pcm_work, pcm, &
    active_components, nlo_types, energy, i_real_fin, model)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    logical, intent(in), dimension(:) :: active_components
    integer, intent(in), dimension(:) :: nlo_types
    real(default), intent(in), dimension(:) :: energy
    integer, intent(in) :: i_real_fin
    class(model_data_t), intent(in) :: model
  end subroutine pcm_nlo_workspace_init_config

<PCM: procedures>+≡
  module subroutine pcm_nlo_workspace_init_config (pcm_work, pcm, &
    active_components, nlo_types, energy, i_real_fin, model)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    logical, intent(in), dimension(:) :: active_components
    integer, intent(in), dimension(:) :: nlo_types
    real(default), intent(in), dimension(:) :: energy
    integer, intent(in) :: i_real_fin
    class(model_data_t), intent(in) :: model
    integer :: i_component
    if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
      "pcm_nlo_workspace_init_config")
    call pcm_work%init_real_and_isr_kinematics (pcm, energy)
    select type (pcm)
    type is (pcm_nlo_t)
      do i_component = 1, size (active_components)
        if (active_components(i_component) .or. &
          pcm%settings%combined_integration) then
          select case (nlo_types(i_component))

```

```

        case (NLO_REAL)
            if (i_component /= i_real_fin) then
                call pcm_work%setup_real_component (pcm, &
                    pcm%settings%fks_template%subtraction_disabled)
            end if
        case (NLO_VIRTUAL)
            call pcm_work%init_virtual (pcm, model)
        case (NLO_MISMATCH)
            call pcm_work%init_soft_mismatch (pcm)
        case (NLO_DGLAP)
            call pcm_work%init_dglap_remnant (pcm)
        end select
    end if
end do
end select
end subroutine pcm_nlo_workspace_init_config

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: setup_real_component => pcm_nlo_workspace_setup_real_component

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_workspace_setup_real_component (pcm_work, pcm, &
        subtraction_disabled)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        class(pcm_t), intent(in) :: pcm
        logical, intent(in) :: subtraction_disabled
    end subroutine pcm_nlo_workspace_setup_real_component

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_workspace_setup_real_component (pcm_work, pcm, &
        subtraction_disabled)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        class(pcm_t), intent(in) :: pcm
        logical, intent(in) :: subtraction_disabled
        select type (pcm)
        type is (pcm_nlo_t)
            call pcm_work%init_real_subtraction (pcm)
            if (subtraction_disabled) call pcm_work%disable_subtraction ()
        end select
    end subroutine pcm_nlo_workspace_setup_real_component

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: init_real_and_isr_kinematics => &
        pcm_nlo_workspace_init_real_and_isr_kinematics

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_workspace_init_real_and_isr_kinematics &
        (pcm_work, pcm, energy)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), dimension(:), intent(in) :: energy
    end subroutine pcm_nlo_workspace_init_real_and_isr_kinematics

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_workspace_init_real_and_isr_kinematics &

```

```

        (pcm_work, pcm, energy)
class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
class(pcm_t), intent(in) :: pcm
real(default), dimension(:), intent(in) :: energy
integer :: n_contr
allocate (pcm_work%real_kinematics)
allocate (pcm_work%isr_kinematics)
select type (pcm)
type is (pcm_nlo_t)
    associate (region_data => pcm%region_data)
        if (allocated (region_data%alr_contributors)) then
            n_contr = size (region_data%alr_contributors)
        else if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
            n_contr = 2
        else
            n_contr = 1
        end if
        call pcm_work%real_kinematics%init &
            (region_data%n_legs_real, region_data%n_phs, &
             region_data%n_regions, n_contr)
        if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) &
            call pcm_work%real_kinematics%init_onshell &
                (region_data%n_legs_real, region_data%n_phs)
        pcm_work%isr_kinematics%n_in = region_data%n_in
    end associate
end select
pcm_work%isr_kinematics%beam_energy = energy
end subroutine pcm_nlo_workspace_init_real_and_isr_kinematics

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: set_real_and_isr_kinematics => &
        pcm_nlo_workspace_set_real_and_isr_kinematics

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_workspace_set_real_and_isr_kinematics &
        (pcm_work, phs_identifiers, sqrts)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(in) :: sqrts
    end subroutine pcm_nlo_workspace_set_real_and_isr_kinematics

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_workspace_set_real_and_isr_kinematics &
        (pcm_work, phs_identifiers, sqrts)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(in) :: sqrts
        call pcm_work%real_sub%set_real_kinematics &
            (pcm_work%real_kinematics)
        call pcm_work%real_sub%set_isr_kinematics &
            (pcm_work%isr_kinematics)
    end subroutine pcm_nlo_workspace_set_real_and_isr_kinematics

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: init_real_subtraction => pcm_nlo_workspace_init_real_subtraction

```


<PCM: sub interfaces>+≡

```

module subroutine pcm_nlo_workspace_init_real_subtraction (pcm_work, pcm)
  class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
  class(pcm_t), intent(in) :: pcm
end subroutine pcm_nlo_workspace_init_real_subtraction

```

<PCM: procedures>+≡

```

module subroutine pcm_nlo_workspace_init_real_subtraction (pcm_work, pcm)
  class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
  class(pcm_t), intent(in) :: pcm
  select type (pcm)
  type is (pcm_nlo_t)
    associate (region_data => pcm%region_data)
      call pcm_work%real_sub%init (region_data, pcm%settings)
      if (allocated (pcm%settings%selected_alr)) then
        associate (selected_alr => pcm%settings%selected_alr)
          if (any (selected_alr < 0)) then
            call msg_fatal ("Fixed alpha region must be non-negative!")
          else if (any (selected_alr > region_data%n_regions)) then
            call msg_fatal ("Fixed alpha region is larger than the"&
              &" total number of singular regions!")
          else
            allocate (pcm_work%real_sub%selected_alr &
              (size (selected_alr)))
            pcm_work%real_sub%selected_alr = selected_alr
          end if
        end associate
      end if
    end associate
  end select
end subroutine pcm_nlo_workspace_init_real_subtraction

```

<PCM: pcm instance: TBP>+≡

```

procedure :: set_momenta_and_scales_virtual => &
  pcm_nlo_workspace_set_momenta_and_scales_virtual

```

<PCM: sub interfaces>+≡

```

module subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual &
  (pcm_work, p, ren_scale, fac_scale, es_scale)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), allocatable, intent(in) :: ren_scale
  real(default), intent(in) :: fac_scale
  real(default), allocatable, intent(in) :: es_scale
end subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual

```

<PCM: procedures>+≡

```

module subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual &
  (pcm_work, p, ren_scale, fac_scale, es_scale)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), allocatable, intent(in) :: ren_scale
  real(default), intent(in) :: fac_scale
  real(default), allocatable, intent(in) :: es_scale
  associate (virtual => pcm_work%virtual)

```

```

        call virtual%set_ren_scale (ren_scale)
        call virtual%set_fac_scale (p, fac_scale)
        call virtual%set_ellis_sexton_scale (es_scale)
    end associate
end subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual

<PCM: pcm instance: TBP>+≡
    procedure :: set_fac_scale => pcm_nlo_workspace_set_fac_scale

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_set_fac_scale (pcm_work, fac_scale)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        real(default), intent(in) :: fac_scale
    end subroutine pcm_nlo_workspace_set_fac_scale

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_set_fac_scale (pcm_work, fac_scale)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        real(default), intent(in) :: fac_scale
        pcm_work%isr_kinematics%fac_scale = fac_scale
    end subroutine pcm_nlo_workspace_set_fac_scale

<PCM: pcm instance: TBP>+≡
    procedure :: set_momenta => pcm_nlo_workspace_set_momenta

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_set_momenta (pcm_work, &
        p_born, p_real, i_phs, cms)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        type(vector4_t), dimension(:), intent(in) :: p_born, p_real
        integer, intent(in) :: i_phs
        logical, intent(in), optional :: cms
    end subroutine pcm_nlo_workspace_set_momenta

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_set_momenta (pcm_work, &
        p_born, p_real, i_phs, cms)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        type(vector4_t), dimension(:), intent(in) :: p_born, p_real
        integer, intent(in) :: i_phs
        logical, intent(in), optional :: cms
        logical :: yorn
        yorn = .false.; if (present (cms)) yorn = cms
        associate (kinematics => pcm_work%real_kinematics)
            if (yorn) then
                if (.not. kinematics%p_born_cms%initialized) &
                    call kinematics%p_born_cms%init (size (p_born), 1)
                if (.not. kinematics%p_real_cms%initialized) &
                    call kinematics%p_real_cms%init (size (p_real), 1)
                kinematics%p_born_cms%phs_point(1) = p_born
                kinematics%p_real_cms%phs_point(i_phs) = p_real
            else
                if (.not. kinematics%p_born_lab%initialized) &
                    call kinematics%p_born_lab%init (size (p_born), 1)
                if (.not. kinematics%p_real_lab%initialized) &

```

```

        call kinematics%p_real_lab%init (size (p_real), 1)
        kinematics%p_born_lab%phs_point(1) = p_born
        kinematics%p_real_lab%phs_point(i_phs) = p_real
    end if
end associate
end subroutine pcm_nlo_workspace_set_momenta

<PCM: pcm instance: TBP>+≡
    procedure :: get_momenta => pcm_nlo_workspace_get_momenta

<PCM: sub interfaces>+≡
    module function pcm_nlo_workspace_get_momenta (pcm_work, pcm, &
        i_phs, born_phsp, cms) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        integer, intent(in) :: i_phs
        logical, intent(in) :: born_phsp
        logical, intent(in), optional :: cms
    end function pcm_nlo_workspace_get_momenta

<PCM: procedures>+≡
    module function pcm_nlo_workspace_get_momenta (pcm_work, pcm, &
        i_phs, born_phsp, cms) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        integer, intent(in) :: i_phs
        logical, intent(in) :: born_phsp
        logical, intent(in), optional :: cms
        logical :: yorn
        yorn = .false.; if (present (cms)) yorn = cms
        select type (pcm)
        type is (pcm_nlo_t)
            if (born_phsp) then
                if (yorn) then
                    p = pcm_work%real_kinematics%p_born_cms%phs_point(1)
                else
                    p = pcm_work%real_kinematics%p_born_lab%phs_point(1)
                end if
            else
                if (yorn) then
                    p = pcm_work%real_kinematics%p_real_cms%phs_point(i_phs)
                else
                    p = pcm_work%real_kinematics%p_real_lab%phs_point(i_phs)
                end if
            end if
        end select
    end function pcm_nlo_workspace_get_momenta

<PCM: pcm instance: TBP>+≡
    procedure :: get_xi_max => pcm_nlo_workspace_get_xi_max

```

```

<PCM: sub interfaces>+≡
    module function pcm_nlo_workspace_get_xi_max (pcm_work, alr) result (xi_max)
        real(default) :: xi_max
        class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        integer, intent(in) :: alr
    end function pcm_nlo_workspace_get_xi_max

<PCM: procedures>+≡
    module function pcm_nlo_workspace_get_xi_max (pcm_work, alr) result (xi_max)
        real(default) :: xi_max
        class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        integer, intent(in) :: alr
        integer :: i_phs
        i_phs = pcm_work%real_kinematics%alr_to_i_phs (alr)
        xi_max = pcm_work%real_kinematics%xi_max (i_phs)
    end function pcm_nlo_workspace_get_xi_max

<PCM: pcm instance: TBP>+≡
    procedure :: set_x_rad => pcm_nlo_workspace_set_x_rad

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_set_x_rad (pcm_work, x_tot)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        real(default), intent(in), dimension(:) :: x_tot
    end subroutine pcm_nlo_workspace_set_x_rad

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_set_x_rad (pcm_work, x_tot)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        real(default), intent(in), dimension(:) :: x_tot
        integer :: n_par
        n_par = size (x_tot)
        if (n_par < 3) then
            pcm_work%real_kinematics%x_rad = zero
        else
            pcm_work%real_kinematics%x_rad = x_tot (n_par - 2 : n_par)
        end if
    end subroutine pcm_nlo_workspace_set_x_rad

<PCM: pcm instance: TBP>+≡
    procedure :: init_virtual => pcm_nlo_workspace_init_virtual

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_init_virtual (pcm_work, pcm, model)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        class(pcm_t), intent(in) :: pcm
        class(model_data_t), intent(in) :: model
    end subroutine pcm_nlo_workspace_init_virtual

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_init_virtual (pcm_work, pcm, model)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        class(pcm_t), intent(in) :: pcm
        class(model_data_t), intent(in) :: model
        select type (pcm)
            type is (pcm_nlo_t)

```

```

        associate (region_data => pcm%region_data)
        call pcm_work%virtual%init (region_data%get_flv_states_born (), &
            region_data%n_in, pcm%settings, model, pcm%has_pdfs)
        end associate
    end select
end subroutine pcm_nlo_workspace_init_virtual

<PCM: pcm instance: TBP>+≡
    procedure :: disable_virtual_subtraction => &
        pcm_nlo_workspace_disable_virtual_subtraction

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_disable_virtual_subtraction (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    end subroutine pcm_nlo_workspace_disable_virtual_subtraction

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_disable_virtual_subtraction (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    end subroutine pcm_nlo_workspace_disable_virtual_subtraction

<PCM: pcm instance: TBP>+≡
    procedure :: compute_sqme_virt => pcm_nlo_workspace_compute_sqme_virt

<PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_compute_sqme_virt (pcm_work, pcm, p, &
        alpha_coupling, separate_uborns, sqme_virt)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_virt
    end subroutine pcm_nlo_workspace_compute_sqme_virt

<PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_compute_sqme_virt (pcm_work, pcm, p, &
        alpha_coupling, separate_uborns, sqme_virt)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_virt
        type(vector4_t), dimension(:), allocatable :: pp
        associate (virtual => pcm_work%virtual)
            allocate (pp (size (p)))
            if (virtual%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
                pp = pcm_work%real_kinematics%p_born_onshell%get_momenta (1)
            else
                pp = p
            end if
            select type (pcm)
            type is (pcm_nlo_t)
                if (separate_uborns) then

```

```

        allocate (sqme_virt (pcm%get_n_flv_born ()))
    else
        allocate (sqme_virt (1))
    end if
    sqme_virt = zero
    call virtual%evaluate (pcm%region_data, &
        alpha_coupling, pp, separate_uborns, sqme_virt)
    end select
end associate
end subroutine pcm_nlo_workspace_compute_sqme_virt

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: compute_sqme_mismatch => pcm_nlo_workspace_compute_sqme_mismatch

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_workspace_compute_sqme_mismatch (pcm_work, pcm, &
        alpha_s, separate_uborns, sqme_mism)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), intent(in) :: alpha_s
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_mism
    end subroutine pcm_nlo_workspace_compute_sqme_mismatch

```

<PCM: procedures>+≡

```

    module subroutine pcm_nlo_workspace_compute_sqme_mismatch (pcm_work, pcm, &
        alpha_s, separate_uborns, sqme_mism)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), intent(in) :: alpha_s
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_mism
        select type (pcm)
        type is (pcm_nlo_t)
            if (separate_uborns) then
                allocate (sqme_mism (pcm%get_n_flv_born ()))
            else
                allocate (sqme_mism (1))
            end if
            sqme_mism = zero
            sqme_mism = pcm_work%soft_mismatch%evaluate (alpha_s)
        end select
    end subroutine pcm_nlo_workspace_compute_sqme_mismatch

```

<PCM: pcm instance: TBP>+≡

```

    procedure :: compute_sqme_dglap_remnant => &
        pcm_nlo_workspace_compute_sqme_dglap_remnant

```

<PCM: sub interfaces>+≡

```

    module subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant (pcm_work, &
        pcm, alpha_coupling, separate_uborns, sqme_dglap)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns

```

```

        real(default), dimension(:), allocatable, intent(inout) :: sqme_dglap
    end subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant

    <PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant (pcm_work, &
        pcm, alpha_coupling, separate_uborns, sqme_dglap)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_dglap
        select type (pcm)
        type is (pcm_nlo_t)
            if (separate_uborns) then
                allocate (sqme_dglap (pcm%get_n_flv_born ()))
            else
                allocate (sqme_dglap (1))
            end if
        end select
        sqme_dglap = zero
        call pcm_work%dglap_remnant%evaluate (alpha_coupling, &
            separate_uborns, sqme_dglap)
    end subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant

    <PCM: pcm instance: TBP>+≡
    procedure :: set_fixed_order_event_mode => &
        pcm_nlo_workspace_set_fixed_order_event_mode

    <PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_set_fixed_order_event_mode (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    end subroutine pcm_nlo_workspace_set_fixed_order_event_mode

    <PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_set_fixed_order_event_mode (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        pcm_work%real_sub%purpose = FIXED_ORDER_EVENTS
    end subroutine pcm_nlo_workspace_set_fixed_order_event_mode

    <PCM: pcm instance: TBP>+≡
    procedure :: init_soft_mismatch => pcm_nlo_workspace_init_soft_mismatch

    <PCM: sub interfaces>+≡
    module subroutine pcm_nlo_workspace_init_soft_mismatch (pcm_work, pcm)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
    end subroutine pcm_nlo_workspace_init_soft_mismatch

    <PCM: procedures>+≡
    module subroutine pcm_nlo_workspace_init_soft_mismatch (pcm_work, pcm)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        select type (pcm)
        type is (pcm_nlo_t)
            call pcm_work%soft_mismatch%init (pcm%region_data, &
                pcm_work%real_kinematics, pcm%settings%factorization_mode)

```

```

        end select
    end subroutine pcm_nlo_workspace_init_soft_mismatch

    <PCM: pcm instance: TBP>+≡
        procedure :: init_dglap_remnant => pcm_nlo_workspace_init_dglap_remnant

    <PCM: sub interfaces>+≡
        module subroutine pcm_nlo_workspace_init_dglap_remnant (pcm_work, pcm)
            class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
            class(pcm_t), intent(in) :: pcm
        end subroutine pcm_nlo_workspace_init_dglap_remnant

    <PCM: procedures>+≡
        module subroutine pcm_nlo_workspace_init_dglap_remnant (pcm_work, pcm)
            class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
            class(pcm_t), intent(in) :: pcm
            select type (pcm)
            type is (pcm_nlo_t)
                call pcm_work%dglap_remnant%init ( &
                    pcm%settings, &
                    pcm%region_data, &
                    pcm_work%isr_kinematics)
            end select
        end subroutine pcm_nlo_workspace_init_dglap_remnant

    <PCM: pcm instance: TBP>+≡
        procedure :: is_fixed_order_nlo_events &
            => pcm_nlo_workspace_is_fixed_order_nlo_events

    <PCM: sub interfaces>+≡
        module function pcm_nlo_workspace_is_fixed_order_nlo_events &
            (pcm_work) result (is_fnlo)
            logical :: is_fnlo
            class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        end function pcm_nlo_workspace_is_fixed_order_nlo_events

    <PCM: procedures>+≡
        module function pcm_nlo_workspace_is_fixed_order_nlo_events &
            (pcm_work) result (is_fnlo)
            logical :: is_fnlo
            class(pcm_nlo_workspace_t), intent(in) :: pcm_work
            is_fnlo = pcm_work%real_sub%purpose == FIXED_ORDER_EVENTS
        end function pcm_nlo_workspace_is_fixed_order_nlo_events

    <PCM: pcm instance: TBP>+≡
        procedure :: final => pcm_nlo_workspace_final

    <PCM: sub interfaces>+≡
        module subroutine pcm_nlo_workspace_final (pcm_work)
            class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        end subroutine pcm_nlo_workspace_final

    <PCM: procedures>+≡
        module subroutine pcm_nlo_workspace_final (pcm_work)
            class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
            call pcm_work%real_sub%final ()

```



```

call pcm_work%virtual%final ()
call pcm_work%soft_mismatch%final ()
call pcm_work%dglaap_remnant%final ()
if (associated (pcm_work%real_kinematics)) then
  call pcm_work%real_kinematics%final ()
  nullify (pcm_work%real_kinematics)
end if
if (associated (pcm_work%isr_kinematics)) then
  nullify (pcm_work%isr_kinematics)
end if
end subroutine pcm_nlo_workspace_final

```

<PCM: pcm instance: TBP>+≡

```

procedure :: is_nlo => pcm_nlo_workspace_is_nlo

```

<PCM: sub interfaces>+≡

```

module function pcm_nlo_workspace_is_nlo (pcm_work) result (is_nlo)
  logical :: is_nlo
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
end function pcm_nlo_workspace_is_nlo

```

<PCM: procedures>+≡

```

module function pcm_nlo_workspace_is_nlo (pcm_work) result (is_nlo)
  logical :: is_nlo
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  is_nlo = .true.
end function pcm_nlo_workspace_is_nlo

```

This routine modifies the kinematic factors applied to the real matrix element for use with POWHEG matching. We need to divide the real matrix element by ξ_{max} to cancel a factor of ξ_{max} applied in `apply_kinematic_factors_radiation`. It comes from the fact that we sample $\tilde{\xi} \in [0, 1]$ when integrating but $\xi \in [p_T^2, \xi_{\text{max}}]$ for POWHEG matching. Thus, we are taking into account that $d\xi = d\tilde{\xi} \frac{\xi}{\xi_{\text{max}}} = d\tilde{\xi}_{\text{max}}$. Additionally, we need to cancel the Jacobian from the random number mapping. We only want the physical part of the Jacobian in our Sudakov splitting function. Furthermore, the real matrix element lacks its flux factor $\frac{1}{2\hat{s}_{\mathcal{R}}}$ and the real Jacobian lacks a factor of $\frac{1}{1-\xi}$. Together, this is a factor of $\frac{1}{2\hat{s}_{\mathcal{B}}}$, i.e. the same as the flux factor of the Born matrix element. We do not correct any of both here, as only the ratio of both will be relevant for the Sudakov.

<PCM: pcm instance: TBP>+≡

```

procedure :: powheg_kinematic_factors_real => &
  pcm_nlo_workspace_powheg_kinematic_factors_real

```

<PCM: sub interfaces>+≡

```

module function pcm_nlo_workspace_powheg_kinematic_factors_real &
  (pcm_work, sqme_real, alr) result (sqme_real_corr)
  real(default) :: sqme_real_corr
  class(pcm_nlo_workspace_t), intent(in) :: pcm_work
  real(default), intent(in) :: sqme_real
  integer, intent(in) :: alr
end function pcm_nlo_workspace_powheg_kinematic_factors_real

```

```

⟨PCM: procedures⟩+≡
  module function pcm_nlo_workspace_powheg_kinematic_factors_real &
    (pcm_work, sqme_real, alr) result (sqme_real_corr)
    real(default) :: sqme_real_corr
    class(pcm_nlo_workspace_t), intent(in) :: pcm_work
    real(default), intent(in) :: sqme_real
    integer, intent(in) :: alr
    real(default) :: xi_max, jac_rand
    integer :: i_phs
    xi_max = pcm_work%get_xi_max (alr)
    i_phs = pcm_work%real_kinematics%alr_to_i_phs (alr)
    jac_rand = pcm_work%real_kinematics%jac_rand (i_phs)
    sqme_real_corr = sqme_real / xi_max / jac_rand
  end function pcm_nlo_workspace_powheg_kinematic_factors_real

```

30.9 Kinematics instance

In this data type we combine all objects (instances) necessary for generating (or recovering) a kinematical configuration. The components work together as an implementation of multi-channel phase space.

sf_chain is an instance of the structure-function chain. It is used both for generating kinematics and, after the proper scale has been determined, evaluating the structure function entries.

phs is an instance of the phase space for the elementary process.

The array **f** contains the products of the Jacobians that originate from parameter mappings in the structure-function chain or in the phase space. We allocate this explicitly if either **sf_chain** or **phs** are explicitly allocated, otherwise we can take over a pointer.

All components are implemented as pointers to (anonymous) targets. For each component, there is a flag that tells whether this component is to be regarded as a proper component (‘owned’ by the object) or as a pointer.

```

⟨kinematics.f90⟩≡
  ⟨File header⟩

```

```

  module kinematics

```

```

    ⟨Use kinds⟩

```

```

    use lorentz
    use physics_defs
    use sf_base
    use phs_base
    use fks_regions
    use mci_base
    use process_config
    use process_mci
    use pcm_base, only: pcm_t, pcm_workspace_t
    use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t

```

```

    ⟨Standard module head⟩

```

```

    <Kinematics: public>

    <Kinematics: types>

    interface
    <Kinematics: sub interfaces>
    end interface

    end module kinematics

    <kinematics_sub.f90>≡
    <File header>

    submodule (kinematics) kinematics_s

    <Use debug>
    use format_utils, only: write_separator
    use diagnostics
    use io_units
    use phs_points, only: assignment(=), size
    use interactions
    use phs_fks
    use ttv_formfactors, only: mis_to_mpole

    implicit none

    contains

    <Kinematics: procedures>

    end submodule kinematics_s

    <Kinematics: public>≡
    public :: kinematics_t

    <Kinematics: types>≡
    type :: kinematics_t
    integer :: n_in = 0
    integer :: n_channel = 0
    integer :: selected_channel = 0
    type(sf_chain_instance_t), pointer :: sf_chain => null ()
    class(phs_t), pointer :: phs => null ()
    real(default), dimension(:), pointer :: f => null ()
    real(default) :: phs_factor
    logical :: sf_chain_allocated = .false.
    logical :: phs_allocated = .false.
    logical :: f_allocated = .false.
    integer :: emitter = -1
    integer :: i_phs = 0
    integer :: i_con = 0
    logical :: only_cm_frame = .false.
    logical :: new_seed = .true.
    logical :: threshold = .false.
    contains
    <Kinematics: kinematics: TBP>

```

```
end type kinematics_t
```

Output. Show only those components which are marked as owned.

```
<Kinematics: kinematics: TBP>≡
  procedure :: write => kinematics_write

<Kinematics: sub interfaces>≡
  module subroutine kinematics_write (object, unit)
    class(kinematics_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine kinematics_write

<Kinematics: procedures>≡
  module subroutine kinematics_write (object, unit)
    class(kinematics_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, c
    u = given_output_unit (unit)
    if (object%f_allocated) then
      write (u, "(1x,A)") "Flux * PHS volume:"
      write (u, "(2x,ES19.12)") object%phs_factor
      write (u, "(1x,A)") "Jacobian factors per channel:"
      do c = 1, size (object%f)
        write (u, "(3x,I0,':',1x,ES14.7)", advance="no") c, object%f(c)
        if (c == object%selected_channel) then
          write (u, "(1x,A)") "[selected]"
        else
          write (u, *)
        end if
      end do
    end if
    if (object%sf_chain_allocated) then
      call write_separator (u)
      call object%sf_chain%write (u)
    end if
    if (object%phs_allocated) then
      call write_separator (u)
      call object%phs%write (u)
    end if
  end subroutine kinematics_write
```

Finalizer. Delete only those components which are marked as owned.

```
<Kinematics: kinematics: TBP>+≡
  procedure :: final => kinematics_final

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_final (object)
    class(kinematics_t), intent(inout) :: object
  end subroutine kinematics_final

<Kinematics: procedures>+≡
  module subroutine kinematics_final (object)
    class(kinematics_t), intent(inout) :: object
    if (object%sf_chain_allocated) then
      call object%sf_chain%final ()
```

```

        deallocate (object%sf_chain)
        object%sf_chain_allocated = .false.
    end if
    if (object%phs_allocated) then
        call object%phs%final ()
        deallocate (object%phs)
        object%phs_allocated = .false.
    end if
    if (object%f_allocated) then
        deallocate (object%f)
        object%f_allocated = .false.
    end if
end subroutine kinematics_final

```

Configure the kinematics object. This consists of several configuration steps which correspond to individual procedures. In essence, we configure the structure-function part, the partonic phase-space part, and various NLO items.

TODO wk 19-03-01: This includes some region-data setup within pcm, hence pcm is intent(inout). This should be moved elsewhere, so pcm can become strictly intent(in).

(Kinematics: kinematics: TBP)+≡

```

    procedure :: configure => kinematics_configure

```

(Kinematics: sub interfaces)+≡

```

    module subroutine kinematics_configure (kin, pcm, pcm_work, &
        sf_chain, beam_config, phs_config, nlo_type, is_i_sub)
        class(kinematics_t), intent(out) :: kin
        class(pcm_t), intent(inout) :: pcm
        class(pcm_workspace_t), intent(in) :: pcm_work
        type(sf_chain_t), intent(in), target :: sf_chain
        type(process_beam_config_t), intent(in), target :: beam_config
        class(phs_config_t), intent(in), target :: phs_config
        integer, intent(in) :: nlo_type
        logical, intent(in) :: is_i_sub
    end subroutine kinematics_configure

```

(Kinematics: procedures)+≡

```

    module subroutine kinematics_configure (kin, pcm, pcm_work, &
        sf_chain, beam_config, phs_config, nlo_type, is_i_sub)
        class(kinematics_t), intent(out) :: kin
        class(pcm_t), intent(inout) :: pcm
        class(pcm_workspace_t), intent(in) :: pcm_work
        type(sf_chain_t), intent(in), target :: sf_chain
        type(process_beam_config_t), intent(in), target :: beam_config
        class(phs_config_t), intent(in), target :: phs_config
        integer, intent(in) :: nlo_type
        logical, intent(in) :: is_i_sub
        logical :: extended_sf
        extended_sf = nlo_type == NLO_DGLAP .or. &
            (nlo_type == NLO_REAL .and. is_i_sub)
        call kin%init_sf_chain (sf_chain, beam_config, &
            extended_sf = pcm%has_pdfs .and. extended_sf)
        !!! Add one for additional Born matrix element
        call kin%init_phs (phs_config)
    end subroutine kinematics_configure

```

```

call kin%set_nlo_info (nlo_type)
select type (phs => kin%phs)
type is (phs_fks_t)
  call phs%allocate_momenta (phs_config, .not. (nlo_type == NLO_REAL))
  select type (pcm)
  type is (pcm_nlo_t)
    call pcm%region_data%init_phs_identifiers (phs%phs_identifiers)
    !!! The triple select type pyramid of doom
    select type (pcm_work)
    type is (pcm_nlo_workspace_t)
      if (allocated (pcm_work%real_kinematics%alr_to_i_phs)) &
        call pcm%region_data%set_alr_to_i_phs (phs%phs_identifiers, &
        pcm_work%real_kinematics%alr_to_i_phs)
    end select
  end select
end select
end subroutine kinematics_configure

```

Set the flags indicating whether the phase space shall be set up for the calculation of the real contribution. For this case, also set the emitter.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: set_nlo_info => kinematics_set_nlo_info

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_set_nlo_info (k, nlo_type)
    class(kinematics_t), intent(inout) :: k
    integer, intent(in) :: nlo_type
    end subroutine kinematics_set_nlo_info

<Kinematics: procedures>+≡
  module subroutine kinematics_set_nlo_info (k, nlo_type)
    class(kinematics_t), intent(inout) :: k
    integer, intent(in) :: nlo_type
    if (nlo_type == NLO_VIRTUAL) k%only_cm_frame = .true.
    end subroutine kinematics_set_nlo_info

<Kinematics: kinematics: TBP>+≡
  procedure :: set_threshold => kinematics_set_threshold

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_set_threshold (kin, factorization_mode)
    class(kinematics_t), intent(inout) :: kin
    integer, intent(in) :: factorization_mode
    end subroutine kinematics_set_threshold

<Kinematics: procedures>+≡
  module subroutine kinematics_set_threshold (kin, factorization_mode)
    class(kinematics_t), intent(inout) :: kin
    integer, intent(in) :: factorization_mode
    kin%threshold = factorization_mode == FACTORIZATION_THRESHOLD
    end subroutine kinematics_set_threshold

```

Allocate the structure-function chain instance, initialize it as a copy of the `sf_chain` template, and prepare it for evaluation.

The `sf_chain` remains a target because the (usually constant) beam momenta are taken from there.

```

(Kinematics: kinematics: TBP)+≡
  procedure :: init_sf_chain => kinematics_init_sf_chain

(Kinematics: sub interfaces)+≡
  module subroutine kinematics_init_sf_chain &
    (k, sf_chain, config, extended_sf)
    class(kinematics_t), intent(inout) :: k
    type(sf_chain_t), intent(in), target :: sf_chain
    type(process_beam_config_t), intent(in) :: config
    logical, intent(in), optional :: extended_sf
  end subroutine kinematics_init_sf_chain

(Kinematics: procedures)+≡
  module subroutine kinematics_init_sf_chain (k, sf_chain, config, extended_sf)
    class(kinematics_t), intent(inout) :: k
    type(sf_chain_t), intent(in), target :: sf_chain
    type(process_beam_config_t), intent(in) :: config
    logical, intent(in), optional :: extended_sf
    integer :: n_strfun, n_channel
    integer :: c
    k%n_in = config%data%get_n_in ()
    n_strfun = config%n_strfun
    n_channel = config%n_channel
    allocate (k%sf_chain)
    k%sf_chain_allocated = .true.
    call k%sf_chain%init (sf_chain, n_channel)
    if (n_strfun /= 0) then
      do c = 1, n_channel
        call k%sf_chain%set_channel (c, config%sf_channel(c))
      end do
    end if
    call k%sf_chain%link_interactions ()
    call k%sf_chain%exchange_mask ()
    call k%sf_chain%init_evaluators (extended_sf = extended_sf)
  end subroutine kinematics_init_sf_chain

```

Allocate and initialize the phase-space part and the array of Jacobian factors.

```

(Kinematics: kinematics: TBP)+≡
  procedure :: init_phs => kinematics_init_phs

(Kinematics: sub interfaces)+≡
  module subroutine kinematics_init_phs (k, config)
    class(kinematics_t), intent(inout) :: k
    class(phs_config_t), intent(in), target :: config
  end subroutine kinematics_init_phs

(Kinematics: procedures)+≡
  module subroutine kinematics_init_phs (k, config)
    class(kinematics_t), intent(inout) :: k
    class(phs_config_t), intent(in), target :: config
    k%n_channel = config%get_n_channel ()
    call config%allocate_instance (k%phs)
    call k%phs%init (config)
  end subroutine kinematics_init_phs

```

```

        k%phs_allocated = .true.
        allocate (k%f (k%n_channel))
        k%f = 0
        k%f_allocated = .true.
    end subroutine kinematics_init_phs

<Kinematics: kinematics: TBP>+≡
    procedure :: evaluate_radiation_kinematics => &
        kinematics_evaluate_radiation_kinematics

<Kinematics: sub interfaces>+≡
    module subroutine kinematics_evaluate_radiation_kinematics (k, r_in)
        class(kinematics_t), intent(inout) :: k
        real(default), intent(in), dimension(:) :: r_in
    end subroutine kinematics_evaluate_radiation_kinematics

<Kinematics: procedures>+≡
    module subroutine kinematics_evaluate_radiation_kinematics (k, r_in)
        class(kinematics_t), intent(inout) :: k
        real(default), intent(in), dimension(:) :: r_in
        select type (phs => k%phs)
            type is (phs_fks_t)
                if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) then
                    call phs%generate_radiation_variables &
                        (r_in(phs%n_r_born + 1 : phs%n_r_born + 3), &
                        threshold = k%threshold)
                    call phs%compute_cms_energy ()
                end if
            end select
    end subroutine kinematics_evaluate_radiation_kinematics

<Kinematics: kinematics: TBP>+≡
    procedure :: generate_fsr_in => kinematics_generate_fsr_in

<Kinematics: sub interfaces>+≡
    module subroutine kinematics_generate_fsr_in (kin)
        class(kinematics_t), intent(inout) :: kin
    end subroutine kinematics_generate_fsr_in

<Kinematics: procedures>+≡
    module subroutine kinematics_generate_fsr_in (kin)
        class(kinematics_t), intent(inout) :: kin
        select type (phs => kin%phs)
            type is (phs_fks_t)
                call phs%generate_fsr_in ()
            end select
    end subroutine kinematics_generate_fsr_in

<Kinematics: kinematics: TBP>+≡
    procedure :: compute_xi_ref_momenta => kinematics_compute_xi_ref_momenta

<Kinematics: sub interfaces>+≡
    module subroutine kinematics_compute_xi_ref_momenta (k, reg_data, nlo_type)
        class(kinematics_t), intent(inout) :: k
        type(region_data_t), intent(in) :: reg_data

```



```

        integer, intent(in) :: nlo_type
    end subroutine kinematics_compute_xi_ref_momenta

<Kinematics: procedures>+≡
module subroutine kinematics_compute_xi_ref_momenta (k, reg_data, nlo_type)
    class(kinematics_t), intent(inout) :: k
    type(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: nlo_type
    logical :: use_contributors
    use_contributors = allocated (reg_data%alr_contributors)
    select type (phs => k%phs)
    type is (phs_fks_t)
        if (use_contributors) then
            call phs%compute_xi_ref_momenta (contributors = reg_data%alr_contributors)
        else if (k%threshold) then
            if (.not. is_subtraction_component (k%emitter, nlo_type)) &
                call phs%compute_xi_ref_momenta_threshold ()
        else
            call phs%compute_xi_ref_momenta ()
        end if
    end select
end subroutine kinematics_compute_xi_ref_momenta

```

Generate kinematics, given a phase-space channel and a MC parameter set. The main result is the momentum array **p**, but we also fill the momentum entries in the structure-function chain and the Jacobian-factor array **f**. Regarding phase space, we fill only the parameter arrays for the selected channel.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: compute_selected_channel => kinematics_compute_selected_channel

<Kinematics: sub interfaces>+≡
    module subroutine kinematics_compute_selected_channel &
        (k, mci_work, phs_channel, p, success)
        class(kinematics_t), intent(inout) :: k
        type(mci_work_t), intent(in) :: mci_work
        integer, intent(in) :: phs_channel
        type(vector4_t), dimension(:), intent(out) :: p
        logical, intent(out) :: success
    end subroutine kinematics_compute_selected_channel

<Kinematics: procedures>+≡
module subroutine kinematics_compute_selected_channel &
    (k, mci_work, phs_channel, p, success)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
    type(vector4_t), dimension(:), intent(out) :: p
    logical, intent(out) :: success
    integer :: sf_channel
    k%selected_channel = phs_channel
    sf_channel = k%phs%config%get_sf_channel (phs_channel)
    call k%sf_chain%compute_kinematics (sf_channel, mci_work%get_x_strfun ())
    call k%sf_chain%get_out_momenta (p(1:k%n_in))
    call k%phs%set_incoming_momenta (p(1:k%n_in))
    call k%phs%compute_flux ()

```

```

call k%phs%select_channel (phs_channel)
call k%phs%evaluate_selected_channel (phs_channel, &
    mci_work%get_x_process ())

select type (phs => k%phs)
type is (phs_fks_t)
    if (debug_on) call msg_debug2 (D_REAL, "phase space is phs_FKS")
    if (phs%q_defined) then
        call phs%get_born_momenta (p)
        if (debug_on) then
            call msg_debug2 (D_REAL, "q is defined")
            call msg_debug2 (D_REAL, "get_born_momenta called")
        end if
        k%phs_factor = phs%get_overall_factor ()
        success = .true.
    else
        k%phs_factor = 0
        success = .false.
    end if
class default
    if (phs%q_defined) then
        call k%phs%get_outgoing_momenta (p(k%n_in + 1 :))
        k%phs_factor = k%phs%get_overall_factor ()
        success = .true.
    else
        k%phs_factor = 0
        success = .false.
    end if
end select
end subroutine kinematics_compute_selected_channel

```

(Kinematics: kinematics: TBP)+≡

```

procedure :: redo_sf_chain => kinematics_redo_sf_chain

```

(Kinematics: sub interfaces)+≡

```

module subroutine kinematics_redo_sf_chain (kin, mci_work, phs_channel)
class(kinematics_t), intent(inout) :: kin
type(mci_work_t), intent(in) :: mci_work
integer, intent(in) :: phs_channel
end subroutine kinematics_redo_sf_chain

```

(Kinematics: procedures)+≡

```

module subroutine kinematics_redo_sf_chain (kin, mci_work, phs_channel)
class(kinematics_t), intent(inout) :: kin
type(mci_work_t), intent(in) :: mci_work
integer, intent(in) :: phs_channel
real(default), dimension(:), allocatable :: x
integer :: sf_channel, n
real(default) :: xi, y
n = size (mci_work%get_x_strfun ())
if (n > 0) then
    allocate (x(n))
    x = mci_work%get_x_strfun ()
    sf_channel = kin%phs%config%get_sf_channel (phs_channel)
    call kin%sf_chain%compute_kinematics (sf_channel, x)
end if
end subroutine kinematics_redo_sf_chain

```

```

end if
end subroutine kinematics_redo_sf_chain

```

Complete kinematics by filling the non-selected phase-space parameter arrays.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: compute_other_channels => kinematics_compute_other_channels

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_compute_other_channels &
    (k, mci_work, phs_channel)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
  end subroutine kinematics_compute_other_channels

<Kinematics: procedures>+≡
  module subroutine kinematics_compute_other_channels (k, mci_work, phs_channel)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
    integer :: c, c_sf
    call k%phs%evaluate_other_channels (phs_channel)
    do c = 1, k%n_channel
      c_sf = k%phs%config%get_sf_channel (c)
      k%f(c) = k%sf_chain%get_f (c_sf) * k%phs%get_f (c)
    end do
  end subroutine kinematics_compute_other_channels

```

Just fetch the outgoing momenta of the `sf_chain` subobject, which become the incoming (seed) momenta of the hard interaction.

This is a stripped down-version of the above which we use when recovering kinematics. Momenta are known, but no MC parameters yet.

(We do not use the `get_out_momenta` method of the chain, since this relies on the structure-function interactions, which are not necessary filled here. We do rely on the momenta of the last evaluator in the chain, however.)

```

<Kinematics: kinematics: TBP>+≡
  procedure :: get_incoming_momenta => kinematics_get_incoming_momenta

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_get_incoming_momenta (k, p)
    class(kinematics_t), intent(in) :: k
    type(vector4_t), dimension(:), intent(out) :: p
  end subroutine kinematics_get_incoming_momenta

<Kinematics: procedures>+≡
  module subroutine kinematics_get_incoming_momenta (k, p)
    class(kinematics_t), intent(in) :: k
    type(vector4_t), dimension(:), intent(out) :: p
    type(interaction_t), pointer :: int
    integer :: i
    int => k%sf_chain%get_out_int_ptr ()
    do i = 1, k%n_in
      p(i) = int%get_momentum (k%sf_chain%get_out_i (i))
    end do
  end subroutine kinematics_get_incoming_momenta

```

```

end subroutine kinematics_get_incoming_momenta

<Kinematics: kinematics: TBP>+=
  procedure :: get_boost_to_lab => kinematics_get_boost_to_lab

<Kinematics: sub interfaces>+=
  module function kinematics_get_boost_to_lab (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
  end function kinematics_get_boost_to_lab

<Kinematics: procedures>+=
  module function kinematics_get_boost_to_lab (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
    lt = kin%phs%get_lorentz_transformation ()
  end function kinematics_get_boost_to_lab

<Kinematics: kinematics: TBP>+=
  procedure :: get_boost_to_cms => kinematics_get_boost_to_cms

<Kinematics: sub interfaces>+=
  module function kinematics_get_boost_to_cms (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
  end function kinematics_get_boost_to_cms

<Kinematics: procedures>+=
  module function kinematics_get_boost_to_cms (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
    lt = inverse (kin%phs%get_lorentz_transformation ())
  end function kinematics_get_boost_to_cms

```

This inverts the remainder of the above `compute` method. We know the momenta and recover the rest, as far as needed. If we select a channel, we can complete the inversion and reconstruct the MC parameter set.

```

<Kinematics: kinematics: TBP>+=
  procedure :: recover_mcpair => kinematics_recover_mcpair

<Kinematics: sub interfaces>+=
  module subroutine kinematics_recover_mcpair (k, mci_work, phs_channel, p)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: phs_channel
    type(vector4_t), dimension(:), intent(in) :: p
  end subroutine kinematics_recover_mcpair

<Kinematics: procedures>+=
  module subroutine kinematics_recover_mcpair (k, mci_work, phs_channel, p)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: phs_channel
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: c, c_sf

```

```

real(default), dimension(:), allocatable :: x_sf, x_phs
c = phs_channel
c_sf = k%phs%config%get_sf_channel (c)
k%selected_channel = c
call k%sf_chain%recover_kinematics (c_sf)
call k%phs%set_incoming_momenta (p(1:k%n_in))
call k%phs%compute_flux ()
call k%phs%set_outgoing_momenta (p(k%n_in+1:))
call k%phs%inverse ()
do c = 1, k%n_channel
    c_sf = k%phs%config%get_sf_channel (c)
    k%f(c) = k%sf_chain%get_f (c_sf) * k%phs%get_f (c)
end do
k%phs_factor = k%phs%get_overall_factor ()
c = phs_channel
c_sf = k%phs%config%get_sf_channel (c)
allocate (x_sf (k%sf_chain%config%get_n_bound ()))
allocate (x_phs (k%phs%config%get_n_par ()))
call k%phs%select_channel (c)
call k%sf_chain%get_mcpair (c_sf, x_sf)
call k%phs%get_mcpair (c, x_phs)
call mci_work%set_x_strfun (x_sf)
call mci_work%set_x_process (x_phs)
end subroutine kinematics_recover_mcpair

```

This first part of `recover_mcpair`: just handle the sfchain.

(Kinematics: kinematics: TBP)+≡

```

procedure :: recover_sfchain => kinematics_recover_sfchain

```

(Kinematics: sub interfaces)+≡

```

module subroutine kinematics_recover_sfchain (k, channel, p)
    class(kinematics_t), intent(inout) :: k
    integer, intent(in) :: channel
    type(vector4_t), dimension(:), intent(in) :: p
end subroutine kinematics_recover_sfchain

```

(Kinematics: procedures)+≡

```

module subroutine kinematics_recover_sfchain (k, channel, p)
    class(kinematics_t), intent(inout) :: k
    integer, intent(in) :: channel
    type(vector4_t), dimension(:), intent(in) :: p
    k%selected_channel = channel
    call k%sf_chain%recover_kinematics (channel)
end subroutine kinematics_recover_sfchain

```

Retrieve the MC input parameter array for a specific channel. We assume that the kinematics is complete, so this is known for all channels.

(Kinematics: kinematics: TBP)+≡

```

procedure :: get_mcpair => kinematics_get_mcpair

```

(Kinematics: sub interfaces)+≡

```

module subroutine kinematics_get_mcpair (k, phs_channel, r)
    class(kinematics_t), intent(in) :: k
    integer, intent(in) :: phs_channel

```

```

        real(default), dimension(:), intent(out) :: r
    end subroutine kinematics_get_mcpair

<Kinematics: procedures>+≡
    module subroutine kinematics_get_mcpair (k, phs_channel, r)
        class(kinematics_t), intent(in) :: k
        integer, intent(in) :: phs_channel
        real(default), dimension(:), intent(out) :: r
        integer :: sf_channel, n_par_sf, n_par_phs
        sf_channel = k%phs%config%get_sf_channel (phs_channel)
        n_par_phs = k%phs%config%get_n_par ()
        n_par_sf = k%sf_chain%config%get_n_bound ()
        if (n_par_sf > 0) then
            call k%sf_chain%get_mcpair (sf_channel, r(1:n_par_sf))
        end if
        if (n_par_phs > 0) then
            call k%phs%get_mcpair (phs_channel, r(n_par_sf+1:))
        end if
    end subroutine kinematics_get_mcpair

```

Evaluate the structure function chain, assuming that kinematics is known.

The status must be precisely SF_DONE_KINEMATICS. We thus avoid evaluating the chain twice via different pointers to the same target.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: evaluate_sf_chain => kinematics_evaluate_sf_chain

<Kinematics: sub interfaces>+≡
    module subroutine kinematics_evaluate_sf_chain &
        (k, fac_scale, negative_sf, sf_rescale)
        class(kinematics_t), intent(inout) :: k
        real(default), intent(in) :: fac_scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(inout), optional :: sf_rescale
    end subroutine kinematics_evaluate_sf_chain

```

```

<Kinematics: procedures>+≡
    module subroutine kinematics_evaluate_sf_chain &
        (k, fac_scale, negative_sf, sf_rescale)
        class(kinematics_t), intent(inout) :: k
        real(default), intent(in) :: fac_scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(inout), optional :: sf_rescale
        select case (k%sf_chain%get_status ())
        case (SF_DONE_KINEMATICS)
            call k%sf_chain%evaluate (fac_scale, negative_sf = negative_sf, &
                sf_rescale = sf_rescale)
        end select
    end subroutine kinematics_evaluate_sf_chain

```

Recover beam momenta, i.e., return the beam momenta stored in the current `sf_chain` to their source. This is a side effect.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: return_beam_momenta => kinematics_return_beam_momenta

```

```

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_return_beam_momenta (k)
    class(kinematics_t), intent(in) :: k
    end subroutine kinematics_return_beam_momenta

```

```

<Kinematics: procedures>+≡
  module subroutine kinematics_return_beam_momenta (k)
    class(kinematics_t), intent(in) :: k
    call k%sf_chain%return_beam_momenta ()
    end subroutine kinematics_return_beam_momenta

```

Check whether the phase space is configured in the center-of-mass frame. Relevant for using the proper momenta input for BLHA matrix elements.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: lab_is_cm => kinematics_lab_is_cm

```

```

<Kinematics: sub interfaces>+≡
  module function kinematics_lab_is_cm (k) result (lab_is_cm)
    logical :: lab_is_cm
    class(kinematics_t), intent(in) :: k
    end function kinematics_lab_is_cm

```

```

<Kinematics: procedures>+≡
  module function kinematics_lab_is_cm (k) result (lab_is_cm)
    logical :: lab_is_cm
    class(kinematics_t), intent(in) :: k
    lab_is_cm = k%phs%config%lab_is_cm
    end function kinematics_lab_is_cm

```

```

<Kinematics: kinematics: TBP>+≡
  procedure :: modify_momenta_for_subtraction => &
    kinematics_modify_momenta_for_subtraction

```

```

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_modify_momenta_for_subtraction (k, p_in, p_out)
    class(kinematics_t), intent(inout) :: k
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:), allocatable :: p_out
    end subroutine kinematics_modify_momenta_for_subtraction

```

```

<Kinematics: procedures>+≡
  module subroutine kinematics_modify_momenta_for_subtraction (k, p_in, p_out)
    class(kinematics_t), intent(inout) :: k
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:), allocatable :: p_out
    allocate (p_out (size (p_in)))
    if (k%threshold) then
      select type (phs => k%phs)
        type is (phs_fks_t)
          p_out = phs%get_onshell_projected_momenta ()
        end select
    else
      p_out = p_in
    end if
    end subroutine kinematics_modify_momenta_for_subtraction

```

```

<Kinematics: kinematics: TBP>+≡
  procedure :: threshold_projection => kinematics_threshold_projection

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_threshold_projection (k, pcm_work, nlo_type)
    class(kinematics_t), intent(inout) :: k
    type(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    integer, intent(in) :: nlo_type
  end subroutine kinematics_threshold_projection

<Kinematics: procedures>+≡
  module subroutine kinematics_threshold_projection (k, pcm_work, nlo_type)
    class(kinematics_t), intent(inout) :: k
    type(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    integer, intent(in) :: nlo_type
    real(default) :: sqrts, mtop
    type(lorentz_transformation_t) :: L_to_cms
    type(vector4_t), dimension(:), allocatable :: p_tot, p_onshell
    integer :: n_tot
    n_tot = k%phs%get_n_tot ()
    allocate (p_tot (size (pcm_work%real_kinematics%p_born_cms%phs_point(1))))
    select type (phs => k%phs)
    type is (phs_fks_t)
      p_tot = pcm_work%real_kinematics%p_born_cms%phs_point(1)
    class default
      p_tot(1 : k%n_in) = phs%p
      p_tot(k%n_in + 1 : n_tot) = phs%q
    end select
    sqrts = sum (p_tot (1:k%n_in))**1
    mtop = m1s_to_mpole (sqrts)
    L_to_cms = get_boost_for_threshold_projection (p_tot, sqrts, mtop)
    call pcm_work%real_kinematics%p_born_cms%set_momenta (1, p_tot)
    p_onshell = pcm_work%real_kinematics%p_born_onshell%phs_point(1)
    call threshold_projection_born (mtop, L_to_cms, p_tot, p_onshell)
    pcm_work%real_kinematics%p_born_onshell%phs_point(1) = p_onshell
    if (debug2_active (D_THRESHOLD)) then
      print *, 'On-shell projected Born: '
      call vector4_write_set (p_onshell)
    end if
  end subroutine kinematics_threshold_projection

<Kinematics: kinematics: TBP>+≡
  procedure :: evaluate_radiation => kinematics_evaluate_radiation

<Kinematics: sub interfaces>+≡
  module subroutine kinematics_evaluate_radiation (k, p_in, p_out, success)
    class(kinematics_t), intent(inout) :: k
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:), allocatable :: p_out
    logical, intent(out) :: success
  end subroutine kinematics_evaluate_radiation

<Kinematics: procedures>+≡
  module subroutine kinematics_evaluate_radiation (k, p_in, p_out, success)
    class(kinematics_t), intent(inout) :: k
    type(vector4_t), intent(in), dimension(:) :: p_in

```



```

type(vector4_t), intent(out), dimension(:), allocatable :: p_out
logical, intent(out) :: success
type(vector4_t), dimension(:), allocatable :: p_real
type(vector4_t), dimension(:), allocatable :: p_born
real(default) :: xi_max_offshell, xi_offshell, y_offshell, jac_rand_dummy, phi
select type (phs => k%phs)
type is (phs_fks_t)
  allocate (p_born (size (p_in)))
  if (k%threshold) then
    p_born = phs%get_onshell_projected_momenta ()
  else
    p_born = p_in
  end if
  if (.not. k%phs%lab_is_cm () .and. .not. k%threshold) then
    p_born = inverse (k%phs%lt_cm_to_lab) * p_born
  end if
  call phs%compute_xi_max (p_born, k%threshold)
  if (k%emitter >= 0) then
    allocate (p_real (size (p_born) + 1))
    allocate (p_out (size (p_born) + 1))
    if (k%emitter <= k%n_in) then
      call phs%generate_isr (k%i_phs, p_real)
    else
      if (k%threshold) then
        jac_rand_dummy = 1._default
        call compute_y_from_emitter (phs%generator%real_kinematics%x_rad (I_Y), &
          phs%generator%real_kinematics%p_born_cms%get_momenta(1), &
          k%n_in, k%emitter, .false., phs%generator%y_max, jac_rand_dummy, &
          y_offshell)
        call phs%compute_xi_max (k%emitter, k%i_phs, y_offshell, &
          phs%generator%real_kinematics%p_born_cms%get_momenta(1), &
          xi_max_offshell)
        xi_offshell = xi_max_offshell * phs%generator%real_kinematics%xi_tilde
        phi = phs%generator%real_kinematics%phi
        call phs%generate_fsr (k%emitter, k%i_phs, p_real, &
          xi_y_phi = [xi_offshell, y_offshell, phi], no_jacobians = .true.)
        call phs%generator%real_kinematics%p_real_cms%set_momenta (k%i_phs, p_real)
        call phs%generate_fsr_threshold (k%emitter, k%i_phs, p_real)
        if (debug2_active (D_SUBTRACTION)) &
          call generate_fsr_threshold_for_other_emitters (k%emitter, k%i_phs)
      else if (k%i_con > 0) then
        call phs%generate_fsr (k%emitter, k%i_phs, p_real, k%i_con)
      else
        call phs%generate_fsr (k%emitter, k%i_phs, p_real)
      end if
    end if
    success = check_scalar_products (p_real)
    if (debug2_active (D_SUBTRACTION)) then
      call msg_debug2 (D_SUBTRACTION, "Real phase-space: ")
      call vector4_write_set (p_real)
    end if
    p_out = p_real
  else
    allocate (p_out (size (p_in))); p_out = p_in
  end if
end select

```

```

        success = .true.
    end if
end select
contains
subroutine generate_fsr_threshold_for_other_emitters (emitter, i_phs)
    integer, intent(in) :: emitter, i_phs
    integer :: ii_phs, this_emitter
    select type (phs => k%phs)
    type is (phs_fks_t)
        do ii_phs = 1, size (phs%phs_identifiers)
            this_emitter = phs%phs_identifiers(ii_phs)%emitter
            if (ii_phs /= i_phs .and. this_emitter /= emitter) &
                call phs%generate_fsr_threshold (this_emitter, i_phs)
        end do
    end select
end subroutine
end subroutine kinematics_evaluate_radiation

```

30.10 Instances

$\langle \text{instances.f90} \rangle \equiv$
 $\langle \text{File header} \rangle$

```

module instances

 $\langle \text{Use kinds} \rangle$ 
 $\langle \text{Use strings} \rangle$ 
    use lorentz
    use mci_base
    use particles
    use sm_qcd, only: qcd_t
    use quantum_numbers
    use interactions
    use model_data
    use variables
    use sf_base
    use pdf, only: pdf_data_t
    use physics_defs
    use process_constants
    use state_matrices
    use phs_base
    use prc_core, only: prc_core_t, prc_core_state_t
    !!! local modules
    use parton_states
    use process_counter
    use pcm_base
    use pcm
    use process_config
    use process_mci
    use process
    use kinematics

```

```

    <Standard module head>

    <Instances: public>

    <Instances: types>

    <Instances: interfaces>

    interface
    <Instances: sub interfaces>
    end interface

contains

    <Instances: main procedures>

end module instances

<instances_sub.f90>≡
    <File header>

submodule (instances) instances_s

    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use constants
    use diagnostics
    use numeric_utils
    use helicities
    use flavors
    use pdg_arrays, only: is_quark, is_charged_lepton, flv_eqv_expr_class

    !!! We should depend less on these modules (move it to pcm_nlo_t e.g.)
    use phs_wood, only: phs_wood_t
    use phs_fks
    use blha_olp_interfaces, only: prc_blha_t
    use blha_config, only: BLHA_AMP_COLOR_C
    use prc_omega, only: prc_omega_t, omega_state_t
    use prc_external, only: prc_external_t, prc_external_state_t
    use prc_threshold, only: prc_threshold_t
    use blha_olp_interfaces, only: blha_result_array_size
    use prc_openloops, only: prc_openloops_t, openloops_state_t
    use prc_recola, only: prc_recola_t
    use blha_olp_interfaces, only: blha_color_c_fill_offdiag, blha_color_c_fill_diag
    use ttv_formfactors, only: mls_to_mpole

    implicit none

contains

    <Instances: procedures>

end submodule instances_s

```

30.10.1 Term instance

A `term_instance_t` object contains all data that describe a term. Each process component consists of one or more distinct terms which may differ in kinematics, but whose squared transition matrices have to be added pointwise.

The `active` flag is set when this term is connected to an active process component. Inactive terms are skipped for kinematics and evaluation.

The `amp` array stores the amplitude values when we get them from evaluating the associated matrix-element code.

The `int_hard` interaction describes the elementary hard process. It receives the momenta and the amplitude entries for each sampling point.

The `isolated` object holds the effective parton state for the elementary interaction. The amplitude entries are computed from `int_hard`.

The `connected` evaluator set convolutes this scattering matrix with the beam (and possibly structure-function) density matrix.

The `checked` flag is set once we have applied cuts on this term. The result of this is stored in the `passed` flag.

Although each `term_instance` carries a `weight`, this currently always keeps the value 1 and is only used to be given to routines to fulfill their signature.

(Instances: types)≡

```

type :: term_instance_t
  type(process_term_t), pointer :: config => null ()
  class(pcm_t), pointer :: pcm => null ()
  class(pcm_workspace_t), pointer :: pcm_work => null ()
  logical :: active = .false.
  complex(default), dimension(:), allocatable :: amp
  type(interaction_t) :: int_hard
  type(isolated_state_t) :: isolated
  type(connected_state_t) :: connected
  class(prc_core_state_t), allocatable :: core_state
  logical :: checked = .false.
  logical :: passed = .false.
  logical, dimension(:), allocatable :: passed_array
  integer, dimension(:), allocatable :: i_flv_to_i_flv_rep
  real(default) :: scale = 0
  real(default), allocatable :: fac_scale
  real(default), allocatable :: ren_scale
  real(default), allocatable :: es_scale
  real(default), allocatable :: alpha_qcd_forced
  real(default) :: weight = 1
  type(vector4_t), dimension(:), allocatable :: p_seed
  type(vector4_t), dimension(:), allocatable :: p_hard
  integer :: nlo_type = BORN
  integer, dimension(:), allocatable :: same_kinematics
  logical :: negative_sf = .false.
  logical :: flv_dep_cut_eval = .false.
contains
  (Instances: term instance: TBP)
end type term_instance_t

```

(Instances: term instance: TBP)≡

```

procedure :: write => term_instance_write

```

<Instances: sub interfaces>≡

```

module subroutine term_instance_write &
  (term, unit, kin, show_eff_state, testflag)
  class(term_instance_t), intent(in) :: term
  integer, intent(in), optional :: unit
  type(kinematics_t), intent(in), optional :: kin
  logical, intent(in), optional :: show_eff_state
  logical, intent(in), optional :: testflag
end subroutine term_instance_write

```

<Instances: procedures>≡

```

module subroutine term_instance_write &
  (term, unit, kin, show_eff_state, testflag)
  class(term_instance_t), intent(in) :: term
  integer, intent(in), optional :: unit
  type(kinematics_t), intent(in), optional :: kin
  logical, intent(in), optional :: show_eff_state
  logical, intent(in), optional :: testflag
  real(default) :: fac_scale, ren_scale
  integer :: u
  logical :: state
  u = given_output_unit (unit)
  state = .true.; if (present (show_eff_state)) state = show_eff_state
  if (term%active) then
    if (associated (term%config)) then
      write (u, "(1x,A,I0,A,I0,A)") "Term #", term%config%i_term, &
        " (component #", term%config%i_component, ")"
    else
      write (u, "(1x,A)") "Term [undefined]"
    end if
  else
    write (u, "(1x,A,I0,A)") "Term #", term%config%i_term, &
      " [inactive]"
  end if
  if (term%checked) then
    write (u, "(3x,A,L1)") "passed cuts" = ", term%passed
  end if
  if (term%passed) then
    write (u, "(3x,A,ES19.12)") "overall scale" = ", term%scale
    write (u, "(3x,A,ES19.12)") "factorization scale" = ", term%get_fac_scale ()
    write (u, "(3x,A,ES19.12)") "renormalization scale" = ", term%get_ren_scale ()
    if (allocated (term%alpha_qcd_forced)) then
      write (u, "(3x,A,ES19.12)") "alpha(QCD) forced" = ", &
        term%alpha_qcd_forced
    end if
    write (u, "(3x,A,ES19.12)") "reweighting factor" = ", term%weight
  end if
  !!! This used to be a member of term_instance
  if (present (kin)) then
    call kin%write (u)
  end if
  call write_separator (u)
  write (u, "(1x,A)") "Amplitude (transition matrix of the &
    &hard interaction):"
  call write_separator (u)

```

```

call term%int_hard%basic_write (u, testflag = testflag)
if (state .and. term%isolated%has_trace) then
  call write_separator (u)
  write (u, "(ix,A)") "Evaluators for the hard interaction:"
  call term%isolated%write (u, testflag = testflag)
end if
if (state .and. term%connected%has_trace) then
  call write_separator (u)
  write (u, "(ix,A)") "Evaluators for the connected process:"
  call term%connected%write (u, testflag = testflag)
end if
end subroutine term_instance_write

```

The interactions and evaluators must be finalized.

(Instances: term instance: TBP)+≡

```

procedure :: final => term_instance_final

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_final (term)
  class(term_instance_t), intent(inout) :: term
end subroutine term_instance_final

```

(Instances: procedures)+≡

```

module subroutine term_instance_final (term)
  class(term_instance_t), intent(inout) :: term
  if (allocated (term%amp)) deallocate (term%amp)
  if (allocated (term%core_state)) deallocate (term%core_state)
  if (allocated (term%ren_scale)) deallocate (term%ren_scale)
  if (allocated (term%fac_scale)) deallocate (term%fac_scale)
  if (allocated (term%es_scale)) deallocate (term%es_scale)
  if (allocated (term%alpha_qcd_forced)) &
    deallocate (term%alpha_qcd_forced)
  if (allocated (term%p_seed)) deallocate (term%p_seed)
  if (allocated (term%p_hard)) deallocate (term%p_hard)
  call term%connected%final ()
  call term%isolated%final ()
  call term%int_hard%final ()
  term%pcm => null ()
  term%pcm_work => null ()
end subroutine term_instance_final

```

For a new term object, we configure the structure-function interface, the phase space, the matrix-element (interaction) interface, etc.

(Instances: term instance: TBP)+≡

```

procedure :: configure => term_instance_configure

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_configure &
  (term_instance, process, i, pcm_work, sf_chain, kin)
  class(term_instance_t), intent(out), target :: term_instance
  type(process_t), intent(in), target :: process
  integer, intent(in) :: i
  class(pcm_workspace_t), intent(in), target :: pcm_work
  type(sf_chain_t), intent(in), target :: sf_chain

```

```

        type(kinematics_t), intent(inout), target :: kin
    end subroutine term_instance_configure

<Instances: procedures>+=
module subroutine term_instance_configure &
    (term_instance, process, i, pcm_work, sf_chain, kin)
    class(term_instance_t), intent(out), target :: term_instance
    type(process_t), intent(in), target :: process
    integer, intent(in) :: i
    class(pcm_workspace_t), intent(in), target :: pcm_work
    type(sf_chain_t), intent(in), target :: sf_chain
    type(kinematics_t), intent(inout), target :: kin
    type(process_term_t) :: term
    integer :: i_component
    logical :: requires_extended_sf
    term = process%get_term_ptr (i)
    i_component = term%i_component
    if (i_component /= 0) then
        call term_instance%init &
            (process%get_pcm_ptr (), pcm_work, process%get_nlo_type_component (i_component))
        requires_extended_sf = term_instance%nlo_type == NLO_DGLAP .or. &
            (term_instance%nlo_type == NLO_REAL .and. process%get_i_sub (i) == i)
        call term_instance%setup_dynamics (process, i, kin, &
            real_finite = process%component_is_real_finite (i_component))
        select type (phs => kin%phs)
        type is (phs_fks_t)
            call term_instance%set_emitter (kin)
            call term_instance%setup_fks_kinematics (kin, &
                process%get_var_list_ptr (), &
                process%get_beam_config_ptr ())
        end select
        select type (pcm => term_instance%pcm)
        type is (pcm_nlo_t)
            call kin%set_threshold (pcm%settings%factorization_mode)
        end select
        call term_instance%setup_expressions (process%get_meta (), process%get_config ())
    end if
end subroutine term_instance_configure

```

First part of term-instance configuration: initialize by assigning pointers to the overall pcm and the associated pcm_workspace objects.

```

<Instances: term instance: TBP>+=
    procedure :: init => term_instance_init

<Instances: sub interfaces>+=
    module subroutine term_instance_init &
        (term_instance, pcm, pcm_work, nlo_type)
        class(term_instance_t), intent(out) :: term_instance
        class(pcm_t), intent(in), target :: pcm
        class(pcm_workspace_t), intent(in), target :: pcm_work
        integer, intent(in) :: nlo_type
    end subroutine term_instance_init

<Instances: procedures>+=
    module subroutine term_instance_init (term_instance, pcm, pcm_work, nlo_type)

```

```

class(term_instance_t), intent(out) :: term_instance
class(pcm_t), intent(in), target :: pcm
class(pcm_workspace_t), intent(in), target :: pcm_work
integer, intent(in) :: nlo_type
term_instance%pcm => pcm
term_instance%pcm_work => pcm_work
term_instance%nlo_type = nlo_type
end subroutine term_instance_init

```

The second part of term-instance configuration concerns dynamics, i.e., the interface to the matrix-element (interaction), and the parton-state objects that combine all kinematics and matrix-element data for evaluation.

The hard interaction (incoming momenta) is linked to the structure function instance. In the isolated state, we either set pointers to both, or we create modified copies (**rearrange**) as effective structure-function chain and interaction, respectively.

Finally, we set up the **subevt** component that will be used for evaluating observables, collecting particles from the trace evaluator in the effective connected state. Their quantum numbers must be determined by following back source links and set explicitly, since they are already eliminated in that trace.

The **rearrange** parts are still commented out; they could become relevant for a NLO algorithm.

```

<Instances: term instance: TBP>+=
  procedure :: setup_dynamics => term_instance_setup_dynamics

<Instances: sub interfaces>+=
  module subroutine term_instance_setup_dynamics &
    (term, process, i_term, kin, real_finite)
    class(term_instance_t), intent(inout), target :: term
    type(process_t), intent(in), target:: process
    integer, intent(in) :: i_term
    type(kinematics_t), intent(in) :: kin
    logical, intent(in), optional :: real_finite
  end subroutine term_instance_setup_dynamics

<Instances: procedures>+=
  module subroutine term_instance_setup_dynamics &
    (term, process, i_term, kin, real_finite)
    class(term_instance_t), intent(inout), target :: term
    type(process_t), intent(in), target:: process
    integer, intent(in) :: i_term
    type(kinematics_t), intent(in) :: kin
    logical, intent(in), optional :: real_finite
    class(prc_core_t), pointer :: core => null ()
    type(process_beam_config_t) :: beam_config
    type(interaction_t), pointer :: sf_chain_int
    type(interaction_t), pointer :: src_int
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_in
    type(state_matrix_t), pointer :: state_matrix
    type(flavor_t), dimension(:), allocatable :: flv_int, flv_src, f_in, f_out
    integer, dimension(:,:), allocatable :: flv_born, flv_real
    type(flavor_t), dimension(:,:), allocatable :: flv_pdf
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_pdf

```



```

integer :: n_in, n_vir, n_out, n_tot, n_sub
integer :: n_flv_born, n_flv_real, n_flv_total
integer :: i, j
logical :: me_already_squared, keep_fs_flavors
logical :: decrease_n_tot
logical :: requires_extended_sf
me_already_squared = .false.
keep_fs_flavors = .false.
term%config => process%get_term_ptr (i_term)
term%int_hard = term%config%int
core => process%get_core_term (i_term)
term%negative_sf = process%get_negative_sf ()
call core%allocate_workspace (term%core_state)
select type (core)
class is (prc_external_t)
    call reduce_interaction (term%int_hard, &
        core%includes_polarization (), .true., .false.)
    me_already_squared = .true.
    allocate (term%amp (term%int_hard%get_n_matrix_elements ()))
class default
    allocate (term%amp (term%config%n_allowed))
end select
if (allocated (term%core_state)) then
    select type (core_state => term%core_state)
    type is (openloops_state_t)
        call core_state%init_threshold (process%get_model_ptr ())
    end select
end if
term%amp = cmplx (0, 0, default)
decrease_n_tot = term%nlo_type == NLO_REAL .and. &
    term%config%i_term_global /= term%config%i_sub
if (present (real_finite)) then
    if (real_finite) decrease_n_tot = .false.
end if
if (decrease_n_tot) then
    allocate (term%p_seed (term%int_hard%get_n_tot () - 1))
else
    allocate (term%p_seed (term%int_hard%get_n_tot ()))
end if
allocate (term%p_hard (term%int_hard%get_n_tot ()))
sf_chain_int => kin%sf_chain%get_out_int_ptr ()
n_in = term%int_hard%get_n_in ()
do j = 1, n_in
    i = kin%sf_chain%get_out_i (j)
    call term%int_hard%set_source_link (j, sf_chain_int, i)
end do
call term%isolated%init (kin%sf_chain, term%int_hard)
allocate (mask_in (n_in))
mask_in = kin%sf_chain%get_out_mask ()
select type (phs => kin%phs)
type is (phs_wood_t)
    if (me_already_squared) then
        call term%isolated%setup_identity_trace &
            (core, mask_in, .true., .false.)
    end if
end select

```

```

else
    call term%isolated%setup_square_trace &
        (core, mask_in, term%config%col, .false.)
end if
type is (phs_fks_t)
select case (phs%mode)
case (PHS_MODE_ADDITIONAL_PARTICLE)
    if (me_already_squared) then
        call term%isolated%setup_identity_trace &
            (core, mask_in, .true., .false.)
    else
        keep_fs_flavors = term%config%data%n_flv > 1
        call term%isolated%setup_square_trace &
            (core, mask_in, term%config%col, &
            keep_fs_flavors)
    end if
case (PHS_MODE_COLLINEAR_REMNANT)
    if (me_already_squared) then
        call term%isolated%setup_identity_trace &
            (core, mask_in, .true., .false.)
    else
        call term%isolated%setup_square_trace &
            (core, mask_in, term%config%col, .false.)
    end if
end select
class default
    call term%isolated%setup_square_trace &
        (core, mask_in, term%config%col, .false.)
end select
if (term%nlo_type == NLO_VIRTUAL .or. (term%nlo_type == NLO_REAL .and. &
    term%config%i_term_global == term%config%i_sub) .or. &
    term%nlo_type == NLO_MISMATCH) then
    n_sub = term%get_n_sub ()
else if (term%nlo_type == NLO_DGLAP) then
    n_sub = n_beams_rescaled + term%get_n_sub ()
else
    !!! No integration of real subtraction in interactions yet
    n_sub = 0
end if
keep_fs_flavors = keep_fs_flavors .or. me_already_squared
requires_extended_sf = term%nlo_type == NLO_DGLAP .or. &
    (term%is_subtraction () .and. process%pcm_contains_pdfs ())
call term%connected%setup_connected_trace (term%isolated, &
    undo_helicities = undo_helicities (core, me_already_squared), &
    keep_fs_flavors = keep_fs_flavors, &
    requires_extended_sf = requires_extended_sf)
associate (int_eff => term%isolated%int_eff)
state_matrix => int_eff%get_state_matrix_ptr ()
n_tot = int_eff%get_n_tot ()
flv_int = quantum_numbers_get_flavor &
    (state_matrix%get_quantum_number (1))
allocate (f_in (n_in))
f_in = flv_int(1:n_in)
deallocate (flv_int)

```

```

end associate
n_in = term%connected%trace%get_n_in ()
n_vir = term%connected%trace%get_n_vir ()
n_out = term%connected%trace%get_n_out ()
allocate (f_out (n_out))
do j = 1, n_out
  call term%connected%trace%find_source &
    (n_in + n_vir + j, src_int, i)
  if (associated (src_int)) then
    state_matrix => src_int%get_state_matrix_ptr ()
    flv_src = quantum_numbers_get_flavor &
      (state_matrix%get_quantum_number (1))
    f_out(j) = flv_src(i)
    deallocate (flv_src)
  end if
end do

beam_config = process%get_beam_config ()
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  term%flv_dep_cut_eval = pcm%settings%nlo_correction_type == "EW" &
    .and. pcm%region_data%alphas_power > 0 &
    .and. any(is_charged_lepton(f_out%get_pdg()))
end select

call term%connected%setup_subevt (term%isolated%sf_chain_eff, &
  beam_config%data%flv, f_in, f_out)
call term%connected%setup_var_list &
  (process%get_var_list_ptr (), beam_config%data)
! Does connected%trace never have any helicity qn?
call term%init_interaction_qn_index (core, term%connected%trace, n_sub, &
  process%get_model_ptr (), is_polarized = .false.)
call term%init_interaction_qn_index &
  (core, term%int_hard, n_sub, process%get_model_ptr ())
call term%init_eqv_expr_classes ()
if (requires_extended_sf) then
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    n_in = pcm%region_data%get_n_in ()
    flv_born = pcm%region_data%get_flv_states_born ()
    flv_real = pcm%region_data%get_flv_states_real ()
    n_flv_born = pcm%region_data%get_n_flv_born ()
    n_flv_real = pcm%region_data%get_n_flv_real ()
    n_flv_total = n_flv_born + n_flv_real
    allocate (flv_pdf(n_in, n_flv_total), &
      qn_pdf(n_in, n_flv_total))
    call flv_pdf(:, :n_flv_born)%init (flv_born(:n_in, :))
    call flv_pdf(:, n_flv_born + 1:n_flv_total)%init (flv_real(:n_in, :))
    call qn_pdf%init (flv_pdf)
    call sf_chain_int%init_qn_index (qn_pdf, n_flv_born, n_flv_real)
  end select
end if
contains

```

```

function undo_helicities (core, me_squared) result (val)
  logical :: val
  class(prc_core_t), intent(in) :: core
  logical, intent(in) :: me_squared
  select type (core)
  class is (prc_external_t)
    val = me_squared .and. .not. core%includes_polarization ()
  class default
    val = .false.
  end select
end function undo_helicities

subroutine reduce_interaction (int, polarized_beams, keep_fs_flavors, &
  keep_colors)
  type(interaction_t), intent(inout) :: int
  logical, intent(in) :: polarized_beams
  logical, intent(in) :: keep_fs_flavors, keep_colors
  type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
  logical, dimension(:), allocatable :: mask_f, mask_c, mask_h
  integer :: n_tot, n_in
  n_in = int%get_n_in (); n_tot = int%get_n_tot ()
  allocate (qn_mask (n_tot))
  allocate (mask_f (n_tot), mask_c (n_tot), mask_h (n_tot))
  mask_c = .not. keep_colors
  mask_f (1 : n_in) = .false.
  if (keep_fs_flavors) then
    mask_f (n_in + 1 : ) = .false.
  else
    mask_f (n_in + 1 : ) = .true.
  end if
  if (polarized_beams) then
    mask_h (1 : n_in) = .false.
  else
    mask_h (1 : n_in) = .true.
  end if
  mask_h (n_in + 1 : ) = .true.
  call qn_mask%init (mask_f, mask_c, mask_h)
  call int%reduce_state_matrix (qn_mask, keep_order = .true.)
end subroutine reduce_interaction
end subroutine term_instance_setup_dynamics

```

Set up index mapping from state matrix to index pair `i_flv`, `i_sub`.

(Instances: public)≡

public :: setup_interaction_qn_index

(Instances: sub interfaces)+≡

```

module subroutine setup_interaction_qn_index &
  (int, data, qn_config, n_sub, is_polarized)
  class(interaction_t), intent(inout) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_config
  integer, intent(in) :: n_sub
  logical, intent(in) :: is_polarized
end subroutine setup_interaction_qn_index

```

<Instances: procedures>+≡

```

module subroutine setup_interaction_qn_index &
  (int, data, qn_config, n_sub, is_polarized)
  class(interaction_t), intent(inout) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_config
  integer, intent(in) :: n_sub
  logical, intent(in) :: is_polarized
  integer :: i
  type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel
  if (is_polarized) then
    call setup_interaction_qn_hel (int, data, qn_hel)
    call int%init_qn_index (qn_config, n_sub, qn_hel)
    call int%set_qn_index_helicity_flip (.true.)
  else
    call int%init_qn_index (qn_config, n_sub)
  end if
end subroutine setup_interaction_qn_index

```

Set up beam polarisation quantum numbers, if beam polarisation is required.

We retrieve the full helicity information from `term%config%data` and reduce the information only to the initial state. Afterwards, we uniquify the initial state polarization by applying an index (hash) table.

The helicity information is fed into an array of quantum numbers to assign flavor, helicity and subtraction indices correctly to their matrix element.

<Instances: public>+≡

```

public :: setup_interaction_qn_hel

```

<Instances: sub interfaces>+≡

```

module subroutine setup_interaction_qn_hel (int, data, qn_hel)
  class(interaction_t), intent(in) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), allocatable, intent(out) :: &
    qn_hel
end subroutine setup_interaction_qn_hel

```

<Instances: procedures>+≡

```

module subroutine setup_interaction_qn_hel (int, data, qn_hel)
  class(interaction_t), intent(in) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), allocatable, intent(out) :: &
    qn_hel
  type(helicity_t), dimension(:), allocatable :: hel
  integer, dimension(:), allocatable :: index_table
  integer, dimension(:, :), allocatable :: hel_state
  integer :: i, j, n_hel_unique
  associate (n_in => int%get_n_in (), n_tot => int%get_n_tot ())
    allocate (hel_state (n_tot, data%get_n_hel ()), &
      source = data%hel_state)
    allocate (index_table (data%get_n_hel ()), &
      source = 0)
    forall (j=1:data%get_n_hel (), i=n_in+1:n_tot) hel_state(i, j) = 0
    n_hel_unique = 0
    HELICITY: do i = 1, data%get_n_hel ()

```

```

do j = 1, data%get_n_hel ()
  if (index_table (j) == 0) then
    index_table(j) = i; n_hel_unique = n_hel_unique + 1
    cycle HELICITY
  else if (all (hel_state(:, i) == &
    hel_state(:, index_table(j)))) then
    cycle HELICITY
  end if
end do
end do HELICITY
allocate (qn_hel (n_tot, n_hel_unique))
allocate (hel (n_tot))
do j = 1, n_hel_unique
  call hel%init (hel_state(:, index_table(j)))
  call qn_hel(:, j)%init (hel)
end do
end associate
end subroutine setup_interaction_qn_hel

```

Initialization of equivalent cut expression classes.

Each flavor index `i_flv` here is assigned to the corresponding one representative for an equivalent cut expression class. This class describes the set of flavor quantum numbers for which the phase space cut expression evaluation yield the same output. The representative `i_flv` for one class correspond to the first flavor quantum numbers of that kind occuring in the state matrix.

(Instances: term instance: TBP)+≡

```

procedure :: init_eqv_expr_classes => term_instance_init_eqv_expr_classes

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_init_eqv_expr_classes (term)
  class(term_instance_t), intent(inout), target :: term
end subroutine term_instance_init_eqv_expr_classes

```

(Instances: procedures)+≡

```

module subroutine term_instance_init_eqv_expr_classes (term)
  class(term_instance_t), intent(inout), target :: term
  type(interaction_t), pointer :: src_int
  type(state_matrix_t), pointer :: state_matrix
  type(flavor_t), dimension(:), allocatable :: flv_src
  logical, dimension(:,:), allocatable :: eqv_expr_class
  logical, dimension (:), allocatable :: evaluated
  integer :: n_in, n_vir, n_out
  integer :: k, j, i
  n_in = term%connected%trace%get_n_in ()
  n_vir = term%connected%trace%get_n_vir ()
  n_out = term%connected%trace%get_n_out ()
  allocate (eqv_expr_class (3, n_out, &
    term%connected%trace%get_qn_index_n_flv ()))
  do k = 1, term%connected%trace%get_qn_index_n_flv ()
    do j = 1, n_out
      call term%connected%trace%find_source &
        (n_in + n_vir + j, src_int, i)
      if (associated (src_int)) then
        state_matrix => src_int%get_state_matrix_ptr ()

```

```

        flv_src = quantum_numbers_get_flavor &
            (state_matrix%get_quantum_number (k))
        eqv_expr_class (:, j, k) = flv_eqv_expr_class (flv_src(i)%get_pdg())
        deallocate (flv_src)
    end if
end do
end do
if (term%flv_dep_cut_eval) then
    allocate (evaluated (term%connected%trace%get_qn_index_n_flv ()))
    evaluated = .false.
    allocate (term%i_flv_to_i_flv_rep (term%connected%trace%get_qn_index_n_flv ()))
    do i = 1, term%connected%trace%get_qn_index_n_flv ()
        if (.not. evaluated (i)) then
            do k = i, term%connected%trace%get_qn_index_n_flv ()
                if (same_eqv_expr_class(eqv_expr_class (:,:,i), eqv_expr_class (:,:,k))) then
                    term%i_flv_to_i_flv_rep (k) = i
                    evaluated (k) = .true.
                end if
            end do
        end if
    end do
end if
end do
end if

contains

function same_eqv_expr_class (flv_mask1, flv_mask2) result (same)
    logical, dimension (:,:), intent(in) :: flv_mask1, flv_mask2
    logical :: same
    integer :: l
    same = .true.
    do l = 1, size (flv_mask1, dim = 2)
        same = same .and. all (flv_mask1(:,l) .eqv. flv_mask2(:,l))
    end do
end function same_eqv_expr_class
end subroutine term_instance_init_eqv_expr_classes

```

<Instances: term instance: TBP>+≡

```

procedure :: init_interaction_qn_index => &
    term_instance_init_interaction_qn_index

```

<Instances: sub interfaces>+≡

```

module subroutine term_instance_init_interaction_qn_index (term, core, &
    int, n_sub, model, is_polarized)
    class(term_instance_t), intent(inout), target :: term
    class(prc_core_t), intent(in) :: core
    class(interaction_t), intent(inout) :: int
    integer, intent(in) :: n_sub
    class(model_data_t), intent(in) :: model
    logical, intent(in), optional :: is_polarized
end subroutine term_instance_init_interaction_qn_index

```

<Instances: procedures>+≡

```

module subroutine term_instance_init_interaction_qn_index (term, core, &
    int, n_sub, model, is_polarized)
    class(term_instance_t), intent(inout), target :: term

```

```

class(prc_core_t), intent(in) :: core
class(interaction_t), intent(inout) :: int
integer, intent(in) :: n_sub
class(model_data_t), intent(in) :: model
logical, intent(in), optional :: is_polarized
logical :: polarized
type(quantum_numbers_t), dimension(:, :), allocatable :: qn_config
integer, dimension(:, :), allocatable :: flv_born
type(flavor_t), dimension(:, :), allocatable :: flv
integer :: i
select type (core)
class is (prc_external_t)
  if (present (is_polarized)) then
    polarized = is_polarized
  else
    polarized = core%includes_polarization ()
  end if
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  associate (is_born => .not. (term%nlo_type == NLO_REAL .and. &
    .not. term%is_subtraction ()))
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      qn_config = pcm%get_qn (is_born)
    end select
    call setup_interaction_qn_index (int, term%config%data, &
      qn_config, n_sub, polarized)
  end associate
class default
  call term%config%data%get_flv_state (flv_born)
  allocate (flv (size (flv_born, dim = 1)))
  allocate (qn_config (size (flv_born, dim = 1), size (flv_born, dim = 2)))
  do i = 1, core%data%n_flv
    call flv%init (flv_born(:, i), model)
    call qn_config(:, i)%init (flv)
  end do
  call setup_interaction_qn_index (int, term%config%data, &
    qn_config, n_sub, polarized)
end select
class default
  call int%init_qn_index ()
end select
end subroutine term_instance_init_interaction_qn_index

```

(Instances: term instance: TBP)+≡

```
procedure :: setup_fks_kinematics => term_instance_setup_fks_kinematics
```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_setup_fks_kinematics &
  (term, kin, var_list, beam_config)
class(term_instance_t), intent(inout), target :: term
type(kinematics_t), intent(inout) :: kin
type(var_list_t), intent(in) :: var_list
type(process_beam_config_t), intent(in) :: beam_config

```



```

end subroutine term_instance_setup_fks_kinematics

(Instances: procedures)+≡
module subroutine term_instance_setup_fks_kinematics &
  (term, kin, var_list, beam_config)
  class(term_instance_t), intent(inout), target :: term
  type(kinematics_t), intent(inout) :: kin
  type(var_list_t), intent(in) :: var_list
  type(process_beam_config_t), intent(in) :: beam_config
  integer :: mode
  logical :: singular_jacobian
  if (.not. (term%nlo_type == NLO_REAL .or. term%nlo_type == NLO_DGLAP .or. &
    term%nlo_type == NLO_MISMATCH)) return
  singular_jacobian = var_list%get_lval &
    (var_str ("?powheg_use_singular_jacobian"))
  if (term%nlo_type == NLO_REAL) then
    mode = check_generator_mode (GEN_REAL_PHASE_SPACE)
  else if (term%nlo_type == NLO_MISMATCH) then
    mode = check_generator_mode (GEN_SOFT_MISMATCH)
  else
    mode = PHS_MODE_UNDEFINED
  end if
  select type (phs => kin%phs)
  type is (phs_fks_t)
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      select type (pcm_work => term%pcm_work)
      type is (pcm_nlo_workspace_t)
        call pcm%setup_phs_generator (pcm_work, &
          phs%generator, phs%config%sqrts, mode, singular_jacobian)
        if (beam_config%has_structure_function ()) then
          pcm_work%isr_kinematics%isr_mode = SQRTS_VAR
        else
          pcm_work%isr_kinematics%isr_mode = SQRTS_FIXED
        end if
        if (debug_on) call msg_debug &
          (D_PHASESPACE, "isr_mode: ", pcm_work%isr_kinematics%isr_mode)
      end select
    end select
  class default
    call msg_fatal ("Phase space should be an FKS phase space!")
  end select
contains
  function check_generator_mode (gen_mode_default) result (gen_mode)
    integer :: gen_mode
    integer, intent(in) :: gen_mode_default
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      associate (settings => pcm%settings)
        if (settings%test_coll_limit .and. settings%test_anti_coll_limit) &
          call msg_fatal ("You cannot check the collinear and anti-collinear limit "&
            &"at the same time!")
        if (settings%test_soft_limit .and. .not. settings%test_coll_limit &
          .and. .not. settings%test_anti_coll_limit) then
          gen_mode = GEN_SOFT_LIMIT_TEST
        end if
      end associate
    end select
  end function
end module

```

```

        else if (.not. settings%test_soft_limit .and. settings%test_coll_limit) then
            gen_mode = GEN_COLL_LIMIT_TEST
        else if (.not. settings%test_soft_limit .and. settings%test_anti_coll_limit) then
            gen_mode = GEN_ANTI_COLL_LIMIT_TEST
        else if (settings%test_soft_limit .and. settings%test_coll_limit) then
            gen_mode = GEN_SOFT_COLL_LIMIT_TEST
        else if (settings%test_soft_limit .and. settings%test_anti_coll_limit) then
            gen_mode = GEN_SOFT_ANTI_COLL_LIMIT_TEST
        else
            gen_mode = gen_mode_default
        end if
    end associate
end select
end function check_generator_mode
end subroutine term_instance_setup_fks_kinematics

```

Set up seed kinematics, starting from the MC parameter set given as argument. As a result, the `k_seed` kinematics object is evaluated (except for the structure-function matrix-element evaluation, which we postpone until we know the factorization scale), and we have a valid `p_seed` momentum array.

```

<Instances: term instance: TBP>+≡
    procedure :: compute_seed_kinematics => term_instance_compute_seed_kinematics

```

```

<Instances: sub interfaces>+≡
    module subroutine term_instance_compute_seed_kinematics &
        (term, kin, mci_work, phs_channel, success)
        class(term_instance_t), intent(inout), target :: term
        type(kinematics_t), intent(inout) :: kin
        type(mci_work_t), intent(in) :: mci_work
        integer, intent(in) :: phs_channel
        logical, intent(out) :: success
    end subroutine term_instance_compute_seed_kinematics

```

```

<Instances: procedures>+≡
    module subroutine term_instance_compute_seed_kinematics &
        (term, kin, mci_work, phs_channel, success)
        class(term_instance_t), intent(inout), target :: term
        type(kinematics_t), intent(inout) :: kin
        type(mci_work_t), intent(in) :: mci_work
        integer, intent(in) :: phs_channel
        logical, intent(out) :: success
        call kin%compute_selected_channel &
            (mci_work, phs_channel, term%p_seed, success)
    end subroutine term_instance_compute_seed_kinematics

```

```

<Instances: term instance: TBP>+≡
    procedure :: evaluate_projections => term_instance_evaluate_projections

```

```

<Instances: sub interfaces>+≡
    module subroutine term_instance_evaluate_projections (term, kin)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
    end subroutine term_instance_evaluate_projections

```

```

<Instances: procedures>+≡
module subroutine term_instance_evaluate_projections (term, kin)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(inout) :: kin
  if (kin%threshold .and. term%nlo_type > BORN) then
    if (debug2_active (D_THRESHOLD)) &
      print *, 'Evaluate on-shell projection: ', &
        char (component_status (term%nlo_type))
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      call kin%threshold_projection (pcm_work, term%nlo_type)
    end select
  end if
end subroutine term_instance_evaluate_projections

```

Compute the momenta in the hard interactions, one for each term that constitutes this process component. In simple cases this amounts to just copying momenta. In more advanced cases, we may generate distinct sets of momenta from the seed kinematics.

The interactions in the term instances are accessed individually. We may choose to calculate all terms at once together with the seed kinematics, use `component%core_state` for storage, and just fill the interactions here.

```

<Instances: term instance: TBP>+≡
  procedure :: compute_hard_kinematics => &
    term_instance_compute_hard_kinematics

<Instances: sub interfaces>+≡
  module subroutine term_instance_compute_hard_kinematics &
    (term, kin, recover, skip_term, success)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    integer, intent(in), optional :: skip_term
    logical, intent(in), optional :: recover
    logical, intent(out) :: success
  end subroutine term_instance_compute_hard_kinematics

<Instances: procedures>+≡
  module subroutine term_instance_compute_hard_kinematics &
    (term, kin, recover, skip_term, success)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    integer, intent(in), optional :: skip_term
    logical, intent(in), optional :: recover
    logical, intent(out) :: success
    type(vector4_t), dimension(:), allocatable :: p
    if (allocated (term%core_state)) &
      call term%core_state%reset_new_kinematics ()
    if (present (skip_term)) then
      if (term%config%i_term_global == skip_term) return
    end if

    if (present (recover)) then
      if (recover) return
    end if

```

```

if (term%nlo_type == NLO_REAL .and. kin%emitter >= 0) then
  call kin%evaluate_radiation (term%p_seed, p, success)
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    if (pcm%dalitz_plot%active) then
      if (kin%emitter > kin%n_in) then
        if (p(kin%emitter)**2 > tiny_07) &
          call pcm%register_dalitz_plot (kin%emitter, p)
        end if
      end if
    end select
  else if (is_subtraction_component (kin%emitter, term%nlo_type)) then
    call kin%modify_momenta_for_subtraction (term%p_seed, p)
    success = .true.
  else
    allocate (p (size (term%p_seed))); p = term%p_seed
    success = .true.
  end if
  call term%int_hard%set_momenta (p)
  if (debug_on) then
    call msg_debug2 (D_REAL, "inside compute_hard_kinematics")
    if (debug2_active (D_REAL)) call vector4_write_set (p)
  end if
end subroutine term_instance_compute_hard_kinematics

```

Here, we invert this. We fetch the incoming momenta which reside in the appropriate `sf_chain` object, stored within the `k_seed` subobject. On the other hand, we have the outgoing momenta of the effective interaction. We rely on the process core to compute the remaining seed momenta and to fill the momenta within the hard interaction. (The latter is trivial if hard and effective interaction coincide.)

After this is done, the incoming momenta in the trace evaluator that corresponds to the hard (effective) interaction, are still left undefined. We remedy this by calling `receive_kinematics` once.

(Instances: term instance: TBP)+≡

```

procedure :: recover_seed_kinematics => &
  term_instance_recover_seed_kinematics

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_recover_seed_kinematics &
  (term, kin, p_seed_ref)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(in) :: kin
  type(vector4_t), dimension(:), intent(in), optional :: p_seed_ref
end subroutine term_instance_recover_seed_kinematics

```

(Instances: procedures)+≡

```

module subroutine term_instance_recover_seed_kinematics &
  (term, kin, p_seed_ref)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(in) :: kin
  integer :: n_in
  type(vector4_t), dimension(:), intent(in), optional :: p_seed_ref
  n_in = kin%n_in

```

```

call kin%get_incoming_momenta (term%p_seed(1:n_in))
associate (int_eff => term%isolated%int_eff)
  call int_eff%set_momenta (term%p_seed(1:n_in), outgoing = .false.)
  if (present (p_seed_ref)) then
    term%p_seed(n_in + 1 : ) = p_seed_ref
  else
    term%p_seed(n_in + 1 : ) = int_eff%get_momenta (outgoing = .true.)
  end if
end associate
call term%isolated%receive_kinematics ()
end subroutine term_instance_recover_seed_kinematics

```

Compute the integration parameters for all channels except the selected one.
 JRR: Obsolete now.

```

<XXX Instances: term instance: TBP>≡
  procedure :: compute_other_channels => &
    term_instance_compute_other_channels

<XXX Instances: procedures>≡
  subroutine term_instance_compute_other_channels &
    (term, mci_work, phs_channel)
    class(term_instance_t), intent(inout), target :: term
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
    call term%k_term%compute_other_channels (mci_work, phs_channel)
  end subroutine term_instance_compute_other_channels

```

Recover beam momenta, i.e., return the beam momenta as currently stored in the kinematics subobject to their source. This is a side effect. JRR: Obsolete now.

```

<XXX Instances: term instance: TBP>+≡
  procedure :: return_beam_momenta => term_instance_return_beam_momenta

<XXX Instances: procedures>+≡
  subroutine term_instance_return_beam_momenta (term)
    class(term_instance_t), intent(in) :: term
    call term%k_term%return_beam_momenta ()
  end subroutine term_instance_return_beam_momenta

```

Applies the real partition by computing the real partition function $F(\Phi)$ and multiplying either $\mathcal{R}_{\text{sin}} = \mathcal{R} \cdot F$ or $\mathcal{R}_{\text{fin}} = \mathcal{R} \cdot (1 - F)$.

```

<Instances: term instance: TBP>+≡
  procedure :: apply_real_partition => term_instance_apply_real_partition

<Instances: sub interfaces>+≡
  module subroutine term_instance_apply_real_partition (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(in) :: kin
  end subroutine term_instance_apply_real_partition

<Instances: procedures>+≡
  module subroutine term_instance_apply_real_partition (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(in) :: kin

```

```

real(default) :: f, sqme
integer :: i_component
integer :: i_amp, n_amps, qn_index
logical :: is_subtraction
i_component = term%config%i_component
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  if (pcm%component_selected (i_component) .and. &
      pcm%nlo_type (i_component) == NLO_REAL) then
    is_subtraction = pcm%component_type (i_component) == &
        COMP_REAL_SING .and. kin%emitter < 0
  if (is_subtraction) return
  select case (pcm%component_type (i_component))
  case (COMP_REAL_FIN)
    call term%connected%trace%set_duplicate_flv_zero()
  end select
  f = pcm%real_partition%get_f (term%p_hard)
  n_amps = term%connected%trace%get_n_matrix_elements ()
  do i_amp = 1, n_amps
    qn_index = term%connected%trace%get_qn_index (i_amp, i_sub = 0)
    if (term%passed_array(i_amp) .or. .not. term%passed) then
      sqme = real (term%connected%trace%get_matrix_element (qn_index))
    else
      sqme = zero
    end if
    if (debug_on) call msg_debug2 &
        (D_PROCESS_INTEGRATION, "term_instance_apply_real_partition")
    select case (pcm%component_type (i_component))
    case (COMP_REAL_FIN)
      if (debug_on) call msg_debug2 &
          (D_PROCESS_INTEGRATION, "Real finite")
      sqme = sqme * (one - f)
    case (COMP_REAL_SING)
      if (debug_on) call msg_debug2 &
          (D_PROCESS_INTEGRATION, "Real singular")
      sqme = sqme * f
    end select
    if (debug_on) call msg_debug2 &
        (D_PROCESS_INTEGRATION, "apply_damping: sqme", sqme)
    call term%connected%trace%set_matrix_element &
        (qn_index, cmplx (sqme, zero, default))
  end do
end if
end select
end subroutine term_instance_apply_real_partition

```

<Instances: term instance: TBP>+≡

```

procedure :: get_p_hard => term_instance_get_p_hard

```

<Instances: sub interfaces>+≡

```

pure module function term_instance_get_p_hard &
  (term_instance) result (p_hard)
  type(vector4_t), dimension(:), allocatable :: p_hard
  class(term_instance_t), intent(in) :: term_instance

```

```

end function term_instance_get_p_hard

<Instances: procedures>+≡
pure module function term_instance_get_p_hard (term_instance) result (p_hard)
  type(vector4_t), dimension(:), allocatable :: p_hard
  class(term_instance_t), intent(in) :: term_instance
  allocate (p_hard (size (term_instance%p_hard)))
  p_hard = term_instance%p_hard
end function term_instance_get_p_hard

<Instances: term instance: TBP>+≡
procedure :: set_emitter => term_instance_set_emitter

<Instances: sub interfaces>+≡
module subroutine term_instance_set_emitter (term, kin)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(inout) :: kin
end subroutine term_instance_set_emitter

<Instances: procedures>+≡
module subroutine term_instance_set_emitter (term, kin)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(inout) :: kin
  integer :: i_phs
  logical :: set_emitter
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    select type (phs => kin%phs)
    type is (phs_fks_t)
      !!! Without resonances, i_alr = i_phs
      i_phs = term%config%i_term
      kin%i_phs = i_phs
      set_emitter = i_phs <= pcm%region_data%n_phs .and. &
        term%nlo_type == NLO_REAL
    if (set_emitter) then
      kin%emitter = phs%phs_identifiers(i_phs)%emitter
      select type (pcm => term%pcm)
      type is (pcm_nlo_t)
        if (allocated (pcm%region_data%i_phs_to_i_con)) &
          kin%i_con = pcm%region_data%i_phs_to_i_con (i_phs)
        end select
      end if
    end select
  end select
end subroutine term_instance_set_emitter

```

For initializing the expressions, we need the local variable list and the parse trees.

```

<Instances: term instance: TBP>+≡
procedure :: setup_expressions => term_instance_setup_expressions

<Instances: sub interfaces>+≡
module subroutine term_instance_setup_expressions (term, meta, config)
  class(term_instance_t), intent(inout), target :: term
  type(process_metadata_t), intent(in), target :: meta

```

```

    type(process_config_data_t), intent(in) :: config
end subroutine term_instance_setup_expressions

```

(Instances: procedures)+≡

```

module subroutine term_instance_setup_expressions (term, meta, config)
  class(term_instance_t), intent(inout), target :: term
  type(process_metadata_t), intent(in), target :: meta
  type(process_config_data_t), intent(in) :: config
  if (allocated (config%ef_cuts)) &
    call term%connected%setup_cuts (config%ef_cuts)
  if (allocated (config%ef_scale)) &
    call term%connected%setup_scale (config%ef_scale)
  if (allocated (config%ef_fac_scale)) &
    call term%connected%setup_fac_scale (config%ef_fac_scale)
  if (allocated (config%ef_ren_scale)) &
    call term%connected%setup_ren_scale (config%ef_ren_scale)
  if (allocated (config%ef_weight)) &
    call term%connected%setup_weight (config%ef_weight)
end subroutine term_instance_setup_expressions

```

Prepare the extra evaluators that we need for processing events.

The matrix elements we get from OpenLoops and GoSam are already squared and summed over color and helicity. They should not be squared again.

(Instances: term instance: TBP)+≡

```

  procedure :: setup_event_data => term_instance_setup_event_data

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_setup_event_data (term, kin, core, model)
  class(term_instance_t), intent(inout), target :: term
  type(kinematics_t), intent(in) :: kin
  class(prc_core_t), intent(in) :: core
  class(model_data_t), intent(in), target :: model
end subroutine term_instance_setup_event_data

```

(Instances: procedures)+≡

```

module subroutine term_instance_setup_event_data (term, kin, core, model)
  class(term_instance_t), intent(inout), target :: term
  type(kinematics_t), intent(in) :: kin
  class(prc_core_t), intent(in) :: core
  class(model_data_t), intent(in), target :: model
  integer :: n_in
  logical :: mask_color
  type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_in
  n_in = term%int_hard%get_n_in ()
  allocate (mask_in (n_in))
  mask_in = kin%sf_chain%get_out_mask ()
  call setup_isolated (term%isolated, core, model, mask_in, term%config%col)
  select type (pcm_work => term%pcm_work)
  type is (pcm_nlo_workspace_t)
    mask_color = pcm_work%is_fixed_order_nlo_events ()
  class default
    mask_color = .false.
  end select
  call setup_connected (term%connected, term%isolated, core, &
    term%nlo_type, mask_color)

```



```

contains
  subroutine setup_isolated (isolated, core, model, mask, color)
    type(isolated_state_t), intent(inout), target :: isolated
    class(prc_core_t), intent(in) :: core
    class(model_data_t), intent(in), target :: model
    type(quantum_numbers_mask_t), intent(in), dimension(:) :: mask
    integer, intent(in), dimension(:) :: color
    select type (core)
    class is (prc_blha_t)
      call isolated%matrix%init_identity(isolated%int_eff)
      isolated%has_matrix = .true.
    class default
      call isolated%setup_square_matrix (core, model, mask, color)
    end select
    !!! TODO (PS-09-10-20) We should not square the flows
    !!! if they come from BLHA either
    call isolated%setup_square_flows (core, model, mask)
  end subroutine setup_isolated

  subroutine setup_connected (connected, isolated, core, nlo_type, mask_color)
    type(connected_state_t), intent(inout), target :: connected
    type(isolated_state_t), intent(in), target :: isolated
    class(prc_core_t), intent(in) :: core
    integer, intent(in) :: nlo_type
    logical, intent(in) :: mask_color
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
    call connected%setup_connected_matrix (isolated)
    if (term%nlo_type == NLO_VIRTUAL .or. (term%nlo_type == NLO_REAL &
      .and. term%config%i_term_global == term%config%i_sub) &
      .or. term%nlo_type == NLO_DGLAP) then
      !!! We do not care about the subtraction matrix elements in
      !!! connected%matrix, because all entries there are supposed
      !!! to be squared. To be able to match with flavor quantum numbers,
      !!! we remove the subtraction quantum entries from the state matrix.
      allocate (mask (connected%matrix%get_n_tot()))
      call mask%set_sub (1)
      call connected%matrix%reduce_state_matrix (mask, keep_order = .true.)
    end if
    call term%init_interaction_qn_index (core, connected%matrix, 0, model, &
      is_polarized = .false.)
    select type (core)
    class is (prc_blha_t)
      call connected%setup_connected_flows &
        (isolated, mask_color = mask_color)
    class default
      call connected%setup_connected_flows (isolated)
    end select
    call connected%setup_state_flv (isolated%get_n_out ())
  end subroutine setup_connected
end subroutine term_instance_setup_event_data

```

Color-correlated matrix elements should be obtained from the external BLHA provider. According to the standard, the matrix elements output is a one-

dimensional array. For FKS subtraction, we require the matrix B_{ij} . BLHA prescribes a mapping $(i, j) \rightarrow k$, where k is the index of the matrix element in the output array. It focusses on the off-diagonal entries, i.e. $i \neq j$. The subroutine `blha_color_c_fill_offdiag` realizes this mapping. The diagonal entries can simply be obtained as the product of the Born matrix element and either C_A or C_F , which is achieved by `blha_color_c_fill_diag`. For simple processes, i.e. those with only one color line, it is $B_{ij} = C_F \cdot B$. For those, we keep the possibility of computing color correlations by a multiplication of the Born matrix element with C_F . It is triggered by the `use_internal_color_correlations` flag and should be used only for testing purposes. However, it is also used for the threshold computation where the process is well-defined and fixed.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_color_correlations => &
    term_instance_evaluate_color_correlations
```

(Instances: sub interfaces)+≡

```
module subroutine term_instance_evaluate_color_correlations (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
end subroutine term_instance_evaluate_color_correlations
```

(Instances: procedures)+≡

```
module subroutine term_instance_evaluate_color_correlations (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    integer :: i_flv_born
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            if (debug_on) call msg_debug2 (D_SUBTRACTION, &
                "term_instance_evaluate_color_correlations: " // &
                "use_internal_color_correlations:", &
                pcm%settings%use_internal_color_correlations)
            if (debug_on) call msg_debug2 (D_SUBTRACTION, "fac_scale", term%get_fac_scale ())
            do i_flv_born = 1, pcm%region_data%n_flv_born
                select case (term%nlo_type)
                case (NLO_REAL)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%real_sub%sqme_born (i_flv_born), &
                        pcm_work%real_sub%sqme_born_color_c (:, :, i_flv_born))
                case (NLO_MISMATCH)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%soft_mismatch%sqme_born (i_flv_born), &
                        pcm_work%soft_mismatch%sqme_born_color_c (:, :, i_flv_born))
                case (NLO_VIRTUAL)
                    !!! This is just a copy of the above with a different offset and can for sure be u
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        -one, pcm_work%virtual%sqme_color_c (:, :, i_flv_born))
                case (NLO_DGLAP)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%dglap_remnant%sqme_born (i_flv_born), &
                        pcm_work%dglap_remnant%sqme_color_c_extra (:, :, i_flv_born))
                end select
            end do
        end select
    end select
```

```

        end do
    end select
end select
contains
function get_trivial_cf_factors (n_tot, flv, factorization_mode) result (beta_ij)
    integer, intent(in) :: n_tot, factorization_mode
    integer, intent(in), dimension(:) :: flv
    real(default), dimension(n_tot, n_tot) :: beta_ij
    if (factorization_mode == NO_FACTORIZATION) then
        beta_ij = get_trivial_cf_factors_default (n_tot, flv)
    else
        beta_ij = get_trivial_cf_factors_threshold (n_tot, flv)
    end if
end function get_trivial_cf_factors

function get_trivial_cf_factors_default (n_tot, flv) result (beta_ij)
    integer, intent(in) :: n_tot
    integer, intent(in), dimension(:) :: flv
    real(default), dimension(n_tot, n_tot) :: beta_ij
    integer :: i, j
    beta_ij = zero
    if (count (is_quark (flv)) == 2) then
        do i = 1, n_tot
            do j = 1, n_tot
                if (is_quark(flv(i)) .and. is_quark(flv(j))) then
                    if (i == j) then
                        beta_ij(i,j) = -cf
                    else
                        beta_ij(i,j) = cf
                    end if
                end if
            end do
        end do
    end if
end function get_trivial_cf_factors_default

function get_trivial_cf_factors_threshold (n_tot, flv) result (beta_ij)
    integer, intent(in) :: n_tot
    integer, intent(in), dimension(:) :: flv
    real(default), dimension(n_tot, n_tot) :: beta_ij
    integer :: i
    beta_ij = zero
    do i = 1, 4
        beta_ij(i,i) = -cf
    end do
    beta_ij(1,2) = cf; beta_ij(2,1) = cf
    beta_ij(3,4) = cf; beta_ij(4,3) = cf
end function get_trivial_cf_factors_threshold

subroutine transfer_me_array_to_bij (pcm, i_flv, &
    sqme_born, sqme_color_c)
    type(pcm_nlo_t), intent(in) :: pcm
    integer, intent(in) :: i_flv
    real(default), intent(in) :: sqme_born

```

```

real(default), dimension(:, :), intent(inout) :: sqme_color_c
logical :: special_case_interferences
integer :: i_color_c, i_sub, n_offset, i_qn
real(default), dimension(:), allocatable :: sqme
real(default) :: sqme_born_c
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "transfer_me_array_to_bij")
if (pcm%settings%use_internal_color_correlations) then
  !!! A negative value for sqme_born indicates that the Born matrix
  !!! element is multiplied at a different place, e.g. in the case
  !!! of the virtual component
  sqme_color_c = get_trivial_cf_factors &
    (pcm%region_data%get_n_legs_born (), &
    pcm%region_data%get_flv_states_born (i_flv), &
    pcm%settings%factorization_mode)
  if (sqme_born > zero) then
    sqme_color_c = sqme_born * sqme_color_c
  else if (sqme_born == zero) then
    sqme_color_c = zero
  end if
else
  special_case_interferences = &
    pcm%region_data%nlo_correction_type == "EW"
  n_offset = 0
  if (term%nlo_type == NLO_VIRTUAL) then
    n_offset = 1
  else if (pcm%has_pdfs .and. (term%is_subtraction () &
    .or. term%nlo_type == NLO_DGLAP)) then
    n_offset = n_beams_rescaled
  end if
  allocate (sqme (term%get_n_sub_color ()), source = zero)
  do i_sub = 1, term%get_n_sub_color ()
    i_qn = term%connected%trace%get_qn_index (i_flv, i_sub = i_sub + n_offset)
    if (term%passed_array(i_flv) .or. .not. term%passed) then
      sqme(i_sub) = real(term%connected%trace%get_matrix_element (i_qn), default)
    else
      sqme(i_sub) = zero
    end if
  end do
  call blha_color_c_fill_offdiag (pcm%region_data%n_legs_born, &
    sqme, sqme_color_c)
  i_qn = term%connected%trace%get_qn_index (i_flv, i_sub = 0)
  if (term%passed_array(i_flv) .or. .not. term%passed) then
    sqme_born_c = real(term%connected%trace%get_matrix_element (i_qn), default)
  else
    sqme_born_c = zero
  end if
  call blha_color_c_fill_diag (sqme_born_c, &
    pcm%region_data%get_flv_states_born (i_flv), &
    sqme_color_c, special_case_interferences)
end if
end subroutine transfer_me_array_to_bij
end subroutine term_instance_evaluate_color_correlations

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_charge_correlations => &
    term_instance_evaluate_charge_correlations

<Instances: sub interfaces>+≡
    module subroutine term_instance_evaluate_charge_correlations (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(inout) :: core
    end subroutine term_instance_evaluate_charge_correlations

<Instances: procedures>+≡
    module subroutine term_instance_evaluate_charge_correlations (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(inout) :: core
        integer :: i_flv_born
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                do i_flv_born = 1, pcm%region_data%n_flv_born
                    select case (term%nlo_type)
                    case (NLO_REAL)
                        call transfer_me_array_to_bij (pcm, i_flv_born, &
                            pcm_work%real_sub%sqme_born (i_flv_born), &
                            pcm_work%real_sub%sqme_born_charge_c (:, :, i_flv_born))
                    case (NLO_MISMATCH)
                        call transfer_me_array_to_bij (pcm, i_flv_born, &
                            pcm_work%soft_mismatch%sqme_born (i_flv_born), &
                            pcm_work%soft_mismatch%sqme_born_charge_c (:, :, i_flv_born))
                    case (NLO_VIRTUAL)
                        call transfer_me_array_to_bij (pcm, i_flv_born, &
                            one, pcm_work%virtual%sqme_charge_c (:, :, i_flv_born))
                    end select
                end do
            end select
        end select
    contains
        subroutine transfer_me_array_to_bij (pcm, i_flv, sqme_born, sqme_charge_c)
            type(pcm_nlo_t), intent(in) :: pcm
            integer, intent(in) :: i_flv
            real(default), intent(in) :: sqme_born
            real(default), dimension(:,:), intent(inout) :: sqme_charge_c
            integer :: n_legs_born, i, j
            real(default), dimension(:), allocatable :: sigma
            real(default), dimension(:), allocatable :: Q
            n_legs_born = pcm%region_data%n_legs_born
            associate (flv_born => pcm%region_data%flv_born(i_flv))
                allocate (sigma (n_legs_born), Q (size (flv_born%charge)))
                Q = flv_born%charge
                sigma(1:flv_born%n_in) = -one
                sigma(flv_born%n_in + 1: ) = one
            end associate
            do i = 1, n_legs_born
                do j = 1, n_legs_born
                    sqme_charge_c(i, j) = sigma(i) * sigma(j) * Q(i) * Q(j) * (-one)
                end do
            end do
        end subroutine transfer_me_array_to_bij
    end module

```

```

end do
sqme_charge_c = sqme_charge_c * sqme_born
end subroutine transfer_me_array_to_bij
end subroutine term_instance_evaluate_charge_correlations

```

The information about spin correlations is not stored in the `nlo_settings` because it is only available after the `fks_regions` have been created.

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_spin_correlations => &
term_instance_evaluate_spin_correlations

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_evaluate_spin_correlations (term, core)
class(term_instance_t), intent(inout) :: term
class(prc_core_t), intent(inout) :: core
end subroutine term_instance_evaluate_spin_correlations

```

(Instances: procedures)+≡

```

module subroutine term_instance_evaluate_spin_correlations (term, core)
class(term_instance_t), intent(inout) :: term
class(prc_core_t), intent(inout) :: core
integer :: i_flv, i_sub, i_emitter, emitter, i_qn
integer :: n_flv, n_sub_color, n_sub_spin, n_offset, i, j
real(default), dimension(1:3, 1:3) :: sqme_spin_c
real(default), dimension(:), allocatable :: sqme_spin_c_all
real(default), dimension(:), allocatable :: sqme_spin_c_arr
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
"term_instance_evaluate_spin_correlations")
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
if (pcm_work%real_sub%requires_spin_correlations () &
.and. term%nlo_type == NLO_REAL) then
select type (core)
type is (prc_openloops_t)
select type (pcm => term%pcm)
type is (pcm_nlo_t)
n_flv = term%connected%trace%get_qn_index_n_flv ()
n_sub_color = term%get_n_sub_color ()
n_sub_spin = term%get_n_sub_spin ()
n_offset = 0; if (pcm%has_pdfs) n_offset = n_beams_rescaled
allocate (sqme_spin_c_arr(6))
do i_flv = 1, n_flv
allocate (sqme_spin_c_all(n_sub_spin))
do i_sub = 1, n_sub_spin
i_qn = term%connected%trace%get_qn_index (i_flv, &
i_sub = i_sub + n_offset + n_sub_color)
if (term%passed_array(i_flv) .or. .not. term%passed) then
sqme_spin_c_all(i_sub) = &
real(term%connected%trace%get_matrix_element (i_qn), default)
else
sqme_spin_c_all(i_sub) = zero
end if
end do
do i_emitter = 1, pcm%region_data%n_emitters
emitter = pcm%region_data%emitters(i_emitter)

```

```

        if (emitter > 0) then
            call split_array (sqme_spin_c_all, sqme_spin_c_arr)
            do j = 1, size (sqme_spin_c, dim=2)
                do i = j, size (sqme_spin_c, dim=1)
                    !!! Restoring the symmetric matrix packed into a 1-dim array
                    !!! c.f. [[prc_openloops_compute_sqme_spin_c]]
                    sqme_spin_c(i,j) = sqme_spin_c_arr(j + i * (i - 1) / 2)
                    if (i /= j) sqme_spin_c(j,i) = sqme_spin_c(i,j)
                end do
            end do
            pcm_work%real_sub%sqme_born_spin_c(:, :, emitter, i_flg) = sqme_spin_c
        end if
    end do
    deallocate (sqme_spin_c_all)
end do
end select
class default
    call msg_fatal &
        ("Spin correlations so far only supported by OpenLoops.")
end select
end if
end select
end subroutine term_instance_evaluate_spin_correlations

```

<Instances: term instance: TBP>+≡

```

    procedure :: apply_fks => term_instance_apply_fks

```

<Instances: sub interfaces>+≡

```

    module subroutine term_instance_apply_fks &
        (term, kin, alpha_s_sub, alpha_qed_sub)
        class(term_instance_t), intent(inout) :: term
        class(kinematics_t), intent(inout) :: kin
        real(default), intent(in) :: alpha_s_sub, alpha_qed_sub
    end subroutine term_instance_apply_fks

```

<Instances: procedures>+≡

```

    module subroutine term_instance_apply_fks &
        (term, kin, alpha_s_sub, alpha_qed_sub)
        class(term_instance_t), intent(inout) :: term
        class(kinematics_t), intent(inout) :: kin
        real(default), intent(in) :: alpha_s_sub, alpha_qed_sub
        real(default), dimension(:), allocatable :: sqme
        integer :: i, i_phs, emitter, i_qn
        logical :: is_subtraction
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                if (term%connected%has_matrix) then
                    allocate (sqme (pcm%get_n_alr ()))
                else
                    allocate (sqme (1))
                end if
            end select
            sqme = zero
            select type (phs => kin%phs)

```

```

type is (phs_fks_t)
  if (pcm%has_pdfs .and. &
    pcm%settings%use_internal_color_correlations) then
    call msg_fatal ("Color correlations for proton processes " // &
      "so far only supported by OpenLoops.")
  end if
  call pcm_work%set_real_and_isr_kinematics &
    (phs%phs_identifiers, kin%phs%get_sqrts ())
  if (kin%emitter < 0) then
    call pcm_work%set_subtraction_event ()
    do i_phs = 1, pcm%region_data%n_phs
      emitter = phs%phs_identifiers(i_phs)%emitter
      call pcm_work%real_sub%compute (emitter, &
        i_phs, alpha_s_sub, alpha_qed_sub, term%connected%has_matrix, sqme)
    end do
  else
    call pcm_work%set_radiation_event ()
    emitter = kin%emitter; i_phs = kin%i_phs
    do i = 1, term%connected%trace%get_qn_index_n_flv ()
      i_qn = term%connected%trace%get_qn_index (i)
      if (term%passed_array(i) .or. .not. term%passed) then
        pcm_work%real_sub%sqme_real_non_sub (i, i_phs) = &
          real (term%connected%trace%get_matrix_element (i_qn))
      else
        pcm_work%real_sub%sqme_real_non_sub (i, i_phs) = zero
      end if
    end do
    call pcm_work%real_sub%compute (emitter, i_phs, alpha_s_sub, &
      alpha_qed_sub, term%connected%has_matrix, sqme)
  end if
end select
end select
end select
if (term%connected%has_trace) &
  call term%connected%trace%set_only_matrix_element &
    (1, cmplx (sum(sqme), 0, default))
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  is_subtraction = kin%emitter < 0
  if (term%connected%has_matrix) &
    call refill_evaluator (cmplx (sqme * term%weight, 0, default), &
      pcm%get_qn (is_subtraction), &
      pcm%region_data%get_flavor_indices (is_subtraction), &
      term%connected%matrix)
  if (term%connected%has_flows) &
    call refill_evaluator (cmplx (sqme * term%weight, 0, default), &
      pcm%get_qn (is_subtraction), &
      pcm%region_data%get_flavor_indices (is_subtraction), &
      term%connected%flows)
  end select
end subroutine term_instance_apply_fks

```

(Instances: term instance: TBP)+=

```
procedure :: evaluate_sqme_virt => term_instance_evaluate_sqme_virt
```


(Instances: sub interfaces)+≡

```

module subroutine term_instance_evaluate_sqme_virt &
  (term, alpha_s, alpha_qed)
  class(term_instance_t), intent(inout) :: term
  real(default), intent(in) :: alpha_s, alpha_qed
end subroutine term_instance_evaluate_sqme_virt

```

(Instances: procedures)+≡

```

module subroutine term_instance_evaluate_sqme_virt (term, alpha_s, alpha_qed)
  class(term_instance_t), intent(inout) :: term
  real(default), intent(in) :: alpha_s, alpha_qed
  real(default), dimension(2) :: alpha_coupling
  type(vector4_t), dimension(:), allocatable :: p_born
  real(default), dimension(:), allocatable :: sqme_virt
  integer :: i_flv, i_qn_born, i_qn_virt
  if (term%nlo_type /= NLO_VIRTUAL) call msg_fatal ("Trying to " // &
    "evaluate virtual matrix element with unsuited term_instance.")
  if (debug2_active (D_VIRTUAL)) then
    call msg_debug2 &
      (D_VIRTUAL, "Evaluating virtual-subtracted matrix elements")
    print *, 'ren_scale: ', term%get_ren_scale ()
    print *, 'fac_scale: ', term%get_fac_scale ()
    if (allocated (term%es_scale)) then
      print *, 'ES scale: ', term%es_scale
    else
      print *, 'ES scale: ', term%get_ren_scale ()
    end if
  end if
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      alpha_coupling = [alpha_s, alpha_qed]
      if (debug2_active (D_VIRTUAL)) then
        print *, 'alpha_s: ', alpha_coupling (1)
        print *, 'alpha_qed: ', alpha_coupling (2)
      end if
      allocate (p_born (pcm%region_data%n_legs_born))
      if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
        p_born = pcm_work%real_kinematics%p_born_onshell%get_momenta(1)
      else
        p_born = term%int_hard%get_momenta ()
      end if
      call pcm_work%set_momenta_and_scales_virtual &
        (p_born, term%ren_scale, term%get_fac_scale (), &
          term%es_scale)
      select type (pcm_work => term%pcm_work)
      type is (pcm_nlo_workspace_t)
        associate (virtual => pcm_work%virtual)
          do i_flv = 1, term%connected%trace%get_qn_index_n_flv ()
            i_qn_born = term%connected%trace%get_qn_index (i_flv, i_sub = 0)
            i_qn_virt = term%connected%trace%get_qn_index (i_flv, i_sub = 1)
            if (term%passed_array(i_flv) .or. .not. term%passed) then
              virtual%sqme_born(i_flv) = &
                real (term%connected%trace%get_matrix_element (i_qn_born))
            end if
          end do
        end associate
      end if
    end if
  end select
end subroutine term_instance_evaluate_sqme_virt

```

```

        virtual%sqme_virt_fin(i_flg) = &
            real (term%connected%trace%get_matrix_element (i_qn_virt))
    else
        virtual%sqme_born(i_flg) = zero
        virtual%sqme_virt_fin(i_flg) = zero
    end if
end do
end associate
end select
call pcm_work%compute_sqme_virt (term%pcm, term%p_hard, &
    alpha_coupling, term%connected%has_matrix, sqme_virt)
call term%connected%trace%set_only_matrix_element &
    (1, cmplx (sum(sqme_virt), 0, default))
if (term%connected%has_matrix) &
    call refill_evaluator (cmplx (sqme_virt * term%weight, &
        0, default), pcm%get_qn (.true.), &
        remove_duplicates_from_int_array ( &
            pcm%region_data%get_flavor_indices (.true.)), &
            term%connected%matrix)
if (term%connected%has_flows) &
    call refill_evaluator (cmplx (sqme_virt * term%weight, &
        0, default), pcm%get_qn (.true.), &
        remove_duplicates_from_int_array ( &
            pcm%region_data%get_flavor_indices (.true.)), &
            term%connected%flows)
end select
end select
end subroutine term_instance_evaluate_sqme_virt

```

Needs generalization to electroweak corrections.

```

<Instances: term instance: TBP>+≡
    procedure :: evaluate_sqme_mismatch => term_instance_evaluate_sqme_mismatch

<Instances: sub interfaces>+≡
    module subroutine term_instance_evaluate_sqme_mismatch (term, alpha_s)
        class(term_instance_t), intent(inout) :: term
        real(default), intent(in) :: alpha_s
    end subroutine term_instance_evaluate_sqme_mismatch

<Instances: procedures>+≡
    module subroutine term_instance_evaluate_sqme_mismatch (term, alpha_s)
        class(term_instance_t), intent(inout) :: term
        real(default), intent(in) :: alpha_s
        real(default), dimension(:), allocatable :: sqme_mism
        if (term%nlo_type /= NLO_MISMATCH) call msg_fatal &
            ("Trying to evaluate soft mismatch with unsuited term_instance.")
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            call pcm_work%compute_sqme_mismatch &
                (term%pcm, alpha_s, term%connected%has_matrix, sqme_mism)
        end select
        call term%connected%trace%set_only_matrix_element &
            (1, cmplx (sum (sqme_mism) * term%weight, 0, default))
        if (term%connected%has_matrix) then
            select type (pcm => term%pcm)

```

```

type is (pcm_nlo_t)
  if (term%connected%has_matrix) &
    call refill_evaluator (cmplx (sqme_mism * term%weight, 0, default), &
      pcm%get_qn (.true.), &
      remove_duplicates_from_int_array ( &
        pcm%region_data%get_flavor_indices (.true.)), &
      term%connected%matrix)
  if (term%connected%has_flows) &
    call refill_evaluator (cmplx (sqme_mism * term%weight, 0, default), &
      pcm%get_qn (.true.), &
      remove_duplicates_from_int_array ( &
        pcm%region_data%get_flavor_indices (.true.)), &
      term%connected%flows)
  end select
end if
end subroutine term_instance_evaluate_sqme_mismatch

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_sqme_dglap => term_instance_evaluate_sqme_dglap

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_evaluate_sqme_dglap &
  (term, alpha_s, alpha_qed)
  class(term_instance_t), intent(inout) :: term
  real(default), intent(in) :: alpha_s, alpha_qed
end subroutine term_instance_evaluate_sqme_dglap

```

(Instances: procedures)+≡

```

module subroutine term_instance_evaluate_sqme_dglap (term, alpha_s, alpha_qed)
  class(term_instance_t), intent(inout) :: term
  real(default), intent(in) :: alpha_s, alpha_qed
  real(default), dimension(2) :: alpha_coupling
  real(default), dimension(:), allocatable :: sqme_dglap
  integer :: i_flv
  if (term%nlo_type /= NLO_DGLAP) call msg_fatal &
    ("Trying to evaluate DGLAP remnant with unsuited term_instance.")
  if (debug_on) call msg_debug2 &
    (D_PROCESS_INTEGRATION, "term_instance_evaluate_sqme_dglap")
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      alpha_coupling = [alpha_s, alpha_qed]
      if (debug2_active (D_PROCESS_INTEGRATION)) then
        associate (n_flv => pcm_work%dglap_remnant%reg_data%n_flv_born)
          print *, "size(sqme_born) = ", &
            size (pcm_work%dglap_remnant%sqme_born)
          call term%connected%trace%write ()
        end associate
      end if
      call pcm_work%compute_sqme_dglap_remnant (pcm, alpha_coupling, &
        term%connected%has_matrix, sqme_dglap)
    end select
  end select
  call term%connected%trace%set_only_matrix_element &

```

```

        (1, cmplx (sum (sqme_dglap) * term%weight, 0, default))
    if (term%connected%has_matrix) then
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            call refill_evaluator (cmplx (sqme_dglap * term%weight, 0, default), &
                pcm%get_qn (.true.), &
                remove_duplicates_from_int_array ( &
                    pcm%region_data%get_flavor_indices (.true.), &
                    term%connected%matrix)
            if (term%connected%has_flows) then
                call refill_evaluator &
                    (cmplx (sqme_dglap * term%weight, 0, default), &
                    pcm%get_qn (.true.), &
                    remove_duplicates_from_int_array ( &
                        pcm%region_data%get_flavor_indices (.true.), &
                        term%connected%flows)
            end if
        end select
    end if
end subroutine term_instance_evaluate_sqme_dglap

```

Reset the term instance: clear the parton-state expressions and deactivate.

(Instances: term instance: TBP)+≡

```

    procedure :: reset => term_instance_reset

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_reset (term)
        class(term_instance_t), intent(inout) :: term
    end subroutine term_instance_reset

```

(Instances: procedures)+≡

```

    module subroutine term_instance_reset (term)
        class(term_instance_t), intent(inout) :: term
        call term%connected%reset_expressions ()
        if (allocated (term%alpha_qcd_forced)) deallocate (term%alpha_qcd_forced)
        term%active = .false.
    end subroutine term_instance_reset

```

Force an α_s value that should be used in the matrix-element calculation.

(Instances: term instance: TBP)+≡

```

    procedure :: set_alpha_qcd_forced => term_instance_set_alpha_qcd_forced

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_set_alpha_qcd_forced (term, alpha_qcd)
        class(term_instance_t), intent(inout) :: term
        real(default), intent(in) :: alpha_qcd
    end subroutine term_instance_set_alpha_qcd_forced

```

(Instances: procedures)+≡

```

    module subroutine term_instance_set_alpha_qcd_forced (term, alpha_qcd)
        class(term_instance_t), intent(inout) :: term
        real(default), intent(in) :: alpha_qcd
        if (allocated (term%alpha_qcd_forced)) then
            term%alpha_qcd_forced = alpha_qcd
        else

```

```

        allocate (term%alpha_qcd_forced, source = alpha_qcd)
    end if
end subroutine term_instance_set_alpha_qcd_forced

```

Complete the kinematics computation for the effective parton states.

We assume that the `compute_hard_kinematics` method of the process component instance has already been called, so the `int_hard` contains the correct hard kinematics. The duty of this procedure is first to compute the effective kinematics and store this in the `int_eff` effective interaction inside the `isolated` parton state. The effective kinematics may differ from the kinematics in the hard interaction. It may involve parton recombination or parton splitting. The `rearrange_partons` method is responsible for this part.

We may also call a method to compute the effective structure-function chain at this point. This is not implemented yet.

In the simple case that no rearrangement is necessary, as indicated by the `rearrange` flag, the effective interaction is a pointer to the hard interaction, and we can skip the rearrangement method. Similarly for the effective structure-function chain.

The final step of kinematics setup is to transfer the effective kinematics to the evaluators and to the `subevt`.

```

<Instances: term instance: TBP>+≡
    procedure :: compute_eff_kinematics => &
        term_instance_compute_eff_kinematics

<Instances: sub interfaces>+≡
    module subroutine term_instance_compute_eff_kinematics (term)
        class(term_instance_t), intent(inout) :: term
    end subroutine term_instance_compute_eff_kinematics

<Instances: procedures>+≡
    module subroutine term_instance_compute_eff_kinematics (term)
        class(term_instance_t), intent(inout) :: term
        term%checked = .false.
        term%passed = .false.
        call term%isolated%receive_kinematics ()
        call term%connected%receive_kinematics ()
    end subroutine term_instance_compute_eff_kinematics

```

Inverse. Reconstruct the connected state from the momenta in the trace evaluator (which we assume to be set), then reconstruct the isolated state as far as possible. The second part finalizes the momentum configuration, using the incoming seed momenta

```

<Instances: term instance: TBP>+≡
    procedure :: recover_hard_kinematics => &
        term_instance_recover_hard_kinematics

<Instances: sub interfaces>+≡
    module subroutine term_instance_recover_hard_kinematics (term)
        class(term_instance_t), intent(inout) :: term
    end subroutine term_instance_recover_hard_kinematics

```

```

<Instances: procedures>+≡
module subroutine term_instance_recover_hard_kinematics (term)
  class(term_instance_t), intent(inout) :: term
  term%checked = .false.
  term%passed = .false.
  call term%connected%send_kinematics ()
  call term%isolated%send_kinematics ()
end subroutine term_instance_recover_hard_kinematics

```

Check the term whether it passes cuts and, if successful, evaluate scales and weights. The factorization scale is also given to the term kinematics, enabling structure-function evaluation.

```

<Instances: term instance: TBP>+≡
procedure :: evaluate_expressions => &
  term_instance_evaluate_expressions

```

```

<Instances: sub interfaces>+≡
module subroutine term_instance_evaluate_expressions &
  (term, config, scale_forced)
  class(term_instance_t), intent(inout) :: term
  type(process_beam_config_t), intent(in) :: config
  real(default), intent(in), allocatable, optional :: scale_forced
end subroutine term_instance_evaluate_expressions

```

```

<Instances: procedures>+≡
module subroutine term_instance_evaluate_expressions &
  (term, config, scale_forced)
  class(term_instance_t), intent(inout) :: term
  type(process_beam_config_t), intent(in) :: config
  real(default), intent(in), allocatable, optional :: scale_forced
  real(default) :: scale = 0
  real(default) :: weight = 1
  real(default), allocatable :: fac_scale, ren_scale
  type(interaction_t), pointer :: src_int
  type(state_matrix_t), pointer :: state_matrix
  type(flavor_t), dimension(:), allocatable :: flv_int, flv_src, f_in, f_out
  logical :: passed
  integer :: n_in, n_vir, n_out, n_tot, n_flv
  integer :: i, j, k
  n_flv = term%connected%trace%get_qn_index_n_flv ()
  if (.not. allocated (term%passed_array)) allocate (term%passed_array(n_flv))
  if (term%flv_dep_cut_eval) then
    do k = 1, n_flv
      if (k == term%i_flv_to_i_flv_rep(k)) then
        n_in = term%int_hard%get_n_in ()
        associate (int_eff => term%isolated%int_eff)
          state_matrix => int_eff%get_state_matrix_ptr ()
          n_tot = int_eff%get_n_tot ()
          flv_int = quantum_numbers_get_flavor &
            (state_matrix%get_quantum_number (k))
          allocate (f_in (n_in))
          f_in = flv_int(1:n_in)
          deallocate (flv_int)
        end associate
      end if
    end do
  end if
end subroutine term_instance_evaluate_expressions

```

```

n_in = term%connected%trace%get_n_in ()
n_vir = term%connected%trace%get_n_vir ()
n_out = term%connected%trace%get_n_out ()
allocate (f_out (n_out))
do j = 1, n_out
  call term%connected%trace%find_source &
    (n_in + n_vir + j, src_int, i)
  if (associated (src_int)) then
    state_matrix => src_int%get_state_matrix_ptr ()
    flv_src = quantum_numbers_get_flavor &
      (state_matrix%get_quantum_number (k))
    f_out(j) = flv_src(i)
    deallocate (flv_src)
  end if
end do

call term%connected%renew_flv_content_subevt &
  (term%isolated%sf_chain_eff, &
   config%data%flv, f_in, f_out)
call term%connected%evaluate_expressions (passed, &
  scale, fac_scale, ren_scale, weight, &
  scale_forced, force_evaluation = .true.)
if (k == 1) then
  term%scale = scale
  if (allocated (fac_scale)) then
    if (.not. allocated (term%fac_scale)) then
      allocate (term%fac_scale, source = fac_scale)
    else
      term%fac_scale = fac_scale
    end if
  end if
  if (allocated (ren_scale)) then
    if (.not. allocated (term%ren_scale)) then
      allocate (term%ren_scale, source = ren_scale)
    else
      term%ren_scale = ren_scale
    end if
  end if
  term%weight = weight
end if
term%passed_array(k) = passed
deallocate (f_in)
deallocate (f_out)
else
  term%passed_array(k) = term%passed_array(term%i_flv_to_i_flv_rep(k))
end if
end do
term%passed = any (term%passed_array)
else
  call term%connected%evaluate_expressions (term%passed, &
    term%scale, term%fac_scale, term%ren_scale, term%weight, &
    scale_forced, force_evaluation = .true.)
  term%passed_array = term%passed
end if

```

```

    term%checked = .true.
end subroutine term_instance_evaluate_expressions

```

Evaluate the trace: first evaluate the hard interaction, then the trace evaluator. We use the `evaluate_interaction` method of the process component which generated this term. The `subevt` and `cut` expressions are not yet filled.

The `component` argument is `intent(inout)` because the `compute_amplitude` method may modify the `core_state` workspace object.

(Instances: term instance: TBP)+≡

```

    procedure :: evaluate_interaction => term_instance_evaluate_interaction

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_evaluate_interaction (term, core, kin)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in), pointer :: core
        type(kinematics_t), intent(inout) :: kin
    end subroutine term_instance_evaluate_interaction

```

(Instances: procedures)+≡

```

    module subroutine term_instance_evaluate_interaction (term, core, kin)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in), pointer :: core
        type(kinematics_t), intent(inout) :: kin
        if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
            "term_instance_evaluate_interaction")
        if (kin%only_cm_frame .and. (.not. kin%lab_is_cm())) then
            term%p_hard = kin%get_boost_to_cms () * term%int_hard%get_momenta ()
        else
            term%p_hard = term%int_hard%get_momenta ()
        end if
        select type (core)
        class is (prc_external_t)
            call term%evaluate_interaction_external (core, kin)
        class default
            call term%evaluate_interaction_default (core)
        end select
        call term%int_hard%set_matrix_element (term%amp)
    end subroutine term_instance_evaluate_interaction

```

(Instances: term instance: TBP)+≡

```

    procedure :: evaluate_interaction_default &
        => term_instance_evaluate_interaction_default

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_evaluate_interaction_default (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in) :: core
    end subroutine term_instance_evaluate_interaction_default

```

(Instances: procedures)+≡

```

    module subroutine term_instance_evaluate_interaction_default (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in) :: core
        real(default) :: fac_scale, ren_scale
        integer :: i

```



```

if (allocated (term%fac_scale)) then
  fac_scale = term%fac_scale
else
  fac_scale = term%scale
end if
if (allocated (term%ren_scale)) then
  ren_scale = term%ren_scale
else
  ren_scale = term%scale
end if
do i = 1, term%config%n_allowed
  term%amp(i) = core%compute_amplitude (term%config%i_term, term%p_hard, &
    term%config%flv(i), term%config%hel(i), term%config%col(i), &
    fac_scale, ren_scale, term%alpha_qcd_forced, &
    term%core_state)
end do
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  call pcm_work%set_fac_scale (fac_scale)
end select
end subroutine term_instance_evaluate_interaction_default

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_interaction_external &
=> term_instance_evaluate_interaction_external

```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_evaluate_interaction_external &
  (term, core, kin)
  class(term_instance_t), intent(inout) :: term
  class(prc_core_t), intent(inout) :: core
  type(kinematics_t), intent(inout) :: kin
end subroutine term_instance_evaluate_interaction_external

```

(Instances: procedures)+≡

```

module subroutine term_instance_evaluate_interaction_external &
  (term, core, kin)
  class(term_instance_t), intent(inout) :: term
  class(prc_core_t), intent(inout) :: core
  type(kinematics_t), intent(inout) :: kin
  if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
    "term_instance_evaluate_interaction_external")
  select type (core_state => term%core_state)
  type is (openloops_state_t)
    select type (core)
    type is (prc_openloops_t)
      call core%compute_alpha_s (core_state, term%get_ren_scale ())
      if (allocated (core_state%threshold_data)) &
        call evaluate_threshold_parameters (core_state, core, kin%phs%get_sqrts ())
    end select
  class is (prc_external_state_t)
    select type (core)
    class is (prc_external_t)
      call core%compute_alpha_s (core_state, term%get_ren_scale ())
    end select
  end select

```

```

end select
call evaluate_threshold_interaction ()
if (term%nlo_type == NLO_VIRTUAL) then
    call term%evaluate_interaction_external_loop (core)
else
    call term%evaluate_interaction_external_tree (core)
end if
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
    call pcm_work%set_fac_scale (term%get_fac_scale ())
end select

contains

subroutine evaluate_threshold_parameters (core_state, core, sqrts)
    type(openloops_state_t), intent(inout) :: core_state
    type(prc_openloops_t), intent(inout) :: core
    real(default), intent(in) :: sqrts
    real(default) :: mtop, wtop
    mtop = mls_to_mpole (sqrts)
    wtop = core_state%threshold_data%compute_top_width &
        (mtop, core_state%alpha_qcd)
    call core%set_mass_and_width (6, mtop, wtop)
end subroutine

subroutine evaluate_threshold_interaction ()
    integer :: leg
    select type (core)
    type is (prc_threshold_t)
        if (term%nlo_type > BORN) then
            select type (pcm_work => term%pcm_work)
            type is (pcm_nlo_workspace_t)
                if (kin%emitter >= 0) then
                    call core%set_offshell_momenta &
                        (pcm_work%real_kinematics%p_real_cms%get_momenta(term%config%i_term))
                    leg = thr_leg (kin%emitter)
                    call core%set_leg (leg)
                    call core%set_onshell_momenta &
                        (pcm_work%real_kinematics%p_real_onshell(leg)%get_momenta(term%config%i_te
                else
                    call core%set_leg (0)
                    call core%set_offshell_momenta &
                        (pcm_work%real_kinematics%p_born_cms%get_momenta(1))
                end if
            end select
        else
            call core%set_leg (-1)
            call core%set_offshell_momenta (term%p_hard)
        end if
    end select
end subroutine evaluate_threshold_interaction
end subroutine term_instance_evaluate_interaction_external

```

Retrieve the matrix elements from a matrix element provider and place them into term%amp.

For the handling of NLO calculations, FKS applies a book keeping handling flavor and/or particle type (e.g. for QCD: quark/gluon and quark flavor) in order to calculate the subtraction terms. Therefore, we have to insert the calculated matrix elements correctly into the state matrix where each entry corresponds to a set of quantum numbers. We apply a mapping `hard_qn_ind` from a list of quantum numbers provided by FKS to the hard process `int_hard`.

The calculated matrix elements are insert into `term%amp` in the following way. The first `n_born` particles are the matrix element of the hard process. In non-trivial beams, we store another `n_beams_rescaled` copies of these matrix elements as the first `n_beams_rescaled` subtractions. This is a remnant from times before the method `term_instance_set_sf_factors` and these entries are not used anymore. However, eliminating these entries involves deeper changes in how the connection tables for the evaluator product are set up and should therefore be part of a larger refactoring of the interactions & state matrices. The next $n_{\text{born}} \times n_{\text{subcolor}}$ are color-correlated Born matrix elements, with then again the next $n_{\text{born}} \times n_{\text{emitters}} \times n_{\text{subspin}}$ being spin-correlated Born matrix elements.

If two or more flavor structures would produce the same amplitude we only compute one and use the `eqv_index` determined by the `prc_core` and just copy the result to improve performance.

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_interaction_external_tree &
    => term_instance_evaluate_interaction_external_tree

<Instances: sub interfaces>+≡
  module subroutine term_instance_evaluate_interaction_external_tree &
    (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
  end subroutine term_instance_evaluate_interaction_external_tree

<Instances: procedures>+≡
  module subroutine term_instance_evaluate_interaction_external_tree &
    (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    real(default) :: sqme
    real(default), dimension(:), allocatable :: sqme_color_c
    real(default), dimension(:), allocatable :: sqme_spin_c
    real(default), dimension(6) :: sqme_spin_c_tmp
    integer :: n_flv, n_hel, n_sub_color, n_sub_spin, n_pdf_off
    integer :: i_flv, i_hel, i_sub, i_color_c, i_color_c_eqv, &
      i_spin_c, i_spin_c_eqv
    integer :: i_flv_eqv, i_hel_eqv
    integer :: emitter, i_emitter
    logical :: bad_point, bp
    logical, dimension(:,:), allocatable :: eqv_me_evaluated
    if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
      "term_instance_evaluate_interaction_external_tree")
    allocate (sqme_color_c (blha_result_array_size &
      (term%int_hard%get_n_tot (), BLHA_AMP_COLOR_C)))
    n_flv = term%int_hard%get_qn_index_n_flv ()
    n_hel = term%int_hard%get_qn_index_n_hel ()

```

```

n_sub_color = term%get_n_sub_color ()
n_sub_spin = term%get_n_sub_spin ()
allocate (eqv_me_evaluated(n_flv,n_hel))
eqv_me_evaluated = .false.
do i_flv = 1, n_flv
  if (.not. term%passed_array(i_flv) .and. term%passed) cycle
  do i_hel = 1, n_hel
    i_flv_eqv = core%data%eqv_flv_index(i_flv)
    i_hel_eqv = core%data%eqv_hel_index(i_hel)
    if (.not. eqv_me_evaluated(i_flv_eqv, i_hel_eqv)) then
      select type (core)
      class is (prc_external_t)
        call core%update_alpha_s (term%core_state, term%get_ren_scale ())
        call core%compute_sqme (i_flv, i_hel, term%p_hard, &
          term%get_ren_scale (), sqme, bad_point)
        call term%pcm_work%set_bad_point (bad_point)
        associate (i_int => term%int_hard%get_qn_index &
          (i_flv = i_flv, i_hel = i_hel, i_sub = 0))
          term%amp(i_int) = cmplx (sqme, 0, default)
        end associate
      end select
      n_pdf_off = 0
      if (term%pcm%has_pdfs .and. &
        (term%is_subtraction () .or. term%nlo_type == NLO_DGLAP)) then
        n_pdf_off = n_pdf_off + n_beams_rescaled
        do i_sub = 1, n_pdf_off
          term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub)) = &
            term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub = 0))
        end do
      end if
      if (term%pcm%has_pdfs .and. term%nlo_type == NLO_DGLAP) then
        sqme_color_c = zero
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
          if (pcm%settings%nlo_correction_type == "EW" .and. &
            pcm%region_data%alphas_power > 0) then
            select type (core)
            class is (prc_blha_t)
              call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                term%p_hard, term%get_ren_scale (), sqme_color_c, &
                bad_point)
              call term%pcm_work%set_bad_point (bad_point)
            class is (prc_recola_t)
              call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                term%p_hard, term%get_ren_scale (), sqme_color_c, &
                bad_point)
              call term%pcm_work%set_bad_point (bad_point)
            end select
          end if
        end select
        do i_sub = 1, n_sub_color
          i_color_c = term%int_hard%get_qn_index &
            (i_flv, i_hel, i_sub + n_pdf_off)
          term%amp(i_color_c) = cmplx (sqme_color_c(i_sub), 0, default)
        end do
      end if
    end if
  end do
end do

```

```

        end do
    end if
    if ((term%nlo_type == NLO_REAL .and. term%is_subtraction ()) .or. &
        term%nlo_type == NLO_MISMATCH) then
        sqme_color_c = zero
        select type (core)
        class is (prc_blha_t)
            call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                term%p_hard, term%get_ren_scale (), sqme_color_c, bad_point)
            call term%pcm_work%set_bad_point (bad_point)
        class is (prc_recola_t)
            call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                term%p_hard, term%get_ren_scale (), sqme_color_c, bad_point)
            call term%pcm_work%set_bad_point (bad_point)
        end select
        do i_sub = 1, n_sub_color
            i_color_c = term%int_hard%get_qn_index &
                (i_flv, i_hel, i_sub + n_pdf_off)
            term%amp(i_color_c) = cmplx (sqme_color_c(i_sub), 0, default)
        end do
        if (n_sub_spin > 0) then
            bad_point = .false.
            allocate (sqme_spin_c(0))
            select type (core)
            type is (prc_openloops_t)
                select type (pcm => term%pcm)
                type is (pcm_nlo_t)
                    do i_emitter = 1, pcm%region_data%n_emitters
                        emitter = pcm%region_data%emitters(i_emitter)
                        if (emitter > 0) then
                            call core%compute_sqme_spin_c &
                                (i_flv, &
                                    i_hel, &
                                    emitter, &
                                    term%p_hard, &
                                    term%get_ren_scale (), &
                                    sqme_spin_c_tmp, &
                                    bp)
                            sqme_spin_c = [sqme_spin_c, sqme_spin_c_tmp]
                            bad_point = bad_point .or. bp
                        end if
                    end do
                end select
            end select
            do i_sub = 1, n_sub_spin
                i_spin_c = term%int_hard%get_qn_index (i_flv, i_hel, &
                    i_sub + n_pdf_off + n_sub_color)
                term%amp(i_spin_c) = cmplx &
                    (sqme_spin_c(i_sub), 0, default)
            end do
        end select
        deallocate (sqme_spin_c)
    end if
end if
eqv_me_evaluated(i_flv_eqv, i_hel_eqv) = .true.

```

```

else
  associate (i_int => term%int_hard%get_qn_index &
    (i_flv = i_flv, i_hel = i_hel, i_sub = 0), &
    i_int_eqv => term%int_hard%get_qn_index &
    (i_flv = i_flv_eqv, i_hel = i_hel_eqv, i_sub = 0))
    term%amp(i_int) = term%amp(i_int_eqv)
  end associate
  n_pdf_off = 0
  if (term%pcm%has_pdfs .and. &
    (term%is_subtraction () .or. term%nlo_type == NLO_DGLAP)) then
    n_pdf_off = n_pdf_off + n_beams_rescaled
    do i_sub = 1, n_pdf_off
      term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub)) = &
        term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub = 0))
    end do
  end if
  if (term%pcm%has_pdfs .and. term%nlo_type == NLO_DGLAP) then
    do i_sub = 1, n_sub_color
      i_color_c = term%int_hard%get_qn_index &
        (i_flv, i_hel, i_sub + n_pdf_off)
      i_color_c_eqv = term%int_hard%get_qn_index &
        (i_flv_eqv, i_hel_eqv, i_sub + n_pdf_off)
      term%amp(i_color_c) = term%amp(i_color_c_eqv)
    end do
  end if
  if ((term%nlo_type == NLO_REAL .and. term%is_subtraction ()) .or. &
    term%nlo_type == NLO_MISMATCH) then
    do i_sub = 1, n_sub_color
      i_color_c = term%int_hard%get_qn_index &
        (i_flv, i_hel, i_sub + n_pdf_off)
      i_color_c_eqv = term%int_hard%get_qn_index &
        (i_flv_eqv, i_hel_eqv, i_sub + n_pdf_off)
      term%amp(i_color_c) = term%amp(i_color_c_eqv)
    end do
    do i_sub = 1, n_sub_spin
      i_spin_c = term%int_hard%get_qn_index (i_flv, i_hel, &
        i_sub + n_pdf_off + n_sub_color)
      i_spin_c_eqv = term%int_hard%get_qn_index (i_flv_eqv, i_hel_eqv, &
        i_sub + n_pdf_off + n_sub_color)
      term%amp(i_spin_c) = term%amp(i_spin_c_eqv)
    end do
  end if
end if
end do
end do
end subroutine term_instance_evaluate_interaction_external_tree

```

Same as for `term_instance_evaluate_interaction_external_tree`, but for the integrated-subtraction and finite one-loop terms. We only need color-correlated Born matrix elements, but an additional entry per flavor structure for the finite one-loop contribution. We thus have $2 + n_{sub_color}$ entries in the `term%amp` for each `i_flv` and `i_hel` combination.

If two or more flavor structures would produce the same amplitude we only

compute one and use the `eqv_index` determined by the `prc_core` and just copy the result to improve performance.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_interaction_external_loop &
=> term_instance_evaluate_interaction_external_loop
```

(Instances: sub interfaces)+≡

```
module subroutine term_instance_evaluate_interaction_external_loop &
  (term, core)
  class(term_instance_t), intent(inout) :: term
  class(prc_core_t), intent(in) :: core
end subroutine term_instance_evaluate_interaction_external_loop
```

(Instances: procedures)+≡

```
module subroutine term_instance_evaluate_interaction_external_loop &
  (term, core)
  class(term_instance_t), intent(inout) :: term
  class(prc_core_t), intent(in) :: core
  integer :: n_hel, n_sub, n_flv
  integer :: i, i_flv, i_hel, i_sub, i_virt, i_color_c, i_color_c_eqv
  integer :: i_flv_eqv, i_hel_eqv
  real(default), dimension(4) :: sqme_virt
  real(default), dimension(:), allocatable :: sqme_color_c
  real(default) :: es_scale
  logical :: bad_point
  logical, dimension(:,:), allocatable :: eqv_me_evaluated
  if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
    "term_instance_evaluate_interaction_external_loop")
  allocate (sqme_color_c (blha_result_array_size &
    (term%int_hard%get_n_tot (), BLHA_AMP_COLOR_C)))
  n_flv = term%int_hard%get_qn_index_n_flv ()
  n_hel = term%int_hard%get_qn_index_n_hel ()
  n_sub = term%int_hard%get_qn_index_n_sub ()
  allocate (eqv_me_evaluated(n_flv,n_hel))
  eqv_me_evaluated = .false.
  i_virt = 1
  do i_flv = 1, n_flv
    if (.not. term%passed_array(i_flv) .and. term%passed) cycle
    do i_hel = 1, n_hel
      i_flv_eqv = core%data%eqv_flv_index(i_flv)
      i_hel_eqv = core%data%eqv_hel_index(i_hel)
      if (.not. eqv_me_evaluated(i_flv_eqv, i_hel_eqv)) then
        select type (core)
        class is (prc_external_t)
          if (allocated (term%es_scale)) then
            es_scale = term%es_scale
          else
            es_scale = term%get_ren_scale ()
          end if
          call core%compute_sqme_virt (i_flv, i_hel, term%p_hard, &
            term%get_ren_scale (), es_scale, &
            term%pcm%blha_defaults%loop_method, &
            sqme_virt, bad_point)
          call term%pcm_work%set_bad_point (bad_point)
        end select
      end if
    end do
  end do
```

```

associate (i_born => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = 0), &
  i_loop => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = i_virt))
  term%amp(i_loop) = cmplx (sqme_virt(3), 0, default)
  term%amp(i_born) = cmplx (sqme_virt(4), 0, default)
end associate
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  select type (core)
  class is (prc_blha_t)
    call core%compute_sqme_color_c_raw (i_flv, i_hel, &
      term%p_hard, term%get_ren_scale (), &
      sqme_color_c, bad_point)
    call term%pcm_work%set_bad_point (bad_point)
    do i_sub = 1 + i_virt, n_sub
      i_color_c = term%int_hard%get_qn_index &
        (i_flv, i_hel = i_hel, i_sub = i_sub)
      ! Index shift: i_sub - i_virt
      term%amp(i_color_c) = &
        cmplx (sqme_color_c(i_sub - i_virt), 0, default)
    end do
  type is (prc_recola_t)
    call core%compute_sqme_color_c_raw (i_flv, i_hel, &
      term%p_hard, term%get_ren_scale (), sqme_color_c, bad_point)
    call term%pcm_work%set_bad_point (bad_point)
    do i_sub = 1 + i_virt, n_sub
      i_color_c = term%int_hard%get_qn_index &
        (i_flv, i_hel = i_hel, i_sub = i_sub)
      ! Index shift: i_sub - i_virt
      term%amp(i_color_c) = &
        cmplx (sqme_color_c(i_sub - i_virt), 0, default)
    end do
  end select
end select
eqv_me_evaluated(i_flv_eqv, i_hel_eqv) = .true.
else
  associate (i_born => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = 0), &
    i_loop => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = i_virt), &
    i_born_eqv => term%int_hard%get_qn_index &
      (i_flv_eqv, i_hel = i_hel_eqv, i_sub = 0), &
    i_loop_eqv => term%int_hard%get_qn_index &
      (i_flv_eqv, i_hel = i_hel_eqv, i_sub = 1))
    term%amp(i_loop) = term%amp(i_loop_eqv)
    term%amp(i_born) = term%amp(i_born_eqv)
  end associate
  do i_sub = 1 + i_virt, n_sub
    i_color_c = term%int_hard%get_qn_index &
      (i_flv, i_hel = i_hel, i_sub = i_sub)
    i_color_c_eqv = term%int_hard%get_qn_index &
      (i_flv_eqv, i_hel = i_hel_eqv, i_sub = i_sub)
    ! Index shift: i_sub - i_virt
    term%amp(i_color_c) = term%amp(i_color_c_eqv)
  end do
end if
end do

```



```

end do
end subroutine term_instance_evaluate_interaction_external_loop

```

Evaluate the trace. First evaluate the structure-function chain (i.e., the density matrix of the incoming partons). Do this twice, in case the sf-chain instances within `kin` and `isolated` differ. Next, evaluate the hard interaction, then compute the convolution with the initial state.

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_trace => term_instance_evaluate_trace

<Instances: sub interfaces>+≡
  module subroutine term_instance_evaluate_trace (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
  end subroutine term_instance_evaluate_trace

<Instances: procedures>+≡
  module subroutine term_instance_evaluate_trace (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    real(default) :: fac_scale
    if (allocated (term%fac_scale)) then
      fac_scale = term%fac_scale
    else
      fac_scale = term%scale
    end if
    call kin%evaluate_sf_chain (fac_scale, term%negative_sf)
    call term%evaluate_scaled_sf_chains (kin)
    call term%isolated%evaluate_sf_chain (fac_scale)
    call term%isolated%evaluate_trace ()
    call term%connected%evaluate_trace ()
  end subroutine term_instance_evaluate_trace

```

Include rescaled structure functions due to NLO calculation. We rescale the structure function for the real subtraction `sf_rescale_collinear`, the collinear counter terms `sf_rescale_dglap_t` and for the case, in which we have an emitter in the initial state, we rescale the kinematics for it using `sf_rescale_real_t`. The references are arXiv:0709.2092, Eqs. (2.35)-(2.42).

Obviously, it is completely irrelevant, which beam is treated. It becomes problematic when handling *ep* collisions. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_scaled_sf_chains => &
    term_instance_evaluate_scaled_sf_chains

<Instances: main procedures>≡
  subroutine term_instance_evaluate_scaled_sf_chains (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    class(sf_rescale_t), allocatable :: sf_rescale
    if (.not. term%pcm%has_pdfs) return
    if (term%nlo_type == NLO_REAL) then
      if (term%is_subtraction ()) then

```

```

allocate (sf_rescale_collinear_t :: sf_rescale)
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  select type (sf_rescale)
  type is (sf_rescale_collinear_t)
    call sf_rescale%set (pcm_work%real_kinematics%xi_tilde)
  end select
end select
call kin%sf_chain%evaluate (term%get_fac_scale (), &
  term%negative_sf, sf_rescale)
deallocate (sf_rescale)
else if (kin%emitter >= 0 .and. kin%emitter <= kin%n_in) then
allocate (sf_rescale_real_t :: sf_rescale)
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  select type (sf_rescale)
  type is (sf_rescale_real_t)
    call sf_rescale%set (pcm_work%real_kinematics%xi_tilde * &
      pcm_work%real_kinematics%xi_max (kin%i_phs), &
      pcm_work%real_kinematics%y (kin%i_phs))
  end select
end select
call kin%sf_chain%evaluate (term%get_fac_scale (), &
  term%negative_sf, sf_rescale)
deallocate (sf_rescale)
else
  call kin%sf_chain%evaluate (term%get_fac_scale (), term%negative_sf)
end if
else if (term%nlo_type == NLO_DGLAP) then
allocate (sf_rescale_dglap_t :: sf_rescale)
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  select type (sf_rescale)
  type is (sf_rescale_dglap_t)
    call sf_rescale%set (pcm_work%isr_kinematics%z)
  end select
end select
call kin%sf_chain%evaluate (term%get_fac_scale (), &
  term%negative_sf, sf_rescale)
deallocate (sf_rescale)
end if
end subroutine term_instance_evaluate_scaled_sf_chains

```

Evaluate the extra data that we need for processing the object as a physical event.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_event_data => term_instance_evaluate_event_data
```

(Instances: sub interfaces)+≡

```

module subroutine term_instance_evaluate_event_data (term)
  class(term_instance_t), intent(inout) :: term
end subroutine term_instance_evaluate_event_data

```

(Instances: procedures)+≡

```
module subroutine term_instance_evaluate_event_data (term)
```

```

class(term_instance_t), intent(inout) :: term
logical :: only_momenta
only_momenta = term%nlo_type > BORN
call term%isolated%evaluate_event_data (only_momenta)
call term%connected%evaluate_event_data (only_momenta)
end subroutine term_instance_evaluate_event_data

```

<Instances: term instance: TBP>+≡

```

procedure :: set_fac_scale => term_instance_set_fac_scale

```

<Instances: sub interfaces>+≡

```

module subroutine term_instance_set_fac_scale (term, fac_scale)
class(term_instance_t), intent(inout) :: term
real(default), intent(in) :: fac_scale
end subroutine term_instance_set_fac_scale

```

<Instances: procedures>+≡

```

module subroutine term_instance_set_fac_scale (term, fac_scale)
class(term_instance_t), intent(inout) :: term
real(default), intent(in) :: fac_scale
term%fac_scale = fac_scale
end subroutine term_instance_set_fac_scale

```

Return data that might be useful for external processing. The factorization scale and renormalization scale are identical to the general scale if not explicitly set:

<Instances: term instance: TBP>+≡

```

procedure :: get_fac_scale => term_instance_get_fac_scale
procedure :: get_ren_scale => term_instance_get_ren_scale

```

<Instances: sub interfaces>+≡

```

module function term_instance_get_fac_scale (term) result (fac_scale)
class(term_instance_t), intent(in) :: term
real(default) :: fac_scale
end function term_instance_get_fac_scale
module function term_instance_get_ren_scale (term) result (ren_scale)
class(term_instance_t), intent(in) :: term
real(default) :: ren_scale
end function term_instance_get_ren_scale

```

<Instances: procedures>+≡

```

module function term_instance_get_fac_scale (term) result (fac_scale)
class(term_instance_t), intent(in) :: term
real(default) :: fac_scale
if (allocated (term%fac_scale)) then
fac_scale = term%fac_scale
else
fac_scale = term%scale
end if
end function term_instance_get_fac_scale

```

```

module function term_instance_get_ren_scale (term) result (ren_scale)
class(term_instance_t), intent(in) :: term
real(default) :: ren_scale
if (allocated (term%ren_scale)) then

```

```

        ren_scale = term%ren_scale
    else
        ren_scale = term%scale
    end if
end function term_instance_get_ren_scale

```

We take the strong coupling from the process core. The value is calculated when a new event is requested, so we should call it only after the event has been evaluated. If it is not available there (a negative number is returned), we take the value stored in the term configuration, which should be determined by the model. If the model does not provide a value, the result is zero.

```

<Instances: term instance: TBP>+≡
    procedure :: get_alpha_s => term_instance_get_alpha_s

<Instances: sub interfaces>+≡
    module function term_instance_get_alpha_s (term, core) result (alpha_s)
        class(term_instance_t), intent(in) :: term
        class(prc_core_t), intent(in) :: core
        real(default) :: alpha_s
    end function term_instance_get_alpha_s

<Instances: procedures>+≡
    module function term_instance_get_alpha_s (term, core) result (alpha_s)
        class(term_instance_t), intent(in) :: term
        class(prc_core_t), intent(in) :: core
        real(default) :: alpha_s
        alpha_s = core%get_alpha_s (term%core_state)
        if (alpha_s < zero) alpha_s = term%config%alpha_s
    end function term_instance_get_alpha_s

```

The second helicity for `helicities` comes with a minus sign because OpenLoops inverts the helicity index of antiparticles.

```

<Instances: term instance: TBP>+≡
    procedure :: get_helicities_for_openloops => &
        term_instance_get_helicities_for_openloops

<Instances: sub interfaces>+≡
    module subroutine term_instance_get_helicities_for_openloops &
        (term, helicities)
        class(term_instance_t), intent(in) :: term
        integer, dimension(:,:), allocatable, intent(out) :: helicities
    end subroutine term_instance_get_helicities_for_openloops

<Instances: procedures>+≡
    module subroutine term_instance_get_helicities_for_openloops &
        (term, helicities)
        class(term_instance_t), intent(in) :: term
        integer, dimension(:,:), allocatable, intent(out) :: helicities
        type(helicity_t), dimension(:), allocatable :: hel
        type(quantum_numbers_t), dimension(:,:), allocatable :: qn
        type(quantum_numbers_mask_t) :: qn_mask
        integer :: h, i, j, n_in
        call qn_mask%set_sub (1)
        call term%isolated%trace%get_quantum_numbers_mask (qn_mask, qn)
    end subroutine term_instance_get_helicities_for_openloops

```

```

n_in = term%int_hard%get_n_in ()
allocate (helicities (size (qn, dim=1), n_in))
allocate (hel (n_in))
do i = 1, size (qn, dim=1)
  do j = 1, n_in
    hel(j) = qn(i, j)%get_helicity ()
    call hel(j)%diagonalize ()
    call hel(j)%get_indices (h, h)
    helicities (i, j) = h
  end do
end do
end subroutine term_instance_get_helicities_for_openloops

```

<Instances: term instance: TBP>+≡
 procedure :: get_i_term_global => term_instance_get_i_term_global

<Instances: sub interfaces>+≡
 elemental module function term_instance_get_i_term_global &
 (term) result (i_term)
 integer :: i_term
 class(term_instance_t), intent(in) :: term
end function term_instance_get_i_term_global

<Instances: procedures>+≡
 elemental module function term_instance_get_i_term_global &
 (term) result (i_term)
 integer :: i_term
 class(term_instance_t), intent(in) :: term
 i_term = term%config%i_term_global
end function term_instance_get_i_term_global

<Instances: term instance: TBP>+≡
 procedure :: is_subtraction => term_instance_is_subtraction

<Instances: sub interfaces>+≡
 elemental module function term_instance_is_subtraction (term) result (sub)
 logical :: sub
 class(term_instance_t), intent(in) :: term
end function term_instance_is_subtraction

<Instances: procedures>+≡
 elemental module function term_instance_is_subtraction (term) result (sub)
 logical :: sub
 class(term_instance_t), intent(in) :: term
 sub = term%config%i_term_global == term%config%i_sub
end function term_instance_is_subtraction

Retrieve n_sub which was calculated in process_term_setup_interaction.

<Instances: term instance: TBP>+≡
 procedure :: get_n_sub => term_instance_get_n_sub
 procedure :: get_n_sub_color => term_instance_get_n_sub_color
 procedure :: get_n_sub_spin => term_instance_get_n_sub_spin

```

<Instances: sub interfaces>+≡
    module function term_instance_get_n_sub (term) result (n_sub)
        integer :: n_sub
        class(term_instance_t), intent(in) :: term
    end function term_instance_get_n_sub
    module function term_instance_get_n_sub_color (term) result (n_sub_color)
        integer :: n_sub_color
        class(term_instance_t), intent(in) :: term
    end function term_instance_get_n_sub_color
    module function term_instance_get_n_sub_spin (term) result (n_sub_spin)
        integer :: n_sub_spin
        class(term_instance_t), intent(in) :: term
    end function term_instance_get_n_sub_spin

<Instances: procedures>+≡
    module function term_instance_get_n_sub (term) result (n_sub)
        integer :: n_sub
        class(term_instance_t), intent(in) :: term
        n_sub = term%config%n_sub
    end function term_instance_get_n_sub

    module function term_instance_get_n_sub_color (term) result (n_sub_color)
        integer :: n_sub_color
        class(term_instance_t), intent(in) :: term
        n_sub_color = term%config%n_sub_color
    end function term_instance_get_n_sub_color

    module function term_instance_get_n_sub_spin (term) result (n_sub_spin)
        integer :: n_sub_spin
        class(term_instance_t), intent(in) :: term
        n_sub_spin = term%config%n_sub_spin
    end function term_instance_get_n_sub_spin

```

30.10.2 The process instance

NOTE: The description below represents the intended structure after refactoring and disentangling the FKS-NLO vs. LO algorithm dependencies.

A process instance contains all process data that depend on the sampling point and thus change often. In essence, it is an event record at the elementary (parton) level. We do not call it such, to avoid confusion with the actual event records. If decays are involved, the latter are compositions of several elementary processes (i.e., their instances).

We implement the process instance as an extension of the `mci_sampler_t` that we need for computing integrals and generate events.

The base type contains: the `integrand`, the `selected_channel`, the two-dimensional array `x` of parameters, and the one-dimensional array `f` of Jacobians. These subobjects are public and used for communicating with the multi-channel integrator.

The `process` pointer accesses the process of which this record is an instance. It is required whenever the calculation needs invariant configuration data, therefore the process should stay in memory for the whole lifetime of its instances.

The **pcm** pointer is a shortcut to the **pcm** (process-component manager) component of the associated process, which we need wherever the calculation depends on the overall algorithm.

The **pcm_work** component is the workspace for the **pcm** object referenced above.

The **evaluation_status** code is used to check the current status. In particular, failure at various stages is recorded there.

The **count** object records process evaluations, broken down according to status.

The **sqme** value is the single real number that results from evaluating and tracing the kinematics and matrix elements. This is the number that is handed over to an integration routine.

The **weight** value is the event weight. It is defined when an event has been generated from the process instance, either weighted or unweighted. The value is the **sqme** value times Jacobian weights from the integration, or unity, respectively.

The **i_mci** index chooses a subset of components that are associated with a common parameter set and integrator, i.e., that are added coherently.

The **sf_chain** subobject is a realization of the beam and structure-function configuration in the **process** object. It is not used for calculation directly but serves as the template for the sf-chain instances that are contained in the **component** objects.

The **kinematics** array contains the set of phase-space points that are associated with the current calculation. The entries may correspond to different process components and terms. (TODO wk 19-02-22: Not implemented yet.)

TODO wk 19-02-22: May include extra arrays for storing (squared) amplitude data. The **term** data set may be reduced to just results, or be removed altogether.

The **term** subobjects are workspace for evaluating kinematics, matrix elements, cuts etc. The array entries correspond to the **term** configuration entries in the associated process object.

The **mci_work** subobject contains the array of real input parameters (random numbers) that generates the kinematical point. It also contains the workspace for the MC integrators. The active entry of the **mci_work** array is selected by the **i_mci** index above.

The **hook** pointer accesses a list of after evaluate objects which are evaluated after the matrix element.

```

<Instances: public>+≡
    public :: process_instance_t

<Instances: types>+≡
    type, extends (mci_sampler_t) :: process_instance_t
        type(process_t), pointer :: process => null ()
        class(pcm_t), pointer :: pcm => null ()
        class(pcm_workspace_t), allocatable :: pcm_work
        integer :: evaluation_status = STAT_UNDEFINED
        real(default) :: sqme = 0
        real(default) :: weight = 0
        real(default) :: excess = 0
        integer :: n_dropped = 0
        integer :: i_mci = 0

```

```

integer :: selected_channel = 0
type(sf_chain_t) :: sf_chain
type(kinematics_t), dimension(:), allocatable :: kin
type(term_instance_t), dimension(:), allocatable :: term
type(mci_work_t), dimension(:), allocatable :: mci_work
class(process_instance_hook_t), pointer :: hook => null ()
contains
  <Instances: process instance: TBP>
end type process_instance_t

```

Wrapper type for storing pointers to process instance objects in arrays.

```

<Instances: public>+≡
  public :: process_instance_ptr_t
<Instances: types>+≡
  type :: process_instance_ptr_t
  type(process_instance_t), pointer :: p => null ()
end type process_instance_ptr_t

```

The process hooks are first-in-last-out list of objects which are evaluated after the phase space and matrixelement are evaluated. It is possible to retrieve the sampler object and read the sampler information.

The hook object are part of the `process_instance` and therefore, share a common lifetime. A data transfer, after the usual lifetime of the `process_instance`, is not provided, as such the finalisation procedure has to take care of this! E.g. write the object to file from which later the collected information can then be retrieved.

```

<Instances: public>+≡
  public :: process_instance_hook_t
<Instances: types>+≡
  type, abstract :: process_instance_hook_t
  class(process_instance_hook_t), pointer :: next => null ()
  contains
    procedure(process_instance_hook_init), deferred :: init
    procedure(process_instance_hook_final), deferred :: final
    procedure(process_instance_hook_evaluate), deferred :: evaluate
  end type process_instance_hook_t

```

We have to provide an `init`, a `final` procedure and, for after evaluation, the `evaluate` procedure.

The `init` procedures accesses `var_list` and current instance object.

```

<Instances: public>+≡
  public :: process_instance_hook_final, process_instance_hook_evaluate
<Instances: interfaces>≡
  abstract interface
    subroutine process_instance_hook_init (hook, var_list, instance, pdf_data)
      import :: process_instance_hook_t, var_list_t, process_instance_t, pdf_data_t
      class(process_instance_hook_t), intent(inout), target :: hook
      type(var_list_t), intent(in) :: var_list
      class(process_instance_t), intent(in), target :: instance
      type(pdf_data_t), intent(in), optional :: pdf_data
    end subroutine
  end interface

```



```

end subroutine process_instance_hook_init

subroutine process_instance_hook_final (hook)
  import :: process_instance_hook_t
  class(process_instance_hook_t), intent(inout) :: hook
end subroutine process_instance_hook_final

subroutine process_instance_hook_evaluate (hook, instance)
  import :: process_instance_hook_t, process_instance_t
  class(process_instance_hook_t), intent(inout) :: hook
  class(process_instance_t), intent(in), target :: instance
end subroutine process_instance_hook_evaluate
end interface

```

The output routine contains a header with the most relevant information about the process, copied from `process_metadata_write`. We mark the active components by an asterisk.

The next section is the MC parameter input. The following sections are written only if the evaluation status is beyond setting the parameters, or if the `verbose` option is set.

```

<Instances: process instance: TBP>≡
  procedure :: write_header => process_instance_write_header
  procedure :: write => process_instance_write

<Instances: sub interfaces>+≡
  module subroutine process_instance_write_header (object, unit, testflag)
    class(process_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine process_instance_write_header
  module subroutine process_instance_write (object, unit, testflag)
    class(process_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine process_instance_write

<Instances: procedures>+≡
  module subroutine process_instance_write_header (object, unit, testflag)
    class(process_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    if (associated (object%process)) then
      call object%process%write_meta (u, testflag)
    else
      write (u, "(1x,A)") "Process instance [undefined process]"
      return
    end if
    write (u, "(3x,A)", advance = "no") "status = "
    select case (object%evaluation_status)
    case (STAT_INITIAL);           write (u, "(A)") "initialized"
    case (STAT_ACTIVATED);        write (u, "(A)") "activated"

```

```

case (STAT_BEAM_MOMENTA);      write (u, "(A)") "beam momenta set"
case (STAT_FAILED_KINEMATICS); write (u, "(A)") "failed kinematics"
case (STAT_SEED_KINEMATICS);  write (u, "(A)") "seed kinematics"
case (STAT_HARD_KINEMATICS);  write (u, "(A)") "hard kinematics"
case (STAT_EFF_KINEMATICS);   write (u, "(A)") "effective kinematics"
case (STAT_FAILED_CUTS);      write (u, "(A)") "failed cuts"
case (STAT_PASSED_CUTS);      write (u, "(A)") "passed cuts"
case (STAT_EVALUATED_TRACE);  write (u, "(A)") "evaluated trace"
    call write_separator (u)
    write (u, "(3x,A,ES19.12)") "sqme = ", object%sqme
case (STAT_EVENT_COMPLETE);   write (u, "(A)") "event complete"
    call write_separator (u)
    write (u, "(3x,A,ES19.12)") "sqme = ", object%sqme
    write (u, "(3x,A,ES19.12)") "weight = ", object%weight
    if (.not. vanishes (object%excess)) &
        write (u, "(3x,A,ES19.12)") "excess = ", object%excess
case default;                  write (u, "(A)") "undefined"
end select
if (object%i_mci /= 0) then
    call write_separator (u)
    call object%mc_i_work(object%i_mci)%write (u, testflag)
end if
call write_separator (u, 2)
end subroutine process_instance_write_header

module subroutine process_instance_write (object, unit, testflag)
    class(process_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u, i
    u = given_output_unit (unit)
    call object%write_header (u)
    if (object%evaluation_status >= STAT_BEAM_MOMENTA) then
        call object%sf_chain%write (u)
        call write_separator (u, 2)
        if (object%evaluation_status >= STAT_SEED_KINEMATICS) then
            if (object%evaluation_status >= STAT_HARD_KINEMATICS) then
                call write_separator (u, 2)
                write (u, "(1x,A)") "Active terms:"
                if (any (object%term%active)) then
                    do i = 1, size (object%term)
                        if (object%term(i)%active) then
                            call write_separator (u)
                            call object%term(i)%write (u, &
                                kin = object%kin(i), &
                                show_eff_state = &
                                object%evaluation_status >= STAT_EFF_KINEMATICS, &
                                testflag = testflag)
                        end if
                    end do
                end if
            end if
        end if
        call write_separator (u, 2)
    end if
end module process_instance_write

```

```

        end if
    end subroutine process_instance_write

```

Initialization connects the instance with a process. All initial information is transferred from the process object. The process object contains templates for the interaction subobjects (beam and term), but no evaluators. The initialization routine creates evaluators for the matrix element trace, other evaluators are left untouched.

Before we start generating, we double-check if the process library has been updated after the process was initialized (`check_library_sanity`). This may happen if between integration and event generation the library has been recompiled, so all links become broken.

The `instance` object must have the `target` attribute (also in any caller) since the initialization routine assigns various pointers to subobject of `instance`.

```

<Instances: process instance: TBP>+≡
    procedure :: init => process_instance_init

<Instances: sub interfaces>+≡
    module subroutine process_instance_init (instance, process)
        class(process_instance_t), intent(out), target :: instance
        type(process_t), intent(inout), target :: process
    end subroutine process_instance_init

<Instances: procedures>+≡
    module subroutine process_instance_init (instance, process)
        class(process_instance_t), intent(out), target :: instance
        type(process_t), intent(inout), target :: process
        integer :: i
        class(pcm_t), pointer :: pcm
        type(process_term_t), pointer :: term
        type(var_list_t), pointer :: var_list
        integer :: i_born, i_real, i_real_fin, i_component
        if (debug_on) call msg_debug &
            (D_PROCESS_INTEGRATION, "process_instance_init")
        instance%process => process
        instance%pcm => process%get_pcm_ptr ()
        call instance%process%check_library_sanity ()
        call instance%setup_sf_chain (process%get_beam_config_ptr ())
        allocate (instance%mci_work (process%get_n_mci ()))
        do i = 1, size (instance%mci_work)
            call instance%process%init_mci_work (instance%mci_work(i), i)
        end do
        call instance%process%reset_selected_cores ()
        pcm => instance%process%get_pcm_ptr ()
        call pcm%allocate_workspace (instance%pcm_work)
        select type (pcm)
        type is (pcm_nlo_t)
            !!! The process is kept when the integration is finalized, but not the
            !!! process_instance. Thus, we check whether pcm has been initialized
            !!! but set up the pcm_work each time.
            i_real_fin = process%get_associated_real_fin (1)
            if (.not. pcm%initialized) then
                i_born = pcm%get_i_core (pcm%i_born)
                i_real = pcm%get_i_core (pcm%i_real)

```

```

        call pcm%init_qn (process%get_model_ptr ())
        if (i_real_fin > 0) call pcm%allocate_ps_matching ()
        var_list => process%get_var_list_ptr ()
        if (var_list%get_sval (var_str ("$dalitz_plot")) /= var_str ('')) &
            call pcm%activate_dalitz_plot (var_list%get_sval (var_str ("$dalitz_plot")))
    end if
    pcm%initialized = .true.
    select type (pcm_work => instance%pcm_work)
    type is (pcm_nlo_workspace_t)
        call pcm_work%init_config (pcm, &
            process%component_can_be_integrated (), &
            process%get_nlo_type_component (), process%get_energy (), &
            i_real_fin, process%get_model_ptr ())
    end select
end select
! TODO wk-03-01 n_terms will eventually acquire a different meaning
allocate (instance%kin (process%get_n_terms ()))
do i = 1, process%get_n_terms ()
    term => process%get_term_ptr (i)
    i_component = term%i_component
    call instance%kin(i)%configure (pcm, instance%pcm_work, &
        instance%sf_chain, &
        process%get_beam_config_ptr (), &
        process%get_phs_config (i_component), &
        process%get_nlo_type_component (i_component), &
        term%i_sub == i)
end do
! TODO wk-03-01 n_terms will eventually acquire a different meaning
allocate (instance%term (process%get_n_terms ()))
do i = 1, process%get_n_terms ()
    call instance%term(i)%configure (process, i, instance%pcm_work, &
        instance%sf_chain, instance%kin(i))
end do
call instance%set_i_mci_to_real_component ()
call instance%find_same_kinematics ()
instance%evaluation_status = STAT_INITIAL
end subroutine process_instance_init

```

Finalize all subobjects that may contain allocated pointers.

(Instances: process instance: TBP)+≡

```

    procedure :: final => process_instance_final

```

(Instances: sub interfaces)+≡

```

    module subroutine process_instance_final (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_final

```

(Instances: procedures)+≡

```

    module subroutine process_instance_final (instance)
        class(process_instance_t), intent(inout) :: instance
        class(process_instance_hook_t), pointer :: current
        integer :: i
        instance%process => null ()
        if (allocated (instance%mci_work)) then
            do i = 1, size (instance%mci_work)

```

```

        call instance%mci_work(i)%final ()
    end do
    deallocate (instance%mci_work)
end if
call instance%sf_chain%final ()
if (allocated (instance%kin)) then
    do i = 1, size (instance%kin)
        call instance%kin(i)%final ()
    end do
    deallocate (instance%kin)
end if
if (allocated (instance%term)) then
    do i = 1, size (instance%term)
        call instance%term(i)%final ()
    end do
    deallocate (instance%term)
end if
call instance%pcm_work%final ()
instance%evaluation_status = STAT_UNDEFINED
do while (associated (instance%hook))
    current => instance%hook
    call current%final ()
    instance%hook => current%next
    deallocate (current)
end do
instance%hook => null ()
end subroutine process_instance_final

```

Revert the process instance to initial state. We do not deallocate anything, just reset the state index and deactivate all components and terms.

We do not reset the choice of the MCI set *i_mci* unless this is required explicitly.

```

<Instances: process instance: TBP>+≡
    procedure :: reset => process_instance_reset

<Instances: sub interfaces>+≡
    module subroutine process_instance_reset (instance, reset_mci)
        class(process_instance_t), intent(inout), target :: instance
        logical, intent(in), optional :: reset_mci
    end subroutine process_instance_reset

<Instances: procedures>+≡
    module subroutine process_instance_reset (instance, reset_mci)
        class(process_instance_t), intent(inout), target :: instance
        logical, intent(in), optional :: reset_mci
        integer :: i
        call instance%process%reset_selected_cores ()
        do i = 1, size (instance%term)
            call instance%term(i)%reset ()
        end do
        instance%term%checked = .false.
        instance%term%passed = .false.
        instance%kin%new_seed = .true.
        if (present (reset_mci)) then

```

```

        if (reset_mci) instance%i_mci = 0
    end if
    instance%selected_channel = 0
    instance%evaluation_status = STAT_INITIAL
end subroutine process_instance_reset

```

Integration and event generation

The sampler test should just evaluate the squared matrix element `n_calls` times, discarding the results, and return. This can be done before integration, e.g., for timing estimates.

```

<Instances: process instance: TBP>+≡
    procedure :: sampler_test => process_instance_sampler_test

<Instances: sub interfaces>+≡
    module subroutine process_instance_sampler_test (instance, i_mci, n_calls)
        class(process_instance_t), intent(inout), target :: instance
        integer, intent(in) :: i_mci
        integer, intent(in) :: n_calls
    end subroutine process_instance_sampler_test

<Instances: procedures>+≡
    module subroutine process_instance_sampler_test (instance, i_mci, n_calls)
        class(process_instance_t), intent(inout), target :: instance
        integer, intent(in) :: i_mci
        integer, intent(in) :: n_calls
        integer :: i_mci_work
        i_mci_work = instance%process%get_i_mci_work (i_mci)
        call instance%choose_mci (i_mci_work)
        call instance%reset_counter ()
        call instance%process%sampler_test (instance, n_calls, i_mci_work)
        call instance%process%set_counter_mci_entry (i_mci_work, instance%get_counter ())
    end subroutine process_instance_sampler_test

```

Generate a weighted event. We select one of the available MCI integrators by its index `i_mci` and thus generate an event for the associated (group of) process component(s). The arguments exactly correspond to the initializer and finalizer above.

The resulting event is stored in the `process_instance` object, which also holds the workspace of the integrator.

Note: The `process` object contains the random-number state, which changes for each event. Otherwise, all volatile data are inside the `instance` object.

```

<Instances: process instance: TBP>+≡
    procedure :: generate_weighted_event => &
        process_instance_generate_weighted_event

<Instances: sub interfaces>+≡
    module subroutine process_instance_generate_weighted_event (instance, i_mci)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_mci
    end subroutine process_instance_generate_weighted_event

```

```

<Instances: procedures>+≡
module subroutine process_instance_generate_weighted_event (instance, i_mci)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer :: i_mci_work
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  associate (mci_work => instance%mci_work(i_mci_work))
    call instance%process%generate_weighted_event &
      (i_mci_work, mci_work, instance, &
        instance%keep_failed_events ())
  end associate
end subroutine process_instance_generate_weighted_event

```

```

<Instances: process instance: TBP>+≡
procedure :: generate_unweighted_event => &
  process_instance_generate_unweighted_event

```

```

<Instances: sub interfaces>+≡
module subroutine process_instance_generate_unweighted_event &
  (instance, i_mci)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
end subroutine process_instance_generate_unweighted_event

```

```

<Instances: procedures>+≡
module subroutine process_instance_generate_unweighted_event (instance, i_mci)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer :: i_mci_work
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  associate (mci_work => instance%mci_work(i_mci_work))
    call instance%process%generate_unweighted_event &
      (i_mci_work, mci_work, instance)
  end associate
end subroutine process_instance_generate_unweighted_event

```

This replaces the event generation methods for the situation that the process instance object has been filled by other means (i.e., reading and/or recalculating its contents). We just have to fill in missing MCI data, especially the event weight.

```

<Instances: process instance: TBP>+≡
procedure :: recover_event => process_instance_recover_event

```

```

<Instances: sub interfaces>+≡
module subroutine process_instance_recover_event (instance)
  class(process_instance_t), intent(inout) :: instance
end subroutine process_instance_recover_event

```

```

<Instances: procedures>+≡
module subroutine process_instance_recover_event (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i_mci
  i_mci = instance%i_mci

```

```

call instance%process%set_i_mci_work (i_mci)
associate (mci_instance => instance%mci_work(i_mci)%mci)
    call mci_instance%fetch (instance, instance%selected_channel)
end associate
end subroutine process_instance_recover_event

```

Activate the components and terms that correspond to a currently selected MCI parameter set.

```

<Instances: process instance: TBP>+≡
    procedure :: activate => process_instance_activate

<Instances: sub interfaces>+≡
    module subroutine process_instance_activate (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_activate

<Instances: procedures>+≡
    module subroutine process_instance_activate (instance)
        class(process_instance_t), intent(inout) :: instance
        integer :: i, j
        integer, dimension(:), allocatable :: i_term
        associate (mci_work => instance%mci_work(instance%i_mci))
            call instance%process%select_components &
                (mci_work%get_active_components ())
        end associate
        associate (process => instance%process)
            do i = 1, instance%process%get_n_components ()
                if (instance%process%component_is_selected (i)) then
                    allocate (i_term (size (process%get_component_i_terms (i))))
                    i_term = process%get_component_i_terms (i)
                    do j = 1, size (i_term)
                        instance%term(i_term(j))%active = .true.
                    end do
                end if
                if (allocated (i_term)) deallocate (i_term)
            end do
        end associate
        instance%evaluation_status = STAT_ACTIVATED
    end subroutine process_instance_activate

<Instances: process instance: TBP>+≡
    procedure :: find_same_kinematics => process_instance_find_same_kinematics

<Instances: sub interfaces>+≡
    module subroutine process_instance_find_same_kinematics (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_find_same_kinematics

<Instances: procedures>+≡
    module subroutine process_instance_find_same_kinematics (instance)
        class(process_instance_t), intent(inout) :: instance
        integer :: i_term1, i_term2, k, n_same
        do i_term1 = 1, size (instance%term)
            if (.not. allocated (instance%term(i_term1)%same_kinematics)) then
                n_same = 1 !!! Index group includes the index of its term_instance
            end if
        end do
    end subroutine process_instance_find_same_kinematics

```



```

do i_term2 = 1, size (instance%term)
  if (i_term1 == i_term2) cycle
  if (compare_md5s (i_term1, i_term2)) n_same = n_same + 1
end do
allocate (instance%term(i_term1)%same_kinematics (n_same))
associate (same_kinematics1 => instance%term(i_term1)%same_kinematics)
  same_kinematics1 = 0
  k = 1
  do i_term2 = 1, size (instance%term)
    if (compare_md5s (i_term1, i_term2)) then
      same_kinematics1(k) = i_term2
      k = k + 1
    end if
  end do
  do k = 1, size (same_kinematics1)
    if (same_kinematics1(k) == i_term1) cycle
    i_term2 = same_kinematics1(k)
    allocate (instance%term(i_term2)%same_kinematics (n_same))
    instance%term(i_term2)%same_kinematics = same_kinematics1
  end do
end associate
end if
end do
contains
function compare_md5s (i, j) result (same)
  logical :: same
  integer, intent(in) :: i, j
  character(32) :: md5sum_1, md5sum_2
  integer :: mode_1, mode_2
  mode_1 = 0; mode_2 = 0
  select type (phs => instance%kin(i)%phs%config)
  type is (phs_fks_config_t)
    md5sum_1 = phs%md5sum_born_config
    mode_1 = phs%mode
  class default
    md5sum_1 = phs%md5sum_phs_config
  end select
  select type (phs => instance%kin(j)%phs%config)
  type is (phs_fks_config_t)
    md5sum_2 = phs%md5sum_born_config
    mode_2 = phs%mode
  class default
    md5sum_2 = phs%md5sum_phs_config
  end select
  same = (md5sum_1 == md5sum_2) .and. (mode_1 == mode_2)
end function compare_md5s
end subroutine process_instance_find_same_kinematics

```

(Instances: process instance: TBP)+≡

```

procedure :: transfer_same_kinematics => &
  process_instance_transfer_same_kinematics

```

(Instances: sub interfaces)+≡

```

module subroutine process_instance_transfer_same_kinematics &

```

```

        (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
    end subroutine process_instance_transfer_same_kinematics

<Instances: procedures>+≡
module subroutine process_instance_transfer_same_kinematics (instance, i_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term
    integer :: i, i_term_same
    associate (same_kinematics => instance%term(i_term)%same_kinematics)
        do i = 1, size (same_kinematics)
            i_term_same = same_kinematics(i)
            instance%term(i_term_same)%p_seed = instance%term(i_term)%p_seed
            associate (phs => instance%kin(i_term_same)%phs)
                call phs%set_lorentz_transformation &
                    (instance%kin(i_term)%phs%get_lorentz_transformation ())
            select type (phs)
            type is (phs_fks_t)
                call phs%set_momenta (instance%term(i_term_same)%p_seed)
                if (i_term_same /= i_term) then
                    call phs%set_reference_frames (.false.)
                end if
            end select
            end associate
            instance%kin(i_term_same)%new_seed = .false.
        end do
    end associate
end subroutine process_instance_transfer_same_kinematics

<Instances: process instance: TBP>+≡
procedure :: redo_sf_chains => process_instance_redo_sf_chains

<Instances: sub interfaces>+≡
module subroutine process_instance_redo_sf_chains &
    (instance, i_term, phs_channel)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), dimension(:) :: i_term
    integer, intent(in) :: phs_channel
end subroutine process_instance_redo_sf_chains

<Instances: procedures>+≡
module subroutine process_instance_redo_sf_chains &
    (instance, i_term, phs_channel)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), dimension(:) :: i_term
    integer, intent(in) :: phs_channel
    integer :: i
    do i = 1, size (i_term)
        call instance%kin(i_term(i))%redo_sf_chain &
            (instance%mc_i_work(instance%i_mci), phs_channel)
    end do
end subroutine process_instance_redo_sf_chains

```

Integrate the process, using a previously initialized process instance. We select one of the available MCI integrators by its index `i_mci` and thus integrate over (structure functions and) phase space for the associated (group of) process component(s).

(Instances: process instance: TBP)+≡

```
procedure :: integrate => process_instance_integrate
```

(Instances: sub interfaces)+≡

```
module subroutine process_instance_integrate (instance, i_mci, &
      n_it, n_calls, adapt_grids, adapt_weights, final, pacify)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer, intent(in) :: n_it
  integer, intent(in) :: n_calls
  logical, intent(in), optional :: adapt_grids
  logical, intent(in), optional :: adapt_weights
  logical, intent(in), optional :: final, pacify
end subroutine process_instance_integrate
```

(Instances: procedures)+≡

```
module subroutine process_instance_integrate (instance, i_mci, &
      n_it, n_calls, adapt_grids, adapt_weights, final, pacify)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer, intent(in) :: n_it
  integer, intent(in) :: n_calls
  logical, intent(in), optional :: adapt_grids
  logical, intent(in), optional :: adapt_weights
  logical, intent(in), optional :: final, pacify
  integer :: nlo_type, i_mci_work
  nlo_type = instance%process%get_component_nlo_type (i_mci)
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  call instance%reset_counter ()
  associate (mci_work => instance%mci_work(i_mci_work), &
        process => instance%process)
    call process%integrate (i_mci_work, mci_work, &
      instance, n_it, n_calls, adapt_grids, adapt_weights, &
      final, pacify, nlo_type = nlo_type)
    call process%set_counter_mci_entry (i_mci_work, instance%get_counter ())
  end associate
end subroutine process_instance_integrate
```

Subroutine of the initialization above: initialize the beam and structure-function chain template. We establish pointers to the configuration data, so `beam_config` must have a `target` attribute.

The resulting chain is not used directly for calculation. It will acquire instances which are stored in the process-component instance objects.

(Instances: process instance: TBP)+≡

```
procedure :: setup_sf_chain => process_instance_setup_sf_chain
```

(Instances: sub interfaces)+≡

```
module subroutine process_instance_setup_sf_chain (instance, config)
  class(process_instance_t), intent(inout) :: instance
```

```

        type(process_beam_config_t), intent(in), target :: config
    end subroutine process_instance_setup_sf_chain
<Instances: procedures>+≡
    module subroutine process_instance_setup_sf_chain (instance, config)
        class(process_instance_t), intent(inout) :: instance
        type(process_beam_config_t), intent(in), target :: config
        integer :: n_strfun
        n_strfun = config%n_strfun
        if (n_strfun /= 0) then
            call instance%sf_chain%init (config%data, config%sf)
        else
            call instance%sf_chain%init (config%data)
        end if
        if (config%sf_trace) then
            call instance%sf_chain%setup_tracing (config%sf_trace_file)
        end if
    end subroutine process_instance_setup_sf_chain

```

This initialization routine should be called only for process instances which we intend as a source for physical events. It initializes the evaluators in the parton states of the terms. They describe the (semi-)exclusive transition matrix and the distribution of color flow for the partonic process, convoluted with the beam and structure-function chain.

If the model is not provided explicitly, we may use the model instance that belongs to the process. However, an explicit model allows us to override particle settings.

```

<Instances: process instance: TBP>+≡
    procedure :: setup_event_data => process_instance_setup_event_data
<Instances: sub interfaces>+≡
    module subroutine process_instance_setup_event_data &
        (instance, model, i_core)
        class(process_instance_t), intent(inout), target :: instance
        class(model_data_t), intent(in), optional, target :: model
        integer, intent(in), optional :: i_core
    end subroutine process_instance_setup_event_data
<Instances: procedures>+≡
    module subroutine process_instance_setup_event_data (instance, model, i_core)
        class(process_instance_t), intent(inout), target :: instance
        class(model_data_t), intent(in), optional, target :: model
        integer, intent(in), optional :: i_core
        class(model_data_t), pointer :: current_model
        integer :: i
        class(prc_core_t), pointer :: core => null ()
        if (present (model)) then
            current_model => model
        else
            current_model => instance%process%get_model_ptr ()
        end if
        do i = 1, size (instance%term)
            associate (term => instance%term(i), kin => instance%kin(i))
                if (associated (term%config)) then
                    core => instance%process%get_core_term (i)
                end if
            end associate
        end do
    end subroutine process_instance_setup_event_data

```

```

        call term%setup_event_data (kin, core, current_model)
    end if
end associate
end do
core => null ()
end subroutine process_instance_setup_event_data

```

Choose a MC parameter set and the corresponding integrator. The choice persists beyond calls of the `reset` method above. This method is automatically called here.

```

<Instances: process instance: TBP>+≡
    procedure :: choose_mci => process_instance_choose_mci

<Instances: sub interfaces>+≡
    module subroutine process_instance_choose_mci (instance, i_mci)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_mci
    end subroutine process_instance_choose_mci

<Instances: procedures>+≡
    module subroutine process_instance_choose_mci (instance, i_mci)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_mci
        instance%i_mci = i_mci
        call instance%reset ()
    end subroutine process_instance_choose_mci

```

Explicitly set a MC parameter set. Works only if we are in initial state. We assume that the length of the parameter set is correct.

After setting the parameters, activate the components and terms that correspond to the chosen MC parameter set.

The `warmup_flag` is used when a dummy phase-space point is computed for the warmup of e.g. OpenLoops helicities. The setting of the `evaluation_status` has to be avoided then.

```

<Instances: process instance: TBP>+≡
    procedure :: set_mcpair => process_instance_set_mcpair

<Instances: sub interfaces>+≡
    module subroutine process_instance_set_mcpair (instance, x, warmup_flag)
        class(process_instance_t), intent(inout) :: instance
        real(default), dimension(:), intent(in) :: x
        logical, intent(in), optional :: warmup_flag
    end subroutine process_instance_set_mcpair

<Instances: procedures>+≡
    module subroutine process_instance_set_mcpair (instance, x, warmup_flag)
        class(process_instance_t), intent(inout) :: instance
        real(default), dimension(:), intent(in) :: x
        logical, intent(in), optional :: warmup_flag
        logical :: activate
        activate = .true.; if (present (warmup_flag)) activate = .not. warmup_flag
        if (instance%evaluation_status == STAT_INITIAL) then
            associate (mci_work => instance%mci_work(instance%i_mci))
                call mci_work%set (x)
            end associate
        end if
    end subroutine process_instance_set_mcpair

```

```

        end associate
        if (activate) call instance%activate ()
    end if
end subroutine process_instance_set_mcpair

```

Receive the beam momentum/momenta from a source interaction. This applies to a cascade decay process instance, where the ‘beam’ momentum varies event by event.

The master beam momentum array is contained in the main structure function chain subobject `sf_chain`. The sf-chain instance that reside in the components will take their beam momenta from there.

The procedure transforms the instance status into `STAT_BEAM_MOMENTA`. For process instance with fixed beam, this intermediate status is skipped.

```

<Instances: process instance: TBP>+≡
    procedure :: receive_beam_momenta => process_instance_receive_beam_momenta

<Instances: sub interfaces>+≡
    module subroutine process_instance_receive_beam_momenta (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_receive_beam_momenta

<Instances: procedures>+≡
    module subroutine process_instance_receive_beam_momenta (instance)
        class(process_instance_t), intent(inout) :: instance
        if (instance%evaluation_status >= STAT_INITIAL) then
            call instance%sf_chain%receive_beam_momenta ()
            instance%evaluation_status = STAT_BEAM_MOMENTA
        end if
    end subroutine process_instance_receive_beam_momenta

```

Set the beam momentum/momenta explicitly. Otherwise, analogous to the previous procedure.

```

<Instances: process instance: TBP>+≡
    procedure :: set_beam_momenta => process_instance_set_beam_momenta

<Instances: sub interfaces>+≡
    module subroutine process_instance_set_beam_momenta (instance, p)
        class(process_instance_t), intent(inout) :: instance
        type(vector4_t), dimension(:), intent(in) :: p
    end subroutine process_instance_set_beam_momenta

<Instances: procedures>+≡
    module subroutine process_instance_set_beam_momenta (instance, p)
        class(process_instance_t), intent(inout) :: instance
        type(vector4_t), dimension(:), intent(in) :: p
        if (instance%evaluation_status >= STAT_INITIAL) then
            call instance%sf_chain%set_beam_momenta (p)
            instance%evaluation_status = STAT_BEAM_MOMENTA
        end if
    end subroutine process_instance_set_beam_momenta

```

Recover the initial beam momenta (those in the `sf_chain` component), given a valid (recovered) `sf_chain_instance` in one of the active components. We need

to do this only if the lab frame is not the c.m. frame, otherwise those beams would be fixed anyway.

```

<Instances: process instance: TBP>+≡
  procedure :: recover_beam_momenta => process_instance_recover_beam_momenta
<Instances: sub interfaces>+≡
  module subroutine process_instance_recover_beam_momenta (instance, i_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term
  end subroutine process_instance_recover_beam_momenta
<Instances: procedures>+≡
  module subroutine process_instance_recover_beam_momenta (instance, i_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term
    if (.not. instance%process%lab_is_cm ()) then
      if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
        call instance%kin(i_term)%return_beam_momenta ()
      end if
    end if
  end subroutine process_instance_recover_beam_momenta

```

Explicitly choose MC integration channel. We assume here that the channel count is identical for all active components.

```

<Instances: process instance: TBP>+≡
  procedure :: select_channel => process_instance_select_channel
<Instances: sub interfaces>+≡
  module subroutine process_instance_select_channel (instance, channel)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
  end subroutine process_instance_select_channel
<Instances: procedures>+≡
  module subroutine process_instance_select_channel (instance, channel)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    instance%selected_channel = channel
  end subroutine process_instance_select_channel

```

First step of process evaluation: set up seed kinematics. That is, for each active process component, compute a momentum array from the MC input parameters.

If `skip_term` is set, we skip the component that accesses this term. We can assume that the associated data have already been recovered, and we are just computing the rest.

```

<Instances: process instance: TBP>+≡
  procedure :: compute_seed_kinematics => &
    process_instance_compute_seed_kinematics
<Instances: sub interfaces>+≡
  module subroutine process_instance_compute_seed_kinematics &
    (instance, recover, skip_term)
    class(process_instance_t), intent(inout) :: instance
    logical, intent(in), optional :: recover
    integer, intent(in), optional :: skip_term
  end subroutine process_instance_compute_seed_kinematics

```

(Instances: procedures)+≡

```

module subroutine process_instance_compute_seed_kinematics &
  (instance, recover, skip_term)
  class(process_instance_t), intent(inout) :: instance
  logical, intent(in), optional :: recover
  integer, intent(in), optional :: skip_term
  integer :: channel, skip_component, i, j
  logical :: success
  integer, dimension(:), allocatable :: i_term
  channel = instance%selected_channel
  if (channel == 0) then
    call msg_bug ("Compute seed kinematics: undefined integration channel")
  end if
  if (present (skip_term)) then
    skip_component = instance%term(skip_term)%config%i_component
  else
    skip_component = 0
  end if
  if (present (recover)) then
    if (recover) return
  end if
  if (instance%evaluation_status >= STAT_ACTIVATED) then
    success = .true.
    do i = 1, instance%process%get_n_components ()
      if (i == skip_component) cycle
      if (instance%process%component_is_selected (i)) then
        allocate (i_term (size (instance%process%get_component_i_terms (i))))
        i_term = instance%process%get_component_i_terms (i)
        do j = 1, size (i_term)
          associate (term => instance%term(i_term(j)), kin => instance%kin(i_term(j)))
            if (kin%new_seed) then
              call term%compute_seed_kinematics (kin, &
                instance%mci_work(instance%i_mci), channel, success)
              call instance%transfer_same_kinematics (i_term(j))
            end if
            if (.not. success) exit
          end associate
        end do
        select type (pcm => instance%pcm)
        class is (pcm_nlo_t)
          call term%evaluate_projections (kin)
          call kin%evaluate_radiation_kinematics &
            (instance%mci_work(instance%i_mci)%get_x_process ())
          call kin%generate_fsr_in ()
          call kin%compute_xi_ref_momenta (pcm%region_data, term%nlo_type)
        end select
      end associate
    end do
    if (allocated (i_term)) deallocate (i_term)
  end do
  if (success) then
    instance%evaluation_status = STAT_SEED_KINEMATICS
  else
    instance%evaluation_status = STAT_FAILED_KINEMATICS
  end if
end if

```



```

end if
associate (mci_work => instance%mci_work(instance%i_mci))
  select type (pcm_work => instance%pcm_work)
    class is (pcm_nlo_workspace_t)
      call pcm_work%set_x_rad (mci_work%get_x_process ())
    end select
  end associate
end subroutine process_instance_compute_seed_kinematics

```

(Instances: process instance: TBP)+≡

```

procedure :: get_x_process => process_instance_get_x_process

```

(Instances: sub interfaces)+≡

```

pure module function process_instance_get_x_process (instance) result (x)
  real(default), dimension(:), allocatable :: x
  class(process_instance_t), intent(in) :: instance
end function process_instance_get_x_process

```

(Instances: procedures)+≡

```

pure module function process_instance_get_x_process (instance) result (x)
  real(default), dimension(:), allocatable :: x
  class(process_instance_t), intent(in) :: instance
  allocate (x(size (instance%mci_work(instance%i_mci)%get_x_process ())))
  x = instance%mci_work(instance%i_mci)%get_x_process ()
end function process_instance_get_x_process

```

(Instances: process instance: TBP)+≡

```

procedure :: get_active_component_type => &
  process_instance_get_active_component_type

```

(Instances: sub interfaces)+≡

```

pure module function process_instance_get_active_component_type &
  (instance) result (nlo_type)
  integer :: nlo_type
  class(process_instance_t), intent(in) :: instance
end function process_instance_get_active_component_type

```

(Instances: procedures)+≡

```

pure module function process_instance_get_active_component_type &
  (instance) result (nlo_type)
  integer :: nlo_type
  class(process_instance_t), intent(in) :: instance
  nlo_type = instance%process%get_component_nlo_type (instance%i_mci)
end function process_instance_get_active_component_type

```

Inverse: recover missing parts of the kinematics from the momentum configuration, which we know for a single term and component. Given a channel, reconstruct the MC parameter set.

(Instances: process instance: TBP)+≡

```

procedure :: recover_mcpair => process_instance_recover_mcpair

```

(Instances: sub interfaces)+≡

```

module subroutine process_instance_recover_mcpair (instance, i_term)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
end subroutine process_instance_recover_mcpair

```

<Instances: procedures>+≡

```

module subroutine process_instance_recover_mcpair (instance, i_term)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
  integer :: channel, i
  if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
    channel = instance%selected_channel
    if (channel == 0) then
      call msg_bug ("Recover MC parameters: undefined integration channel")
    end if
    call instance%kin(i_term)%recover_mcpair &
      (instance%mc_i_work(instance%i_mci), channel, instance%term(i_term)%p_seed)
    if (instance%term(i_term)%nlo_type == NLO_REAL) then
      do i = 1, size (instance%term)
        if (i /= i_term .and. instance%term(i)%nlo_type == NLO_REAL) then
          if (instance%term(i)%active) then
            call instance%kin(i)%recover_mcpair &
              (instance%mc_i_work(instance%i_mci), channel, &
               instance%term(i)%p_seed)
          end if
        end if
      end do
    end if
  end if
end subroutine process_instance_recover_mcpair

```

This is part of `recover_mcpair`, extracted for the case when there is no phase space and parameters to recover, but we still need the structure function kinematics for evaluation.

<Instances: process instance: TBP>+≡

```

procedure :: recover_sfchain => process_instance_recover_sfchain

```

<Instances: sub interfaces>+≡

```

module subroutine process_instance_recover_sfchain (instance, i_term)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
end subroutine process_instance_recover_sfchain

```

<Instances: procedures>+≡

```

module subroutine process_instance_recover_sfchain (instance, i_term)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
  integer :: channel
  if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
    channel = instance%selected_channel
    if (channel == 0) then
      call msg_bug ("Recover sfchain: undefined integration channel")
    end if
    call instance%kin(i_term)%recover_sfchain &
      (channel, instance%term(i_term)%p_seed)
  end if
end subroutine process_instance_recover_sfchain

```

Second step of process evaluation: compute all momenta, for all active components, from the seed kinematics.

```

<Instances: process instance: TBP>+≡
  procedure :: compute_hard_kinematics => &
    process_instance_compute_hard_kinematics

<Instances: sub interfaces>+≡
  module subroutine process_instance_compute_hard_kinematics &
    (instance, recover, skip_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), optional :: skip_term
    logical, intent(in), optional :: recover
  end subroutine process_instance_compute_hard_kinematics

<Instances: procedures>+≡
  module subroutine process_instance_compute_hard_kinematics &
    (instance, recover, skip_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), optional :: skip_term
    logical, intent(in), optional :: recover
    integer :: i
    logical :: success
    success = .true.
    if (instance%evaluation_status >= STAT_SEED_KINEMATICS) then
      do i = 1, size (instance%term)
        associate (term => instance%term(i), kin => instance%kin(i))
          if (term%active) then
            call term%compute_hard_kinematics &
              (kin, recover, skip_term, success)
            if (.not. success) exit
            !!! Ren scale is zero when this is commented out! Understand!
            if (term%nlo_type == NLO_REAL) &
              call kin%redo_sf_chain (instance%mc_work(instance%i_mci), &
                instance%selected_channel)
          end if
        end associate
      end do
      if (success) then
        instance%evaluation_status = STAT_HARD_KINEMATICS
      else
        instance%evaluation_status = STAT_FAILED_KINEMATICS
      end if
    end if
  end subroutine process_instance_compute_hard_kinematics

```

Inverse: recover seed kinematics. We know the beam momentum configuration and the outgoing momenta of the effective interaction, for one specific term.

```

<Instances: process instance: TBP>+≡
  procedure :: recover_seed_kinematics => &
    process_instance_recover_seed_kinematics

<Instances: sub interfaces>+≡
  module subroutine process_instance_recover_seed_kinematics &
    (instance, i_term)
    class(process_instance_t), intent(inout) :: instance

```

```

        integer, intent(in) :: i_term
    end subroutine process_instance_recover_seed_kinematics

    <Instances: procedures>+=
    module subroutine process_instance_recover_seed_kinematics (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        type(vector4_t), dimension(:), allocatable :: p_seed_ref
        integer :: i
        if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
            call instance%term(i_term)%recover_seed_kinematics (instance%kin(i_term))
            if (instance%term(i_term)%nlo_type == NLO_REAL) then
                allocate (p_seed_ref &
                    (instance%term(i_term)%isolated%int_eff%get_n_out ()))
                p_seed_ref = instance%term(i_term)%isolated%int_eff%get_momenta &
                    (outgoing = .true.)
                do i = 1, size (instance%term)
                    if (i /= i_term .and. instance%term(i)%nlo_type == NLO_REAL) then
                        if (instance%term(i)%active) then
                            call instance%term(i)%recover_seed_kinematics &
                                (instance%kin(i), p_seed_ref)
                        end if
                    end if
                end do
            end if
        end if
    end subroutine process_instance_recover_seed_kinematics

```

Third step of process evaluation: compute the effective momentum configurations, for all active terms, from the hard kinematics.

```

    <Instances: process instance: TBP>+=
    procedure :: compute_eff_kinematics => &
        process_instance_compute_eff_kinematics

    <Instances: sub interfaces>+=
    module subroutine process_instance_compute_eff_kinematics &
        (instance, skip_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in), optional :: skip_term
    end subroutine process_instance_compute_eff_kinematics

    <Instances: procedures>+=
    module subroutine process_instance_compute_eff_kinematics &
        (instance, skip_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in), optional :: skip_term
        integer :: i
        if (instance%evaluation_status >= STAT_HARD_KINEMATICS) then
            do i = 1, size (instance%term)
                if (present (skip_term)) then
                    if (i == skip_term) cycle
                end if
                if (instance%term(i)%active) then
                    call instance%term(i)%compute_eff_kinematics ()
                end if
            end do
        end if
    end subroutine process_instance_compute_eff_kinematics

```

```

        end do
        instance%evaluation_status = STAT_EFF_KINEMATICS
    end if
end subroutine process_instance_compute_eff_kinematics

```

Inverse: recover the hard kinematics from effective kinematics for one term, then compute effective kinematics for the other terms.

```

<Instances: process instance: TBP>+≡
    procedure :: recover_hard_kinematics => &
        process_instance_recover_hard_kinematics

<Instances: sub interfaces>+≡
    module subroutine process_instance_recover_hard_kinematics &
        (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
    end subroutine process_instance_recover_hard_kinematics

<Instances: procedures>+≡
    module subroutine process_instance_recover_hard_kinematics (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        integer :: i
        if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
            call instance%term(i_term)%recover_hard_kinematics ()
            do i = 1, size (instance%term)
                if (i /= i_term) then
                    if (instance%term(i)%active) then
                        call instance%term(i)%compute_eff_kinematics ()
                    end if
                end if
            end do
            instance%evaluation_status = STAT_EFF_KINEMATICS
        end if
    end subroutine process_instance_recover_hard_kinematics

```

Fourth step of process evaluation: check cuts for all terms. Where successful, compute any scales and weights. Otherwise, deactivate the term. If any of the terms has passed, set the state to STAT_PASSED_CUTS.

The argument `scale_forced`, if present, will override the scale calculation in the term expressions.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_expressions => &
        process_instance_evaluate_expressions

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate_expressions &
        (instance, scale_forced)
        class(process_instance_t), intent(inout) :: instance
        real(default), intent(in), allocatable, optional :: scale_forced
    end subroutine process_instance_evaluate_expressions

<Instances: procedures>+≡
    module subroutine process_instance_evaluate_expressions &

```

```

        (instance, scale_forced)
class(process_instance_t), intent(inout) :: instance
real(default), intent(in), allocatable, optional :: scale_forced
integer :: i
logical :: passed_real
if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
    do i = 1, size (instance%term)
        if (instance%term(i)%active) then
            call instance%term(i)%evaluate_expressions &
                (instance%process%get_beam_config (), scale_forced)
        end if
    end do
    call evaluate_real_scales_and_cuts ()
    call set_ellis_sexton_scale ()
    if (.not. passed_real) then
        instance%evaluation_status = STAT_FAILED_CUTS
    else
        if (any (instance%term%passed)) then
            instance%evaluation_status = STAT_PASSED_CUTS
        else
            instance%evaluation_status = STAT_FAILED_CUTS
        end if
    end if
end if
contains
subroutine evaluate_real_scales_and_cuts ()
    integer :: i
    passed_real = .true.
    select type (pcm => instance%pcm)
    type is (pcm_nlo_t)
        do i = 1, size (instance%term)
            if (instance%term(i)%active .and. instance%term(i)%nlo_type == NLO_REAL) then
                if (pcm%settings%cut_all_real_sqmes) &
                    passed_real = passed_real .and. instance%term(i)%passed
                if (pcm%settings%use_born_scale) &
                    call replace_scales (instance%term(i))
            end if
        end do
    end select
end subroutine evaluate_real_scales_and_cuts

subroutine replace_scales (this_term)
    type(term_instance_t), intent(inout) :: this_term
    integer :: i_sub
    i_sub = this_term%config%i_sub
    if (this_term%config%i_term_global /= i_sub .and. i_sub > 0) then
        this_term%ren_scale = instance%term(i_sub)%ren_scale
        this_term%fac_scale = instance%term(i_sub)%fac_scale
    end if
end subroutine replace_scales

subroutine set_ellis_sexton_scale ()
    real(default) :: es_scale
    type(var_list_t), pointer :: var_list

```

```

integer :: i
var_list => instance%process%get_var_list_ptr ()
es_scale = var_list%get_rval (var_str ("ellis_sexton_scale"))
do i = 1, size (instance%term)
  if (instance%term(i)%active .and. instance%term(i)%nlo_type == NLO_VIRTUAL) then
    if (es_scale > zero) then
      if (allocated (instance%term(i)%es_scale)) then
        instance%term(i)%es_scale = es_scale
      else
        allocate (instance%term(i)%es_scale, source=es_scale)
      end if
    end if
  end if
end do
end subroutine set_ellis_sexton_scale
end subroutine process_instance_evaluate_expressions

```

Fifth step of process evaluation: fill the parameters for the non-selected channels, that have not been used for seeding. We should do this after evaluating cuts, since we may save some expensive calculations if the phase space point fails the cuts.

If `skip_term` is set, we skip the component that accesses this term. We can assume that the associated data have already been recovered, and we are just computing the rest.

```

<Instances: process instance: TBP>+=
  procedure :: compute_other_channels => &
    process_instance_compute_other_channels

<Instances: sub interfaces>+=
  module subroutine process_instance_compute_other_channels &
    (instance, skip_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), optional :: skip_term
  end subroutine process_instance_compute_other_channels

<Instances: procedures>+=
  module subroutine process_instance_compute_other_channels &
    (instance, skip_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), optional :: skip_term
    integer :: channel, skip_component, i, j
    integer, dimension(:), allocatable :: i_term
    channel = instance%selected_channel
    if (channel == 0) then
      call msg_bug ("Compute other channels: undefined integration channel")
    end if
    if (present (skip_term)) then
      skip_component = instance%term(skip_term)%config%i_component
    else
      skip_component = 0
    end if
    if (instance%evaluation_status >= STAT_PASSED_CUTS) then
      do i = 1, instance%process%get_n_components ()
        if (i == skip_component) cycle

```

```

        if (instance%process%component_is_selected (i)) then
            allocate (i_term (size (instance%process%get_component_i_terms (i))))
            i_term = instance%process%get_component_i_terms (i)
            do j = 1, size (i_term)
                call instance%kin(i_term(j))%compute_other_channels &
                    (instance%mci_work(instance%i_mci), channel)
            end do
        end if
        if (allocated (i_term)) deallocate (i_term)
    end do
end if
end subroutine process_instance_compute_other_channels

```

If not done otherwise, we flag the kinematics as new for the core state, such that the routine below will actually compute the matrix element and not just look it up.

```

<Instances: process instance: TBP>+≡
    procedure :: reset_core_kinematics => process_instance_reset_core_kinematics

<Instances: sub interfaces>+≡
    module subroutine process_instance_reset_core_kinematics (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_reset_core_kinematics

<Instances: procedures>+≡
    module subroutine process_instance_reset_core_kinematics (instance)
        class(process_instance_t), intent(inout) :: instance
        integer :: i
        if (instance%evaluation_status >= STAT_PASSED_CUTS) then
            do i = 1, size (instance%term)
                associate (term => instance%term(i))
                    if (term%active .and. term%passed) then
                        if (allocated (term%core_state)) &
                            call term%core_state%reset_new_kinematics ()
                    end if
                end associate
            end do
        end if
    end subroutine process_instance_reset_core_kinematics

```

Sixth step of process evaluation: evaluate the matrix elements, and compute the trace (summed over quantum numbers) for all terms. Finally, sum up the terms, iterating over all active process components.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_trace => process_instance_evaluate_trace

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate_trace (instance, recover)
        class(process_instance_t), intent(inout) :: instance
        logical, intent(in), optional :: recover
    end subroutine process_instance_evaluate_trace

<Instances: procedures>+≡
    module subroutine process_instance_evaluate_trace (instance, recover)
        class(process_instance_t), intent(inout) :: instance

```



```

logical, intent(in), optional :: recover
class(prc_core_t), pointer :: core => null ()
integer :: i, i_real_fin, i_core, i_qn, i_flg
real(default) :: alpha_s, alpha_qcd, pt
class(prc_core_t), pointer :: core_sub => null ()
class(model_data_t), pointer :: model => null ()
logical :: has_pdfs
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "process_instance_evaluate_trace")
has_pdfs = instance%process%pcm_contains_pdfs ()
instance%sqme = zero
select type (pcm_work => instance%pcm_work)
type is (pcm_nlo_workspace_t)
    if (allocated(pcm_work%real_sub%sqme_real_arr)) then
        pcm_work%real_sub%sqme_real_arr = zero
    end if
end select
call instance%reset_matrix_elements ()
if (instance%evaluation_status >= STAT_PASSED_CUTS) then
    do i = 1, size (instance%term)
        associate (term => instance%term(i), kin => instance%kin(i))
            if (term%active .and. term%passed) then
                core => instance%process%get_core_term (i)
                select type (pcm => instance%process%get_pcm_ptr ())
                class is (pcm_nlo_t)
                    i_core = pcm%get_i_core (pcm%i_sub)
                    core_sub => instance%process%get_core_ptr (i_core)
                end select
                call term%evaluate_interaction (core, kin)
                call term%evaluate_trace (kin)
                i_real_fin = instance%process%get_associated_real_fin (1)
                if (instance%process%uses_real_partition ()) &
                    call term%apply_real_partition (kin)
                if (term%config%i_component == i_real_fin) then
                    if (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction ()) then
                        !!! Force the scale pT into the events for the real finite
                        associate (p_hard => term%p_hard)
                            !!! This is only the correct pt for ISR
                            pt = transverse_part(p_hard(size(p_hard)))
                            call term%set_fac_scale (pt)
                            select type (core)
                            class is (prc_external_t)
                                select type (core_state => term%core_state)
                                class is (prc_external_state_t)
                                    core_state%alpha_qcd = core%qcd%alpha%get (pt)
                                end select
                            type is (prc_omega_t)
                                select type (core_state => term%core_state)
                                type is (omega_state_t)
                                    core_state%alpha_qcd = core%qcd%alpha%get (pt)
                                end select
                            end select
                        end select
                    end associate
                end if
            end if
        end do
    else

```

```

if (term%nlo_type == BORN) then
  do i_flg = 1, term%connected%trace%get_qn_index_n_flg ( )
    i_qn = term%connected%trace%get_qn_index (i_flg, i_sub = 0)
    if (.not. term%passed_array(i_flg)) then
      call term%connected%trace%set_matrix_element &
        (i_qn, cmplx (zero, zero, default))
    end if
  end do
end if
if ((term%nlo_type == NLO_REAL .and. kin%emitter < 0) &
  .or. term%nlo_type == NLO_MISMATCH &
  .or. term%nlo_type == NLO_DGLAP) &
  call term%set_born_sqmes (core)
if (term%is_subtraction ( ) .or. &
  term%nlo_type == NLO_DGLAP) &
  call term%set_sf_factors (kin, has_pdfs)
if (term%nlo_type > BORN) then
  if (.not. (term%nlo_type == NLO_REAL .and. &
    kin%emitter >= 0)) then
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      if (char (pcm%settings%nlo_correction_type) == "QCD" .or. &
        char (pcm%settings%nlo_correction_type) == "Full") &
        call term%evaluate_color_correlations (core_sub)
      if (char (pcm%settings%nlo_correction_type) == "EW" .or. &
        char (pcm%settings%nlo_correction_type) == "Full") then
        call term%evaluate_charge_correlations (core_sub)
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
          associate (reg_data => pcm%region_data)
            if (reg_data%alphas_power > 0) &
              call term%evaluate_color_correlations (core_sub)
          end associate
        end select
      end if
    end select
  end if
  if (term%is_subtraction ( )) then
    call term%evaluate_spin_correlations (core_sub)
  end if
end if
alpha_s = core%get_alpha_s (term%core_state)
alpha_qed = core%get_alpha_qed (term%core_state)
if (term%nlo_type > BORN) then
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    if (alpha_qed == -1 .and. (&
      char (pcm%settings%nlo_correction_type) == "EW" .or. &
      char (pcm%settings%nlo_correction_type) == "Full")) then
      call msg_bug("Attempting to compute EW corrections with alpha_qed = -1")
    end if
  end select
end if
if (present (recover)) then

```

```

        if (recover) return
    end if
    select case (term%nlo_type)
    case (NLO_REAL)
        call term%apply_fks (kin, alpha_s, alpha_qed)
    case (NLO_VIRTUAL)
        call term%evaluate_sqme_virt (alpha_s, alpha_qed)
    case (NLO_MISMATCH)
        call term%evaluate_sqme_mismatch (alpha_s)
    case (NLO_DGLAP)
        call term%evaluate_sqme_dglap (alpha_s, alpha_qed)
    end select
    end if
    end if
    core_sub => null ()
    instance%sqme = instance%sqme + real (sum (&
        term%connected%trace%get_matrix_element () * &
        term%weight))
    end associate
end do
core => null ()
if (instance%pcm_work%is_valid ()) then
    instance%evaluation_status = STAT_EVALUATED_TRACE
else
    instance%evaluation_status = STAT_FAILED_KINEMATICS
end if
else
    !!! Failed kinematics or failed cuts: set sqme to zero
    instance%sqme = zero
end if
end subroutine process_instance_evaluate_trace

```

(Instances: term instance: TBP)+≡

```

    procedure :: set_born_sqmes => term_instance_set_born_sqmes

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_set_born_sqmes (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in) :: core
    end subroutine term_instance_set_born_sqmes

```

(Instances: procedures)+≡

```

    module subroutine term_instance_set_born_sqmes (term, core)
        class(term_instance_t), intent(inout) :: term
        class(prc_core_t), intent(in) :: core
        integer :: i_flv, ii_flv
        real(default) :: sqme
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            do i_flv = 1, term%connected%trace%get_qn_index_n_flv ()
                ii_flv = term%connected%trace%get_qn_index (i_flv, i_sub = 0)
                if (term%passed_array (i_flv) .or. .not. term%passed) then
                    sqme = real (term%connected%trace%get_matrix_element (ii_flv))
                else
                    sqme = zero
                end if
            end do
        end select
    end subroutine term_instance_set_born_sqmes

```

```

        end if
        select case (term%nlo_type)
        case (NLO_REAL)
            pcm_work%real_sub%sqme_born(i_flg) = sqme
        case (NLO_MISMATCH)
            pcm_work%soft_mismatch%sqme_born(i_flg) = sqme
        case (NLO_DGLAP)
            pcm_work%dglap_remnant%sqme_born(i_flg) = sqme
        end select
    end do
end select
end subroutine term_instance_set_born_sqmes

```

Calculates and then saves the ratio of the value of the (rescaled) real structure function chain of each ISR alpha region over the value of the corresponding underlying born flavor structure. In the case of emitter 0 we also need the rescaled ratio for emitter 1 and 2 in that region for the (soft-)collinear limits. If the emitter is 1 or 2 in some cases, e. g. for EW corrections where a photon in the proton is required, there can be the possibility of soft radiation off the initial state. For that purpose the unrescaled ratio is needed and as a default we always save these numbers in `sf_factors(:,0)`. Although this procedure is implying functionality for general structure functions, it should be reviewed for anything else besides PDFs, as there might be complications in the details. The general idea of getting the ratio in this way should hold up in these cases as well, however.

(Instances: term instance: TBP)+≡

```

    procedure :: set_sf_factors => term_instance_set_sf_factors

```

(Instances: sub interfaces)+≡

```

    module subroutine term_instance_set_sf_factors (term, kin, has_pdfs)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
        logical, intent(in) :: has_pdfs
    end subroutine term_instance_set_sf_factors

```

(Instances: procedures)+≡

```

    module subroutine term_instance_set_sf_factors (term, kin, has_pdfs)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
        logical, intent(in) :: has_pdfs
        type(interaction_t), pointer :: sf_chain_int
        real(default) :: factor_born, factor_real
        integer :: n_in, alr, em
        integer :: i_born, i_real
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            if (.not. has_pdfs) then
                pcm_work%real_sub%sf_factors = one
                return
            end if
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                sf_chain_int => kin%sf_chain%get_out_int_ptr ()
                associate (reg_data => pcm%region_data)

```

```

n_in = reg_data%get_n_in ()
do alr = 1, reg_data%n_regions
  em = reg_data%regions(alr)%emitter
  if (em <= n_in) then
    i_born = reg_data%regions(alr)%uborn_index
    i_real = reg_data%regions(alr)%real_index
    factor_born = sf_chain_int%get_matrix_element &
      (sf_chain_int%get_sf_qn_index_born (i_born, i_sub = 0))
    factor_real = sf_chain_int%get_matrix_element &
      (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = em))
    call set_factor (pcm_work, alr, em, factor_born, factor_real)
    if (em == 0) then
      do em = 1, 2
        factor_real = sf_chain_int%get_matrix_element &
          (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = em))
        call set_factor (pcm_work, alr, em, factor_born, factor_real)
      end do
    else
      factor_real = sf_chain_int%get_matrix_element &
        (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = 0))
      call set_factor (pcm_work, alr, 0, factor_born, factor_real)
    end if
  end if
end do
end associate
end select
end select
contains
subroutine set_factor (pcm_work, alr, em, factor_born, factor_real)
  type(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
  integer, intent(in) :: alr, em
  real(default), intent(in) :: factor_born, factor_real
  real(default) :: factor
  if (any (vanishes ([factor_real, factor_born], tiny(1._default), tiny(1._default)))) then
    factor = zero
  else
    factor = factor_real / factor_born
  end if
  select case (term%nlo_type)
  case (NLO_REAL)
    pcm_work%real_sub%sf_factors(alr, em) = factor
  case (NLO_DGLAP)
    pcm_work%dglap_remnant%sf_factors(alr, em) = factor
  end select
end subroutine
end subroutine term_instance_set_sf_factors

```

<Instances: process instance: TBP>+≡

```
procedure :: apply_real_partition => process_instance_apply_real_partition
```

<Instances: sub interfaces>+≡

```

module subroutine process_instance_apply_real_partition (instance)
  class(process_instance_t), intent(inout) :: instance
end subroutine process_instance_apply_real_partition

```

<Instances: procedures>+≡

```

module subroutine process_instance_apply_real_partition (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i_component, i_term
  integer, dimension(:), allocatable :: i_terms
  associate (process => instance%process)
    i_component = process%get_first_real_component ()
    if (process%component_is_selected (i_component) .and. &
        process%get_component_nlo_type (i_component) == NLO_REAL) then
      allocate (i_terms, source=process%get_component_i_terms (i_component))
      do i_term = 1, size (i_terms)
        call instance%term(i_terms(i_term))%apply_real_partition ( &
            instance%kin(i_terms(i_term)))
      end do
    end if
    if (allocated (i_terms)) deallocate (i_terms)
  end associate
end subroutine process_instance_apply_real_partition

```

<Instances: process instance: TBP>+≡

```

procedure :: set_i_mci_to_real_component => &
  process_instance_set_i_mci_to_real_component

```

<Instances: sub interfaces>+≡

```

module subroutine process_instance_set_i_mci_to_real_component (instance)
  class(process_instance_t), intent(inout) :: instance
  end subroutine process_instance_set_i_mci_to_real_component

```

<Instances: procedures>+≡

```

module subroutine process_instance_set_i_mci_to_real_component (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i_mci, i_component
  type(process_component_t), pointer :: component => null ()
  select type (pcm_work => instance%pcm_work)
  type is (pcm_nlo_workspace_t)
    if (allocated (pcm_work%i_mci_to_real_component)) then
      call msg_warning &
        ("i_mci_to_real_component already allocated - replace it")
      deallocate (pcm_work%i_mci_to_real_component)
    end if
    allocate (pcm_work%i_mci_to_real_component (size (instance%pcm_work)))
    do i_mci = 1, size (instance%pcm_work)
      do i_component = 1, instance%process%get_n_components ()
        component => instance%process%get_component_ptr (i_component)
        if (component%i_mci /= i_mci) cycle
        select case (component%component_type)
        case (COMP_MASTER, COMP_REAL)
          pcm_work%i_mci_to_real_component (i_mci) = &
            component%config%get_associated_real ()
        case (COMP_REAL_FIN)
          pcm_work%i_mci_to_real_component (i_mci) = &
            component%config%get_associated_real_fin ()
        case (COMP_REAL_SING)
          pcm_work%i_mci_to_real_component (i_mci) = &
            component%config%get_associated_real_sing ()
        end select
      end do
    end do
  end select
end subroutine process_instance_set_i_mci_to_real_component

```

```

        end select
    end do
    end do
    component => null ()
end select
end subroutine process_instance_set_i_mci_to_real_component

```

Final step of process evaluation: evaluate the matrix elements, and compute the trace (summed over quantum numbers) for all terms. Finally, sum up the terms, iterating over all active process components.

If **weight** is provided, we already know the kinematical event weight (the MCI weight which depends on the kinematics sampling algorithm, but not on the matrix element), so we do not need to take it from the MCI record.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_event_data => process_instance_evaluate_event_data

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate_event_data (instance, weight)
        class(process_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: weight
    end subroutine process_instance_evaluate_event_data

<Instances: procedures>+≡
    module subroutine process_instance_evaluate_event_data (instance, weight)
        class(process_instance_t), intent(inout) :: instance
        real(default), intent(in), optional :: weight
        integer :: i
        if (instance%evaluation_status >= STAT_EVALUATED_TRACE) then
            do i = 1, size (instance%term)
                associate (term => instance%term(i))
                    if (term%active) then
                        call term%evaluate_event_data ()
                    end if
                end associate
            end do
            if (present (weight)) then
                instance%weight = weight
            else
                instance%weight = &
                    instance%mci_work(instance%i_mci)%mci%get_event_weight ()
                instance%excess = &
                    instance%mci_work(instance%i_mci)%mci%get_event_excess ()
            end if
            instance%n_dropped = &
                instance%mci_work(instance%i_mci)%mci%get_n_event_dropped ()
            instance%evaluation_status = STAT_EVENT_COMPLETE
        else
            !!! failed kinematics etc.: set weight to zero
            instance%weight = zero
            !!! Maybe we want to process and keep the event nevertheless
            if (instance%keep_failed_events ()) then
                do i = 1, size (instance%term)
                    associate (term => instance%term(i))
                        if (term%active) then

```

```

        call term%evaluate_event_data ()
    end if
    end associate
end do
!      do i = 1, size (instance%term)
!          instance%term(i)%fac_scale = zero
!      end do
    instance%evaluation_status = STAT_EVENT_COMPLETE
end if
end if
end subroutine process_instance_evaluate_event_data

```

Computes the real-emission matrix element for externally supplied momenta for the term instance with index `i_term` and a phase space point set with index `i_phs`. In addition, for the real emission, each term instance corresponds to one emitter. There is the possibility to supply an external α_s as well as an external scale to override the scale set in the Sindarin, e.g. for POWHEG matching.

(Instances: process instance: TBP)+≡

```

    procedure :: compute_sqme_rad => process_instance_compute_sqme_rad

```

(Instances: sub interfaces)+≡

```

    module subroutine process_instance_compute_sqme_rad (instance, &
        i_term, i_phs, is_subtraction, alpha_s_external, scale_forced)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term, i_phs
    logical, intent(in) :: is_subtraction
    real(default), intent(in), optional :: alpha_s_external
    real(default), intent(in), allocatable, optional :: scale_forced
    end subroutine process_instance_compute_sqme_rad

```

(Instances: procedures)+≡

```

    module subroutine process_instance_compute_sqme_rad (instance, &
        i_term, i_phs, is_subtraction, alpha_s_external, scale_forced)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term, i_phs
    logical, intent(in) :: is_subtraction
    real(default), intent(in), optional :: alpha_s_external
    real(default), intent(in), allocatable, optional :: scale_forced
    class(prc_core_t), pointer :: core
    integer :: i_real_fin
    logical :: has_pdfs
    has_pdfs = instance%process%pcm_contains_pdfs ()
    select type (pcm_work => instance%pcm_work)
    type is (pcm_nlo_workspace_t)
        if (allocated(pcm_work%real_sub%sqme_real_arr)) then
            pcm_work%real_sub%sqme_real_arr = zero
        end if
    end select
    if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "process_instance_compute_sqme_rad")
    select type (pcm_work => instance%pcm_work)
    type is (pcm_nlo_workspace_t)
        associate (term => instance%term(i_term), kin => instance%kin(i_term))
            core => instance%process%get_core_term (i_term)
            if (is_subtraction) then

```



```

        call pcm_work%set_subtraction_event ()
    else
        call pcm_work%set_radiation_event ()
    end if
    call term%int_hard%set_momenta (pcm_work%get_momenta &
        (term%pcm, i_phs = i_phs, born_phsp = is_subtraction))
    if (allocated (term%core_state)) &
        call term%core_state%reset_new_kinematics ()
    if (present (alpha_s_external)) then
        call term%set_alpha_qcd_forced (alpha_s_external)
    end if
    call term%compute_eff_kinematics ()
    call term%evaluate_expressions &
        (instance%process%get_beam_config (), scale_forced)
    call term%evaluate_interaction (core, kin)
    call term%evaluate_trace (kin)
    if (term%is_subtraction ()) then
        call term%set_sf_factors (kin, has_pdfs)
        select type (pcm => instance%pcm)
        type is (pcm_nlo_t)
            if (char (pcm%settings%nlo_correction_type) == "QCD" .or. &
                char (pcm%settings%nlo_correction_type) == "Full") &
                call term%evaluate_color_correlations (core)
            if (char (pcm%settings%nlo_correction_type) == "EW" .or. &
                char (pcm%settings%nlo_correction_type) == "Full") &
                call term%evaluate_charge_correlations (core)
        end select
        call term%evaluate_spin_correlations (core)
    end if
    i_real_fin = instance%process%get_associated_real_fin (1)
    if (term%config%i_component /= i_real_fin) &
        call term%apply_fks (kin, core%get_alpha_s (term%core_state), &
            core%get_alpha_qed (term%core_state))
    if (instance%process%uses_real_partition ()) &
        call instance%apply_real_partition ()
    end associate
end select
core => null ()
end subroutine process_instance_compute_sqme_rad

```

For unweighted event generation, we should reset the reported event weight to unity (signed) or zero. The latter case is appropriate for an event which failed for whatever reason.

```

<Instances: process instance: TBP>+≡
    procedure :: normalize_weight => process_instance_normalize_weight

<Instances: sub interfaces>+≡
    module subroutine process_instance_normalize_weight (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_normalize_weight

<Instances: procedures>+≡
    module subroutine process_instance_normalize_weight (instance)
        class(process_instance_t), intent(inout) :: instance

```

```

    if (.not. vanishes (instance%weight)) then
        instance%weight = sign (1._default, instance%weight)
    end if
end subroutine process_instance_normalize_weight

```

This is a convenience routine that performs the computations of the steps 1 to 5 in a single step. The arguments are the input for `set_mcp`. After this, the evaluation status should be either `STAT_FAILED_KINEMATICS`, `STAT_FAILED_CUTS` or `STAT_EVALUATED_TRACE`.

Before calling this, we should call `choose_mci`.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_sqme => process_instance_evaluate_sqme

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate_sqme (instance, channel, x)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: channel
        real(default), dimension(:), intent(in) :: x
    end subroutine process_instance_evaluate_sqme

<Instances: procedures>+≡
    module subroutine process_instance_evaluate_sqme (instance, channel, x)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: channel
        real(default), dimension(:), intent(in) :: x
        call instance%reset ()
        call instance%set_mcp (x)
        call instance%select_channel (channel)
        call instance%compute_seed_kinematics ()
        call instance%compute_hard_kinematics ()
        call instance%compute_eff_kinematics ()
        call instance%evaluate_expressions ()
        call instance%compute_other_channels ()
        call instance%evaluate_trace ()
    end subroutine process_instance_evaluate_sqme

```

This is the inverse. Assuming that the final trace evaluator contains a valid momentum configuration, recover kinematics and recalculate the matrix elements and their trace.

To be precise, we first recover kinematics for the given term and associated component, then recalculate from that all other terms and active components. The `channel` is not really required to obtain the matrix element, but it allows us to reconstruct the exact MC parameter set that corresponds to the given phase space point.

Before calling this, we should call `choose_mci`.

```

<Instances: process instance: TBP>+≡
    procedure :: recover => process_instance_recover

<Instances: sub interfaces>+≡
    module subroutine process_instance_recover &
        (instance, channel, i_term, update_sqme, recover_phs, scale_forced)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: channel

```

```

        integer, intent(in) :: i_term
        logical, intent(in) :: update_sqme
        logical, intent(in) :: recover_phs
        real(default), intent(in), allocatable, optional :: scale_forced
    end subroutine process_instance_recover

<Instances: procedures>+≡
    module subroutine process_instance_recover &
        (instance, channel, i_term, update_sqme, recover_phs, scale_forced)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    integer, intent(in) :: i_term
    logical, intent(in) :: update_sqme
    logical, intent(in) :: recover_phs
    real(default), intent(in), allocatable, optional :: scale_forced
    logical :: skip_phs, recover
    call instance%activate ()
    instance%evaluation_status = STAT_EFF_KINEMATICS
    call instance%recover_hard_kinematics (i_term)
    call instance%recover_seed_kinematics (i_term)
    call instance%select_channel (channel)
    recover = instance%pcm_work%is_nlo ()
    if (recover_phs) then
        call instance%recover_mcpair (i_term)
        call instance%recover_beam_momenta (i_term)
        call instance%compute_seed_kinematics &
            (recover = recover, skip_term = i_term)
        call instance%compute_hard_kinematics &
            (recover = recover, skip_term = i_term)
        call instance%compute_eff_kinematics (i_term)
        call instance%compute_other_channels (i_term)
    else
        call instance%recover_sfchain (i_term)
    end if
    call instance%evaluate_expressions (scale_forced)
    if (update_sqme) then
        call instance%reset_core_kinematics ()
        call instance%evaluate_trace (recover)
    end if
end subroutine process_instance_recover

```

The `evaluate` method is required by the `sampler_t` base type of which the process instance is an extension.

The requirement is that after the process instance is evaluated, the integrand, the selected channel, the x array, and the f Jacobian array are exposed by the `sampler_t` object.

We allow for the additional hook to be called, if associated, for outlying object to access information from the current state of the `sampler`.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate => process_instance_evaluate

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate (sampler, c, x_in, val, x, f)
    class(process_instance_t), intent(inout) :: sampler

```

```

integer, intent(in) :: c
real(default), dimension(:), intent(in) :: x_in
real(default), intent(out) :: val
real(default), dimension(:, :), intent(out) :: x
real(default), dimension(:), intent(out) :: f
end subroutine process_instance_evaluate

```

(Instances: procedures)+≡

```

module subroutine process_instance_evaluate (sampler, c, x_in, val, x, f)
  class(process_instance_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(out) :: val
  real(default), dimension(:, :), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call sampler%evaluate_sqme (c, x_in)
  if (sampler%is_valid ()) then
    call sampler%fetch (val, x, f)
  end if
  call sampler%record_call ()
  call sampler%evaluate_after_hook ()
end subroutine process_instance_evaluate

```

The phase-space point is valid if the event has valid kinematics and has passed the cuts.

(Instances: process instance: TBP)+≡

```

procedure :: is_valid => process_instance_is_valid

```

(Instances: sub interfaces)+≡

```

module function process_instance_is_valid (sampler) result (valid)
  class(process_instance_t), intent(in) :: sampler
  logical :: valid
end function process_instance_is_valid

```

(Instances: procedures)+≡

```

module function process_instance_is_valid (sampler) result (valid)
  class(process_instance_t), intent(in) :: sampler
  logical :: valid
  valid = sampler%evaluation_status >= STAT_PASSED_CUTS
end function process_instance_is_valid

```

Add a process_instance_hook object..

(Instances: process instance: TBP)+≡

```

procedure :: append_after_hook => process_instance_append_after_hook

```

(Instances: sub interfaces)+≡

```

module subroutine process_instance_append_after_hook (sampler, new_hook)
  class(process_instance_t), intent(inout), target :: sampler
  class(process_instance_hook_t), intent(inout), target :: new_hook
end subroutine process_instance_append_after_hook

```

(Instances: procedures)+≡

```

module subroutine process_instance_append_after_hook (sampler, new_hook)
  class(process_instance_t), intent(inout), target :: sampler
  class(process_instance_hook_t), intent(inout), target :: new_hook

```

```

class(process_instance_hook_t), pointer :: last
if (associated (new_hook%next)) then
    call msg_bug ("process_instance_append_after_hook: " // &
        "reuse of SAME hook object is forbidden.")
end if
if (associated (sampler%hook)) then
    last => sampler%hook
    do while (associated (last%next))
        last => last%next
    end do
    last%next => new_hook
else
    sampler%hook => new_hook
end if
end subroutine process_instance_append_after_hook

```

Evaluate the after hook as first in, last out.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_after_hook => process_instance_evaluate_after_hook

<Instances: sub interfaces>+≡
    module subroutine process_instance_evaluate_after_hook (sampler)
        class(process_instance_t), intent(in) :: sampler
    end subroutine process_instance_evaluate_after_hook

<Instances: procedures>+≡
    module subroutine process_instance_evaluate_after_hook (sampler)
        class(process_instance_t), intent(in) :: sampler
        class(process_instance_hook_t), pointer :: current
        current => sampler%hook
        do while (associated(current))
            call current%evaluate (sampler)
            current => current%next
        end do
    end subroutine process_instance_evaluate_after_hook

```

The `rebuild` method should rebuild the kinematics section out of the `x_in` parameter set. The integrand value `val` should not be computed, but is provided as input.

```

<Instances: process instance: TBP>+≡
    procedure :: rebuild => process_instance_rebuild

<Instances: sub interfaces>+≡
    module subroutine process_instance_rebuild (sampler, c, x_in, val, x, f)
        class(process_instance_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
    end subroutine process_instance_rebuild

<Instances: procedures>+≡
    module subroutine process_instance_rebuild (sampler, c, x_in, val, x, f)
        class(process_instance_t), intent(inout) :: sampler

```

```

integer, intent(in) :: c
real(default), dimension(:), intent(in) :: x_in
real(default), intent(in) :: val
real(default), dimension(:,:), intent(out) :: x
real(default), dimension(:), intent(out) :: f
call msg_bug ("process_instance_rebuild not implemented yet")
x = 0
f = 0
end subroutine process_instance_rebuild

```

This is another method required by the `sampler_t` base type: fetch the data that are relevant for the MCI record.

(Instances: process instance: TBP)+≡

```

procedure :: fetch => process_instance_fetch

```

(Instances: sub interfaces)+≡

```

module subroutine process_instance_fetch (sampler, val, x, f)
  class(process_instance_t), intent(in) :: sampler
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
end subroutine process_instance_fetch

```

(Instances: procedures)+≡

```

module subroutine process_instance_fetch (sampler, val, x, f)
  class(process_instance_t), intent(in) :: sampler
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  integer, dimension(:), allocatable :: i_terms
  integer :: i, i_term_base, cc
  integer :: n_channel

  val = 0
  associate (process => sampler%process)
    FIND_COMPONENT: do i = 1, process%get_n_components ()
      if (sampler%process%component_is_selected (i)) then
        allocate (i_terms (size (process%get_component_i_terms (i))))
        i_terms = process%get_component_i_terms (i)
        i_term_base = i_terms(1)
        associate (k => sampler%kin(i_term_base))
          n_channel = k%n_channel
          do cc = 1, n_channel
            call k%get_mcpair (cc, x(:,cc))
          end do
          f = k%f
          val = sampler%sqme * k%phs_factor
        end associate
        if (allocated (i_terms)) deallocate (i_terms)
        exit FIND_COMPONENT
      end if
    end do FIND_COMPONENT
  end associate
end subroutine process_instance_fetch

```

Initialize and finalize event generation for the specified MCI entry.

```

<Instances: process instance: TBP>+≡
  procedure :: init_simulation => process_instance_init_simulation
  procedure :: final_simulation => process_instance_final_simulation

<Instances: sub interfaces>+≡
  module subroutine process_instance_init_simulation (instance, i_mci, &
    safety_factor, keep_failed_events)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    real(default), intent(in), optional :: safety_factor
    logical, intent(in), optional :: keep_failed_events
  end subroutine process_instance_init_simulation
  module subroutine process_instance_final_simulation (instance, i_mci)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
  end subroutine process_instance_final_simulation

<Instances: procedures>+≡
  module subroutine process_instance_init_simulation (instance, i_mci, &
    safety_factor, keep_failed_events)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    real(default), intent(in), optional :: safety_factor
    logical, intent(in), optional :: keep_failed_events
    call instance%mci_work(i_mci)%init_simulation &
      (safety_factor, keep_failed_events)
  end subroutine process_instance_init_simulation

  module subroutine process_instance_final_simulation (instance, i_mci)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    call instance%mci_work(i_mci)%final_simulation ()
  end subroutine process_instance_final_simulation

```

Accessing the process instance

Once the seed kinematics is complete, we can retrieve the MC input parameters for all channels, not just the seed channel.

Note: We choose the first active component. This makes sense only if the seed kinematics is identical for all active components.

```

<Instances: process instance: TBP>+≡
  procedure :: get_mcpair => process_instance_get_mcpair

<Instances: sub interfaces>+≡
  module subroutine process_instance_get_mcpair (instance, channel, x)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    real(default), dimension(:), intent(out) :: x
  end subroutine process_instance_get_mcpair

<Instances: procedures>+≡
  module subroutine process_instance_get_mcpair (instance, channel, x)
    class(process_instance_t), intent(inout) :: instance

```

```

integer, intent(in) :: channel
real(default), dimension(:), intent(out) :: x
integer :: i
if (instance%evaluation_status >= STAT_SEED_KINEMATICS) then
  do i = 1, size (instance%term)
    if (instance%term(i)%active) then
      call instance%kin(i)%get_mcpair (channel, x)
      return
    end if
  end do
  call msg_bug ("Process instance: get_mcpair: no active channels")
else
  call msg_bug ("Process instance: get_mcpair: no seed kinematics")
end if
end subroutine process_instance_get_mcpair

```

Return true if the `sqme` value is known. This also implies that the event is kinematically valid and has passed all cuts.

```

<Instances: process instance: TBP>+≡
  procedure :: has_evaluated_trace => process_instance_has_evaluated_trace

<Instances: sub interfaces>+≡
  module function process_instance_has_evaluated_trace &
    (instance) result (flag)
    class(process_instance_t), intent(in) :: instance
    logical :: flag
  end function process_instance_has_evaluated_trace

<Instances: procedures>+≡
  module function process_instance_has_evaluated_trace (instance) result (flag)
    class(process_instance_t), intent(in) :: instance
    logical :: flag
    flag = instance%evaluation_status >= STAT_EVALUATED_TRACE
  end function process_instance_has_evaluated_trace

```

Return true if the event is complete. In particular, the event must be kinematically valid, passed all cuts, and the event data have been computed.

```

<Instances: process instance: TBP>+≡
  procedure :: is_complete_event => process_instance_is_complete_event

<Instances: sub interfaces>+≡
  module function process_instance_is_complete_event (instance) result (flag)
    class(process_instance_t), intent(in) :: instance
    logical :: flag
  end function process_instance_is_complete_event

<Instances: procedures>+≡
  module function process_instance_is_complete_event (instance) result (flag)
    class(process_instance_t), intent(in) :: instance
    logical :: flag
    flag = instance%evaluation_status >= STAT_EVENT_COMPLETE
  end function process_instance_is_complete_event

```


Select the term for the process instance that will provide the basic event record (used in `evt_trivial_make_particle_set`). It might be necessary to write out additional events corresponding to other terms (done in `evt_nlo`).

```

<Instances: process instance: TBP>+≡
  procedure :: select_i_term => process_instance_select_i_term

<Instances: sub interfaces>+≡
  module function process_instance_select_i_term (instance) result (i_term)
    integer :: i_term
    class(process_instance_t), intent(in) :: instance
  end function process_instance_select_i_term

<Instances: procedures>+≡
  module function process_instance_select_i_term (instance) result (i_term)
    integer :: i_term
    class(process_instance_t), intent(in) :: instance
    integer :: i_mci
    i_mci = instance%i_mci
    i_term = instance%process%select_i_term (i_mci)
  end function process_instance_select_i_term

```

Return pointer to the master beam interaction.

```

<Instances: process instance: TBP>+≡
  procedure :: get_beam_int_ptr => process_instance_get_beam_int_ptr

<Instances: sub interfaces>+≡
  module function process_instance_get_beam_int_ptr (instance) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    type(interaction_t), pointer :: ptr
  end function process_instance_get_beam_int_ptr

<Instances: procedures>+≡
  module function process_instance_get_beam_int_ptr (instance) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    type(interaction_t), pointer :: ptr
    ptr => instance%sf_chain%get_beam_int_ptr ()
  end function process_instance_get_beam_int_ptr

```

Return pointers to the matrix and flows interactions, given a term index.

```

<Instances: process instance: TBP>+≡
  procedure :: get_trace_int_ptr => process_instance_get_trace_int_ptr
  procedure :: get_matrix_int_ptr => process_instance_get_matrix_int_ptr
  procedure :: get_flows_int_ptr => process_instance_get_flows_int_ptr

<Instances: sub interfaces>+≡
  module function process_instance_get_trace_int_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(interaction_t), pointer :: ptr
  end function process_instance_get_trace_int_ptr
  module function process_instance_get_matrix_int_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term

```

```

        type(interaction_t), pointer :: ptr
    end function process_instance_get_matrix_int_ptr
    module function process_instance_get_flows_int_ptr &
        (instance, i_term) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(interaction_t), pointer :: ptr
    end function process_instance_get_flows_int_ptr
<Instances: procedures>+≡
    module function process_instance_get_trace_int_ptr &
        (instance, i_term) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(interaction_t), pointer :: ptr
        ptr => instance%term(i_term)%connected%get_trace_int_ptr ()
    end function process_instance_get_trace_int_ptr

    module function process_instance_get_matrix_int_ptr &
        (instance, i_term) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(interaction_t), pointer :: ptr
        ptr => instance%term(i_term)%connected%get_matrix_int_ptr ()
    end function process_instance_get_matrix_int_ptr

    module function process_instance_get_flows_int_ptr &
        (instance, i_term) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(interaction_t), pointer :: ptr
        ptr => instance%term(i_term)%connected%get_flows_int_ptr ()
    end function process_instance_get_flows_int_ptr

```

Return the complete account of flavor combinations in the underlying interaction object, including beams, radiation, and hard interaction.

```

<Instances: process instance: TBP>+≡
    procedure :: get_state_flv => process_instance_get_state_flv
<Instances: sub interfaces>+≡
    module function process_instance_get_state_flv &
        (instance, i_term) result (state_flv)
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        type(state_flv_content_t) :: state_flv
    end function process_instance_get_state_flv
<Instances: procedures>+≡
    module function process_instance_get_state_flv &
        (instance, i_term) result (state_flv)
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        type(state_flv_content_t) :: state_flv
        state_flv = instance%term(i_term)%connected%get_state_flv ()
    end function process_instance_get_state_flv

```

Return pointers to the parton states of a selected term.

```

<Instances: process instance: TBP>+≡
  procedure :: get_isolated_state_ptr => &
    process_instance_get_isolated_state_ptr
  procedure :: get_connected_state_ptr => &
    process_instance_get_connected_state_ptr

<Instances: sub interfaces>+≡
  module function process_instance_get_isolated_state_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(isolated_state_t), pointer :: ptr
  end function process_instance_get_isolated_state_ptr
  module function process_instance_get_connected_state_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(connected_state_t), pointer :: ptr
  end function process_instance_get_connected_state_ptr

<Instances: procedures>+≡
  module function process_instance_get_isolated_state_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(isolated_state_t), pointer :: ptr
    ptr => instance%term(i_term)%isolated
  end function process_instance_get_isolated_state_ptr

  module function process_instance_get_connected_state_ptr &
    (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(connected_state_t), pointer :: ptr
    ptr => instance%term(i_term)%connected
  end function process_instance_get_connected_state_ptr

```

Return the indices of the beam particles and incoming partons within the currently active state matrix, respectively.

```

<Instances: process instance: TBP>+≡
  procedure :: get_beam_index => process_instance_get_beam_index
  procedure :: get_in_index => process_instance_get_in_index

<Instances: sub interfaces>+≡
  module subroutine process_instance_get_beam_index (instance, i_term, i_beam)
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
    integer, dimension(:), intent(out) :: i_beam
  end subroutine process_instance_get_beam_index
  module subroutine process_instance_get_in_index (instance, i_term, i_in)
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
    integer, dimension(:), intent(out) :: i_in
  end subroutine process_instance_get_in_index

```

(Instances: procedures)+≡

```

module subroutine process_instance_get_beam_index (instance, i_term, i_beam)
  class(process_instance_t), intent(in) :: instance
  integer, intent(in) :: i_term
  integer, dimension(:), intent(out) :: i_beam
  call instance%term(i_term)%connected%get_beam_index (i_beam)
end subroutine process_instance_get_beam_index

module subroutine process_instance_get_in_index (instance, i_term, i_in)
  class(process_instance_t), intent(in) :: instance
  integer, intent(in) :: i_term
  integer, dimension(:), intent(out) :: i_in
  call instance%term(i_term)%connected%get_in_index (i_in)
end subroutine process_instance_get_in_index

```

Return squared matrix element and event weight, and event weight excess where applicable. `n_dropped` is a number that can be nonzero when a weighted event has been generated, dropping events with zero weight (failed cuts) on the fly. If `i_term` is provided for `get_sqme`, we take the first matrix element as we also set the first matrix element with `set_only_matrix_element` when computing the real, the dglap or the virtual contribution.

(Instances: process instance: TBP)+≡

```

procedure :: get_sqme => process_instance_get_sqme
procedure :: get_weight => process_instance_get_weight
procedure :: get_excess => process_instance_get_excess
procedure :: get_n_dropped => process_instance_get_n_dropped

```

(Instances: sub interfaces)+≡

```

module function process_instance_get_sqme (instance, i_term) result (sqme)
  real(default) :: sqme
  class(process_instance_t), intent(in) :: instance
  integer, intent(in), optional :: i_term
end function process_instance_get_sqme
module function process_instance_get_weight (instance) result (weight)
  real(default) :: weight
  class(process_instance_t), intent(in) :: instance
end function process_instance_get_weight
module function process_instance_get_excess (instance) result (excess)
  real(default) :: excess
  class(process_instance_t), intent(in) :: instance
end function process_instance_get_excess
module function process_instance_get_n_dropped (instance) result (n_dropped)
  integer :: n_dropped
  class(process_instance_t), intent(in) :: instance
end function process_instance_get_n_dropped

```

(Instances: procedures)+≡

```

module function process_instance_get_sqme (instance, i_term) result (sqme)
  real(default) :: sqme
  class(process_instance_t), intent(in) :: instance
  integer, intent(in), optional :: i_term
  if (instance%evaluation_status >= STAT_EVALUATED_TRACE) then
    if (present (i_term)) then
      sqme = instance%term(i_term)%connected%trace%get_matrix_element (1)
    end if
  end if
end function process_instance_get_sqme

```

```

        else
            sqme = instance%sqme
        end if
    else
        sqme = 0
    end if
end function process_instance_get_sqme

module function process_instance_get_weight (instance) result (weight)
    real(default) :: weight
    class(process_instance_t), intent(in) :: instance
    if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
        weight = instance%weight
    else
        weight = 0
    end if
end function process_instance_get_weight

module function process_instance_get_excess (instance) result (excess)
    real(default) :: excess
    class(process_instance_t), intent(in) :: instance
    if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
        excess = instance%excess
    else
        excess = 0
    end if
end function process_instance_get_excess

module function process_instance_get_n_dropped (instance) result (n_dropped)
    integer :: n_dropped
    class(process_instance_t), intent(in) :: instance
    if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
        n_dropped = instance%n_dropped
    else
        n_dropped = 0
    end if
end function process_instance_get_n_dropped

```

Return the currently selected MCI channel.

(Instances: process instance: TBP)+≡

```

    procedure :: get_channel => process_instance_get_channel

```

(Instances: sub interfaces)+≡

```

    module function process_instance_get_channel (instance) result (channel)
        integer :: channel
        class(process_instance_t), intent(in) :: instance
    end function process_instance_get_channel

```

(Instances: procedures)+≡

```

    module function process_instance_get_channel (instance) result (channel)
        integer :: channel
        class(process_instance_t), intent(in) :: instance
        channel = instance%selected_channel
    end function process_instance_get_channel

```

```

<Instances: process instance: TBP>+≡
  procedure :: set_fac_scale => process_instance_set_fac_scale

<Instances: sub interfaces>+≡
  module subroutine process_instance_set_fac_scale (instance, fac_scale)
    class(process_instance_t), intent(inout) :: instance
    real(default), intent(in) :: fac_scale
  end subroutine process_instance_set_fac_scale

<Instances: procedures>+≡
  module subroutine process_instance_set_fac_scale (instance, fac_scale)
    class(process_instance_t), intent(inout) :: instance
    real(default), intent(in) :: fac_scale
    integer :: i_term
    i_term = 1
    call instance%term(i_term)%set_fac_scale (fac_scale)
  end subroutine process_instance_set_fac_scale

```

Return factorization scale and strong coupling. We have to select a term instance.

```

<Instances: process instance: TBP>+≡
  procedure :: get_fac_scale => process_instance_get_fac_scale
  procedure :: get_alpha_s => process_instance_get_alpha_s

<Instances: sub interfaces>+≡
  module function process_instance_get_fac_scale &
    (instance, i_term) result (fac_scale)
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
    real(default) :: fac_scale
  end function process_instance_get_fac_scale
  module function process_instance_get_alpha_s &
    (instance, i_term) result (alpha_s)
    real(default) :: alpha_s
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
  end function process_instance_get_alpha_s

<Instances: procedures>+≡
  module function process_instance_get_fac_scale &
    (instance, i_term) result (fac_scale)
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
    real(default) :: fac_scale
    fac_scale = instance%term(i_term)%get_fac_scale ()
  end function process_instance_get_fac_scale

  module function process_instance_get_alpha_s &
    (instance, i_term) result (alpha_s)
    real(default) :: alpha_s
    class(process_instance_t), intent(in) :: instance
    integer, intent(in) :: i_term
    class(prc_core_t), pointer :: core => null ()
    core => instance%process%get_core_term (i_term)
    alpha_s = instance%term(i_term)%get_alpha_s (core)
    core => null ()

```

```

end function process_instance_get_alpha_s

<Instances: process instance: TBP>+≡
  procedure :: get_qcd => process_instance_get_qcd

<Instances: sub interfaces>+≡
  module function process_instance_get_qcd (process_instance) result (qcd)
    type(qcd_t) :: qcd
    class(process_instance_t), intent(in) :: process_instance
  end function process_instance_get_qcd

<Instances: procedures>+≡
  module function process_instance_get_qcd (process_instance) result (qcd)
    type(qcd_t) :: qcd
    class(process_instance_t), intent(in) :: process_instance
    qcd = process_instance%process%get_qcd ()
  end function process_instance_get_qcd

Counter.

<Instances: process instance: TBP>+≡
  procedure :: reset_counter => process_instance_reset_counter
  procedure :: record_call => process_instance_record_call
  procedure :: get_counter => process_instance_get_counter

<Instances: sub interfaces>+≡
  module subroutine process_instance_reset_counter (process_instance)
    class(process_instance_t), intent(inout) :: process_instance
  end subroutine process_instance_reset_counter
  module subroutine process_instance_record_call (process_instance)
    class(process_instance_t), intent(inout) :: process_instance
  end subroutine process_instance_record_call
  pure module function process_instance_get_counter &
    (process_instance) result (counter)
    class(process_instance_t), intent(in) :: process_instance
    type(process_counter_t) :: counter
  end function process_instance_get_counter

<Instances: procedures>+≡
  module subroutine process_instance_reset_counter (process_instance)
    class(process_instance_t), intent(inout) :: process_instance
    call process_instance%mci_work(process_instance%i_mci)%reset_counter ()
  end subroutine process_instance_reset_counter

  module subroutine process_instance_record_call (process_instance)
    class(process_instance_t), intent(inout) :: process_instance
    call process_instance%mci_work(process_instance%i_mci)%record_call &
      (process_instance%evaluation_status)
  end subroutine process_instance_record_call

  pure module function process_instance_get_counter &
    (process_instance) result (counter)
    class(process_instance_t), intent(in) :: process_instance
    type(process_counter_t) :: counter
    counter = process_instance%mci_work(process_instance%i_mci)%get_counter ()
  end function process_instance_get_counter

```

Sum up the total number of calls for all MCI records.

```

<Instances: process instance: TBP>+≡
    procedure :: get_actual_calls_total => process_instance_get_actual_calls_total

<Instances: sub interfaces>+≡
    pure module function process_instance_get_actual_calls_total &
        (process_instance) result (n)
        class(process_instance_t), intent(in) :: process_instance
        integer :: n
    end function process_instance_get_actual_calls_total

<Instances: procedures>+≡
    pure module function process_instance_get_actual_calls_total &
        (process_instance) result (n)
        class(process_instance_t), intent(in) :: process_instance
        integer :: n
        integer :: i
        type(process_counter_t) :: counter
        n = 0
        do i = 1, size (process_instance%mci_work)
            counter = process_instance%mci_work(i)%get_counter ()
            n = n + counter%total
        end do
    end function process_instance_get_actual_calls_total

<Instances: process instance: TBP>+≡
    procedure :: reset_matrix_elements => process_instance_reset_matrix_elements

<Instances: sub interfaces>+≡
    module subroutine process_instance_reset_matrix_elements (instance)
        class(process_instance_t), intent(inout) :: instance
    end subroutine process_instance_reset_matrix_elements

<Instances: procedures>+≡
    module subroutine process_instance_reset_matrix_elements (instance)
        class(process_instance_t), intent(inout) :: instance
        integer :: i_term
        do i_term = 1, size (instance%term)
            call instance%term(i_term)%connected%trace%set_matrix_element &
                (cmplx (0, 0, default))
            call instance%term(i_term)%connected%matrix%set_matrix_element &
                (cmplx (0, 0, default))
        end do
    end subroutine process_instance_reset_matrix_elements

<Instances: process instance: TBP>+≡
    procedure :: get_test_phase_space_point &
        => process_instance_get_test_phase_space_point

<Instances: sub interfaces>+≡
    module subroutine process_instance_get_test_phase_space_point (instance, &
        i_component, i_core, p)
        type(vector4_t), dimension(:), allocatable, intent(out) :: p
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_component, i_core
    end subroutine process_instance_get_test_phase_space_point

```



```

<Instances: procedures>+≡
module subroutine process_instance_get_test_phase_space_point (instance, &
    i_component, i_core, p)
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_component, i_core
    real(default), dimension(:), allocatable :: x
    logical :: success
    integer :: i_term
    instance%i_mci = i_component
    i_term = instance%process%get_i_term (i_core)
    associate (term => instance%term(i_term), kin => instance%kin(i_term))
        allocate (x (instance%kin%work(i_component)%config%n_par))
        x = 0.5_default
        call instance%set_mcpair (x, .true.)
        call instance%select_channel (i)
        call term%compute_seed_kinematics &
            (kin, instance%kin%work(i_component), 1, success)
        call kin%evaluate_radiation_kinematics &
            (instance%kin%work(instance%i_mci)%get_x_process ())
        call term%compute_hard_kinematics (kin, success = success)
        allocate (p (size (term%p_hard)))
        p = term%int_hard%get_momenta ()
    end associate
end subroutine process_instance_get_test_phase_space_point

```

```

<Instances: process instance: TBP>+≡
procedure :: get_p_hard => process_instance_get_p_hard

```

```

<Instances: sub interfaces>+≡
pure module function process_instance_get_p_hard &
    (process_instance, i_term) result (p_hard)
    type(vector4_t), dimension(:), allocatable :: p_hard
    class(process_instance_t), intent(in) :: process_instance
    integer, intent(in) :: i_term
end function process_instance_get_p_hard

```

```

<Instances: procedures>+≡
pure module function process_instance_get_p_hard &
    (process_instance, i_term) result (p_hard)
    type(vector4_t), dimension(:), allocatable :: p_hard
    class(process_instance_t), intent(in) :: process_instance
    integer, intent(in) :: i_term
    allocate (p_hard (size (process_instance%term(i_term)%get_p_hard ())))
    p_hard = process_instance%term(i_term)%get_p_hard ()
end function process_instance_get_p_hard

```

```

<Instances: process instance: TBP>+≡
procedure :: get_first_active_i_term => &
    process_instance_get_first_active_i_term

```

```

<Instances: sub interfaces>+≡
module function process_instance_get_first_active_i_term &
    (instance) result (i_term)
    integer :: i_term

```

```

        class(process_instance_t), intent(in) :: instance
    end function process_instance_get_first_active_i_term

<Instances: procedures>+=
    module function process_instance_get_first_active_i_term &
        (instance) result (i_term)
        integer :: i_term
        class(process_instance_t), intent(in) :: instance
        integer :: i
        i_term = 0
        do i = 1, size (instance%term)
            if (instance%term(i)%active) then
                i_term = i
                exit
            end if
        end do
    end function process_instance_get_first_active_i_term

<Instances: process instance: TBP>+=
    procedure :: get_real_of_mci => process_instance_get_real_of_mci

<Instances: sub interfaces>+=
    module function process_instance_get_real_of_mci (instance) result (i_real)
        integer :: i_real
        class(process_instance_t), intent(in) :: instance
    end function process_instance_get_real_of_mci

<Instances: procedures>+=
    module function process_instance_get_real_of_mci (instance) result (i_real)
        integer :: i_real
        class(process_instance_t), intent(in) :: instance
        select type (pcm_work => instance%pcm_work)
        type is (pcm_nlo_workspace_t)
            i_real = pcm_work%i_mci_to_real_component (instance%i_mci)
        end select
    end function process_instance_get_real_of_mci

<Instances: process instance: TBP>+=
    procedure :: get_connected_states => process_instance_get_connected_states

<Instances: sub interfaces>+=
    module function process_instance_get_connected_states &
        (instance, i_component) result (connected)
        type(connected_state_t), dimension(:), allocatable :: connected
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_component
    end function process_instance_get_connected_states

<Instances: procedures>+=
    module function process_instance_get_connected_states &
        (instance, i_component) result (connected)
        type(connected_state_t), dimension(:), allocatable :: connected
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_component
        connected = instance%process%get_connected_states (i_component, &
            instance%term(:)%connected)
    end function process_instance_get_connected_states

```

```
end function process_instance_get_connected_states
```

Get the hadronic center-of-mass energy

<Instances: process instance: TBP>+≡

```
procedure :: get_sqrts => process_instance_get_sqrts
```

<Instances: sub interfaces>+≡

```
module function process_instance_get_sqrts (instance) result (sqrts)
  class(process_instance_t), intent(in) :: instance
  real(default) :: sqrts
end function process_instance_get_sqrts
```

<Instances: procedures>+≡

```
module function process_instance_get_sqrts (instance) result (sqrts)
  class(process_instance_t), intent(in) :: instance
  real(default) :: sqrts
  sqrts = instance%process%get_sqrts ()
end function process_instance_get_sqrts
```

Get the polarizations

<Instances: process instance: TBP>+≡

```
procedure :: get_polarization => process_instance_get_polarization
```

<Instances: sub interfaces>+≡

```
module function process_instance_get_polarization (instance) result (pol)
  class(process_instance_t), intent(in) :: instance
  real(default), dimension(:), allocatable :: pol
end function process_instance_get_polarization
```

<Instances: procedures>+≡

```
module function process_instance_get_polarization (instance) result (pol)
  class(process_instance_t), intent(in) :: instance
  real(default), dimension(:), allocatable :: pol
  pol = instance%process%get_polarization ()
end function process_instance_get_polarization
```

Get the beam spectrum

<Instances: process instance: TBP>+≡

```
procedure :: get_beam_file => process_instance_get_beam_file
```

<Instances: sub interfaces>+≡

```
module function process_instance_get_beam_file (instance) result (file)
  class(process_instance_t), intent(in) :: instance
  type(string_t) :: file
end function process_instance_get_beam_file
```

<Instances: procedures>+≡

```
module function process_instance_get_beam_file (instance) result (file)
  class(process_instance_t), intent(in) :: instance
  type(string_t) :: file
  file = instance%process%get_beam_file ()
end function process_instance_get_beam_file
```

Get the process name

<Instances: process instance: TBP>+≡

```
procedure :: get_process_name => process_instance_get_process_name
```

```

<Instances: sub interfaces>+≡
    module function process_instance_get_process_name (instance) result (name)
        class(process_instance_t), intent(in) :: instance
        type(string_t) :: name
    end function process_instance_get_process_name

<Instances: procedures>+≡
    module function process_instance_get_process_name (instance) result (name)
        class(process_instance_t), intent(in) :: instance
        type(string_t) :: name
        name = instance%process%get_id ()
    end function process_instance_get_process_name

```

Particle sets

Here we provide two procedures that convert the process instance from/to a particle set. The conversion applies to the trace evaluator which has no quantum-number information, thus it involves only the momenta and the parent-child relations. We keep virtual particles.

If `n_incoming` is provided, the status code of the first `n_incoming` particles will be reset to incoming. Otherwise, they would be classified as virtual.

Nevertheless, it is possible to reconstruct the complete structure from a particle set. The reconstruction implies a re-evaluation of the structure function and matrix-element codes.

The `i_term` index is needed for both input and output, to select among different active trace evaluators.

In both cases, the `instance` object must be properly initialized.

NB: The `recover_beams` option should be used only when the particle set originates from an external event file, and the user has asked for it. It should be switched off when reading from raw event file.

```

<Instances: process instance: TBP>+≡
    procedure :: get_trace => process_instance_get_trace
    procedure :: set_trace => process_instance_set_trace

<Instances: sub interfaces>+≡
    module subroutine process_instance_get_trace &
        (instance, pset, i_term, n_incoming)
        class(process_instance_t), intent(in), target :: instance
        type(particle_set_t), intent(out) :: pset
        integer, intent(in) :: i_term
        integer, intent(in), optional :: n_incoming
    end subroutine process_instance_get_trace
    module subroutine process_instance_set_trace &
        (instance, pset, i_term, recover_beams, check_match, success)
        class(process_instance_t), intent(inout), target :: instance
        type(particle_set_t), intent(in) :: pset
        integer, intent(in) :: i_term
        logical, intent(in), optional :: recover_beams, check_match
        logical, intent(out), optional :: success
    end subroutine process_instance_set_trace

```

(Instances: procedures)+≡

```

module subroutine process_instance_get_trace &
  (instance, pset, i_term, n_incoming)
  class(process_instance_t), intent(in), target :: instance
  type(particle_set_t), intent(out) :: pset
  integer, intent(in) :: i_term
  integer, intent(in), optional :: n_incoming
  type(interaction_t), pointer :: int
  logical :: ok
  int => instance%get_trace_int_ptr (i_term)
  call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true., n_incoming)
end subroutine process_instance_get_trace

module subroutine process_instance_set_trace &
  (instance, pset, i_term, recover_beams, check_match, success)
  class(process_instance_t), intent(inout), target :: instance
  type(particle_set_t), intent(in) :: pset
  integer, intent(in) :: i_term
  logical, intent(in), optional :: recover_beams, check_match
  logical, intent(out), optional :: success
  type(interaction_t), pointer :: int
  integer :: n_in
  int => instance%get_trace_int_ptr (i_term)
  n_in = instance%process%get_n_in ()
  call pset%fill_interaction (int, n_in, &
    recover_beams = recover_beams, &
    check_match = check_match, &
    state_flg = instance%get_state_flg (i_term), &
    success = success)
end subroutine process_instance_set_trace

```

This procedure allows us to override any QCD setting of the WHIZARD process and directly set the coupling value that comes together with a particle set.

(Instances: process instance: TBP)+≡

```

procedure :: set_alpha_qcd_forced => process_instance_set_alpha_qcd_forced

```

(Instances: sub interfaces)+≡

```

module subroutine process_instance_set_alpha_qcd_forced &
  (instance, i_term, alpha_qcd)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
  real(default), intent(in) :: alpha_qcd
end subroutine process_instance_set_alpha_qcd_forced

```

(Instances: procedures)+≡

```

module subroutine process_instance_set_alpha_qcd_forced &
  (instance, i_term, alpha_qcd)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
  real(default), intent(in) :: alpha_qcd
  call instance%term(i_term)%set_alpha_qcd_forced (alpha_qcd)
end subroutine process_instance_set_alpha_qcd_forced

```

```

<Instances: process instance: TBP>+≡
    procedure :: has_nlo_component => process_instance_has_nlo_component

<Instances: sub interfaces>+≡
    module function process_instance_has_nlo_component (instance) result (nlo)
        class(process_instance_t), intent(in) :: instance
        logical :: nlo
    end function process_instance_has_nlo_component

<Instances: procedures>+≡
    module function process_instance_has_nlo_component (instance) result (nlo)
        class(process_instance_t), intent(in) :: instance
        logical :: nlo
        nlo = instance%process%is_nlo_calculation ()
    end function process_instance_has_nlo_component

<Instances: process instance: TBP>+≡
    procedure :: keep_failed_events => process_instance_keep_failed_events

<Instances: sub interfaces>+≡
    module function process_instance_keep_failed_events (instance) result (keep)
        logical :: keep
        class(process_instance_t), intent(in) :: instance
    end function process_instance_keep_failed_events

<Instances: procedures>+≡
    module function process_instance_keep_failed_events (instance) result (keep)
        logical :: keep
        class(process_instance_t), intent(in) :: instance
        keep = instance%mci_work(instance%i_mci)%keep_failed_events
    end function process_instance_keep_failed_events

<Instances: process instance: TBP>+≡
    procedure :: get_term_indices => process_instance_get_term_indices

<Instances: sub interfaces>+≡
    module function process_instance_get_term_indices &
        (instance, nlo_type) result (i_term)
        integer, dimension(:), allocatable :: i_term
        class(process_instance_t), intent(in) :: instance
        integer :: nlo_type
    end function process_instance_get_term_indices

<Instances: procedures>+≡
    module function process_instance_get_term_indices &
        (instance, nlo_type) result (i_term)
        integer, dimension(:), allocatable :: i_term
        class(process_instance_t), intent(in) :: instance
        integer :: nlo_type
        allocate (i_term (count (instance%term%nlo_type == nlo_type)))
        i_term = pack (instance%term%get_i_term_global (), &
            instance%term%nlo_type == nlo_type)
    end function process_instance_get_term_indices

<Instances: process instance: TBP>+≡
    procedure :: get_boost_to_lab => process_instance_get_boost_to_lab

```

```

<Instances: sub interfaces>+≡
    module function process_instance_get_boost_to_lab &
        (instance, i_term) result (lt)
        type(lorentz_transformation_t) :: lt
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
    end function process_instance_get_boost_to_lab

<Instances: procedures>+≡
    module function process_instance_get_boost_to_lab &
        (instance, i_term) result (lt)
        type(lorentz_transformation_t) :: lt
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        lt = instance%kin(i_term)%get_boost_to_lab ()
    end function process_instance_get_boost_to_lab

<Instances: process instance: TBP>+≡
    procedure :: get_boost_to_cms => process_instance_get_boost_to_cms

<Instances: sub interfaces>+≡
    module function process_instance_get_boost_to_cms &
        (instance, i_term) result (lt)
        type(lorentz_transformation_t) :: lt
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
    end function process_instance_get_boost_to_cms

<Instances: procedures>+≡
    module function process_instance_get_boost_to_cms &
        (instance, i_term) result (lt)
        type(lorentz_transformation_t) :: lt
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        lt = instance%kin(i_term)%get_boost_to_cms ()
    end function process_instance_get_boost_to_cms

<Instances: process instance: TBP>+≡
    procedure :: lab_is_cm => process_instance_lab_is_cm

<Instances: sub interfaces>+≡
    module function process_instance_lab_is_cm &
        (instance, i_term) result (lab_is_cm)
        logical :: lab_is_cm
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
    end function process_instance_lab_is_cm

<Instances: procedures>+≡
    module function process_instance_lab_is_cm &
        (instance, i_term) result (lab_is_cm)
        logical :: lab_is_cm
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        lab_is_cm = instance%kin(i_term)%phs%lab_is_cm ()
    end function process_instance_lab_is_cm

```

The `pacify` subroutine has the purpose of setting numbers to zero which are (by comparing with a `tolerance` parameter) considered equivalent with zero. We do this in some unit tests. Here, we apply this to the phase space subobject of the process instance.

```

<Instances: public>+≡
    public :: pacify

<Instances: interfaces>+≡
    interface pacify
        module procedure pacify_process_instance
    end interface pacify

<Instances: sub interfaces>+≡
    module subroutine pacify_process_instance (instance)
        type(process_instance_t), intent(inout) :: instance
    end subroutine pacify_process_instance

<Instances: procedures>+≡
    module subroutine pacify_process_instance (instance)
        type(process_instance_t), intent(inout) :: instance
        integer :: i
        do i = 1, size (instance%kin)
            call pacify (instance%kin(i)%phs)
        end do
    end subroutine pacify_process_instance

```

30.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<processes_ut.f90>≡
    <File header>

    module processes_ut
        use unit_tests
        use processes_uti

    <Standard module head>

    <Processes: public test>

    <Processes: public test auxiliary>

    contains

    <Processes: test driver>

    end module processes_ut

<processes_uti.f90>≡
    <File header>

    module processes_uti

```



```

<Use kinds>
<Use strings>
  use format_utils, only: write_separator
  use constants, only: TWOPI4
  use physics_defs, only: CONV
  use os_interface
  use sm_qcd
  use lorentz
  use pdg_arrays
  use model_data
  use models
  use var_base, only: vars_t
  use variables, only: var_list_t
  use model_testbed, only: prepare_model
  use particle_specifiers, only: new_prt_spec
  use flavors
  use interactions, only: reset_interaction_counter
  use particles
  use rng_base
  use mci_base
  use mci_none, only: mci_none_t
  use mci_midpoint
  use sf_mappings
  use sf_base
  use phs_base
  use phs_single
  use phs_forests, only: syntax_phs_forest_init, syntax_phs_forest_final
  use phs_wood, only: phs_wood_config_t
  use resonances, only: resonance_history_set_t
  use process_constants
  use prc_core_def, only: prc_core_def_t
  use prc_core
  use prc_test, only: prc_test_create_library
  use prc_template_me, only: template_me_def_t
  use process_libraries
  use prc_test_core
  use pdf, only: pdf_data_t

  use process_counter
  use process_config, only: process_term_t
  use process, only: process_t
  use instances, only: process_instance_t, process_instance_hook_t

  use rng_base_ut, only: rng_test_factory_t
  use sf_base_ut, only: sf_test_data_t
  use mci_base_ut, only: mci_test_t
  use phs_base_ut, only: phs_test_config_t

<Standard module head>

<Processes: public test auxiliary>

<Processes: test declarations>

```

```

    <Processes: test types>

contains

    <Processes: tests>

    <Processes: test auxiliary>

end module processes_util

```

API: driver for the unit tests below.

```

<Processes: public test>≡
    public :: processes_test

<Processes: test driver>≡
    subroutine processes_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Processes: execute tests>
    end subroutine processes_test

```

Write an empty process object

The most trivial test is to write an uninitialized process object.

```

<Processes: execute tests>≡
    call test (processes_1, "processes_1", &
        "write an empty process object", &
        u, results)

<Processes: test declarations>≡
    public :: processes_1

<Processes: tests>≡
    subroutine processes_1 (u)
        integer, intent(in) :: u
        type(process_t) :: process

        write (u, "(A)")  "* Test output: processes_1"
        write (u, "(A)")  "* Purpose: display an empty process object"
        write (u, "(A)")

        call process%write (.false., u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: processes_1"

    end subroutine processes_1

```

Initialize a process object

Initialize a process and display it.

```

<Processes: execute tests>+≡

```

```

    call test (processes_2, "processes_2", &
        "initialize a simple process object", &
        u, results)
<Processes: test declarations>+≡
    public :: processes_2
<Processes: tests>+≡
    subroutine processes_2 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable :: process
        class(mci_t), allocatable :: mci_template
        class(phs_config_t), allocatable :: phs_config_template

        write (u, "(A)")  "* Test output: processes_2"
        write (u, "(A)")  "* Purpose: initialize a simple process object"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a test library with one process"
        write (u, "(A)")

        libname = "processes2"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib)

        write (u, "(A)")  "* Initialize a process object"
        write (u, "(A)")

        call model%init_test ()

        allocate (process)
        call process%init (procname, lib, os_data, model)
        call process%set_run_id (var_str ("run_2"))
        call process%setup_test_cores ()

        allocate (phs_test_config_t :: phs_config_template)
        call process%init_components (phs_config_template)

        call process%setup_mci (dispatch_mci_empty)

        call process%write (.false., u)

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call process%final ()
        deallocate (process)

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_2"

end subroutine processes_2

```

Trivial for testing: do not allocate the MCI record.

```

<Processes: test auxiliary>≡
subroutine dispatch_mci_empty (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
end subroutine dispatch_mci_empty

```

Compute a trivial matrix element

Initialize a process, retrieve some information and compute a matrix element.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Processes: execute tests>+≡
call test (processes_3, "processes_3", &
  "retrieve a trivial matrix element", &
  u, results)

<Processes: test declarations>+≡
public :: processes_3

<Processes: tests>+≡
subroutine processes_3 (u)
  integer, intent(in) :: u
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), target :: model
  type(process_t), allocatable :: process
  class(phs_config_t), allocatable :: phs_config_template
  type(process_constants_t) :: data
  type(vector4_t), dimension(:), allocatable :: p

  write (u, "(A)")  "* Test output: processes_3"
  write (u, "(A)")  "* Purpose: create a process &
    &and compute a matrix element"
  write (u, "(A)")

  write (u, "(A)")  "* Build and load a test library with one process"
  write (u, "(A)")

  libname = "processes3"
  procname = libname

```

```

call os_data%init ()
call prc_test_create_library (libname, lib)

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)
call process%setup_test_cores ()

allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)
call process%setup_mci (dispatch_mci_test3)

write (u, "(A)")  "* Return the number of process components"
write (u, "(A)")

write (u, "(A,I0)")  "n_components = ", process%get_n_components ()

write (u, "(A)")
write (u, "(A)")  "* Return the number of flavor states"
write (u, "(A)")

data = process%get_constants (1)

write (u, "(A,I0)")  "n_flv(1) = ", data%n_flv

write (u, "(A)")
write (u, "(A)")  "* Return the first flavor state"
write (u, "(A)")

write (u, "(A,4(1x,I0))")  "flv_state(1) =", data%flv_state (:,1)

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics &
    &[arbitrary, the matrix element is constant]"

allocate (p (4))

write (u, "(A)")
write (u, "(A)")  "* Retrieve the matrix element"
write (u, "(A)")

write (u, "(A,F5.3,' + ',F5.3,' I')")  "me (1, p, 1, 1, 1) = ", &
    process%compute_amplitude (1, 1, 1, p, 1, 1, 1)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_3"

end subroutine processes_3

```

MCI record with some contents.

```

<Processes: test auxiliary>+≡
subroutine dispatch_mci_test3 (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_test_t :: mci)
  select type (mci)
  type is (mci_test_t)
    call mci%set_dimensions (2, 2)
    call mci%set_divisions (100)
  end select
end subroutine dispatch_mci_test3

```

Generate a process instance

Initialize a process and process instance, choose a sampling point and fill the process instance.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Processes: execute tests>+≡
call test (processes_4, "processes_4", &
  "create and fill a process instance (partonic event)", &
  u, results)

<Processes: test declarations>+≡
public :: processes_4

<Processes: tests>+≡
subroutine processes_4 (u)
  integer, intent(in) :: u
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), target :: model
  type(process_t), allocatable, target :: process
  class(phs_config_t), allocatable :: phs_config_template
  real(default) :: sqrts
  type(process_instance_t), allocatable, target :: process_instance
  type(particle_set_t) :: pset

  write (u, "(A)")  "* Test output: processes_4"
  write (u, "(A)")  "* Purpose: create a process &
    &and fill a process instance"
  write (u, "(A)")

```

```

write (u, "(A)")  "* Build and initialize a test process"
write (u, "(A)")

libname = "processes4"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpars ([0._default, 0._default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

```

```

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)

call process_instance%activate ()
process_instance%evaluation_status = STAT_EFF_KINEMATICS
call process_instance%recover_hard_kinematics (i_term = 1)
call process_instance%recover_seed_kinematics (i_term = 1)
call process_instance%select_channel (1)
call process_instance%recover_mcpair (i_term = 1)

call process_instance%compute_seed_kinematics (skip_term = 1)
call process_instance%compute_hard_kinematics (skip_term = 1)
call process_instance%compute_eff_kinematics (skip_term = 1)

call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels (skip_term = 1)
call process_instance%evaluate_trace ()
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```



```

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_4"

end subroutine processes_4

```

Structure function configuration

Configure structure functions (multi-channel) in a process object.

```

<Processes: execute tests>+≡
  call test (processes_7, "processes_7", &
    "process configuration with structure functions", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_7

<Processes: tests>+≡
  subroutine processes_7 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_channel_t), dimension(2) :: sf_channel

    write (u, "(A)")  "* Test output: processes_7"
    write (u, "(A)")  "* Purpose: initialize a process with &
      &structure functions"
    write (u, "(A)")

    write (u, "(A)")  "* Build and initialize a process object"
    write (u, "(A)")

    libname = "processes7"
    procname = libname

    call os_data%init ()
    call prc_test_create_library (libname, lib)

```

```

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%test_allocate_sf_channels (3)

call sf_channel(1)%init (2)
call sf_channel(1)%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel(1))

call sf_channel(2)%init (2)
call sf_channel(2)%set_s_mapping ([1,2])
call process%set_sf_channel (3, sf_channel(2))

call process%setup_mci (dispatch_mci_empty)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_7"

```

```
end subroutine processes_7
```

Evaluating a process with structure function

Configure structure functions (single-channel) in a process object, create an instance, compute kinematics and evaluate.

Note the order of operations when setting up structure functions and phase space. The beams are first, they determine the `sqrts` value. We can also set up the chain of structure functions. We then configure the phase space. From this, we can obtain information about special configurations (resonances, etc.), which we need for allocating the possible structure-function channels (parameterizations and mappings). Finally, we match phase-space channels onto structure-function channels.

In the current example, this matching is trivial; we only have one structure-function channel.

```
<Processes: execute tests>+≡
  call test (processes_8, "processes_8", &
    "process evaluation with structure functions", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_8

<Processes: tests>+≡
  subroutine processes_8 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t), allocatable, target :: process_instance
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_channel_t) :: sf_channel
    type(particle_set_t) :: pset

    write (u, "(A)")  "* Test output: processes_8"
    write (u, "(A)")  "* Purpose: evaluate a process with &
      &structure functions"
    write (u, "(A)")

    write (u, "(A)")  "* Build and initialize a process object"
    write (u, "(A)")

    libname = "processes8"
    procname = libname
```

```

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%configure_phs ()

call process%test_allocate_sf_channels (1)

call sf_channel%init (2)
call sf_channel%activate_mapping ([1,2])
call process%set_sf_channel (1, sf_channel)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_mci (dispatch_mci_empty)
call process%setup_terms ()

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)

```

```

call process_instance%init (process)

write (u, "(A)")  "* Set up kinematics and evaluate"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, &
    [0.8_default, 0.8_default, 0.1_default, 0.2_default])
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pacify (pset)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (2)

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 1, i_term = 1, update_sqme = .true., recover_phs = .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_8"

```

```
end subroutine processes_8
```

Multi-channel phase space and structure function

This is an extension of the previous example. This time, we have two distinct structure-function channels which are matched to the two distinct phase-space channels.

```
(Processes: execute tests)+≡
  call test (processes_9, "processes_9", &
    "multichannel kinematics and structure functions", &
    u, results)

(Processes: test declarations)+≡
  public :: processes_9

(Processes: tests)+≡
  subroutine processes_9 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t), allocatable, target :: process_instance
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_channel_t) :: sf_channel
    real(default), dimension(4) :: x_saved
    type(particle_set_t) :: pset

    write (u, "(A)")  "* Test output: processes_9"
    write (u, "(A)")  "*   Purpose: evaluate a process with &
      &structure functions"
    write (u, "(A)")  "*               in a multi-channel configuration"
    write (u, "(A)")

    write (u, "(A)")  "* Build and initialize a process object"
    write (u, "(A)")

    libname = "processes9"
    procname = libname

    call os_data%init ()
    call prc_test_create_library (libname, lib)

    call reset_interaction_counter ()

    call model%init_test ()
```

```

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%configure_phs ()

call process%test_allocate_sf_channels (2)

call sf_channel%init (2)
call process%set_sf_channel (1, sf_channel)

call sf_channel%init (2)
call sf_channel%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel)

call process%test_set_component_sf_channel ([1, 2])

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_mci (dispatch_mci_empty)
call process%setup_terms ()

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

```

```

write (u, "(A)")  "* Set up kinematics in channel 1 and evaluate"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, &
    [0.8_default, 0.8_default, 0.1_default, 0.2_default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract MC input parameters"
write (u, "(A)")

write (u, "(A)")  "Channel 1:"
call process_instance%get_mcpair (1, x_saved)
write (u, "(2x,9(1x,F7.5))")  x_saved

write (u, "(A)")  "Channel 2:"
call process_instance%get_mcpair (2, x_saved)
write (u, "(2x,9(1x,F7.5))")  x_saved

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics in channel 2 and evaluate"
write (u, "(A)")

call process_instance%evaluate_sqme (2, x_saved)
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance for channel 2"
write (u, "(A)")

call reset_interaction_counter (2)

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 2, i_term = 1, update_sqme = .true., recover_phs = .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()

call process_instance%final ()
deallocate (process_instance)

```



```

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_9"

end subroutine processes_9

```

Event generation

Activate the MC integrator for the process object and use it to generate a single event. Note that the test integrator does not require integration in preparation for generating events.

```

<Processes: execute tests>+≡
  call test (processes_10, "processes_10", &
    "event generation", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_10

<Processes: tests>+≡
  subroutine processes_10 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(mci_t), pointer :: mci
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t), allocatable, target :: process_instance

    write (u, "(A)")  "* Test output: processes_10"
    write (u, "(A)")  "* Purpose: generate events for a process without &
      &structure functions"
    write (u, "(A)")  "*           in a multi-channel configuration"
    write (u, "(A)")

    write (u, "(A)")  "* Build and initialize a process object"
    write (u, "(A)")

    libname = "processes10"
    procname = libname

    call os_data%init ()
    call prc_test_create_library (libname, lib)

    call reset_interaction_counter ()

```

```

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()

call process%setup_mci (dispatch_mci_test10)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call process%test_get_mci_ptr (mci)
select type (mci)
type is (mci_test_t)
! This ensures that the next 'random' numbers are 0.3, 0.5, 0.7
call mci%rng%init (3)
! Include the constant PHS factor in the stored maximum of the integrand
call mci%set_max_factor (conv * twopi4 &
/ (2 * sqrt (lambda (sqrt_s **2, 125._default**2, 125._default**2)))
end select

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call process_instance%generate_unweighted_event (1)
call process%test_get_mci_ptr (mci)

```

```

select type (mci)
type is (mci_test_t)
    write (u, "(A,I0)") " Success in try ", mci%tries
    write (u, "(A)")
end select

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_10"

end subroutine processes_10

```

MCI record with some contents.

```

<Processes: test auxiliary>+≡
subroutine dispatch_mci_test10 (mci, var_list, process_id, is_nlo)
    class(mci_t), allocatable, intent(out) :: mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    logical, intent(in), optional :: is_nlo
    allocate (mci_test_t :: mci)
    select type (mci)
    type is (mci_test_t); call mci%set_divisions (100)
    end select
end subroutine dispatch_mci_test10

```

Integration

Activate the MC integrator for the process object and use it to integrate over phase space.

```

<Processes: execute tests>+≡
    call test (processes_11, "processes_11", &
        "integration", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_11

<Processes: tests>+≡
subroutine processes_11 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib

```

```

type(string_t) :: libname
type(string_t) :: procname
type(os_data_t) :: os_data
type(model_t), target :: model
type(process_t), allocatable, target :: process
class(mci_t), allocatable :: mci_template
class(phs_config_t), allocatable :: phs_config_template
real(default) :: sqrts
type(process_instance_t), allocatable, target :: process_instance

write (u, "(A)")  "* Test output: processes_11"
write (u, "(A)")  "*   Purpose: integrate a process without &
                    &structure functions"
write (u, "(A)")  "*               in a multi-channel configuration"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes11"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()

allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

call process%setup_mci (dispatch_mci_test10)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"

```

```

write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Integrate with default test parameters"
write (u, "(A)")

call process_instance%integrate (1, n_it=1, n_calls=10000)
call process%final_integration (1)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A,ES13.7)")  " Integral divided by phs factor = ", &
    process%get_integral (1) &
    / process_instance%kin(1)%phs_factor

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_11"

end subroutine processes_11

```

Complete events

For the purpose of simplifying further tests, we implement a convenience routine that initializes a process and prepares a single event. This is a wrapup of the test `processes_10`.

The procedure is re-exported by the `processes_ut` module.

```

<Processes: public test auxiliary>≡
  public :: prepare_test_process

<Processes: test auxiliary>+≡
  subroutine prepare_test_process &
    (process, process_instance, model, var_list, run_id)
    type(process_t), intent(out), target :: process
    type(process_instance_t), intent(out), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(var_list_t), intent(inout), optional :: var_list
    type(string_t), intent(in), optional :: run_id
    type(process_library_t), target :: lib
    type(string_t) :: libname

```

```

type(string_t) :: procname
type(os_data_t) :: os_data
type(model_t), allocatable, target :: process_model
class(mci_t), pointer :: mci
class(phs_config_t), allocatable :: phs_config_template
real(default) :: sqrts
libname = "processes_test"
procname = libname
call os_data%init ()
call prc_test_create_library (libname, lib)
call reset_interaction_counter ()
allocate (process_model)
call process_model%init (model%get_name (), &
    model%get_n_real (), &
    model%get_n_complex (), &
    model%get_n_field (), &
    model%get_n_vtx ())
call process_model%copy_from (model)
call process%init (procname, lib, os_data, process_model, var_list)
if (present (run_id)) call process%set_run_id (run_id)
call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)
sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_test10)
call process%setup_terms ()
call process_instance%init (process)
call process%test_get_mci_ptr (mci)
select type (mci)
type is (mci_test_t)
    ! This ensures that the next 'random' numbers are 0.3, 0.5, 0.7
    call mci%rng%init (3)
    ! Include the constant PHS factor in the stored maximum of the integrand
    call mci%set_max_factor (conv * twopi4 &
        / (2 * sqrt (lambda (sqrts **2, 125._default**2, 125._default**2))))
end select
call process%reset_library_ptr () ! avoid dangling pointer
call process_model%final ()
end subroutine prepare_test_process

```

Here we do the cleanup of the process and process instance emitted by the previous routine.

```

<Processes: public test auxiliary>+≡
    public :: cleanup_test_process

<Processes: test auxiliary>+≡
    subroutine cleanup_test_process (process, process_instance)
        type(process_t), intent(inout) :: process
        type(process_instance_t), intent(inout) :: process_instance
        call process_instance%final ()
        call process%final ()
    end subroutine cleanup_test_process

```

This is the actual test. Prepare the test process and event, fill all evaluators, and display the results. Use a particle set as temporary storage, read kinematics and recalculate the event.

```

<Processes: execute tests>+≡
    call test (processes_12, "processes_12", &
               "event post-processing", &
               u, results)

<Processes: test declarations>+≡
    public :: processes_12

<Processes: tests>+≡
    subroutine processes_12 (u)
        integer, intent(in) :: u
        type(process_t), allocatable, target :: process
        type(process_instance_t), allocatable, target :: process_instance
        type(particle_set_t) :: pset
        type(model_data_t), target :: model

        write (u, "(A)")  "* Test output: processes_12"
        write (u, "(A)")  "* Purpose: generate a complete partonic event"
        write (u, "(A)")

        call model%init_test ()

        write (u, "(A)")  "* Build and initialize process and process instance &
                           &and generate event"
        write (u, "(A)")

        allocate (process)
        allocate (process_instance)
        call prepare_test_process (process, process_instance, model, &
                                   run_id = var_str ("run_12"))
        call process_instance%setup_event_data (i_core = 1)

        call process%prepare_simulation (1)
        call process_instance%init_simulation (1)
        call process_instance%generate_weighted_event (1)
        call process_instance%evaluate_event_data ()

        call process_instance%write (u)

        call process_instance%get_trace (pset, 1)

        call process_instance%final_simulation (1)
        call process_instance%final ()
        deallocate (process_instance)

        write (u, "(A)")
        write (u, "(A)")  "* Recover kinematics and recalculate"
        write (u, "(A)")

        call reset_interaction_counter (2)

```

```

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 1, i_term = 1, update_sqme = .true., recover_phs = .true.)

call process_instance%recover_event ()
call process_instance%evaluate_event_data ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_12"

end subroutine processes_12

```

Colored interaction

This test specifically checks the transformation of process data (flavor, helicity, and color) into an interaction in a process term.

We use the `test_t` process core (which has no nontrivial particles), but call only the `is_allowed` method, which always returns true.

```

<Processes: execute tests>+≡
    call test (processes_13, "processes_13", &
        "colored interaction", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_13

<Processes: tests>+≡
    subroutine processes_13 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_data_t), target :: model
        type(process_term_t) :: term
        class(prc_core_t), allocatable :: core

        write (u, "(A)")  "* Test output: processes_13"
    end subroutine

```



```

write (u, "(A)")  "*"   Purpose: initialized a colored interaction"
write (u, "(A)")

write (u, "(A)")  "*" Set up a process constants block"
write (u, "(A)")

call os_data%init ()
call model%init_sm_test ()

allocate (test_t :: core)

associate (data => term%data)
  data%n_in = 2
  data%n_out = 3
  data%n_flv = 2
  data%n_hel = 2
  data%n_col = 2
  data%n_cin = 2

  allocate (data%flv_state (5, 2))
  data%flv_state (:,1) = [ 1, 21, 1, 21, 21]
  data%flv_state (:,2) = [ 2, 21, 2, 21, 21]

  allocate (data%hel_state (5, 2))
  data%hel_state (:,1) = [1, 1, 1, 1, 0]
  data%hel_state (:,2) = [1,-1, 1,-1, 0]

  allocate (data%col_state (2, 5, 2))
  data%col_state (:,:,1) = &
    reshape ([[1, 0], [2,-1], [3, 0], [2,-3], [0,0]], [2,5])
  data%col_state (:,:,2) = &
    reshape ([[1, 0], [2,-3], [3, 0], [2,-1], [0,0]], [2,5])

  allocate (data%ghost_flag (5, 2))
  data%ghost_flag(1:4,:) = .false.
  data%ghost_flag(5,:) = .true.

end associate

write (u, "(A)")  "*" Set up the interaction"
write (u, "(A)")

call reset_interaction_counter ()
call term%setup_interaction (core, model)
call term%int%basic_write (u)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: processes_13"
end subroutine processes_13

```

MD5 sums

Configure a process with structure functions (multi-channel) and compute MD5 sums

```
(Processes: execute tests)+≡
    call test (processes_14, "processes_14", &
               "process configuration and MD5 sum", &
               u, results)

(Processes: test declarations)+≡
    public :: processes_14

(Processes: tests)+≡
    subroutine processes_14 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        type(sf_config_t), dimension(:), allocatable :: sf_config
        type(sf_channel_t), dimension(3) :: sf_channel

        write (u, "(A)")  "* Test output: processes_14"
        write (u, "(A)")  "*   Purpose: initialize a process with &
                           &structure functions"
        write (u, "(A)")  "*                           and compute MD5 sum"
        write (u, "(A)")

        write (u, "(A)")  "* Build and initialize a process object"
        write (u, "(A)")

        libname = "processes7"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib)
        call lib%compute_md5sum ()

        call model%init_test ()

        allocate (process)
        call process%init (procname, lib, os_data, model)

        call process%setup_test_cores ()
        allocate (phs_test_config_t :: phs_config_template)
        call process%init_components (phs_config_template)

        write (u, "(A)")  "* Set beam, structure functions, and mappings"
        write (u, "(A)")
```

```

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

call process%test_allocate_sf_channels (3)

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call sf_channel(1)%init (2)
call process%set_sf_channel (1, sf_channel(1))

call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel(2))

call sf_channel(3)%init (2)
call sf_channel(3)%set_s_mapping ([1,2])
call process%set_sf_channel (3, sf_channel(3))

call process%setup_mci (dispatch_mci_empty)

call process%compute_md5sum ()

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_14"

end subroutine processes_14

```

Decay Process Evaluation

Initialize and evaluate a decay process.

```

<Processes: execute tests>+≡
    call test (processes_15, "processes_15", &
        "decay process", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_15

<Processes: tests>+≡
    subroutine processes_15 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        type(process_instance_t), allocatable, target :: process_instance
        type(particle_set_t) :: pset

        write (u, "(A)")  "* Test output: processes_15"
        write (u, "(A)")  "* Purpose: initialize a decay process object"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a test library with one process"
        write (u, "(A)")

        libname = "processes15"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib, scattering = .false., &
            decay = .true.)

        call model%init_test ()
        call model%set_par (var_str ("ff"), 0.4_default)
        call model%set_par (var_str ("mf"), &
            model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

        write (u, "(A)")  "* Initialize a process object"
        write (u, "(A)")

        allocate (process)
        call process%init (procname, lib, os_data, model)

        call process%setup_test_cores ()
        allocate (phs_single_config_t :: phs_config_template)
        call process%init_components (phs_config_template)

        write (u, "(A)")  "* Prepare a trivial beam setup"
        write (u, "(A)")

        call process%setup_beams_decay (i_core = 1)
        call process%configure_phs ()

```

```

call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpair ([0._default, 0._default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover (1, 1, .true., .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_15"

end subroutine processes_15

```

Integration: decay

Activate the MC integrator for the decay object and use it to integrate over phase space.

```

<Processes: execute tests>+≡
  call test (processes_16, "processes_16", &
    "decay integration", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_16

<Processes: tests>+≡
  subroutine processes_16 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template

```

```

type(process_instance_t), allocatable, target :: process_instance

write (u, "(A)")  "* Test output: processes_16"
write (u, "(A)")  "*   Purpose: integrate a process without &
                    &structure functions"
write (u, "(A)")  "*               in a multi-channel configuration"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes16"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib, scattering = .false., &
                             decay = .true.)

call reset_interaction_counter ()

call model%init_test ()
call model%set_par (var_str ("ff"), 0.4_default)
call model%set_par (var_str ("mf"), &
                    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

call process%setup_beams_decay (i_core = 1)
call process%configure_phs ()

call process%setup_mci (dispatch_mci_test_midpoint)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Integrate with default test parameters"

```

```

write (u, "(A)")

call process_instance%integrate (1, n_it=1, n_calls=10000)
call process%final_integration (1)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A,ES13.7)") " Integral divided by phs factor = ", &
    process%get_integral (1) &
    / process_instance%kin(1)%phs_factor

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_16"

end subroutine processes_16

```

MCI record prepared for midpoint integrator.

```

<Processes: test auxiliary>+≡
subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
class(mci_t), allocatable, intent(out) :: mci
type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_id
logical, intent(in), optional :: is_nlo
allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

Decay Process Evaluation

Initialize and evaluate a decay process for a moving particle.

```

<Processes: execute tests>+≡
call test (processes_17, "processes_17", &
    "decay of moving particle", &
    u, results)

<Processes: test declarations>+≡
public :: processes_17

<Processes: tests>+≡
subroutine processes_17 (u)
integer, intent(in) :: u
type(process_library_t), target :: lib

```



```

type(string_t) :: libname
type(string_t) :: procname
type(os_data_t) :: os_data
type(model_t), target :: model
type(process_t), allocatable, target :: process
class(phs_config_t), allocatable :: phs_config_template
type(process_instance_t), allocatable, target :: process_instance
type(particle_set_t) :: pset
type(flavor_t) :: flv_beam
real(default) :: m, p, E

write (u, "(A)")  "* Test output: processes_17"
write (u, "(A)")  "* Purpose: initialize a decay process object"
write (u, "(A)")

write (u, "(A)")  "* Build and load a test library with one process"
write (u, "(A)")

libname = "processes17"
procname = libname

call os_data%init ()

call prc_test_create_library (libname, lib, scattering = .false., &
    decay = .true.)

write (u, "(A)")  "* Initialize a process object"
write (u, "(A)")

call model%init_test ()
call model%set_par (var_str ("ff"), 0.4_default)
call model%set_par (var_str ("mf"), &
    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

call process%setup_beams_decay (rest_frame = .false., i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set parent momentum and random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpair ([0._default, 0._default])

call flv_beam%init (25, process%get_model_ptr ())
m = flv_beam%get_mass ()
p = 3 * m / 4
E = sqrt (m**2 + p**2)
call process_instance%set_beam_momenta ([vector4_moving (E, p, 3)])

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover (1, 1, .true., .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_17"

end subroutine processes_17

```

Resonances in Phase Space

This test demonstrates the extraction of the resonance-history set from the generated phase space. We need a nontrivial process, but no matrix element. This is provided by the `prc_template` method, using the `SM` model. We also need the `phs_wood` method, otherwise we would not have resonances in the phase space configuration.

```

<Processes: execute tests>+≡
  call test (processes_18, "processes_18", &
    "extract resonance history set", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_18

<Processes: tests>+≡
  subroutine processes_18 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(string_t) :: model_name

```

```

type(os_data_t) :: os_data
class(model_data_t), pointer :: model
class(vars_t), pointer :: vars
type(process_t), pointer :: process
type(resonance_history_set_t) :: res_set
integer :: i

write (u, "(A)")  "* Test output: processes_18"
write (u, "(A)")  "* Purpose: extra resonance histories"
write (u, "(A)")

write (u, "(A)")  "* Build and load a test library with one process"
write (u, "(A)")

libname = "processes_18_lib"
procname = "processes_18_p"

call os_data%init ()

call syntax_phs_forest_init ()

model_name = "SM"
model => null ()
call prepare_model (model, model_name, vars)

write (u, "(A)")  "* Initialize a process library with one process"
write (u, "(A)")

select type (model)
class is (model_t)
    call prepare_resonance_test_library (lib, libname, procname, model, os_data, u)
end select

write (u, "(A)")
write (u, "(A)")  "* Initialize a process object with phase space"

allocate (process)
select type (model)
class is (model_t)
    call prepare_resonance_test_process (process, lib, procname, model, os_data)
end select

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call process%extract_resonance_history_set (res_set)
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

```

```

call model%final ()
deallocate (model)

call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_18"

end subroutine processes_18

```

Auxiliary subroutine that constructs the process library for the above test.

(Processes: test auxiliary)+≡

```

subroutine prepare_resonance_test_library &
  (lib, libname, procname, model, os_data, u)
  type(process_library_t), target, intent(out) :: lib
  type(string_t), intent(in) :: libname
  type(string_t), intent(in) :: procname
  type(model_t), intent(in), target :: model
  type(os_data_t), intent(in) :: os_data
  integer, intent(in) :: u
  type(string_t), dimension(:), allocatable :: prt_in, prt_out
  class(prc_core_def_t), allocatable :: def
  type(process_def_entry_t), pointer :: entry

  call lib%init (libname)

  allocate (prt_in (2), prt_out (3))
  prt_in = [var_str ("e+"), var_str ("e-")]
  prt_out = [var_str ("d"), var_str ("ubar"), var_str ("W+")]

  allocate (template_me_def_t :: def)
  select type (def)
  type is (template_me_def_t)
    call def%init (model, prt_in, prt_out, unity = .false.)
  end select
  allocate (entry)
  call entry%init (procname, &
    model_name = model%get_name (), &
    n_in = 2, n_components = 1)
  call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template"), &
    variant = def)
  call entry%write (u)

  call lib%append (entry)

  call lib%configure (os_data)
  call lib%write_makefile (os_data, force = .true., verbose = .false.)
  call lib%clean (os_data, distclean = .false.)
  call lib%write_driver (force = .true.)

```

```

        call lib%load (os_data)

    end subroutine prepare_resonance_test_library

```

We want a test process which has been initialized up to the point where we can evaluate the matrix element. This is in fact rather complicated. We copy the steps from `integration_setup_process` in the `integrate` module, which is not available at this point.

```

(Processes: test auxiliary)+≡
subroutine prepare_resonance_test_process &
    (process, lib, procname, model, os_data)
    class(process_t), intent(out), target :: process
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: procname
    type(model_t), intent(in), target :: model
    type(os_data_t), intent(in) :: os_data
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts

    call process%init (procname, lib, os_data, model)

    allocate (phs_config_t :: phs_config_template)
    call process%init_components (phs_config_template)

    call process%setup_test_cores (type_string = var_str ("template"))

    sqrts = 1000
    call process%setup_beams_sqrts (sqrts, i_core = 1)
    call process%configure_phs ()
    call process%setup_mci (dispatch_mci_none)

    call process%setup_terms ()

end subroutine prepare_resonance_test_process

```

MCI record prepared for the none (dummy) integrator.

```

(Processes: test auxiliary)+≡
subroutine dispatch_mci_none (mci, var_list, process_id, is_nlo)
    class(mci_t), allocatable, intent(out) :: mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    logical, intent(in), optional :: is_nlo
    allocate (mci_none_t :: mci)
end subroutine dispatch_mci_none

```

Add after evaluate hook(s)

Initialize a process and process instance, add a trivial process hook, choose a sampling point and fill the process instance.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

<Processes: test types>+≡

```

type, extends(process_instance_hook_t) :: process_instance_hook_test_t
    integer :: unit
    character(len=15) :: name
contains
    procedure :: init => process_instance_hook_test_init
    procedure :: final => process_instance_hook_test_final
    procedure :: evaluate => process_instance_hook_test_evaluate
end type process_instance_hook_test_t

```

<Processes: test auxiliary>+≡

```

subroutine process_instance_hook_test_init (hook, var_list, instance, pdf_data)
    class(process_instance_hook_test_t), intent(inout), target :: hook
    type(var_list_t), intent(in) :: var_list
    class(process_instance_t), intent(in), target :: instance
    type(pdf_data_t), intent(in), optional :: pdf_data
end subroutine process_instance_hook_test_init

subroutine process_instance_hook_test_final (hook)
    class(process_instance_hook_test_t), intent(inout) :: hook
end subroutine process_instance_hook_test_final

subroutine process_instance_hook_test_evaluate (hook, instance)
    class(process_instance_hook_test_t), intent(inout) :: hook
    class(process_instance_t), intent(in), target :: instance
    write (hook%unit, "(A)") "Execute hook:"
    write (hook%unit, "(2X,A,1X,A,I0,A)") hook%name, "(", len (trim (hook%name)), ")"
end subroutine process_instance_hook_test_evaluate

```

<Processes: execute tests>+≡

```

call test (processes_19, "processes_19", &
    "add trivial hooks to a process instance ", &
    u, results)

```

<Processes: test declarations>+≡

```

public :: processes_19

```

<Processes: tests>+≡

```

subroutine processes_19 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t) :: process_instance
    class(process_instance_hook_t), allocatable, target :: process_instance_hook, process_instance_hook_test_t
    type(particle_set_t) :: pset

    write (u, "(A)")  "*" Test output: processes_19"
    write (u, "(A)")  "*"  Purpose: allocate process instance &

```

```

        &and add an after evaluate hook"
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Allocate a process instance"
write (u, "(A)")

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate hook and add to process instance"
write (u, "(A)")

allocate (process_instance_hook_test_t :: process_instance_hook)
call process_instance%append_after_hook (process_instance_hook)

allocate (process_instance_hook_test_t :: process_instance_hook2)
call process_instance%append_after_hook (process_instance_hook2)

select type (process_instance_hook)
type is (process_instance_hook_test_t)
    process_instance_hook%unit = u
    process_instance_hook%name = "Hook 1"
end select
select type (process_instance_hook2)
type is (process_instance_hook_test_t)
    process_instance_hook2%unit = u
    process_instance_hook2%name = "Hook 2"
end select

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%evaluate_after_hook ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance_hook%final ()
deallocate (process_instance_hook)

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_19"

end subroutine processes_19

```

30.12 Process Stacks

For storing and handling multiple processes, we define process stacks. These are ordinary stacks where new process entries are pushed onto the top. We allow for multiple entries with identical process ID, but distinct run ID.

The implementation is essentially identical to the `prclib_stacks` module above. Unfortunately, Fortran supports no generic programming, so we do not make use of this fact.

When searching for a specific process ID, we will get (a pointer to) the top-most process entry with that ID on the stack, which was entered last. Usually, this is the best version of the process (in terms of integral, etc.) Thus the stack terminology makes sense.

```

<process_stacks.f90>≡
  <File header>

  module process_stacks

    <Use kinds>
    <Use strings>
    use variables
    use process

    <Standard module head>

    <Process stacks: public>

    <Process stacks: types>

    interface
    <Process stacks: sub interfaces>
    end interface

  end module process_stacks

<process_stacks_sub.f90>≡
  <File header>

  submodule (process_stacks) process_stacks_s

    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use observables

    implicit none

  contains

    <Process stacks: procedures>

  end submodule process_stacks_s

```

30.12.1 The process entry type

A process entry is a process object, augmented by a pointer to the next entry. We do not need specific methods, all relevant methods are inherited.

On higher level, processes should be prepared as process entry objects.

```

<Process stacks: public>≡
    public :: process_entry_t

<Process stacks: types>≡
    type, extends (process_t) :: process_entry_t
        type(process_entry_t), pointer :: next => null ()
    end type process_entry_t

```

30.12.2 The process stack type

For easy conversion and lookup it is useful to store the filling number in the object. The content is stored as a linked list.

The `var_list` component stores process-specific results, so they can be retrieved as (pseudo) variables.

The process stack can be linked to another one. This allows us to work with stacks of local scope.

```

<Process stacks: public>+≡
    public :: process_stack_t

<Process stacks: types>+≡
    type :: process_stack_t
        integer :: n = 0
        type(process_entry_t), pointer :: first => null ()
        type(var_list_t), pointer :: var_list => null ()
        type(process_stack_t), pointer :: next => null ()
    contains
        <Process stacks: process stack: TBP>
    end type process_stack_t

```

Finalize partly: deallocate the process stack and variable list entries, but keep the variable list as an empty object. This way, the variable list links are kept.

```

<Process stacks: process stack: TBP>≡
    procedure :: clear => process_stack_clear

<Process stacks: sub interfaces>≡
    module subroutine process_stack_clear (stack)
        class(process_stack_t), intent(inout) :: stack
    end subroutine process_stack_clear

<Process stacks: procedures>≡
    module subroutine process_stack_clear (stack)
        class(process_stack_t), intent(inout) :: stack
        type(process_entry_t), pointer :: process
        if (associated (stack%var_list)) then
            call stack%var_list%final ()
        end if
        do while (associated (stack%first))
            process => stack%first
            stack%first => process%next
            call process%final ()
            deallocate (process)
        end do
    end subroutine process_stack_clear

```

```

        stack%n = 0
    end subroutine process_stack_clear

```

Finalizer. Clear and deallocate the variable list.

```

<Process stacks: process stack: TBP>+≡
    procedure :: final => process_stack_final

<Process stacks: sub interfaces>+≡
    module subroutine process_stack_final (object)
        class(process_stack_t), intent(inout) :: object
    end subroutine process_stack_final

<Process stacks: procedures>+≡
    module subroutine process_stack_final (object)
        class(process_stack_t), intent(inout) :: object
        call object%clear ()
        if (associated (object%var_list)) then
            deallocate (object%var_list)
        end if
    end subroutine process_stack_final

```

Output. The processes on the stack will be ordered LIFO, i.e., backwards.

```

<Process stacks: process stack: TBP>+≡
    procedure :: write => process_stack_write

<Process stacks: sub interfaces>+≡
    recursive module subroutine process_stack_write (object, unit, pacify)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
    end subroutine process_stack_write

<Process stacks: procedures>+≡
    recursive module subroutine process_stack_write (object, unit, pacify)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        type(process_entry_t), pointer :: process
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        select case (object%n)
        case (0)
            write (u, "(1x,A)") "Process stack: [empty]"
            call write_separator (u, 2)
        case default
            write (u, "(1x,A)") "Process stack:"
            process => object%first
            do while (associated (process))
                call process%write (.false., u, pacify = pacify)
                process => process%next
            end do
        end select
        if (associated (object%next)) then
            write (u, "(1x,A)") "[Processes from context environment:]"

```

```

        call object%next%write (u, pacify)
    end if
end subroutine process_stack_write

```

The variable list is printed by a separate routine, since it should be linked to the global variable list, anyway.

```

(Process stacks: process stack: TBP)+≡
    procedure :: write_var_list => process_stack_write_var_list

(Process stacks: sub interfaces)+≡
    module subroutine process_stack_write_var_list (object, unit)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine process_stack_write_var_list

(Process stacks: procedures)+≡
    module subroutine process_stack_write_var_list (object, unit)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        if (associated (object%var_list)) then
            call object%var_list%write (unit)
        end if
    end subroutine process_stack_write_var_list

```

Short output.

Since this is a stack, the default output ordering for each stack will be last-in, first-out. To enable first-in, first-out, which is more likely to be requested, there is an optional `fifo` argument.

```

(Process stacks: process stack: TBP)+≡
    procedure :: show => process_stack_show

(Process stacks: sub interfaces)+≡
    recursive module subroutine process_stack_show (object, unit, fifo)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: fifo
    end subroutine process_stack_show

(Process stacks: procedures)+≡
    recursive module subroutine process_stack_show (object, unit, fifo)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: fifo
        type(process_entry_t), pointer :: process
        logical :: reverse
        integer :: u, i, j
        u = given_output_unit (unit)
        reverse = .false.; if (present (fifo)) reverse = fifo
        select case (object%n)
        case (0)
        case default
            if (.not. reverse) then
                process => object%first
                do while (associated (process))
                    call process%show (u, verbose=.false.)

```

```

        process => process%next
    end do
else
    do i = 1, object%n
        process => object%first
        do j = 1, object%n - i
            process => process%next
        end do
        call process%show (u, verbose=.false.)
    end do
end if
end select
if (associated (object%next)) call object%next%show ()
end subroutine process_stack_show

```

30.12.3 Link

Link the current process stack to a global one.

```

<Process stacks: process stack: TBP>+≡
    procedure :: link => process_stack_link

<Process stacks: sub interfaces>+≡
    module subroutine process_stack_link (local_stack, global_stack)
        class(process_stack_t), intent(inout) :: local_stack
        type(process_stack_t), intent(in), target :: global_stack
    end subroutine process_stack_link

<Process stacks: procedures>+≡
    module subroutine process_stack_link (local_stack, global_stack)
        class(process_stack_t), intent(inout) :: local_stack
        type(process_stack_t), intent(in), target :: global_stack
        local_stack%next => global_stack
    end subroutine process_stack_link

```

Initialize the process variable list and link the main variable list to it.

```

<Process stacks: process stack: TBP>+≡
    procedure :: init_var_list => process_stack_init_var_list

<Process stacks: sub interfaces>+≡
    module subroutine process_stack_init_var_list (stack, var_list)
        class(process_stack_t), intent(inout) :: stack
        type(var_list_t), intent(inout), optional :: var_list
    end subroutine process_stack_init_var_list

<Process stacks: procedures>+≡
    module subroutine process_stack_init_var_list (stack, var_list)
        class(process_stack_t), intent(inout) :: stack
        type(var_list_t), intent(inout), optional :: var_list
        allocate (stack%var_list)
        if (present (var_list)) call var_list%link (stack%var_list)
    end subroutine process_stack_init_var_list

```

Link the process variable list to a global variable list.

```

(Process stacks: process stack: TBP)+≡
    procedure :: link_var_list => process_stack_link_var_list

(Process stacks: sub interfaces)+≡
    module subroutine process_stack_link_var_list (stack, var_list)
        class(process_stack_t), intent(inout) :: stack
        type(var_list_t), intent(in), target :: var_list
    end subroutine process_stack_link_var_list

(Process stacks: procedures)+≡
    module subroutine process_stack_link_var_list (stack, var_list)
        class(process_stack_t), intent(inout) :: stack
        type(var_list_t), intent(in), target :: var_list
        call stack%var_list%link (var_list)
    end subroutine process_stack_link_var_list

```

30.12.4 Push

We take a process pointer and push it onto the stack. The previous pointer is nullified. Subsequently, the process is ‘owned’ by the stack and will be finalized when the stack is deleted.

```

(Process stacks: process stack: TBP)+≡
    procedure :: push => process_stack_push

(Process stacks: sub interfaces)+≡
    module subroutine process_stack_push (stack, process)
        class(process_stack_t), intent(inout) :: stack
        type(process_entry_t), intent(inout), pointer :: process
    end subroutine process_stack_push

(Process stacks: procedures)+≡
    module subroutine process_stack_push (stack, process)
        class(process_stack_t), intent(inout) :: stack
        type(process_entry_t), intent(inout), pointer :: process
        process%next => stack%first
        stack%first => process
        process => null ()
        stack%n = stack%n + 1
    end subroutine process_stack_push

```

Inverse: Remove the last process pointer in the list and return it.

```

(Process stacks: process stack: TBP)+≡
    procedure :: pop_last => process_stack_pop_last

(Process stacks: sub interfaces)+≡
    module subroutine process_stack_pop_last (stack, process)
        class(process_stack_t), intent(inout) :: stack
        type(process_entry_t), intent(inout), pointer :: process
    end subroutine process_stack_pop_last

```

```

<Process stacks: procedures>+≡
module subroutine process_stack_pop_last (stack, process)
  class(process_stack_t), intent(inout) :: stack
  type(process_entry_t), intent(inout), pointer :: process
  type(process_entry_t), pointer :: previous
  integer :: i
  select case (stack%n)
  case (:0)
    process => null ()
  case (1)
    process => stack%first
    stack%first => null ()
    stack%n = 0
  case (2:)
    process => stack%first
    do i = 2, stack%n
      previous => process
      process => process%next
    end do
    previous%next => null ()
    stack%n = stack%n - 1
  end select
end subroutine process_stack_pop_last

```

Initialize process variables for a given process ID, without setting values.

```

<Process stacks: process stack: TBP>+≡
  procedure :: init_result_vars => process_stack_init_result_vars

<Process stacks: sub interfaces>+≡
  module subroutine process_stack_init_result_vars (stack, id)
    class(process_stack_t), intent(inout) :: stack
    type(string_t), intent(in) :: id
  end subroutine process_stack_init_result_vars

<Process stacks: procedures>+≡
  module subroutine process_stack_init_result_vars (stack, id)
    class(process_stack_t), intent(inout) :: stack
    type(string_t), intent(in) :: id
    call var_list_init_num_id (stack%var_list, id)
    call var_list_init_process_results (stack%var_list, id)
  end subroutine process_stack_init_result_vars

```

Fill process variables with values. This is executed after the integration pass.

Note: We set only integral and error. With multiple MCI records possible, the results for `n_calls`, `chi2` etc. are not necessarily unique. (We might set the efficiency, though.)

```

<Process stacks: process stack: TBP>+≡
  procedure :: fill_result_vars => process_stack_fill_result_vars

<Process stacks: sub interfaces>+≡
  module subroutine process_stack_fill_result_vars (stack, id)
    class(process_stack_t), intent(inout) :: stack
    type(string_t), intent(in) :: id
  end subroutine process_stack_fill_result_vars

```

```

<Process stacks: procedures>+≡
module subroutine process_stack_fill_result_vars (stack, id)
  class(process_stack_t), intent(inout) :: stack
  type(string_t), intent(in) :: id
  type(process_t), pointer :: process
  process => stack%get_process_ptr (id)
  if (associated (process)) then
    call var_list_init_num_id (stack%var_list, id, process%get_num_id ())
    if (process%has_integral ()) then
      call var_list_init_process_results (stack%var_list, id, &
        integral = process%get_integral (), &
        error = process%get_error ())
    end if
  else
    call msg_bug ("process_stack_fill_result_vars: unknown process ID")
  end if
end subroutine process_stack_fill_result_vars

```

If one of the result variables has a local image in `var_list_local`, update the value there as well.

```

<Process stacks: process stack: TBP>+≡
  procedure :: update_result_vars => process_stack_update_result_vars

<Process stacks: sub interfaces>+≡
  module subroutine process_stack_update_result_vars &
    (stack, id, var_list_local)
    class(process_stack_t), intent(inout) :: stack
    type(string_t), intent(in) :: id
    type(var_list_t), intent(inout) :: var_list_local
  end subroutine process_stack_update_result_vars

<Process stacks: procedures>+≡
module subroutine process_stack_update_result_vars (stack, id, var_list_local)
  class(process_stack_t), intent(inout) :: stack
  type(string_t), intent(in) :: id
  type(var_list_t), intent(inout) :: var_list_local
  call update ("integral(" // id // ")")
  call update ("error(" // id // ")")
contains
  subroutine update (var_name)
    type(string_t), intent(in) :: var_name
    real(default) :: value
    if (var_list_local%contains (var_name, follow_link = .false.)) then
      value = stack%var_list%get_rval (var_name)
      call var_list_local%set_real (var_name, value, is_known = .true.)
    end if
  end subroutine update
end subroutine process_stack_update_result_vars

```

30.12.5 Data Access

Tell if a process exists.

```

<Process stacks: process stack: TBP>+≡

```



```

    procedure :: exists => process_stack_exists
<Process stacks: sub interfaces>+≡
    module function process_stack_exists (stack, id) result (flag)
        class(process_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: id
        logical :: flag
    end function process_stack_exists
<Process stacks: procedures>+≡
    module function process_stack_exists (stack, id) result (flag)
        class(process_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: id
        logical :: flag
        type(process_t), pointer :: process
        process => stack%get_process_ptr (id)
        flag = associated (process)
    end function process_stack_exists

```

Return a pointer to a process with specific ID. Look also at a linked stack, if necessary.

```

<Process stacks: process stack: TBP>+≡
    procedure :: get_process_ptr => process_stack_get_process_ptr
<Process stacks: sub interfaces>+≡
    recursive module function process_stack_get_process_ptr &
        (stack, id) result (ptr)
        class(process_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: id
        type(process_t), pointer :: ptr
    end function process_stack_get_process_ptr
<Process stacks: procedures>+≡
    recursive module function process_stack_get_process_ptr &
        (stack, id) result (ptr)
        class(process_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: id
        type(process_t), pointer :: ptr
        type(process_entry_t), pointer :: entry
        ptr => null ()
        entry => stack%first
        do while (associated (entry))
            if (entry%get_id () == id) then
                ptr => entry%process_t
                return
            end if
            entry => entry%next
        end do
        if (associated (stack%next)) ptr => stack%next%get_process_ptr (id)
    end function process_stack_get_process_ptr

```

30.12.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<process_stacks_ut.f90>≡

```

```

    <File header>

    module process_stacks_ut
        use unit_tests
        use process_stacks_util

    <Standard module head>

    <Process stacks: public test>

    contains

    <Process stacks: test driver>

    end module process_stacks_ut
<process_stacks_util.f90>≡
    <File header>

    module process_stacks_util

    <Use strings>
        use os_interface
        use sm_qcd
        use models
        use model_data
        use variables, only: var_list_t
        use process_libraries
        use rng_base
        use prc_test, only: prc_test_create_library
        use process, only: process_t
        use instances, only: process_instance_t
        use processes_ut, only: prepare_test_process

        use process_stacks

        use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <Process stacks: test declarations>

    contains

    <Process stacks: tests>

    end module process_stacks_util

API: driver for the unit tests below.
<Process stacks: public test>≡
    public :: process_stacks_test
<Process stacks: test driver>≡
    subroutine process_stacks_test (u, results)
        integer, intent(in) :: u

```

```

        type(test_results_t), intent(inout) :: results
    <Process stacks: execute tests>≡
end subroutine process_stacks_test

```

Write an empty process stack

The most trivial test is to write an uninitialized process stack.

```

<Process stacks: execute tests>≡
    call test (process_stacks_1, "process_stacks_1", &
        "write an empty process stack", &
        u, results)

<Process stacks: test declarations>≡
    public :: process_stacks_1

<Process stacks: tests>≡
    subroutine process_stacks_1 (u)
        integer, intent(in) :: u
        type(process_stack_t) :: stack

        write (u, "(A)")  "* Test output: process_stacks_1"
        write (u, "(A)")  "* Purpose: display an empty process stack"
        write (u, "(A)")

        call stack%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: process_stacks_1"

    end subroutine process_stacks_1

```

Fill a process stack

Fill a process stack with two (identical) processes.

```

<Process stacks: execute tests>+≡
    call test (process_stacks_2, "process_stacks_2", &
        "fill a process stack", &
        u, results)

<Process stacks: test declarations>+≡
    public :: process_stacks_2

<Process stacks: tests>+≡
    subroutine process_stacks_2 (u)
        integer, intent(in) :: u
        type(process_stack_t) :: stack
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(var_list_t) :: var_list
        type(process_entry_t), pointer :: process => null ()

```

```

write (u, "(A)")  "* Test output: process_stacks_2"
write (u, "(A)")  "* Purpose: fill a process stack"
write (u, "(A)")

write (u, "(A)")  "* Build, initialize and store two test processes"
write (u, "(A)")

libname = "process_stacks2"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call model%init_test ()
call var_list%append_string (var_str ("run_id"))
call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

allocate (process)

call var_list%set_string &
    (var_str ("run_id"), var_str ("run1"), is_known=.true.)
call process%init (procname, lib, os_data, model, var_list)
call stack%push (process)

allocate (process)

call var_list%set_string &
    (var_str ("run_id"), var_str ("run2"), is_known=.true.)
call process%init (procname, lib, os_data, model, var_list)
call stack%push (process)

call stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stack%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_stacks_2"

end subroutine process_stacks_2

```

Fill a process stack

Fill a process stack with two (identical) processes.

(Process stacks: execute tests) +≡

```

call test (process_stacks_3, "process_stacks_3", &
    "process variables", &
    u, results)

```

```

<Process stacks: test declarations>+≡
    public :: process_stacks_3

<Process stacks: tests>+≡
    subroutine process_stacks_3 (u)
        integer, intent(in) :: u
        type(process_stack_t) :: stack
        type(model_t), target :: model
        type(string_t) :: procname
        type(process_entry_t), pointer :: process => null ()
        type(process_instance_t), target :: process_instance

        write (u, "(A)")  "* Test output: process_stacks_3"
        write (u, "(A)")  "*   Purpose: setup process variables"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process variables"
        write (u, "(A)")

        procname = "processes_test"
        call model%init_test ()

        write (u, "(A)")  "* Initialize process variables"
        write (u, "(A)")

        call stack%init_var_list ()
        call stack%init_result_vars (procname)
        call stack%write_var_list (u)

        write (u, "(A)")
        write (u, "(A)")  "* Build and integrate a test process"
        write (u, "(A)")

        allocate (process)
        call prepare_test_process (process%process_t, process_instance, model)
        call process_instance%integrate (1, 1, 1000)
        call process_instance%final ()
        call process%final_integration (1)
        call stack%push (process)

        write (u, "(A)")  "* Fill process variables"
        write (u, "(A)")

        call stack%fill_result_vars (procname)
        call stack%write_var_list (u)

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call stack%final ()
        call model%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: process_stacks_3"

```

```
end subroutine process_stacks_3
```

Linked a process stack

Fill two process stack, linked to each other.

```
<Process stacks: execute tests>+≡
  call test (process_stacks_4, "process_stacks_4", &
    "linked stacks", &
    u, results)

<Process stacks: test declarations>+≡
  public :: process_stacks_4

<Process stacks: tests>+≡
  subroutine process_stacks_4 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(process_stack_t), target :: stack1, stack2
    type(model_t), target :: model
    type(string_t) :: libname
    type(string_t) :: procname1, procname2
    type(os_data_t) :: os_data
    type(process_entry_t), pointer :: process => null ()

    write (u, "(A)")  "* Test output: process_stacks_4"
    write (u, "(A)")  "* Purpose: link process stacks"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process variables"
    write (u, "(A)")

    libname = "process_stacks_4_lib"
    procname1 = "process_stacks_4a"
    procname2 = "process_stacks_4b"

    call os_data%init ()

    write (u, "(A)")  "* Initialize first process"
    write (u, "(A)")

    call prc_test_create_library (procname1, lib)

    call model%init_test ()

    allocate (process)
    call process%init (procname1, lib, os_data, model)
    call stack1%push (process)

    write (u, "(A)")  "* Initialize second process"
    write (u, "(A)")

    call stack2%link (stack1)

    call prc_test_create_library (procname2, lib)
```

```

allocate (process)

call process%init (procname2, lib, os_data, model)
call stack2%push (process)

write (u, "(A)")  "* Show linked stacks"
write (u, "(A)")

call stack2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stack2%final ()
call stack1%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_stacks_4"

end subroutine process_stacks_4

```

Chapter 31

Matching

```
<matching_base.f90>≡  
  <File header>  
  
  module matching_base  
  
    <Use strings>  
    use sm_qcd  
    use model_data  
    use particles  
    use variables  
    use shower_base  
    use instances, only: process_instance_t  
    use rng_base  
  
    <Standard module head>  
  
    <Matching base: public>  
  
    <Matching base: parameters>  
  
    <Matching base: types>
```

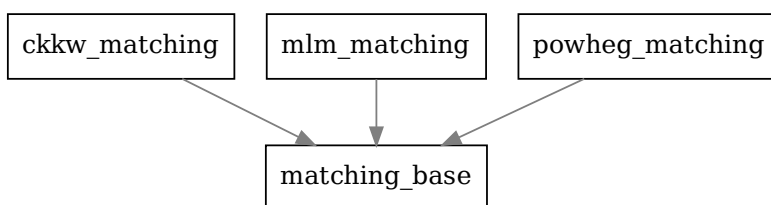


Figure 31.1: Module dependencies in `src/matching`.


```

    <Matching base: interfaces>

    interface
    <Matching base: sub interfaces>
    end interface

    end module matching_base

<matching_base_sub.f90>≡
    <File header>

    submodule (matching_base) matching_base_s

    <Use debug>
    use diagnostics

    implicit none

    contains

    <Matching base: procedures>

    end submodule matching_base_s

```

31.1 Abstract Matching Type

A matching will need access to the `shower` as well as matrix elements that we currently get over `process_instace`. The `model` is intended for the backup `model_hadrons`.

```

<Matching base: public>≡
    public :: matching_t

<Matching base: types>≡
    type, abstract :: matching_t
    logical :: is_hadron_collision = .false.
    type(qcd_t) :: qcd
    class(shower_base_t), pointer :: shower => null ()
    type(process_instance_t), pointer :: process_instance => null ()
    class(model_data_t), pointer :: model => null ()
    class(rng_t), allocatable :: rng
    type(string_t) :: process_name
    contains
    <Matching base: matching: TBP>
    end type matching_t

<Matching base: matching: TBP>≡
    procedure (matching_init), deferred :: init

<Matching base: interfaces>≡
    abstract interface
    subroutine matching_init (matching, var_list, process_name)
    import

```

```

        class(matching_t), intent(out) :: matching
        type(var_list_t), intent(in) :: var_list
        type(string_t), intent(in) :: process_name
    end subroutine matching_init
end interface

```

If we use a polymorphic settings type, this boilerplate wouldn't be necessary but then we introduce `select type` statements all over the place.

```

<default matching init>≡
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_name
    if (debug_on) call msg_debug (D_MATCHING, "matching_init")
    call matching%settings%init (var_list)
    matching%process_name = process_name

<Matching base: matching: TBP>+≡
    procedure (matching_write), deferred :: write

<Matching base: interfaces>+≡
    abstract interface
        subroutine matching_write (matching, unit)
            import
            class(matching_t), intent(in) :: matching
            integer, intent(in), optional :: unit
        end subroutine matching_write
    end interface

<Matching base: matching: TBP>+≡
    procedure :: import_rng => matching_import_rng

<Matching base: sub interfaces>≡
    pure module subroutine matching_import_rng (matching, rng)
        class(matching_t), intent(inout) :: matching
        class(rng_t), allocatable, intent(inout) :: rng
    end subroutine matching_import_rng

<Matching base: procedures>≡
    pure module subroutine matching_import_rng (matching, rng)
        class(matching_t), intent(inout) :: matching
        class(rng_t), allocatable, intent(inout) :: rng
        call move_alloc (from = rng, to = matching%rng)
    end subroutine matching_import_rng

<Matching base: matching: TBP>+≡
    procedure :: connect => matching_connect
    procedure :: base_connect => matching_connect

<Matching base: sub interfaces>+≡
    module subroutine matching_connect &
        (matching, process_instance, model, shower)
        class(matching_t), intent(inout) :: matching
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target, optional :: model
        class(shower_base_t), intent(in), target, optional :: shower
    end subroutine matching_connect

```

```

<Matching base: procedures>+≡
module subroutine matching_connect (matching, process_instance, model, shower)
  class(matching_t), intent(inout) :: matching
  type(process_instance_t), intent(in), target :: process_instance
  class(model_data_t), intent(in), target, optional :: model
  class(shower_base_t), intent(in), target, optional :: shower
  if (debug_on) call msg_debug (D_MATCHING, "matching_connect")
  matching%process_instance => process_instance
  if (present (model)) matching%model => model
  if (present (shower)) matching%shower => shower
end subroutine matching_connect

```

```

<Matching base: matching: TBP>+≡
  procedure (matching_before_shower), deferred :: before_shower

```

```

<Matching base: interfaces>+≡
  abstract interface
    subroutine matching_before_shower (matching, particle_set, vetoed)
      import
      class(matching_t), intent(inout) :: matching
      type(particle_set_t), intent(inout) :: particle_set
      logical, intent(out) :: vetoed
    end subroutine matching_before_shower
  end interface

```

```

<Matching base: matching: TBP>+≡
  procedure (matching_after_shower), deferred :: after_shower

```

```

<Matching base: interfaces>+≡
  abstract interface
    subroutine matching_after_shower (matching, particle_set, vetoed)
      import
      class(matching_t), intent(inout) :: matching
      type(particle_set_t), intent(inout) :: particle_set
      logical, intent(out) :: vetoed
    end subroutine matching_after_shower
  end interface

```

Per default, do nothing here.

```

<Matching base: matching: TBP>+≡
  procedure :: prepare_for_events => matching_prepare_for_events

```

```

<Matching base: sub interfaces>+≡
  module subroutine matching_prepare_for_events (matching)
    class(matching_t), intent(inout), target :: matching
  end subroutine matching_prepare_for_events

```

```

<Matching base: procedures>+≡
  module subroutine matching_prepare_for_events (matching)
    class(matching_t), intent(inout), target :: matching
  end subroutine matching_prepare_for_events

```

```

<Matching base: matching: TBP>+≡
  procedure :: first_event => matching_first_event

```

```

<Matching base: sub interfaces>+≡
    module subroutine matching_first_event (matching)
        class(matching_t), intent(inout), target :: matching
    end subroutine matching_first_event

<Matching base: procedures>+≡
    module subroutine matching_first_event (matching)
        class(matching_t), intent(inout), target :: matching
    end subroutine matching_first_event

<Matching base: matching: TBP>+≡
    procedure (matching_get_method), deferred :: get_method

<Matching base: interfaces>+≡
    abstract interface
        function matching_get_method (matching) result (method)
            import
            type(string_t) :: method
            class(matching_t), intent(in) :: matching
        end function matching_get_method
    end interface

<Matching base: matching: TBP>+≡
    procedure :: final => matching_final

<Matching base: sub interfaces>+≡
    module subroutine matching_final (matching)
        class(matching_t), intent(in) :: matching
    end subroutine matching_final

<Matching base: procedures>+≡
    module subroutine matching_final (matching)
        class(matching_t), intent(in) :: matching
    end subroutine matching_final

```

31.1.1 Matching implementations

```

<Matching base: public>+≡
    public :: MATCH_MLM, MATCH_CKKW, MATCH_POWHEG

<Matching base: parameters>≡
    integer, parameter :: MATCH_MLM = 1
    integer, parameter :: MATCH_CKKW = 2
    integer, parameter :: MATCH_POWHEG = 3
    integer, parameter :: MATCH_UNDEFINED = 17

A dictionary

<Matching base: public>+≡
    public :: matching_method

<Matching base: interfaces>+≡
    interface matching_method
        module procedure matching_method_of_string
        module procedure matching_method_to_string
    end interface

```

```

<Matching base: sub interfaces>+≡
    elemental module function matching_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
    end function matching_method_of_string
    elemental module function matching_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
    end function matching_method_to_string

<Matching base: procedures>+≡
    elemental module function matching_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
        select case (char (string))
            case ("MLM")
                i = MATCH_MLM
            case ("CKKW")
                i = MATCH_CKKW
            case ("POWHEG")
                i = MATCH_POWHEG
            case default
                i = MATCH_UNDEFINED
        end select
    end function matching_method_of_string

    elemental module function matching_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
            case (MATCH_MLM)
                string = "MLM"
            case (MATCH_CKKW)
                string = "CKKW"
            case (MATCH_POWHEG)
                string = "POWHEG"
            case default
                string = "UNDEFINED"
        end select
    end function matching_method_to_string

```

31.2 MLM Matching

```

<mlm_matching.f90>≡
    <File header>

    module mlm_matching

    <Use kinds with double>
    <Use strings>
        use constants
        use lorentz

```

```

    use particles
    use variables
    use matching_base

    <Standard module head>

    <MLM matching: public>

    <MLM matching: types>

    interface
    <MLM matching: sub interfaces>
    end interface

end module mlm_matching

<mlm_matching_sub.f90>≡
<File header>

submodule (mlm_matching) mlm_matching_s

    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use file_utils
    use subevents, only: PRT_OUTGOING
    use shower_base
    use ktclus

    implicit none

contains

    <MLM matching: procedures>

end submodule mlm_matching_s

<MLM matching: public>≡
    public :: mlm_matching_settings_t

<MLM matching: types>≡
    type :: mlm_matching_settings_t
        real(default) :: mlm_Qcut_ME = one
        real(default) :: mlm_Qcut_PS = one
        real(default) :: mlm_ptmin, mlm_etamax, mlm_Rmin, mlm_Emin
        real(default) :: mlm_ETclusfactor = 0.2_default
        real(default) :: mlm_ETclusminE = five
        real(default) :: mlm_etaclusfactor = one
        real(default) :: mlm_Rclusfactor = one
        real(default) :: mlm_Eclusfactor = one
        integer :: kt_imode_hadronic = 4313
        integer :: kt_imode_leptonic = 1111
        integer :: mlm_nmaxMEjets = 0
    contains

```

```

    <MLM matching: mlm matching settings: TBP>
    end type mlm_matching_settings_t

    <MLM matching: mlm matching settings: TBP>≡
    procedure :: init => mlm_matching_settings_init

    <MLM matching: sub interfaces>≡
    module subroutine mlm_matching_settings_init (settings, var_list)
        class(mlm_matching_settings_t), intent(out) :: settings
        type(var_list_t), intent(in) :: var_list
    end subroutine mlm_matching_settings_init

    <MLM matching: procedures>≡
    module subroutine mlm_matching_settings_init (settings, var_list)
        class(mlm_matching_settings_t), intent(out) :: settings
        type(var_list_t), intent(in) :: var_list
        settings%mlm_Qcut_ME = &
            var_list%get_rval (var_str ("mlm_Qcut_ME"))
        settings%mlm_Qcut_PS = &
            var_list%get_rval (var_str ("mlm_Qcut_PS"))
        settings%mlm_ptmin = &
            var_list%get_rval (var_str ("mlm_ptmin"))
        settings%mlm_etamax = &
            var_list%get_rval (var_str ("mlm_etamax"))
        settings%mlm_Rmin = &
            var_list%get_rval (var_str ("mlm_Rmin"))
        settings%mlm_Emin = &
            var_list%get_rval (var_str ("mlm_Emin"))
        settings%mlm_nmaxMEjets = &
            var_list%get_ival (var_str ("mlm_nmaxMEjets"))

        settings%mlm_ETclusfactor = &
            var_list%get_rval (var_str ("mlm_ETclusfactor"))
        settings%mlm_ETclusminE = &
            var_list%get_rval (var_str ("mlm_ETclusminE"))
        settings%mlm_etaclusfactor = &
            var_list%get_rval (var_str ("mlm_etaclusfactor"))
        settings%mlm_Rclusfactor = &
            var_list%get_rval (var_str ("mlm_Rclusfactor"))
        settings%mlm_Eclusfactor = &
            var_list%get_rval (var_str ("mlm_Eclusfactor"))
    end subroutine mlm_matching_settings_init

    <MLM matching: mlm matching settings: TBP>+≡
    procedure :: write => mlm_matching_settings_write

    <MLM matching: sub interfaces>+≡
    module subroutine mlm_matching_settings_write (settings, unit)
        class(mlm_matching_settings_t), intent(in) :: settings
        integer, intent(in), optional :: unit
    end subroutine mlm_matching_settings_write

    <MLM matching: procedures>+≡
    module subroutine mlm_matching_settings_write (settings, unit)
        class(mlm_matching_settings_t), intent(in) :: settings

```

```

integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(3x,A,ES19.12)") &
    "mlm_Qcut_ME" = ", settings%mlm_Qcut_ME
write (u, "(3x,A,ES19.12)") &
    "mlm_Qcut_PS" = ", settings%mlm_Qcut_PS
write (u, "(3x,A,ES19.12)") &
    "mlm_ptmin" = ", settings%mlm_ptmin
write (u, "(3x,A,ES19.12)") &
    "mlm_etamax" = ", settings%mlm_etamax
write (u, "(3x,A,ES19.12)") &
    "mlm_Rmin" = ", settings%mlm_Rmin
write (u, "(3x,A,ES19.12)") &
    "mlm_Emin" = ", settings%mlm_Emin
write (u, "(3x,A,1x,I0)") &
    "mlm_nmaxMEjets" = ", settings%mlm_nmaxMEjets
write (u, "(3x,A,ES19.12)") &
    "mlm_ETclusfactor (D=0.2)" = ", settings%mlm_ETclusfactor
write (u, "(3x,A,ES19.12)") &
    "mlm_ETclusminE (D=5.0)" = ", settings%mlm_ETclusminE
write (u, "(3x,A,ES19.12)") &
    "mlm_etaclusfactor (D=1.0)" = ", settings%mlm_etaClusfactor
write (u, "(3x,A,ES19.12)") &
    "mlm_Rclusfactor (D=1.0)" = ", settings%mlm_RClusfactor
write (u, "(3x,A,ES19.12)") &
    "mlm_Eclusfactor (D=1.0)" = ", settings%mlm_EClusfactor
end subroutine mlm_matching_settings_write

```

This is a container for the (colored) parton momenta as well as the jet momenta.

```

<MLM matching: public>+≡
public :: mlm_matching_t

<MLM matching: types>+≡
type, extends (matching_t) :: mlm_matching_t
    type(vector4_t), dimension(:), allocatable, public :: P_ME
    type(vector4_t), dimension(:), allocatable, public :: P_PS
    type(vector4_t), dimension(:), allocatable, private :: JETS_ME
    type(vector4_t), dimension(:), allocatable, private :: JETS_PS
    type(mlm_matching_settings_t) :: settings
contains
    <MLM matching: mlm matching: TBP>
end type mlm_matching_t

<MLM matching: mlm matching: TBP>≡
procedure :: init => mlm_matching_init

<MLM matching: sub interfaces>+≡
module subroutine mlm_matching_init (matching, var_list, process_name)
    class(mlm_matching_t), intent(out) :: matching
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_name
end subroutine mlm_matching_init

```



```

<MLM matching: procedures>+≡
  module subroutine mlm_matching_init (matching, var_list, process_name)
    class(mlm_matching_t), intent(out) :: matching
    <default matching init>
  end subroutine mlm_matching_init

```

```

<MLM matching: mln matching: TBP>+≡
  procedure :: write => mlm_matching_write

```

```

<MLM matching: sub interfaces>+≡
  module subroutine mlm_matching_write (matching, unit)
    class(mlm_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
  end subroutine mlm_matching_write

```

```

<MLM matching: procedures>+≡
  module subroutine mlm_matching_write (matching, unit)
    class(mlm_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
    integer :: i, u
    u = given_output_unit (unit); if (u < 0) return

    write (u, "(1x,A)") "MLM matching:"
    call matching%settings%write (u)
    write (u, "(3x,A)") "Momenta of ME partons:"
    if (allocated (matching%P_ME)) then
      do i = 1, size (matching%P_ME)
        write (u, "(4x)", advance = "no")
        call vector4_write (matching%P_ME(i), unit = u)
      end do
    else
      write (u, "(5x,A)") "[empty]"
    end if
    call write_separator (u)
    write (u, "(3x,A)") "Momenta of ME jets:"
    if (allocated (matching%JETS_ME)) then
      do i = 1, size (matching%JETS_ME)
        write (u, "(4x)", advance = "no")
        call vector4_write (matching%JETS_ME(i), unit = u)
      end do
    else
      write (u, "(5x,A)") "[empty]"
    end if
    call write_separator (u)
    write(u, "(3x,A)") "Momenta of shower partons:"
    if (allocated (matching%P_PS)) then
      do i = 1, size (matching%P_PS)
        write (u, "(4x)", advance = "no")
        call vector4_write (matching%P_PS(i), unit = u)
      end do
    else
      write (u, "(5x,A)") "[empty]"
    end if
    call write_separator (u)
    write (u, "(3x,A)") "Momenta of shower jets:"

```

```

    if (allocated (matching%JETS_PS)) then
        do i = 1, size (matching%JETS_PS)
            write (u, "(4x)", advance = "no")
            call vector4_write (matching%JETS_PS(i), unit = u)
        end do
    else
        write (u, "(5x,A)") "[empty]"
    end if
    call write_separator (u)
end subroutine mlm_matching_write

```

<MLM matching: mlm matching: TBP>+≡

```

    procedure :: get_method => mlm_matching_get_method

```

<MLM matching: sub interfaces>+≡

```

    module function mlm_matching_get_method (matching) result (method)
        type(string_t) :: method
        class(mlm_matching_t), intent(in) :: matching
    end function mlm_matching_get_method

```

<MLM matching: procedures>+≡

```

    module function mlm_matching_get_method (matching) result (method)
        type(string_t) :: method
        class(mlm_matching_t), intent(in) :: matching
        method = matching_method (MATCH_MLM)
    end function mlm_matching_get_method

```

<MLM matching: mlm matching: TBP>+≡

```

    procedure :: before_shower => mlm_matching_before_shower

```

<MLM matching: sub interfaces>+≡

```

    module subroutine mlm_matching_before_shower &
        (matching, particle_set, vetoed)
        class(mlm_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
    end subroutine mlm_matching_before_shower

```

<MLM matching: procedures>+≡

```

    module subroutine mlm_matching_before_shower &
        (matching, particle_set, vetoed)
        class(mlm_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
        vetoed = .false.
    end subroutine mlm_matching_before_shower

```

<MLM matching: mlm matching: TBP>+≡

```

    procedure :: after_shower => mlm_matching_after_shower

```

<MLM matching: sub interfaces>+≡

```

    module subroutine mlm_matching_after_shower (matching, particle_set, vetoed)
        class(mlm_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
    end subroutine mlm_matching_after_shower

```

<MLM matching: procedures>+≡

```

module subroutine mlm_matching_after_shower (matching, particle_set, vetoed)
  class(mlm_matching_t), intent(inout) :: matching
  type(particle_set_t), intent(inout) :: particle_set
  logical, intent(out) :: vetoed
  if (debug_on) call msg_debug (D_MATCHING, "mlm_matching_after_shower")
  call matching%shower%get_final_colored_ME_momenta (matching%P_ME)
  call matching%fill_P_PS (particle_set)
  !!! MLM stage 3 -> reconstruct and possibly reject
  call matching%apply (vetoed)
  if (debug_active (D_MATCHING)) call matching%write ()
  if (allocated (matching%P_ME)) deallocate (matching%P_ME)
  if (allocated (matching%P_PS)) deallocate (matching%P_PS)
  if (allocated (matching%JETS_ME)) deallocate (matching%JETS_ME)
  if (allocated (matching%JETS_PS)) deallocate (matching%JETS_PS)
end subroutine mlm_matching_after_shower

```

Transfer partons after parton shower to matching%P_PS

<MLM matching: mlm matching: TBP>+≡

```

procedure :: fill_P_PS => mlm_matching_fill_P_PS

```

<MLM matching: sub interfaces>+≡

```

module subroutine mlm_matching_fill_P_PS (matching, particle_set)
  class(mlm_matching_t), intent(inout) :: matching
  type(particle_set_t), intent(in) :: particle_set
end subroutine mlm_matching_fill_P_PS

```

<MLM matching: procedures>+≡

```

module subroutine mlm_matching_fill_P_PS (matching, particle_set)
  class(mlm_matching_t), intent(inout) :: matching
  type(particle_set_t), intent(in) :: particle_set
  integer :: i, j, n_jets_PS
  integer, dimension(2) :: col
  type(particle_t) :: tempprt
  real(double) :: eta
  type(vector4_t) :: p_tmp

  !!! loop over particles and extract final colored ones with eta<etamax
  n_jets_PS = 0
  do i = 1, particle_set%get_n_tot ()
    if (signal_is_pending ()) return
    tempprt = particle_set%get_particle (i)
    if (tempprt%get_status () /= PRT_OUTGOING) cycle
    col = tempprt%get_color ()
    if (all (col == 0)) cycle
! TODO: (bcn 2015-04-28) where is the corresponding part for lepton colliders?
    if (matching%is_hadron_collision) then
      p_tmp = tempprt%get_momentum ()
      if (energy (p_tmp) - longitudinal_part (p_tmp) < 1.E-10_default .or. &
          energy (p_tmp) + longitudinal_part (p_tmp) < 1.E-10_default) then
        eta = pseudorapidity (p_tmp)
      else
        eta = rapidity (p_tmp)
      end if
      if (eta > matching%settings%mlm_etaClusfactor * &

```

```

        matching%settings%mlm_etamax) then
    if (debug_active (D_MATCHING)) then
        call msg_debug (D_MATCHING, "Rejecting this particle")
        call tempprt%write ()
    end if
    cycle
end if
end if
n_jets_PS = n_jets_PS + 1
end do

allocate (matching%P_PS(1:n_jets_PS))
if (debug_on) call msg_debug (D_MATCHING, "n_jets_ps", n_jets_ps)

j = 1
do i = 1, particle_set%get_n_tot ()
    tempprt = particle_set%get_particle (i)
    if (tempprt%get_status () /= PRT_OUTGOING) cycle
    col = tempprt%get_color ()
    if (all(col == 0)) cycle
! TODO: (bcn 2015-04-28) where is the corresponding part for lepton colliders?
    if (matching%is_hadron_collision) then
        p_tmp = tempprt%get_momentum ()
        if (energy (p_tmp) - longitudinal_part (p_tmp) < 1.E-10_default .or. &
            energy (p_tmp) + longitudinal_part (p_tmp) < 1.E-10_default) then
            eta = pseudorapidity (p_tmp)
        else
            eta = rapidity (p_tmp)
        end if
        if (eta > matching%settings%mlm_etaClusfactor * &
            matching%settings%mlm_etamax) cycle
    end if
    matching%P_PS(j) = tempprt%get_momentum ()
    j = j + 1
end do
end subroutine mlm_matching_fill_P_PS

```

<MLM matching: mlm matching: TBP>+≡
 procedure :: apply => mlm_matching_apply

<MLM matching: sub interfaces>+≡
 module subroutine mlm_matching_apply (matching, vetoed)
 class(mlm_matching_t), intent(inout) :: matching
 logical, intent(out) :: vetoed
 end subroutine mlm_matching_apply

<MLM matching: procedures>+≡
 module subroutine mlm_matching_apply (matching, vetoed)
 class(mlm_matching_t), intent(inout) :: matching
 logical, intent(out) :: vetoed
 integer :: i, j
 integer :: n_jets_ME, n_jets_PS, n_jets_PS_atycut
 real(double) :: ycut
 real(double), dimension(:, :), allocatable :: PP
 real(double), dimension(:, :), allocatable :: Y

```

real(double), dimension(:,:), allocatable :: P_JETS
real(double), dimension(:,:), allocatable :: P_ME
integer, dimension(:), allocatable :: JET
integer :: NJET, NSUB
integer :: imode
!!! TODO: (bcn 2014-03-26) Why is ECUT hard coded to 1?
!!! It is the denominator of the KT measure. Candidate for removal
real(double) :: ECUT = 1._double
integer :: ip1,ip2

! KTCLUS COMMON BLOCK
INTEGER NMAX,NUM,HIST
PARAMETER (NMAX=512)
DOUBLE PRECISION P,KT,KTP,KTS,ETOT,RSQ,KTLAST
COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
      KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM

vetoed = .true.
if (signal_is_pending ()) return

<Set n_jets_ME/PS from matching (or equal zero)>

<Jet clustering for partons after matrix element>

<Jet clustering for partons after shower>

<Veto: too many or not enough jets after PS>

<Cluster ME jets with PS jets one at a time>

vetoed = .false.
999 continue
end subroutine mlm_matching_apply

<Set n_jets_ME/PS from matching (or equal zero)>≡
if (allocated (matching%P_ME)) then
  ! print *, "number of partons after ME: ", size(matching%P_ME)
  n_jets_ME = size (matching%P_ME)
else
  n_jets_ME = 0
end if
if (allocated (matching%p_PS)) then
  ! print *, "number of partons after PS: ", size(matching%p_PS)
  n_jets_PS = size (matching%p_PS)
else
  n_jets_PS = 0
end if

<Jet clustering for partons after matrix element>≡
if (n_jets_ME > 0) then
  ycut = (matching%settings%mlm_ptmin)**2
  allocate (PP(1:4, 1:N_jets_ME))
  do i = 1, n_jets_ME
    PP(1:3,i) = matching%p_ME(i)%p(1:3)

```

```

        PP(4,i) = matching%p_ME(i)%p(0)
    end do

    <Set imode for lepton or hadron collisions>

    allocate (P_ME(1:4,1:n_jets_ME))
    allocate (JET(1:n_jets_ME))
    allocate (Y(1:n_jets_ME))

    if (signal_is_pending ()) return
    call KTCLUR (imode, PP, n_jets_ME, &
        dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), ECUT, y, *999)
    call KTRECO (1, PP, n_jets_ME, ECUT, ycut, ycut, P_ME, JET, &
        NJET, NSUB, *999)

    n_jets_ME = NJET
    if (NJET > 0) then
        allocate (matching%JETS_ME (1:NJET))
        do i = 1, NJET
            matching%JETS_ME(i) = vector4_moving (REAL(P_ME(4,i), default), &
                vector3_moving([REAL(P_ME(1,i), default), &
                    REAL(P_ME(2,i), default), REAL(P_ME(3,i), default)]))
        end do
    end if
    deallocate (P_ME)
    deallocate (JET)
    deallocate (Y)
    deallocate (PP)
end if

<Jet clustering for partons after shower>≡
if (n_jets_PS > 0) then
    ycut = (matching%settings%mlm_ptmin + max (matching%settings%mlm_ETclusminE, &
        matching%settings%mlm_ETclusfactor * matching%settings%mlm_ptmin))*2
    allocate (PP(1:4, 1:n_jets_PS))
    do i = 1, n_jets_PS
        PP(1:3,i) = matching%p_PS(i)%p(1:3)
        PP(4,i) = matching%p_PS(i)%p(0)
    end do

    <Set imode for lepton or hadron collisions>

    allocate (P_JETS(1:4,1:n_jets_PS))
    allocate (JET(1:n_jets_PS))
    allocate (Y(1:n_jets_PS))

    if (signal_is_pending ()) return
    call KTCLUR (imode, PP, n_jets_PS, &
        dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), &
        ECUT, y, *999)
    call KTRECO (1, PP, n_jets_PS, ECUT, ycut, ycut, P_JETS, JET, &
        NJET, NSUB, *999)
    n_jets_PS_atycut = NJET
    if (n_jets_ME == matching%settings%mlm_nmaxMEjets .and. NJET > 0) then
        ! print *, " resetting ycut to ", Y(matching%settings%mlm_nmaxMEjets)
    end if
end if

```

```

        ycut = y(matching%settings%mlm_nmaxMEjets)
        call KTRECO (1, PP, n_jets_PS, ECUT, ycut, ycut, P_JETS, JET, &
                     NJET, NSUB, *999)
    end if

    ! !Sample of code for a FastJet interface
    ! palg = 1d0          ! 1.0d0 = kt, 0.0d0 = Cam/Aachen, -1.0d0 = anti-kt
    ! R = 0.7_double     ! radius parameter
    ! f = 0.75_double    ! overlap threshold
    ! !call fastjetppgenkt(PP,n,R,palg,P_JETS,NJET) ! KT-Algorithm
    ! !call fastjetsiscone(PP,n,R,f,P_JETS,NJET)   ! SiSCone-Algorithm

    if (NJET > 0) then
        allocate (matching%JETS_PS(1:NJET))
        do i = 1, NJET
            matching%JETS_PS(i) = vector4_moving (REAL(P_JETS(4,i), default), &
            vector3_moving([REAL(P_JETS(1,i), default), &
            REAL(P_JETS(2,i), default), REAL(P_JETS(3,i), default)]))
        end do
    end if

    deallocate (P_JETS)
    deallocate (JET)
    deallocate (Y)
else
    n_jets_PS_atycut = 0
end if

<Set imode for lepton or hadron collisions>≡
    if (matching%is_hadron_collision) then
        imode = matching%settings%kt_imode_hadronic
    else
        imode = matching%settings%kt_imode_leptonic
    end if

<Veto: too many or not enough jets after PS>≡
    if (n_jets_PS_atycut < n_jets_ME) then
        ! print *, "DISCARDING: Not enough PS jets: ", n_jets_PS_atycut
        return
    end if
    if (n_jets_PS_atycut > n_jets_ME .and. n_jets_ME /= matching%settings%mlm_nmaxMEjets) then
        ! print *, "DISCARDING: Too many PS jets: ", n_jets_PS_atycut
        return
    end if

<Cluster ME jets with PS jets one at a time>≡
    if (allocated(matching%JETS_PS)) then
        ! print *, "number of jets after PS: ", size(matching%JETS_PS)
        n_jets_PS = size (matching%JETS_PS)
    else
        n_jets_PS = 0
    end if
    if (n_jets_ME > 0 .and. n_jets_PS > 0) then
        n_jets_PS = size (matching%JETS_PS)
        if (allocated (PP)) deallocate(PP)
        allocate (PP(1:4, 1:n_jets_PS + 1))
    end if
end if

```

```

do i = 1, n_jets_PS
  if (signal_is_pending ()) return
  PP(1:3,i) = matching%JETS_PS(i)%p(1:3)
  PP(4,i) = matching%JETS_PS(i)%p(0)
end do
if (allocated (Y)) deallocate(Y)
allocate (Y(1:n_jets_PS + 1))
y = zero
do i = 1, n_jets_ME
  PP(1:3,n_jets_PS + 2 - i) = matching%JETS_ME(i)%p(1:3)
  PP(4,n_jets_PS + 2 - i) = matching%JETS_ME(i)%p(0)
  !!! This makes more sense than hardcoding
  ! call KTCLUS (4313, PP, (n_jets_PS + 2 - i), 1.0_double, Y, *999)
  call KTCLUR (imode, PP, (n_jets_PS + 2 - i), &
    dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), &
    ECUT, y, *999)
  if (0.99 * y(n_jets_PS + 1 - (i - 1)).gt.ycut) then
    ! print *, "DISCARDING: Jet ", i, " not clusterd"
    return
  end if
  !!! search for and remove PS jet clustered with ME Jet
  ip1 = HIST(n_jets_PS + 2 - i) / NMAX
  ip2 = mod(hist(n_jets_PS + 2 - i), NMAX)
  if ((ip2 /= n_jets_PS + 2 - i) .or. (ip1 <= 0)) then
    ! print *, "DISCARDING: Jet ", i, " not clustered ", ip1, ip2, &
    ! hist(n_jets_PS + 2 - i)
    return
  else
    ! print *, "PARTON clustered", ip1, ip2, hist(n_jets_PS + 2 - i)
    PP(:,IP1) = zero
    do j = IP1, n_jets_PS - i
      PP(:, j) = PP(:,j + 1)
    end do
  end if
end do
end if

```

31.3 CKKW matching

This module contains the CKKW matching.

The type `ckkw_pseudo_shower_weights_t` gives the (relative) weights for different clusterings of the final particles, as given in Eq. (2.7) of hep-ph/0503281v1. Each particle has a binary labelling (power of 2) (first particle = 1, second particle = 2, third particle = 4, ...). Each recombination therefore corresponds to an integer, that is not a power of 2. For multiple subsequent recombinations, no different weights for different sequences of clustering are stored. It is assumed that the weight of a multiply recombined state is a combination of the states with one fewer recombination and that these states' contributions are proportional to their weights. For a $2 - > n$ event, the weights array thus has the size $2^{(2+n)-1}$. The `weights_by_type` array gives the weights depending on the type of the particle, the first index is the same as for weights, the second index gives the type of the new mother particle:

0: uncolored (γ , Z , W , Higgs)

1: colored (quark)

2: gluon

3: squark

4: gluino

`alphaS` gives the value for α_s used in the generation of the matrix element. This is needed for the reweighting using the values for a running α_s at the scales of the clusterings.

`<ckkw_matching.f90>`≡
<File header>

```
module ckkw_matching
```

```
<Use kinds with double>
```

```
<Use strings>
```

```
  use constants
```

```
  use lorentz
```

```
  use particles
```

```
  use rng_base
```

```
  use shower_base
```

```
  use shower_partons
```

```
  use variables
```

```
  use matching_base
```

```
<Standard module head>
```

```
<CKKW matching: public>
```

```
<CKKW matching: types>
```

```
  interface
```

```
<CKKW matching: sub interfaces>
```

```
  end interface
```

```
end module ckkw_matching
```

`<ckkw_matching_sub.f90>`≡

<File header>

```
submodule (ckkw_matching) ckkw_matching_s
```

```
<Use debug>
```

```
  use io_units
```

```
  use format_utils, only: write_separator
```

```
  use diagnostics
```

```
  use physics_defs
```

```
  use shower_core
```

```
implicit none
```

```

contains

<CKKW matching: procedures>

end submodule ckkw_matching_s

```

The fundamental CKKW matching parameter are defined here:

```

<CKKW matching: public>≡
  public :: ckkw_matching_settings_t

<CKKW matching: types>≡
  type :: ckkw_matching_settings_t
    real(default) :: alphaS = 0.118_default
    real(default) :: Qmin = one
    integer :: n_max_jets = 0
  contains
    <CKKW matching: ckkw matching settings: TBP>
  end type ckkw_matching_settings_t

```

This is empty for the moment.

```

<CKKW matching: ckkw matching settings: TBP>≡
  procedure :: init => ckkw_matching_settings_init

<CKKW matching: sub interfaces>≡
  module subroutine ckkw_matching_settings_init (settings, var_list)
    class(ckkw_matching_settings_t), intent(out) :: settings
    type(var_list_t), intent(in) :: var_list
  end subroutine ckkw_matching_settings_init

<CKKW matching: procedures>≡
  module subroutine ckkw_matching_settings_init (settings, var_list)
    class(ckkw_matching_settings_t), intent(out) :: settings
    type(var_list_t), intent(in) :: var_list
    settings%alphaS = 1.0_default
    settings%Qmin = 1.0_default
    settings%n_max_jets = 3
  end subroutine ckkw_matching_settings_init

<CKKW matching: ckkw matching settings: TBP>+≡
  procedure :: write => ckkw_matching_settings_write

<CKKW matching: sub interfaces>+≡
  module subroutine ckkw_matching_settings_write (settings, unit)
    class(ckkw_matching_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
  end subroutine ckkw_matching_settings_write

<CKKW matching: procedures>+≡
  module subroutine ckkw_matching_settings_write (settings, unit)
    class(ckkw_matching_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "CKKW matching settings:"
    call write_separator (u)

```

```

write (u, "(3x,A,1x,ES19.12)") &
    "alphaS      = ", settings%alphaS
write (u, "(3x,A,1x,ES19.12)") &
    "Qmin        = ", settings%Qmin
write (u, "(3x,A,1x,I0)") &
    "n_max_jets  = ", settings%n_max_jets
end subroutine ckkw_matching_settings_write

<CKKW matching: public>+≡
public :: ckkw_pseudo_shower_weights_t

<CKKW matching: types>+≡
type :: ckkw_pseudo_shower_weights_t
    real(default) :: alphaS
    real(default), dimension(:), allocatable :: weights
    real(default), dimension(:,:), allocatable :: weights_by_type
contains
    <CKKW matching: ckkw pseudo shower weights: TBP>
end type ckkw_pseudo_shower_weights_t

<CKKW matching: ckkw pseudo shower weights: TBP>≡
procedure :: init => ckkw_pseudo_shower_weights_init

<CKKW matching: sub interfaces>+≡
module subroutine ckkw_pseudo_shower_weights_init (weights)
    class(ckkw_pseudo_shower_weights_t), intent(out) :: weights
end subroutine ckkw_pseudo_shower_weights_init

<CKKW matching: procedures>+≡
module subroutine ckkw_pseudo_shower_weights_init (weights)
    class(ckkw_pseudo_shower_weights_t), intent(out) :: weights
    weights%alphaS = zero
end subroutine ckkw_pseudo_shower_weights_init

<CKKW matching: ckkw pseudo shower weights: TBP>+≡
procedure :: write => ckkw_pseudo_shower_weights_write

<CKKW matching: sub interfaces>+≡
module subroutine ckkw_pseudo_shower_weights_write (weights, unit)
    class(ckkw_pseudo_shower_weights_t), intent(in) :: weights
    integer, intent(in), optional :: unit
end subroutine ckkw_pseudo_shower_weights_write

<CKKW matching: procedures>+≡
module subroutine ckkw_pseudo_shower_weights_write (weights, unit)
    class(ckkw_pseudo_shower_weights_t), intent(in) :: weights
    integer, intent(in), optional :: unit
    integer :: s, i, u
    u = given_output_unit (unit); if (u < 0) return
    s = size (weights%weights)
    write (u, "(1x,A)") "CKKW (pseudo) shower weights: "
    do i = 1, s
        write (u, "(3x,I0,2(ES19.12))") i, weights%weights(i), &
            weights%weights_by_type(i,:)
    end do
end do

```

```

        write (u, "(3x,A,1x,I0)") "alphaS =", weights%alphaS
    end subroutine ckkw_pseudo_shower_weights_write

```

Generate fake ckkw weights. This can be dropped, once information from the matrix element generation is available.

```

<CKKW matching: ckkw pseudo shower weights: TBP>+≡
    procedure :: fake => ckkw_pseudo_shower_weights_fake

<CKKW matching: sub interfaces>+≡
    pure module subroutine ckkw_pseudo_shower_weights_fake &
        (weights, particle_set)
        class(ckkw_pseudo_shower_weights_t), intent(inout) :: weights
        type(particle_set_t), intent(in) :: particle_set
    end subroutine ckkw_pseudo_shower_weights_fake

<CKKW matching: procedures>+≡
    pure module subroutine ckkw_pseudo_shower_weights_fake (weights, particle_set)
        class(ckkw_pseudo_shower_weights_t), intent(inout) :: weights
        type(particle_set_t), intent(in) :: particle_set
        integer :: i, j, n
        type(vector4_t) :: momentum
        n = 2**particle_set%n_tot
        if (allocated (weights%weights)) then
            deallocate (weights%weights)
        end if
        allocate (weights%weights (1:n))
        do i = 1, n
            momentum = vector4_null
            do j = 1, particle_set%n_tot
                if (btest (i,j-1)) then
                    momentum = momentum + particle_set%prt(j)%p
                end if
            end do
            if (momentum**1 > 0.0) then
                weights%weights(i) = 1.0 / (momentum**2)
            end if
        end do
        ! equally distribute the weights by type
        if (allocated (weights%weights_by_type)) then
            deallocate (weights%weights_by_type)
        end if
        allocate (weights%weights_by_type (1:n, 0:4))
        do i = 1, n
            do j = 0, 4
                weights%weights_by_type(i,j) = 0.2 * weights%weights(i)
            end do
        end do
    end subroutine ckkw_pseudo_shower_weights_fake

<CKKW matching: public>+≡
    public :: ckkw_matching_t

<CKKW matching: types>+≡
    type, extends (matching_t) :: ckkw_matching_t

```

```

        type(ckkw_matching_settings_t) :: settings
        type(ckkw_pseudo_shower_weights_t) :: weights
contains
    <CKKW matching: ckkw matching: TBP>
end type ckkw_matching_t

<CKKW matching: ckkw matching: TBP>≡
    procedure :: init => ckkw_matching_init

<CKKW matching: sub interfaces>+≡
    module subroutine ckkw_matching_init (matching, var_list, process_name)
        class(ckkw_matching_t), intent(out) :: matching
        type(var_list_t), intent(in) :: var_list
        type(string_t), intent(in) :: process_name
    end subroutine ckkw_matching_init

<CKKW matching: procedures>+≡
    module subroutine ckkw_matching_init (matching, var_list, process_name)
        class(ckkw_matching_t), intent(out) :: matching
    <default matching init>
    end subroutine ckkw_matching_init

<CKKW matching: ckkw matching: TBP>+≡
    procedure :: write => ckkw_matching_write

<CKKW matching: sub interfaces>+≡
    module subroutine ckkw_matching_write (matching, unit)
        class(ckkw_matching_t), intent(in) :: matching
        integer, intent(in), optional :: unit
    end subroutine ckkw_matching_write

<CKKW matching: procedures>+≡
    module subroutine ckkw_matching_write (matching, unit)
        class(ckkw_matching_t), intent(in) :: matching
        integer, intent(in), optional :: unit
        call matching%settings%write (unit)
        call matching%weights%write (unit)
    end subroutine ckkw_matching_write

<CKKW matching: ckkw matching: TBP>+≡
    procedure :: get_method => ckkw_matching_get_method

<CKKW matching: sub interfaces>+≡
    module function ckkw_matching_get_method (matching) result (method)
        type(string_t) :: method
        class(ckkw_matching_t), intent(in) :: matching
    end function ckkw_matching_get_method

<CKKW matching: procedures>+≡
    module function ckkw_matching_get_method (matching) result (method)
        type(string_t) :: method
        class(ckkw_matching_t), intent(in) :: matching
        method = matching_method (MATCH_CKKW)
    end function ckkw_matching_get_method

```

```

<CKKW matching: ckkw matching: TBP>+≡
  procedure :: before_shower => ckkw_matching_before_shower

<CKKW matching: sub interfaces>+≡
  module subroutine ckkw_matching_before_shower &
    (matching, particle_set, vetoed)
    class(ckkw_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
  end subroutine ckkw_matching_before_shower

<CKKW matching: procedures>+≡
  module subroutine ckkw_matching_before_shower &
    (matching, particle_set, vetoed)
    class(ckkw_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    call matching%weights%init ()
    call matching%weights%fake (particle_set)
    select type (shower => matching%shower)
    type is (shower_t)
      call ckkw_matching_apply (shower%partons, &
        matching%settings, &
        matching%weights, matching%rng, vetoed)
    class default
      call msg_bug ("CKKW matching only works with WHIZARD shower.")
    end select
  end subroutine ckkw_matching_before_shower

<CKKW matching: public>+≡
  public :: ckkw_matching_apply

<CKKW matching: sub interfaces>+≡
  module subroutine ckkw_matching_apply &
    (partons, settings, weights, rng, vetoed)
    type(parton_pointer_t), dimension(:), intent(inout), allocatable :: &
      partons
    type(ckkw_matching_settings_t), intent(in) :: settings
    type(ckkw_pseudo_shower_weights_t), intent(in) :: weights
    class(rng_t), intent(inout), allocatable :: rng
    logical, intent(out) :: vetoed
  end subroutine ckkw_matching_apply

<CKKW matching: procedures>+≡
  module subroutine ckkw_matching_apply &
    (partons, settings, weights, rng, vetoed)
    type(parton_pointer_t), dimension(:), intent(inout), allocatable :: &
      partons
    type(ckkw_matching_settings_t), intent(in) :: settings
    type(ckkw_pseudo_shower_weights_t), intent(in) :: weights
    class(rng_t), intent(inout), allocatable :: rng
    logical, intent(out) :: vetoed

    real(default), dimension(:), allocatable :: scales
    real(double) :: weight, sf
    real(default) :: rand

```

```

integer :: i, n_partons

if (signal_is_pending ()) return
weight = one

n_partons = size (partons)

do i = 1, n_partons
  call partons(i)%p%write ()
end do

!!! the pseudo parton shower is already simulated by shower_add_interaction
!!! get the respective clustering scales
allocate (scales (1:n_partons))
do i = 1, n_partons
  if (.not. associated (partons(i)%p)) cycle
  if (partons(i)%p%type == INTERNAL) then
    scales(i) = two * min (partons(i)%p%child1%momentum%p(0), &
                          partons(i)%p%child2%momentum%p(0))*2 * &
                      (1.0 - (space_part (partons(i)%p%child1%momentum) * &
                             space_part (partons(i)%p%child2%momentum)) / &
                      (space_part (partons(i)%p%child1%momentum)**1 * &
                       space_part (partons(i)%p%child2%momentum)**1))
    scales(i) = sqrt (scales(i))
    partons(i)%p%ckkwscale = scales(i)
    print *, scales(i)
  end if
end do

print *, " scales finished"
!!! if (highest multiplicity) -> reweight with PDF(mu_F) / PDF(mu_cut)
do i = 1, n_partons
  call partons(i)%p%write ()
end do

!!! Reweight and possibly veto the whole event

!!! calculate the relative alpha_S weight

!! calculate the Sudakov weights for internal lines
!! calculate the Sudakov weights for external lines
do i = 1, n_partons
  if (signal_is_pending ()) return
  if (.not. associated (partons(i)%p)) cycle
  if (partons(i)%p%type == INTERNAL) then
    !!! get type
    !!! check that all particles involved are colored
    if ((partons(i)%p%is_colored () .or. &
         partons(i)%p%ckkwtype > 0) .and. &
        (partons(i)%p%child1%is_colored () .or. &
         partons(i)%p%child1%ckkwtype > 0) .and. &
        (partons(i)%p%child1%is_colored () .or. &
         partons(i)%p%child1%ckkwtype > 0)) then
      print *, "reweight with alphaS(" , partons(i)%p%ckkwscale, &

```

```

        ") for particle ", partons(i)%p%nr
    if (partons(i)%p%belongstoFSR) then
        print *, "FSR"
        weight = weight * D_alpha_s_fsr (partons(i)%p%ckkwscale**2, &
            partons(i)%p%settings) / settings%alphas
    else
        print *, "ISR"
        weight = weight * &
            D_alpha_s_isr (partons(i)%p%ckkwscale**2, &
            partons(i)%p%settings) / settings%alphas
    end if
else
    print *, "no reweight with alphaS for ", partons(i)%p%nr
end if
if (partons(i)%p%child1%type == INTERNAL) then
    print *, "internal line from ", &
        partons(i)%p%child1%ckkwscale, &
        " to ", partons(i)%p%ckkwscale, &
        " for type ", partons(i)%p%child1%ckkwtype
    if (partons(i)%p%child1%ckkwtype == 0) then
        sf = 1.0
    else if (partons(i)%p%child1%ckkwtype == 1) then
        sf = SudakovQ (partons(i)%p%child1%ckkwscale, &
            partons(i)%p%ckkwscale, &
            partons(i)%p%settings, .true., rng)
        print *, "SFQ = ", sf
    else if (partons(i)%p%child1%ckkwtype == 2) then
        sf = SudakovG (partons(i)%p%child1%ckkwscale, &
            partons(i)%p%ckkwscale, &
            partons(i)%p%settings, .true., rng)
        print *, "SFG = ", sf
    else
        print *, "SUSY not yet implemented"
    end if
    weight = weight * min (one, sf)
else
    print *, "external line from ", settings%Qmin, &
        partons(i)%p%ckkwscale
    if (partons(i)%p%child1%is_quark ()) then
        sf = SudakovQ (settings%Qmin, &
            partons(i)%p%ckkwscale, &
            partons(i)%p%settings, .true., rng)
        print *, "SFQ = ", sf
    else if (partons(i)%p%child1%is_gluon ()) then
        sf = SudakovG (settings%Qmin, &
            partons(i)%p%ckkwscale, &
            partons(i)%p%settings, .true., rng)
        print *, "SFG = ", sf
    else
        print *, "not yet implemented (", &
            partons(i)%p%child2%type, ")"
        sf = one
    end if
    weight = weight * min (one, sf)
end if

```



```

end if
if (partons(i)%p%child2%type == INTERNAL) then
  print *, "internal line from ", partons(i)%p%child2%ckkwscale, &
    " to ", partons(i)%p%ckkwscale, &
    " for type ", partons(i)%p%child2%ckkwtype
  if (partons(i)%p%child2%ckkwtype == 0) then
    sf = 1.0
  else if (partons(i)%p%child2%ckkwtype == 1) then
    sf = SudakovQ (partons(i)%p%child2%ckkwscale, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFQ = ", sf
  else if (partons(i)%p%child2%ckkwtype == 2) then
    sf = SudakovG (partons(i)%p%child2%ckkwscale, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFG = ", sf
  else
    print *, "SUSY not yet implemented"
  end if
  weight = weight * min (one, sf)
else
  print *, "external line from ", settings%Qmin, &
    partons(i)%p%ckkwscale
  if (partons(i)%p%child2%is_quark ()) then
    sf = SudakovQ (settings%Qmin, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFQ = ", sf
  else if (partons(i)%p%child2%is_gluon ()) then
    sf = SudakovG (settings%Qmin, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFG = ", sf
  else
    print *, "not yet implemented (", &
      partons(i)%p%child2%type, ")"
    sf = one
  end if
  weight = weight * min (one, sf)
end if
end if
end do

call rng%generate (rand)

print *, "final weight: ", weight

!!!!!!! WRONG
vetoed = .false.
! vetoed = (rand > weight)
if (vetoed) then
  return
end if

```

```

    !!! finally perform the parton shower
    !!! veto emissions that are too hard

    deallocate (scales)
end subroutine ckkw_matching_apply

<CKKW matching: ckkw matching: TBP>+≡
    procedure :: after_shower => ckkw_matching_after_shower

<CKKW matching: sub interfaces>+≡
    module subroutine ckkw_matching_after_shower &
        (matching, particle_set, vetoed)
        class(ckkw_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
    end subroutine ckkw_matching_after_shower

<CKKW matching: procedures>+≡
    module subroutine ckkw_matching_after_shower (matching, particle_set, vetoed)
        class(ckkw_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
        vetoed = .false.
    end subroutine ckkw_matching_after_shower

<CKKW matching: procedures>+≡
    function GammaQ (smallq, largeq, settings, fsr) result (gamma)
        real(default), intent(in) :: smallq, largeq
        type(shower_settings_t), intent(in) :: settings
        logical, intent(in) :: fsr
        real(default) :: gamma
        gamma = (8._default / three) / (pi * smallq)
        gamma = gamma * (log(largeq / smallq) - 0.75)
        if (fsr) then
            gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
        else
            gamma = gamma * D_alpha_s_isr (smallq**2, settings)
        end if
    end function GammaQ

<CKKW matching: procedures>+≡
    function GammaG (smallq, largeq, settings, fsr) result (gamma)
        real(default), intent(in) :: smallq, largeq
        type(shower_settings_t), intent(in) :: settings
        logical, intent(in) :: fsr
        real(default) :: gamma
        gamma = 6._default / (pi * smallq)
        gamma = gamma * (log(largeq / smallq) - 11.0 / 12.0)
        if (fsr) then
            gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
        else
            gamma = gamma * D_alpha_s_isr (smallq**2, settings)
        end if

```

```
end function GammaG
```

(CKKW matching: procedures)+≡

```
function GammaF (smallq, settings, fsr) result (gamma)
  real(default), intent(in) :: smallq
  type(shower_settings_t), intent(in) :: settings
  logical, intent(in) :: fsr
  real(default) :: gamma
  gamma = number_of_flavors (smallq, settings%max_n_flavors, &
    settings%min_virtuality) / (three * pi * smallq)
  if (fsr) then
    gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
  else
    gamma = gamma * D_alpha_s_isr (smallq**2, settings)
  end if
end function GammaF
```

(CKKW matching: procedures)+≡

```
function SudakovQ (Q1, Q, settings, fsr, rng) result (sf)
  real(default), intent(in) :: Q1, Q
  type(shower_settings_t), intent(in) :: settings
  class(rng_t), intent(inout), allocatable :: rng
  logical, intent(in) :: fsr
  real(default) :: sf
  real(default) :: integral
  integer, parameter :: NTRIES = 100
  integer :: i
  real(default) :: rand
  integral = zero
  do i = 1, NTRIES
    call rng%generate (rand)
    integral = integral + GammaQ (Q1 + rand * (Q - Q1), Q, settings, fsr)
  end do
  integral = integral / NTRIES
  sf = exp (-integral)
end function SudakovQ
```

(CKKW matching: procedures)+≡

```
function SudakovG (Q1, Q, settings, fsr, rng) result (sf)
  real(default), intent(in) :: Q1, Q
  type(shower_settings_t), intent(in) :: settings
  logical, intent(in) :: fsr
  real(default) :: sf
  real(default) :: integral
  class(rng_t), intent(inout), allocatable :: rng
  integer, parameter :: NTRIES = 100
  integer :: i
  real(default) :: rand
  integral = zero
  do i = 1, NTRIES
    call rng%generate (rand)
    integral = integral + &
      GammaG (Q1 + rand * (Q - Q1), Q, settings, fsr) + &
```

```

        GammaF (Q1 + rand * (Q - Q1), settings, fsr)
    end do
    integral = integral / NTRIES
    sf = exp (-integral)
end function SudakovG

```

31.4 POWHEG

This module generates radiation according to the POWHEG Sudakov form factor

$$\Delta^{f_b}(\Phi_n, p_T) = \prod_{\alpha_r \in \{\alpha_r | f_b\}} \Delta_{\alpha_r}^{f_b}(\Phi_n, p_T), \quad (31.1)$$

with

$$\Delta_{\alpha_r}^{f_b}(\Phi_n, p_T) = \exp \left\{ - \left[\int d\Phi_{\text{rad}} \frac{R(\Phi_{n+1})}{B^{f_b}(\Phi_n)} \theta(k_T(\Phi_{n+1}) - p_T) \right]_{\alpha_r}^{\bar{\Phi}_n^{\alpha_r} = \Phi_n} \right\} \quad (31.2)$$

We expect that an underlying Born flavor structure f_b has been generated with a probability proportional to its contribution to the \tilde{B} at the given kinematic point.

```

<powheg_matching.f90>≡
  <File header>

```

```

module powheg_matching

```

```

  use, intrinsic :: iso_fortran_env

```

```

  <Use kinds with double>

```

```

  <Use strings>

```

```

  use diagnostics

```

```

  use constants, only: ZERO, ONE, TWO, THREE, FOUR, FIVE, TINY_07, PI, TWOPI

```

```

  use pdf, only: pdf_data_t

```

```

  use lorentz

```

```

  use phs_points, only: assignment(=), operator(*)

```

```

  use sm_qcd, only: qcd_t, alpha_qcd_from_scale_t, alpha_qcd_from_lambda_t

```

```

  use particles

```

```

  use grids

```

```

  use solver

```

```

  use rng_base

```

```

  use variables

```

```

  use phs_fks, only: phs_fks_generator_t, compute_dalitz_bounds, beta_emitter

```

```

  use phs_fks, only: phs_point_set_t, phs_identifier_t, phs_fks_t

```

```

  use phs_fks, only: get_xi_max_isr

```

```

  use phs_fks, only: I_XI, I_Y, I_PLUS, I_MINUS, UBF_FSR_SIMPLE, UBF_FSR_MASSIVE, UBF_FSR_MASSLESS

```

```

  use matching_base

```

```

  use instances, only: process_instance_t, process_instance_hook_t

```

```

  use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t

```

```

  <Standard module head>

```

```

    <POWHEG matching: public>

    <POWHEG matching: types>

    <POWHEG matching: interfaces>

    interface
    <POWHEG matching: sub interfaces>
    end interface

contains

    <POWHEG matching: main procedures>

end module powheg_matching
<powheg_matching_sub.f90>≡
    <File header>

submodule (powheg_matching) powheg_matching_s

    <Use mpi f08>
    <Use debug>
    use io_units, only: given_output_unit, free_unit
    use format_utils, only: write_separator
    use format_defs, only: FMT_16, FMT_19
    use string_utils, only: str
    use numeric_utils
    use os_interface, only: os_file_exist
    use physics_defs, only: CA, BORN, NLO_REAL, MZ_REF
    use pdg_arrays, only: is_gluon, is_quark
    use sf_lhapdf, only: alpha_qcd_lhapdf_t
    use sm_physics, only: Li2, coeff_b0, lambda_qcd
    use subevents, only: PRT_INCOMING, PRT_OUTGOING
    use colors
    use process_config, only: COMP_REAL_FIN
    use prc_external, only: prc_external_state_t
    use prc_omega, only: omega_state_t

    implicit none

contains

    <POWHEG matching: procedures>

end submodule powheg_matching_s

```

31.4.1 Base types for settings and data

λ is the lowest scale $\Lambda^{(5)}_{\overline{\text{MS}}}$ where the radiation α_s^{rad} is still larger than the true α_s . We relate α_s^{rad} and α_s^{true} at the scale $2\Lambda^{(5)}_{\overline{\text{MS}}}$.

```

<POWHEG matching: public>≡

```

```

    public :: powheg_settings_t
<POWHEG matching: types>≡
    type :: powheg_settings_t
        real(default) :: pt2_min = zero
        real(default) :: lambda = zero
        integer :: size_grid_xi = 0
        integer :: size_grid_y = 0
        integer :: upper_bound_func_type = UBF_FSR_SIMPLE
        logical :: test_sudakov = .false.
        logical :: disable_sudakov = .false.
        logical :: singular_jacobian = .false.
    contains
        <POWHEG matching: powheg settings: TBP>
    end type powheg_settings_t

<POWHEG matching: powheg settings: TBP>≡
    procedure :: init => powheg_settings_init

<POWHEG matching: sub interfaces>≡
    module subroutine powheg_settings_init (settings, var_list)
        class(powheg_settings_t), intent(out) :: settings
        type(var_list_t), intent(in) :: var_list
    end subroutine powheg_settings_init

<POWHEG matching: procedures>≡
    module subroutine powheg_settings_init (settings, var_list)
        class(powheg_settings_t), intent(out) :: settings
        type(var_list_t), intent(in) :: var_list
        settings%pt2_min = &
            var_list%get_rval (var_str ("powheg_pt_min"))**2
        settings%size_grid_xi = &
            var_list%get_ival (var_str ("powheg_grid_size_xi"))
        settings%size_grid_y = &
            var_list%get_ival (var_str ("powheg_grid_size_y"))
        settings%lambda = var_list%get_rval (var_str ("powheg_lambda"))
        settings%singular_jacobian = &
            var_list%get_lval (var_str ("?powheg_use_singular_jacobian"))
        settings%test_sudakov = &
            var_list%get_lval (var_str ("?powheg_test_sudakov"))
        settings%disable_sudakov = &
            var_list%get_lval (var_str ("?powheg_disable_sudakov"))
    end subroutine powheg_settings_init

<POWHEG matching: powheg settings: TBP>+≡
    procedure :: write => powheg_settings_write

<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_settings_write (powheg_settings, unit)
        class(powheg_settings_t), intent(in) :: powheg_settings
        integer, intent(in), optional :: unit
    end subroutine powheg_settings_write

<POWHEG matching: procedures>+≡
    module subroutine powheg_settings_write (powheg_settings, unit)
        class(powheg_settings_t), intent(in) :: powheg_settings

```

```

integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(1X,A)") "POWHEG settings:"
write (u, "(3X,A," // FMT_16 // ")") "pt2_min = ", powheg_settings%pt2_min
write (u, "(3X,A," // FMT_16 // ")") "lambda = ", powheg_settings%lambda
write (u, "(3X,A,I12)") "size_grid_xi = ", powheg_settings%size_grid_xi
write (u, "(3X,A,I12)") "size_grid_y = ", powheg_settings%size_grid_y
write (u, "(3X,A,I12)") "upper_bound_func_type = ", powheg_settings%upper_bound_func_type
end subroutine powheg_settings_write

```

<POWHEG matching: public>+≡

```
public :: radiation_t
```

<POWHEG matching: types>+≡

```

type :: radiation_t
real(default) :: xi, y, phi, pt2
integer :: alr
logical :: valid = .false.
contains
<POWHEG matching: radiation: TBP>
end type radiation_t

```

<POWHEG matching: radiation: TBP>≡

```
procedure :: write => radiation_write
```

<POWHEG matching: sub interfaces>+≡

```

module subroutine radiation_write (radiation, unit)
class(radiation_t), intent(in) :: radiation
integer, intent(in), optional :: unit
end subroutine radiation_write

```

<POWHEG matching: procedures>+≡

```

module subroutine radiation_write (radiation, unit)
class(radiation_t), intent(in) :: radiation
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(1X, A)") "Radiation:"
write (u, "(3X, A," // FMT_16 // ")") "xi = ", radiation%xi
write (u, "(3X, A," // FMT_16 // ")") "y = ", radiation%y
write (u, "(3X, A," // FMT_16 // ")") "phi = ", radiation%phi
write (u, "(3X, A," // FMT_16 // ")") "pt2 = ", radiation%pt2
write (u, "(3X, A, I12)") "alr = ", radiation%alr
end subroutine radiation_write

```

lambda2_gen is the scale used in the (log integrated) upper bounding functions.
It is not equivalent to lambda5MSB which is a reference scale for the α_s evolution.

<POWHEG matching: public>+≡

```
public :: process_deps_t
```

<POWHEG matching: types>+≡

```

type :: process_deps_t
real(default) :: lambda2_gen, lambda5MSB, sqrts

```

```

integer :: n_alr
integer :: alpha_power, alphas_power
logical :: lab_is_cm = .true.
type(pdf_data_t) :: pdf_data
type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
integer, dimension(:), allocatable :: alr_to_i_phs
integer :: i_term_born
integer, dimension(:), allocatable :: i_term_real
contains
  <POWHEG matching: process deps: TBP>
end type process_deps_t

<POWHEG matching: process deps: TBP>≡
  procedure :: write => process_deps_write

<POWHEG matching: sub interfaces>+≡
  module subroutine process_deps_write (process_deps, unit)
    class(process_deps_t), intent(in) :: process_deps
    integer, intent(in), optional :: unit
  end subroutine process_deps_write

<POWHEG matching: procedures>+≡
  module subroutine process_deps_write (process_deps, unit)
    class(process_deps_t), intent(in) :: process_deps
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1X,A)") "Process dependencies:"
    write (u, "(3X,A," // FMT_19 // ")") "lambda2_gen = ", &
      process_deps%lambda2_gen
    write (u, "(3X,A," // FMT_19 // ")") "lambda5MSB = ", &
      process_deps%lambda5MSB
    write (u, "(3X,A, I12)") "n_alr = ", process_deps%n_alr
    write (u, "(3X,A, L12)") "lab_is_cm = ", process_deps%lab_is_cm
    write (u, "(3X,A, I10)") "alpha_power = ", process_deps%alpha_power
    write (u, "(3X,A, I9)") "alphas_power = ", process_deps%alphas_power
    write (u, "(3X,A, I10)") "i_term_born = ", process_deps%i_term_born
    do i = 1, size(process_deps%i_term_real)
      write (u, "(3X,A,I2,A, I6)") "i_term_real(",i,") = ", &
        process_deps%i_term_real(i)
    end do
    call process_deps%pdf_data%write(u)
  end subroutine process_deps_write

<POWHEG matching: public>+≡
  public :: event_deps_t

<POWHEG matching: types>+≡
  type :: event_deps_t
    real(default) :: s_hat
    real(default), dimension(2) :: x_born
    real(default) :: s_had
    type(phs_point_set_t) :: p_born_cms
    type(phs_point_set_t) :: p_born_lab
    type(phs_point_set_t) :: p_real_cms

```



```

        type(phs_point_set_t) :: p_real_lab
        real(default), dimension(:), allocatable :: sqme_born
contains
    <POWHEG matching: event deps: TBP>
end type event_deps_t

<POWHEG matching: event deps: TBP>≡
    procedure :: write => event_deps_write

<POWHEG matching: sub interfaces>+≡
    module subroutine event_deps_write (event_deps, unit)
        class(event_deps_t), intent(in) :: event_deps
        integer, intent(in), optional :: unit
    end subroutine event_deps_write

<POWHEG matching: procedures>+≡
    module subroutine event_deps_write (event_deps, unit)
        class(event_deps_t), intent(in) :: event_deps
        integer, intent(in), optional :: unit
        integer :: u, alr
        u = given_output_unit(unit); if (u < 0) return
        write (u, "(1X,A)") "Event dependencies:"
        write (u, "(3X,A," // FMT_19 // ")") "s_hat = ", event_deps%s_hat
        write (u, "(3X,A," // FMT_19 // ")") "x(+) = ", event_deps%x_born(I_PLUS)
        write (u, "(3X,A," // FMT_19 // ")") "x(-) = ", event_deps%x_born(I_MINUS)
        write (u, "(3X,A," // FMT_19 // ")") "s_had = ", event_deps%s_had
        do alr = 1, size(event_deps%sqme_born)
            write (u, "(3X,A,I3,A," // FMT_19 // ")") "sqme_born(",alr,") = ", &
                event_deps%sqme_born(alr)
        end do
    end subroutine event_deps_write

<POWHEG matching: event deps: TBP>+≡
    procedure :: update => event_deps_update

<POWHEG matching: sub interfaces>+≡
    module subroutine event_deps_update (event_deps, sqme_born, &
        p_born, x_born, lt_lab_to_cms)
        class(event_deps_t), intent(inout) :: event_deps
        real(default), dimension(:), intent(in) :: sqme_born
        type(vector4_t), dimension(:), intent(in) :: p_born
        real(default), dimension(2), intent(in) :: x_born
        type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
    end subroutine event_deps_update

<POWHEG matching: procedures>+≡
    module subroutine event_deps_update (event_deps, sqme_born, &
        p_born, x_born, lt_lab_to_cms)
        class(event_deps_t), intent(inout) :: event_deps
        real(default), dimension(:), intent(in) :: sqme_born
        type(vector4_t), dimension(:), intent(in) :: p_born
        real(default), dimension(2), intent(in) :: x_born
        type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
        integer :: n_born
        if (allocated(event_deps%sqme_born)) then

```

```

        event_deps%sqme_born = sqme_born
    else
        allocate(event_deps%sqme_born, source=sqme_born)
    end if
    n_born = size (p_born)
    if (debug_active (D_MATCHING)) then
        if (n_born /= event_deps%p_born_lab%get_n_particles (1)) then
            call msg_fatal &
                ("event_deps_update: number of born_momenta has changed")
        end if
    end if
    call event_deps%p_born_lab%set_momenta (1, p_born)
    call event_deps%set_cms (lt_lab_to_cms)
    event_deps%x_born = x_born
    event_deps%s_hat = event_deps%s_hat / ( x_born(I_PLUS) * x_born(I_MINUS) )
end subroutine event_deps_update

```

Sets the Born momenta in the CMS boosting them if necessary.

```

<POWHEG matching: event_deps: TBP>+≡
    procedure :: set_cms => event_deps_set_cms

<POWHEG matching: sub interfaces>+≡
    module subroutine event_deps_set_cms (event_deps, lt_lab_to_cms)
        class(event_deps_t), intent(inout) :: event_deps
        type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
    end subroutine event_deps_set_cms

<POWHEG matching: procedures>+≡
    module subroutine event_deps_set_cms (event_deps, lt_lab_to_cms)
        class(event_deps_t), intent(inout) :: event_deps
        type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
        associate (pp => event_deps%p_born_lab%phs_point(1))
            event_deps%s_hat = pp%get_msq ([1,2])
            if (present (lt_lab_to_cms)) then
                event_deps%p_born_cms%phs_point(1) = lt_lab_to_cms * pp
            else
                event_deps%p_born_cms%phs_point(1) = pp
            end if
        end associate
    end subroutine event_deps_set_cms

<POWHEG matching: types>+≡
    type :: veto_counter_t
        integer :: n_ubf = 0
        integer :: n_xi_max = 0
        integer :: n_norm = 0
        integer :: n_sqme = 0
        integer :: n_veto_ubf = 0
        integer :: n_veto_xi_max = 0
        integer :: n_veto_norm = 0
        integer :: n_veto_sqme = 0
        integer :: n_fail_ubf = 0
    contains
        <POWHEG matching: veto counter: TBP>

```

```

end type veto_counter_t

<POWHEG matching: veto counter: TBP>≡
  procedure :: record_ubf => veto_counter_record_ubf

<POWHEG matching: sub interfaces>+≡
  pure module subroutine veto_counter_record_ubf (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
  end subroutine veto_counter_record_ubf

<POWHEG matching: procedures>+≡
  pure module subroutine veto_counter_record_ubf (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_ubf = counter%n_ubf + 1
    if (vetoed) counter%n_veto_ubf = counter%n_veto_ubf + 1
  end subroutine veto_counter_record_ubf

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_xi_max => veto_counter_record_xi_max

<POWHEG matching: sub interfaces>+≡
  module subroutine veto_counter_record_xi_max (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
  end subroutine veto_counter_record_xi_max

<POWHEG matching: procedures>+≡
  module subroutine veto_counter_record_xi_max (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_xi_max = counter%n_xi_max + 1
    if (vetoed) counter%n_veto_xi_max = counter%n_veto_xi_max + 1
  end subroutine veto_counter_record_xi_max

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_norm => veto_counter_record_norm

<POWHEG matching: sub interfaces>+≡
  module subroutine veto_counter_record_norm (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
  end subroutine veto_counter_record_norm

<POWHEG matching: procedures>+≡
  module subroutine veto_counter_record_norm (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_norm = counter%n_norm + 1
    if (vetoed) counter%n_veto_norm = counter%n_veto_norm + 1
  end subroutine veto_counter_record_norm

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_sqme => veto_counter_record_sqme

```

```

<POWHEG matching: sub interfaces>+≡
  module subroutine veto_counter_record_sqme (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
  end subroutine veto_counter_record_sqme

```

```

<POWHEG matching: procedures>+≡
  module subroutine veto_counter_record_sqme (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_sqme = counter%n_sqme + 1
    if (vetoed) counter%n_veto_sqme = counter%n_veto_sqme + 1
  end subroutine veto_counter_record_sqme

```

```

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_ubf_fail => veto_counter_record_ubf_fail

```

```

<POWHEG matching: sub interfaces>+≡
  module subroutine veto_counter_record_ubf_fail (counter)
    class(veto_counter_t), intent(inout) :: counter
  end subroutine veto_counter_record_ubf_fail

```

```

<POWHEG matching: procedures>+≡
  module subroutine veto_counter_record_ubf_fail (counter)
    class(veto_counter_t), intent(inout) :: counter
    counter%n_fail_ubf = counter%n_fail_ubf + 1
  end subroutine veto_counter_record_ubf_fail

```

This routine fills the POWHEG veto log file with content showing how many events have been vetoed in which step of the sudakov veto algorithm.

```

<POWHEG matching: veto counter: TBP>+≡
  procedure :: write => veto_counter_write

```

```

<POWHEG matching: sub interfaces>+≡
  module subroutine veto_counter_write (counter, unit)
    class(veto_counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
  end subroutine veto_counter_write

```

```

<POWHEG matching: procedures>+≡
  module subroutine veto_counter_write (counter, unit)
    class(veto_counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A29,I10)") "Nr. of ubf-veto calls: ", counter%n_ubf
    write (u, "(A29,I10)") "Nr. of ubf-vetos: ", counter%n_veto_ubf
    if (counter%n_ubf > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_ubf / counter%n_ubf * 100, "%"
    call write_separator (u)

    write (u, "(A29,I10)") "Nr. of xi_max-veto calls: ", counter%n_xi_max
    write (u, "(A29,I10)") "Nr. of xi_max-vetos: ", counter%n_veto_xi_max
    if (counter%n_xi_max > 0) &

```

```

        write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
            one * counter%n_veto_xi_max / counter%n_xi_max * 100, "%"
        call write_separator (u)

        write (u, "(A29,I10)") "Nr. of norm-veto calls: ", counter%n_norm
        write (u, "(A29,I10)") "Nr. of norm-vetos: ", counter%n_veto_norm
        if (counter%n_norm > 0) &
            write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
                one * counter%n_veto_norm / counter%n_norm * 100, "%"
        call write_separator (u)

        write (u, "(A29,I10)") "Nr. of sqme-veto calls: ", counter%n_sqme
        write (u, "(A29,I10)") "Nr. of sqme-vetos: ", counter%n_veto_sqme
        if (counter%n_sqme > 0) &
            write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
                one * counter%n_veto_sqme / counter%n_sqme * 100, "%"
        call write_separator (u)
        write (u, "(A29,I10)") "Nr. of upper-bound failures: ", &
            counter%n_fail_ubf
        if (counter%n_sqme > 0) &
            write (u, "(A29,F9.2,A1)") "Fraction of failed points: ", &
                one * counter%n_fail_ubf / counter%n_sqme * 100, "%"
        end subroutine veto_counter_write

```

31.4.2 Upper bounding functions and sudakovs

Abstract version

This contains the pieces that depend on the radiation region α_r

<POWHEG matching: public>+≡

public :: sudakov_t

<POWHEG matching: types>+≡

```

type, abstract, extends (solver_function_t) :: sudakov_t
type(process_deps_t), pointer :: process_deps => null()
type(event_deps_t), pointer :: event_deps => null()
type(powheg_settings_t), pointer :: powheg_settings => null()
type(phs_fks_generator_t), pointer :: phs_fks_generator => null()
type(qcd_t) :: qcd
class(rng_t), pointer :: rng => null()
real(default) :: xi2_max = zero
real(default) :: norm_max = zero
real(default) :: current_pt2_max = zero
real(default) :: sum_log_rands = zero
real(default) :: random = zero
type(veto_counter_t) :: veto_counter
integer :: i_phs = 0
contains
<POWHEG matching: sudakov: TBP>
end type sudakov_t

```

<POWHEG matching: sudakov: TBP>≡

procedure :: write => sudakov_write

<POWHEG matching: sub interfaces>+≡

```
module subroutine sudakov_write (sudakov, unit)
  class(sudakov_t), intent(in) :: sudakov
  integer, intent(in), optional :: unit
end subroutine sudakov_write
```

<POWHEG matching: procedures>+≡

```
module subroutine sudakov_write (sudakov, unit)
  class(sudakov_t), intent(in) :: sudakov
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(3X,A," // FMT_19 // ")") "xi2_max = ", sudakov%xi2_max
  write (u, "(3X,A," // FMT_19 // ")") "norm_max = ", sudakov%norm_max
  write (u, "(3X,A," // FMT_19 // ")") &
    "current_pt2_max = ", sudakov%current_pt2_max
  write (u, "(3X,A," // FMT_19 // ")") "sum_log_rands = ", sudakov%sum_log_rands
  write (u, "(3X,A," // FMT_19 // ")") "random = ", sudakov%random
end subroutine sudakov_write
```

To allow for arrays of this class

<POWHEG matching: public>+≡

```
public :: sudakov_wrapper_t
```

<POWHEG matching: types>+≡

```
type :: sudakov_wrapper_t
  class(sudakov_t), allocatable :: s
end type sudakov_wrapper_t
```

<POWHEG matching: sudakov: TBP>+≡

```
procedure :: init => sudakov_init
```

<POWHEG matching: sub interfaces>+≡

```
module subroutine sudakov_init (sudakov, process_deps, event_deps, &
  powheg_settings, qcd, phs_fks_generator, rng)
  class(sudakov_t), intent(out) :: sudakov
  type(process_deps_t), target, intent(in) :: process_deps
  type(event_deps_t), target, intent(in) :: event_deps
  type(powheg_settings_t), target, intent(in) :: powheg_settings
  type(qcd_t), intent(in) :: qcd
  type(phs_fks_generator_t), target, intent(in) :: phs_fks_generator
  class(rng_t), target, intent(in), optional :: rng
end subroutine sudakov_init
```

<POWHEG matching: procedures>+≡

```
module subroutine sudakov_init (sudakov, process_deps, event_deps, &
  powheg_settings, qcd, phs_fks_generator, rng)
  class(sudakov_t), intent(out) :: sudakov
  type(process_deps_t), target, intent(in) :: process_deps
  type(event_deps_t), target, intent(in) :: event_deps
  type(powheg_settings_t), target, intent(in) :: powheg_settings
  type(qcd_t), intent(in) :: qcd
  type(phs_fks_generator_t), target, intent(in) :: phs_fks_generator
  class(rng_t), target, intent(in), optional :: rng
  sudakov%process_deps => process_deps
```

```

    sudakov%event_deps => event_deps
    sudakov%powheg_settings => powheg_settings
    sudakov%qcd = qcd
    sudakov%phs_fks_generator => phs_fks_generator
    if (present (rng)) sudakov%rng => rng
end subroutine sudakov_init

```

This has to be done after the grids are initialized.

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: set_normalization => sudakov_set_normalization

<POWHEG matching: sub interfaces>+≡
    pure module subroutine sudakov_set_normalization (sudakov, norm_max)
        class(sudakov_t), intent(inout) :: sudakov
        real(default), intent(in) :: norm_max
    end subroutine sudakov_set_normalization

<POWHEG matching: procedures>+≡
    pure module subroutine sudakov_set_normalization (sudakov, norm_max)
        class(sudakov_t), intent(inout) :: sudakov
        real(default), intent(in) :: norm_max
        sudakov%norm_max = norm_max
    end subroutine sudakov_set_normalization

```

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: update_xi2_max => sudakov_update_xi2_max

<POWHEG matching: sub interfaces>+≡
    pure module subroutine sudakov_update_xi2_max (sudakov, xi2_max)
        class(sudakov_t), intent(inout) :: sudakov
        real(default), intent(in) :: xi2_max
    end subroutine sudakov_update_xi2_max

<POWHEG matching: procedures>+≡
    pure module subroutine sudakov_update_xi2_max (sudakov, xi2_max)
        class(sudakov_t), intent(inout) :: sudakov
        real(default), intent(in) :: xi2_max
        sudakov%xi2_max = xi2_max
    end subroutine sudakov_update_xi2_max

```

upper_bound_func does *not* contain the normalization N which is given by the grids. In the notation of 1002.2581, it is thus $\frac{1}{N}U(\xi, y)$

```

<POWHEG matching: sudakov: TBP>+≡
    procedure (sudakov_upper_bound_func), deferred :: upper_bound_func

<POWHEG matching: interfaces>≡
    abstract interface
        pure function sudakov_upper_bound_func (sudakov, xi, y, alpha_s) result (u)
            import
            real(default) :: u
            class(sudakov_t), intent(in) :: sudakov
            real(default), intent(in) :: xi, y, alpha_s
        end function sudakov_upper_bound_func
    end interface

```

Similar to the `upper_bound_func`, this is $-\frac{1}{N} \log \Delta(p_T^2)$ where

$$\Delta^{(U)}(p_T) = \exp \left[-N \int U(\xi, y) \theta(k_T - p_T) d\xi dy d\phi \right] \quad (31.3)$$

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_log_integrated_ubf), deferred :: log_integrated_ubf

<POWHEG matching: interfaces>+≡
  abstract interface
    pure function sudakov_log_integrated_ubf (sudakov, pt2) result (y)
    import
    real(default) :: y
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_log_integrated_ubf
end interface

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_generate_xi_and_y_and_phi), deferred :: generate_xi_and_y_and_phi

<POWHEG matching: interfaces>+≡
  abstract interface
    subroutine sudakov_generate_xi_and_y_and_phi (sudakov, r)
    import
    class(sudakov_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_generate_xi_and_y_and_phi
end interface

Generating  $\phi$  can be performed in a generic way for all UBF types.

<POWHEG matching: sudakov: TBP>+≡
  procedure :: generate_phi => sudakov_generate_phi

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_generate_phi (sudakov, r)
    class(sudakov_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_generate_phi

<POWHEG matching: procedures>+≡
  module subroutine sudakov_generate_phi (sudakov, r)
    class(sudakov_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    call sudakov%rng%generate (sudakov%random)
    r%phi = sudakov%random * twopi
  end subroutine sudakov_generate_phi

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_kt2), deferred :: kt2

<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_kt2 (sudakov, xi, y) result (kt2)
    import

```



```

    real(default) :: kt2
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
end function sudakov_kt2
end interface

```

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_kt2_max), deferred :: kt2_max

<POWHEG matching: interfaces>+≡
  abstract interface
    pure function sudakov_kt2_max (sudakov) result (kt2_max)
    import
    real(default) :: kt2_max
    class(sudakov_t), intent(in) :: sudakov
  end function sudakov_kt2_max
end interface

```

Veto routine for an overestimation of the UBF performed to simplify the log integrated UBF

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_reweight_ubf), deferred :: reweight_ubf

<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_reweight_ubf (sudakov, pt2) result (accepted)
    import
    logical :: accepted
    class(sudakov_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_reweight_ubf
end interface

```

Veto routine to correct for an overestimation of ξ_{\max} performed in the case of massive emitters.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_reweight_xi_max), deferred :: reweight_xi_max

<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_reweight_xi_max (sudakov, xi) result (accepted)
    import
    logical :: accepted
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
  end function sudakov_reweight_xi_max
end interface

```

In the generation of p_T^2 via `log_integrated_ubf`, we use the simplified version α_s^{rad} while the grids take the improved version.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: alpha_s => sudakov_alpha_s

```

```

<POWHEG matching: sub interfaces>+≡
  module function sudakov_alpha_s (sudakov, kT2, use_correct, improve_nll) result (a)
    real(default) :: a
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: kT2
    logical, intent(in), optional :: use_correct, improve_nll
  end function sudakov_alpha_s

<POWHEG matching: procedures>+≡
  module function sudakov_alpha_s (sudakov, kT2, use_correct, improve_nll) result (a)
    real(default) :: a
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: kT2
    logical, intent(in), optional :: use_correct, improve_nll
    logical :: correct, nll
    correct = .false.; if (present (use_correct)) correct = use_correct
    nll = .true.; if (present(improve_nll)) nll = improve_nll
    if (correct) then
      a = get_alpha_s (sudakov%qcd, kT2, improve_nll_opt=nll)
    else
      a = sudakov%alpha_s_rad (kT2)
    end if
  end function sudakov_alpha_s

```

To generate the transverse momentum, we have to solve the equation

$$\frac{\Delta^{(U)}(p_T)}{\Delta^{(U)}(p_T^{\max})} = r_1$$

iteratively for p_T . In log space and with initially $\Delta^{(U)}(p_T^{\max}) = 1$, this is

$$\log \Delta^{(U)}(p_T) = \log r_1$$

If no solution is found, we set $p_T = p_T^{\min}$ to exit the event generation loop and generate an emissionless event. If a solution is found but the current emission is not accepted, we set $p_T = p_T^{\max}$ and thus in the next step it is $\Delta^{(U)}(p_T^{\max}) = r_1$, so that we have to solve the equation

$$\log \Delta^{(U)}(p_T) = \log r_1 + \log r_2$$

using another random number r_2 . We use `sum_log_rands` to remember the sum of the logarithms of all previous random numbers used for this event.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: generate_pt2 => sudakov_generate_pt2

<POWHEG matching: sub interfaces>+≡
  module function sudakov_generate_pt2 (sudakov) result (pt2)
    real(default) :: pt2
    class(sudakov_t), intent(inout) :: sudakov
  end function sudakov_generate_pt2

<POWHEG matching: procedures>+≡
  module function sudakov_generate_pt2 (sudakov) result (pt2)
    real(default) :: pt2
    class(sudakov_t), intent(inout) :: sudakov

```

```

logical :: success
success = .false.
if (sudakov%current_pt2_max > sudakov%powheg_settings%pt2_min) then
  call sudakov%rng%generate (sudakov%random)
  sudakov%sum_log_rands = sudakov%sum_log_rands + log(sudakov%random)
  pt2 = solve_interval (sudakov, &
    sudakov%powheg_settings%pt2_min, &
    sudakov%current_pt2_max, success, &
    0.001_default)
end if
if (.not. success) then
  pt2 = sudakov%powheg_settings%pt2_min
end if
end function sudakov_generate_pt2

```

This could be activated if (debug_active (MATCHING)).

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: check_solution_interval => sudakov_check_solution_interval

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_check_solution_interval (sudakov)
    class(sudakov_t), intent(inout) :: sudakov
  end subroutine sudakov_check_solution_interval

<POWHEG matching: procedures>+≡
  module subroutine sudakov_check_solution_interval (sudakov)
    class(sudakov_t), intent(inout) :: sudakov
    real(default) :: r
    real(default), parameter :: dr = 0.05
    real(default) :: pt2
    logical :: success
    r = 0._default
    do
      r = r + dr
      sudakov%random = r
      pt2 = solve_interval (sudakov, &
        sudakov%powheg_settings%pt2_min, &
        sudakov%current_pt2_max, success, &
        0.001_default)
      if (success) then
        print *, 'r: ', r, ' zero found'
      else
        print *, 'r: ', r, 'no zero found'
      end if
      if (r >= 1._default) exit
    end do
  end subroutine sudakov_check_solution_interval

```

Generates the FKS variables (ξ, y, ϕ) and sets the emission hardness scale. In debug mode, we assert that the `pt2` saved in the `radiation_t` and the massive hardness scale are equal. This should hold as we compute `kt2` with the `y` we got from generating `pt2` so that this is a full circle. It then initiates the generation of the transverse momentum followed by a sequence of veto steps to get the

correct distribution.

(POWHEG matching: sudakov: TBP)+≡

```
procedure :: generate_emission => sudakov_generate_emission
```

(POWHEG matching: sub interfaces)+≡

```
module subroutine sudakov_generate_emission (sudakov, r, r_max)
  class(sudakov_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  type(radiation_t), intent(in) :: r_max
end subroutine sudakov_generate_emission
```

(POWHEG matching: procedures)+≡

```
module subroutine sudakov_generate_emission (sudakov, r, r_max)
  class(sudakov_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  type(radiation_t), intent(in) :: r_max
  logical :: accepted
  sudakov%current_pt2_max = r%pt2
  if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_generate_emission")
  if (debug_on) call msg_debug2 (D_MATCHING, "sqrt (sudakov%current_pt2_max)", &
    sqrt (sudakov%current_pt2_max))
  if (debug_on) call msg_debug2 (D_MATCHING, "sudakov%sum_log_rands", sudakov%sum_log_rands)
  LOOP_UNTIL_ACCEPTED: do
    if (signal_is_pending ()) return
    r%valid = .false.
    r%pt2 = sudakov%generate_pt2 ()
    if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_generate_emission: after generate_pt2")
    if (debug_on) call msg_debug2 (D_MATCHING, "sqrt (r%pt2)", sqrt (r%pt2))
    if (debug_on) call msg_debug2 (D_MATCHING, "sudakov%sum_log_rands", sudakov%sum_log_rands)
    if (r%pt2 <= sudakov%powheg_settings%pt2_min .or. r%pt2 <= r_max%pt2) then
      exit
    end if
    accepted = sudakov%reweight_ubf (r%pt2)
    call sudakov%veto_counter%record_ubf (.not. accepted)
    if (.not. accepted) then
      sudakov%current_pt2_max = r%pt2
      cycle
    end if
    call sudakov%generate_xi_and_y_and_phi (r)
    accepted = sudakov%reweight_xi_max (r%xi)
    call sudakov%veto_counter%record_xi_max (.not. accepted)
    if (.not. accepted) then
      sudakov%current_pt2_max = r%pt2
      cycle
    end if
    if (debug_active (D_MATCHING)) then
      call assert_equal (OUTPUT_UNIT, r%pt2, &
        sudakov%kt2 (r%xi, r%y), &
        "sudakov_generate_xi_and_y_and_phi: pt2 inconsistency")
    end if
    r%valid = .true.
    exit
  end do LOOP_UNTIL_ACCEPTED
end subroutine sudakov_generate_emission
```

Evaluates the Sudakov as needed for `solve_interval` to generate a p_T value.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: evaluate => sudakov_evaluate

<POWHEG matching: sub interfaces>+≡
  module function sudakov_evaluate (solver_f, x) result (f)
    complex(default) :: f
    class(sudakov_t), intent(in) :: solver_f
    real(default), intent(in) :: x
  end function sudakov_evaluate

<POWHEG matching: procedures>+≡
  module function sudakov_evaluate (solver_f, x) result (f)
    complex(default) :: f
    class(sudakov_t), intent(in) :: solver_f
    real(default), intent(in) :: x
    f = solver_f%sum_log_rands + &
        solver_f%norm_max * solver_f%log_integrated_ubf (x)
  end function sudakov_evaluate

<POWHEG matching: sudakov: TBP>+≡
  procedure :: associated_emitter => sudakov_associated_emitter

<POWHEG matching: sub interfaces>+≡
  elemental module function sudakov_associated_emitter &
    (sudakov) result (emitter)
    integer :: emitter
    class(sudakov_t), intent(in) :: sudakov
  end function sudakov_associated_emitter

<POWHEG matching: procedures>+≡
  elemental module function sudakov_associated_emitter &
    (sudakov) result (emitter)
    integer :: emitter
    class(sudakov_t), intent(in) :: sudakov
    emitter = sudakov%process_deps%phs_identifiers(sudakov%i_phs)%emitter
  end function sudakov_associated_emitter

<POWHEG matching: sudakov: TBP>+≡
  procedure :: set_i_phs => sudakov_set_i_phs

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_set_i_phs (sudakov, alr)
    class(sudakov_t), intent(inout) :: sudakov
    integer, intent(in) :: alr
  end subroutine sudakov_set_i_phs

<POWHEG matching: procedures>+≡
  module subroutine sudakov_set_i_phs (sudakov, alr)
    class(sudakov_t), intent(inout) :: sudakov
    integer, intent(in) :: alr
    sudakov%i_phs = sudakov%process_deps%alr_to_i_phs(alr)
  end subroutine sudakov_set_i_phs

```

Simple FSR

This corresponds to Appendix C of 1002.2581.

```

<POWHEG matching: public>+≡
  public :: sudakov_simple_fsr_t

<POWHEG matching: types>+≡
  type, extends (sudakov_t) :: sudakov_simple_fsr_t
  contains
    <POWHEG matching: sudakov simple fsr: TBP>
  end type sudakov_simple_fsr_t

```

The simplest upper bounding function for final-state radiation is

$$\text{upper_bound_func} = \frac{U(\xi, y)}{N} = \frac{\alpha_s}{\xi(1-y)} \quad (31.4)$$

```

<POWHEG matching: sudakov simple fsr: TBP>≡
  procedure :: upper_bound_func => sudakov_simple_fsr_upper_bound_func

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_simple_fsr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
  end function sudakov_simple_fsr_upper_bound_func

<POWHEG matching: procedures>+≡
  pure module function sudakov_simple_fsr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
    u = alpha_s / (xi * (1 - y))
  end function sudakov_simple_fsr_upper_bound_func

```

The above upper bounding function corresponds to the transverse momentum scale

$$k_T^2 = \frac{s}{2} \xi^2 (1-y). \quad (31.5)$$

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: kt2 => sudakov_simple_fsr_kt2

<POWHEG matching: sub interfaces>+≡
  module function sudakov_simple_fsr_kt2 (sudakov, xi, y) result (kt2)
    real(default) :: kt2
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
  end function sudakov_simple_fsr_kt2

<POWHEG matching: procedures>+≡
  module function sudakov_simple_fsr_kt2 (sudakov, xi, y) result (kt2)
    real(default) :: kt2
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y

```

```

    kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
      (sudakov%i_phs, sudakov%associated_emitter (), UBF_FSR_SIMPLE, xi, y)
end function sudakov_simple_fsr_kt2

```

For massless emitters, the upper bound on the radiated energy is

$$t_{\max} = \xi_{\max}^2 \hat{s}$$

We use this as largest possible scale for the radiation.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: kt2_max => sudakov_simple_fsr_kt2_max

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_simple_fsr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
  end function sudakov_simple_fsr_kt2_max

<POWHEG matching: procedures>+≡
  pure module function sudakov_simple_fsr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default) :: s_hat
    s_hat = sudakov%event_deps%s_hat
    kt2_max = sudakov%xi2_max * s_hat
  end function sudakov_simple_fsr_kt2_max

```

This is

$$-\frac{\log \Delta^{(U)}(p_T)}{N} = \frac{\pi}{b_0} \theta \left(\xi_{\max}^2 - \frac{p_T^2}{s} \right) \left[\log \frac{\xi_{\max}^2 s}{\Lambda^2} \log \frac{\log \xi_{\max}^2 s / \Lambda^2}{\log p_T^2 / \Lambda^2} - \log \frac{\xi_{\max}^2 s}{p_T^2} \right] \quad (31.6)$$

with $p_{T,\max}^2 = \xi_{\max}^2 s$.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: log_integrated_ubf => sudakov_simple_fsr_log_integrated_ubf

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_simple_fsr_log_integrated_ubf &
    (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_simple_fsr_log_integrated_ubf

<POWHEG matching: procedures>+≡
  pure module function sudakov_simple_fsr_log_integrated_ubf &
    (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: kt2_max, kt2_max1, pt21
    logical :: within_boundaries
    within_boundaries = pt2 <= sudakov%kt2_max () &
      .and. pt2 >= sudakov%powheg_settings%pt2_min
    if (within_boundaries) then

```

```

      kt2_max = sudakov%kt2_max ()
      kt2_max1 = kt2_max / sudakov%process_deps%lambda2_gen
      pt2l = pt2 / sudakov%process_deps%lambda2_gen
      log_sudakov = pi / b0rad () * (log (kt2_max1) * &
        log (log (kt2_max1) / log (pt2l)) - &
        log (kt2_max / pt2))
    else
      log_sudakov = 0
    end if
  end function sudakov_simple_fsr_log_integrated_ubf

```

For this upper bounding function, we just overestimated α_s .

(POWHEG matching: sudakov simple fsr: TBP)+≡

```

  procedure :: reweight_ubf => sudakov_simple_fsr_reweight_ubf

```

(POWHEG matching: sub interfaces)+≡

```

  module function sudakov_simple_fsr_reweight_ubf &
    (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: alpha_s_true, alpha_s_rad
    logical :: alpha_s_equal
  end function sudakov_simple_fsr_reweight_ubf

```

(POWHEG matching: procedures)+≡

```

  module function sudakov_simple_fsr_reweight_ubf &
    (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: alpha_s_true, alpha_s_rad
    logical :: alpha_s_equal
    if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_simple_fsr_reweight_ubf")
    alpha_s_true = sudakov%alpha_s (pt2, use_correct = .true.)
    alpha_s_rad = sudakov%alpha_s (pt2, use_correct = .false.)
    call sudakov%rng%generate (sudakov%random)
    alpha_s_equal = nearly_equal (alpha_s_true, alpha_s_rad)
    accepted = alpha_s_equal .or. sudakov%random < alpha_s_true / alpha_s_rad
    if (debug2_active (D_MATCHING)) then
      print *, ' sqrt(pt2) = ', sqrt(pt2)
      print *, ' alpha_s_true = ', alpha_s_true
      print *, ' sudakov%process_deps%lambda2_gen = ', &
        sudakov%process_deps%lambda2_gen
      print *, ' alpha_s_rad = ', alpha_s_rad
      print *, ' sudakov%random = ', sudakov%random
      print *, ' accepted = ', accepted
      if (alpha_s_rad < alpha_s_true .and. .not. alpha_s_equal) then
        call msg_fatal ("sudakov_simple_fsr_reweight_ubf: &
          &This should never happen. &
          &Have you chosen a running alpha_s?")
      end if
    end if
  end function sudakov_simple_fsr_reweight_ubf

```



```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: reweight_xi_max => sudakov_simple_fsr_reweight_xi_max

<POWHEG matching: sub interfaces>+≡
  module function sudakov_simple_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
  end function sudakov_simple_fsr_reweight_xi_max

<POWHEG matching: procedures>+≡
  module function sudakov_simple_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = .true.
  end function sudakov_simple_fsr_reweight_xi_max

```

This depends on the choice of p_T and is tested in the assertion.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: generate_xi_and_y_and_phi => &
    sudakov_simple_fsr_generate_xi_and_y_and_phi

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi

<POWHEG matching: procedures>+≡
  module subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: s
    s = sudakov%event_deps%s_hat
    call sudakov%generate_xi (r)
    r%y = one - (two * r%pt2) / (s * r%xi**2)
    call sudakov%generate_phi (r)
  end subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi

```

We generate $\xi \in [\frac{p_T}{\sqrt{s}}, \xi_{\max}]$ with a density $1/\xi$ i.e. uniformly in $\log(\xi)$.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: generate_xi => sudakov_simple_fsr_generate_xi

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_simple_fsr_generate_xi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_simple_fsr_generate_xi

<POWHEG matching: procedures>+≡
  module subroutine sudakov_simple_fsr_generate_xi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r

```

```

real(default) :: s, xi2_max
s = sudakov%event_deps%s_hat
xi2_max = sudakov%xi2_max
call sudakov%rng%generate (sudakov%random)
r%xi = exp (((one - sudakov%random) * log (r%pt2 / s) + &
            sudakov%random * log (xi2_max)) / two)
end subroutine sudakov_simple_fsr_generate_xi

```

Dijet production at lepton colliders

In the POWHEG method paper, $e^+e^- \rightarrow q\bar{q}$ requires a UBF different from the simple one to account for an additional divergence for $(\xi, y) \rightarrow (1, -1)$.

```

<POWHEG matching: public>+≡
public :: sudakov_eeqq_fsr_t

<POWHEG matching: types>+≡
type, extends (sudakov_t) :: sudakov_eeqq_fsr_t
contains
  <POWHEG matching: sudakov eeqq fsr: TBP>
end type sudakov_eeqq_fsr_t

```

This k_T measure is the same as in the case for simple FSR up to $\mathcal{O}(\theta^4)$ when $y = \cos(\theta)$. It differs by just a factor of 2 w.r.t. `sudakov_simple_fsr_kt2`.

```

<POWHEG matching: sudakov eeqq fsr: TBP>≡
procedure :: kt2 => sudakov_eeqq_fsr_kt2

<POWHEG matching: sub interfaces>+≡
module function sudakov_eeqq_fsr_kt2 (sudakov, xi, y) result (kt2)
  real(default) :: kt2
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y
end function sudakov_eeqq_fsr_kt2

<POWHEG matching: procedures>+≡
module function sudakov_eeqq_fsr_kt2 (sudakov, xi, y) result (kt2)
  real(default) :: kt2
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y
  kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
        (sudakov%i_phs, sudakov%associated_emitter(), &
         UBF_FSR_MASSLESS_RECOIL, xi, y)
end function sudakov_eeqq_fsr_kt2

```

For eeqq, the shower starts at $k_{\max} = \frac{q^0}{2}$. (c.f. eq. (7.86) in [0709.2092].)

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: kt2_max => sudakov_eeqq_fsr_kt2_max

<POWHEG matching: sub interfaces>+≡
pure module function sudakov_eeqq_fsr_kt2_max (sudakov) result (kt2_max)
  real(default) :: kt2_max
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
end function sudakov_eeqq_fsr_kt2_max

```

```

<POWHEG matching: procedures>+≡
pure module function sudakov_eeqq_fsr_kt2_max (sudakov) result (kt2_max)
  real(default) :: kt2_max
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  kt2_max = 0.25_default * sudakov%event_deps%s_hat
end function sudakov_eeqq_fsr_kt2_max

```

This covers also the singularity at $(\xi, y) \rightarrow (1, -1)$ that occurs for a massless recoiling system.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: upper_bound_func => sudakov_eeqq_fsr_upper_bound_func

```

```

<POWHEG matching: sub interfaces>+≡
pure module function sudakov_eeqq_fsr_upper_bound_func &
  (sudakov, xi, y, alpha_s) result (u)
  real(default) :: u
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y, alpha_s
end function sudakov_eeqq_fsr_upper_bound_func

```

```

<POWHEG matching: procedures>+≡
pure module function sudakov_eeqq_fsr_upper_bound_func &
  (sudakov, xi, y, alpha_s) result (u)
  real(default) :: u
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y, alpha_s
  u = alpha_s / (xi * (1 - y**2))
end function sudakov_eeqq_fsr_upper_bound_func

```

The logarithmic integrated UBF in the eeqq case as explained in [0709.2092], eq. (7.98), is given by

$$\begin{aligned}
-\frac{1}{N} \log [\Delta^U(p_T)] &= 2\pi \int_0^{k_{\max}} \alpha_s(k_T) \log \left[\frac{4k_{\max}^2}{k_T^2} \right] \theta(k_T - p_T) \frac{dk_T}{k_T} \\
&= \frac{\pi}{b_0} \left(\log \left[\frac{4k_{\max}^2}{k_T^2} \right] \log \left[\frac{\log(k_{\max}^2/\Lambda^2)}{\log(p_T^2/\Lambda^2)} \right] - \log \left[\frac{k_{\max}^2}{p_T^2} \right] \right)
\end{aligned} \tag{31.7}$$

with $k_{\max} = \frac{q^0}{2}$. We see that for these logarithms to be well defined, we need to set a lower bound for the transverse momentum $p_{T,\min} > \Lambda = \text{lambda2_gen}$.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: log_integrated_ubf => sudakov_eeqq_fsr_log_integrated_ubf

```

```

<POWHEG matching: sub interfaces>+≡
pure module function sudakov_eeqq_fsr_log_integrated_ubf &
  (sudakov, pt2) result (log_sudakov)
  real(default) :: log_sudakov
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: pt2
end function sudakov_eeqq_fsr_log_integrated_ubf

```

```

(POWHEG matching: procedures)+≡
pure module function sudakov_eeqq_fsr_log_integrated_ubf &
  (sudakov, pt2) result (log_sudakov)
  real(default) :: log_sudakov
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: pt2
  real(default) :: kt2_max, Lambda2
  logical :: within_boundaries
  kt2_max = sudakov%kt2_max ()
  within_boundaries = pt2 >= sudakov%powheg_settings%pt2_min &
    .and. pt2 <= kt2_max
  if (within_boundaries) then
    Lambda2 = sudakov%process_deps%lambda2_gen
    log_sudakov = pi / b0rad () * ( log (4 * kt2_max / Lambda2) * &
      log (log (kt2_max/Lambda2) / log (pt2/Lambda2)) - log(kt2_max/pt2) )
  else
    log_sudakov = 0
  end if
end function sudakov_eeqq_fsr_log_integrated_ubf

```

In order to arrive at the log integrated Sudakov implemented in `sudakov_eeqq_fsr_log_integrated_ubf`, we overestimated

$$\log \left[\frac{1 + \sqrt{1 - (k_T/k_{\max})^2}}{1 - \sqrt{1 - (k_T/k_{\max})^2}} \right] \leq \log \left[\frac{4k_{\max}^2}{k_T^2} \right]. \quad (31.8)$$

We correct for this in this veto step. Additionally, we correct for overestimating α_s .

```

(POWHEG matching: sudakov eeqq fsr: TBP)+≡
procedure :: reweight_ubf => sudakov_eeqq_fsr_reweight_ubf

(POWHEG matching: sub interfaces)+≡
module function sudakov_eeqq_fsr_reweight_ubf &
  (sudakov, pt2) result (accepted)
  logical :: accepted
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  real(default), intent(in) :: pt2
  end function sudakov_eeqq_fsr_reweight_ubf

(POWHEG matching: procedures)+≡
module function sudakov_eeqq_fsr_reweight_ubf (sudakov, pt2) result (accepted)
  logical :: accepted
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  real(default), intent(in) :: pt2
  real(default) :: log_bound, k_max2
  real(default) :: alpha_s_true, alpha_s_rad
  alpha_s_true = sudakov%alpha_s (pt2, use_correct = .true.)
  alpha_s_rad = sudakov%alpha_s (pt2, use_correct = .false.)
  k_max2 = sudakov%kt2_max ()
  log_bound = log((1 + sqrt(1 - (pt2/k_max2))) &
    / (1 - sqrt(1 - (pt2/k_max2))))
  call sudakov%rng%generate (sudakov%random)
  accepted = sudakov%random * log( 4 * k_max2 / pt2 ) * alpha_s_rad &
    <= log_bound * alpha_s_true

```

```

if (debug2_active (D_MATCHING)) then
  print *, ' sqrt(pt2) = ', sqrt(pt2)
  print *, ' alpha_s_true = ', alpha_s_true
  print *, ' sudakov%process_deps%lambda2_gen = ', &
    sudakov%process_deps%lambda2_gen
  print *, ' alpha_s_rad = ', alpha_s_rad
  print *, ' sudakov%random = ', sudakov%random
  print *, ' accepted = ', accepted
  if (log( 4 * k_max2 / pt2 ) * alpha_s_rad < log_bound * alpha_s_true) then
    call msg_fatal ("sudakov_eeqq_fsr_reweight_ubf: &
      &This should never happen. &
      &Have you chosen a running alpha_s?")
  end if
end if
end function sudakov_eeqq_fsr_reweight_ubf

```

In the eeqq case, we did not overestimate ξ with ξ_{\max} .

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
  procedure :: reweight_xi_max => sudakov_eeqq_fsr_reweight_xi_max

<POWHEG matching: sub interfaces>+=
  module function sudakov_eeqq_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
  end function sudakov_eeqq_fsr_reweight_xi_max

<POWHEG matching: procedures>+=
  module function sudakov_eeqq_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = .true.
  end function sudakov_eeqq_fsr_reweight_xi_max

```

In the eeqq case, we generate y from a random number and afterwards compute $\xi(p_T, y)$ so the sequence is reversed in comparison to the simple case.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
  procedure :: generate_xi_and_y_and_phi => &
    sudakov_eeqq_fsr_generate_xi_and_y_and_phi

<POWHEG matching: sub interfaces>+=
  module subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi

<POWHEG matching: procedures>+=
  module subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    call sudakov%generate_y (r)
    call sudakov%generate_xi (r)
  end subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi

```

```

    call sudakov%generate_phi (r)
end subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi

```

To generate y for the eeqq UBF, we take a random number

$$-\log \left[\frac{1 + \sqrt{1 - (p_T/k_{\max})^2}}{1 - \sqrt{1 - (p_T/k_{\max})^2}} \right] < r_y < \log \left[\frac{1 + \sqrt{1 - (p_T/k_{\max})^2}}{1 - \sqrt{1 - (p_T/k_{\max})^2}} \right] \quad (31.9)$$

and then compute

$$y(r_y) = \frac{e^{r_y} - 1}{e^{r_y} + 1} \quad (31.10)$$

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
  procedure :: generate_y => sudakov_eeqq_fsr_generate_y

<POWHEG matching: sub interfaces>+=
  module subroutine sudakov_eeqq_fsr_generate_y (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_eeqq_fsr_generate_y

<POWHEG matching: procedures>+=
  module subroutine sudakov_eeqq_fsr_generate_y (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: k_max2, log_bound, r_y
    k_max2 = sudakov%kt2_max ()
    call sudakov%rng%generate (sudakov%random)
    log_bound = log((1 + sqrt(1 - (r%pt2/k_max2))) &
                   / (1 - sqrt(1 - (r%pt2/k_max2))))
    r_y = -log_bound + sudakov%random * (two * log_bound)
    r%y = (exp(r_y) - 1) / (exp(r_y) + 1)
  end subroutine sudakov_eeqq_fsr_generate_y

```

We generate ξ for the eeqq UBF according to

$$\xi(p_T, y) = \frac{2p_T}{\sqrt{s}\sqrt{1-y^2}} \quad (31.11)$$

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
  procedure :: generate_xi => sudakov_eeqq_fsr_generate_xi

<POWHEG matching: sub interfaces>+=
  module subroutine sudakov_eeqq_fsr_generate_xi (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_eeqq_fsr_generate_xi

<POWHEG matching: procedures>+=
  module subroutine sudakov_eeqq_fsr_generate_xi (sudakov, r)
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: q0
    q0 = sqrt(sudakov%event_deps%s_hat)
    r%xi = (2 * sqrt(r%pt2)) / (q0 * sqrt(1 - r%y**2))
  end subroutine sudakov_eeqq_fsr_generate_xi

```

Massive FSR

```

<POWHEG matching: public>+≡
  public :: sudakov_massive_fsr_t

<POWHEG matching: types>+≡
  type, extends (sudakov_t) :: sudakov_massive_fsr_t
  real(default) :: z, z1, z2 = 0._default
  real(default) :: xi_1, xi_min, xi_m = 0._default
  real(default) :: xi_max_extended = 1._default
  contains
  <POWHEG matching: sudakov massive fsr: TBP>
  end type sudakov_massive_fsr_t

```

According to eq. A.42 1202.0465, during the radiation generation, an alternative expression for ξ_{\max} ,

$$\xi_{\max} = 1 - \frac{(m + m_{\text{rec}})^2}{q^2},$$

is used, which corresponds to an extended Dalitz region. Phase space points outside of the original Dalitz region will be vetoed afterwards in `sudakov_massive_fsr_reweight_xi_max`.

```

<POWHEG matching: sudakov massive fsr: TBP>≡
  procedure :: compute_xi_max_extended &
    => sudakov_massive_fsr_compute_xi_max_extended

<POWHEG matching: sub interfaces>+≡
  module subroutine sudakov_massive_fsr_compute_xi_max_extended &
    (sudakov)
    class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  end subroutine sudakov_massive_fsr_compute_xi_max_extended

<POWHEG matching: procedures>+≡
  module subroutine sudakov_massive_fsr_compute_xi_max_extended (sudakov)
    class(sudakov_massive_fsr_t), intent(inout) :: sudakov
    real(default) :: m, mrec
    real(default) :: q0
    type(vector4_t) :: p
    q0 = sqrt(sudakov%event_deps%s_hat)
    p = sudakov%event_deps%p_born_lab%get_momentum &
      (1, sudakov%associated_emitter())
    m = p**1
    mrec = sqrt ((q0 - p%p(0))**2 - p%p(1)**2 - p%p(2)**2 - p%p(3)**2)
    sudakov%xi_max_extended = one - (m + mrec)**2 / q0**2
  end subroutine sudakov_massive_fsr_compute_xi_max_extended

```

As described in 1202.0465, App. A.5., for massive emitters, the radiation variable ξ is constructed as follows. First,

$$\xi_{\min}(K_T^2) = \frac{\sqrt{K_T^2 (K_T^2 z_2^2 + 8\bar{p}^0 q(1 - z_2)) - K_T^2 z_2}}{2q^2(1 - z_2)} \quad (31.12)$$

is computed where K_T is a hardness scale for the radiation that determines the upper limit of the integral for the Sudakov form factor and coincides with the usual one, i.e. the transverse momentum of the radiated particle, in the massless

limit. Then ξ_1 is computed according to the same equation with $z_2 \leftrightarrow z_1$. Finally, ξ is generated according to

$$\xi = \frac{1}{q^2} \left(\exp \left[\log (\xi_{\min} q^2 - K_T^2) + r \log \frac{\xi_m q^2 - K_T^2}{\xi_{\min} q^2 - K_T^2} \right] + K_T^2 \right), \quad (31.13)$$

where $\xi_m = \min (\xi_{\max}, \xi_1)$.

(POWHEG matching: sudakov massive fsr: TBP)+≡

```
procedure :: generate_xi => sudakov_massive_fsr_generate_xi
```

(POWHEG matching: sub interfaces)+≡

```
module subroutine sudakov_massive_fsr_generate_xi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
end subroutine sudakov_massive_fsr_generate_xi
```

(POWHEG matching: procedures)+≡

```
module subroutine sudakov_massive_fsr_generate_xi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: pt2, q0, q02
  real(default) :: E_em, xi_max_ext
  real(default) :: xi_1, xi_min, xi_m
  pt2 = r%pt2
  E_em = sudakov%event_deps%p_born_lab%get_energy &
    (1, sudakov%associated_emitter())
  q02 = sudakov%event_deps%s_hat; q0 = sqrt(q02)
  xi_max_ext = sudakov%xi_max_extended
  associate (z1 => sudakov%z1, z2 => sudakov%z2)
    xi_1 = (sqrt(pt2 * (pt2 * z1**2 + 8 * E_em * q0 * (one - z1))) - pt2 * z1) / &
      (two * q02 * (one - z1))
    xi_min = (sqrt(pt2 * (pt2 * z2**2 + 8 * E_em * q0 * (one - z2))) - pt2 * z2) / &
      (two * q02 * (one - z2))
  end associate
  xi_m = min (xi_max_ext, xi_1)
  call sudakov%rng%generate (sudakov%random)
  r%xi = (exp (log(xi_min * q02 - pt2) + sudakov%random * &
    log((xi_m * q02 - pt2) / (xi_min * q02 - pt2))) + pt2) / q02
end subroutine sudakov_massive_fsr_generate_xi
```

Generates the FKS variables in the case of a massive emitter and additionally computes z and $z_{1/2}$ as well as ξ_{\max} to be stored in the Sudakov for later use when reweighting ξ_{\max} and retrieving the norm from the POWHEG grid. The corresponding derivations can be found in 1202.0465, App. A.

(POWHEG matching: sudakov massive fsr: TBP)+≡

```
procedure :: generate_xi_and_y_and_phi => &
  sudakov_massive_fsr_generate_xi_and_y_and_phi
```

(POWHEG matching: sub interfaces)+≡

```
module subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
end subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi
```


(POWHEG matching: procedures)+≡

```

module subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: q0
  real(default) :: m2, mrec2, k0_rec_max
  real(default) :: E_em
  type(vector4_t) :: p_emitter

  q0 = sqrt (sudakov%event_deps%s_hat)
  p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
    (1, sudakov%associated_emitter())
  associate (p => p_emitter%p)
    mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
    E_em = p(0)
  end associate
  m2 = p_emitter**2
  call compute_dalitz_bounds (q0, m2, mrec2, sudakov%z1, sudakov%z2, k0_rec_max)
  call sudakov%generate_xi (r)

  sudakov%z = (two * r%pt2 * E_em - r%xi**2 * q0**3) / &
    (r%pt2 * r%xi * q0 - r%xi**2 * q0**3)
  sudakov%xi2_max = - (q0**2 * sudakov%z**2 - two * q0 * k0_rec_max * sudakov%z + mrec2) / &
    (q0**2 * sudakov%z * (one - sudakov%z))
  sudakov%xi2_max = sudakov%xi2_max**2
  r%y = two * (sudakov%z2 - sudakov%z) / (sudakov%z2 - sudakov%z1) - one
  call sudakov%generate_phi (r)
end subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi

```

Computes the hardness scale as discussed in 1202.0465, App. A.2.

$$K_T^2 = \frac{\xi^2 q^3 (1-z)}{2\bar{p}_{\text{em}}^0 - z\xi q} \quad (31.14)$$

(POWHEG matching: sudakov massive fsr: TBP)+≡

```

procedure :: kt2 => sudakov_massive_fsr_kt2

```

(POWHEG matching: sub interfaces)+≡

```

module function sudakov_massive_fsr_kt2 (sudakov, xi, y) result (kt2)
  real(default) :: kt2
  class(sudakov_massive_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y
end function sudakov_massive_fsr_kt2

```

(POWHEG matching: procedures)+≡

```

module function sudakov_massive_fsr_kt2 (sudakov, xi, y) result (kt2)
  real(default) :: kt2
  class(sudakov_massive_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y
  kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
    (sudakov%i_phs, sudakov%associated_emitter(), UBF_FSR_MASSIVE, xi, y)
end function sudakov_massive_fsr_kt2

```

For massive emitters, the upper bound on the radiated p_T is

$$t_{\max} = \frac{\xi_{\max}^2 q^3 (1 - z_2)}{2 \cdot \bar{p}^0 - z_2 \xi_{\max} q}$$

For this, we have to compute z_2 from the Dalitz bounds as `sudakov%z2` has not yet been set for the current event.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
  procedure :: kt2_max => sudakov_massive_fsr_kt2_max

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_massive_fsr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
  end function sudakov_massive_fsr_kt2_max

<POWHEG matching: procedures>+≡
  pure module function sudakov_massive_fsr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default) :: q0, E_em, xi_max, z1, z2, m2, mrec2, k0_rec_max
    type(vector4_t) :: p_emitter
    q0 = sqrt(sudakov%event_deps%s_hat)
    p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
      (1, sudakov%associated_emitter())
    associate (p => p_emitter%p)
      mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
      E_em = p(0)
    end associate
    m2 = p_emitter**2
    call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
    xi_max = sudakov%xi_max_extended
    kt2_max = (xi_max**2 * q0**3 * (one - z2)) / (two * E_em - z2 * xi_max * q0)
  end function sudakov_massive_fsr_kt2_max

```

The upper bounding function for massive emitters according to Eq. A.56 in [1202.0465] (disregarding a possible factor of α_s) is

$$U(\xi, y) \sim \frac{\sqrt{s}}{\bar{p}_{\text{em}}} \frac{1}{\xi(1-z)} \quad (31.15)$$

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
  procedure :: upper_bound_func => sudakov_massive_fsr_upper_bound_func

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_massive_fsr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
  end function sudakov_massive_fsr_upper_bound_func

<POWHEG matching: procedures>+≡
  pure module function sudakov_massive_fsr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u

```

```

class(sudakov_massive_fsr_t), intent(in) :: sudakov
real(default), intent(in) :: xi, y, alpha_s
real(default) :: q, p_em
q = sqrt (sudakov%event_deps%s_hat)
p_em = space_part_norm &
      (sudakov%event_deps%p_born_lab%get_momentum (1, &
      sudakov%associated_emitter()))
u = alpha_s * q / p_em * one / (xi * (one - sudakov%z))
end function sudakov_massive_fsr_upper_bound_func

```

The integrated upper-bounding function for massive final-state emitters is given by

$$\begin{aligned}
I(t) = & \frac{q}{\bar{p}_{\text{em}}} \left[\log \xi \log \left[(1 - z_2) \frac{q}{k_T^2} \right] + \frac{1}{2} \log^2 \xi + G(-k_T^2, q^2, \xi) - G(2\bar{p}_{\text{em}}, -q, \xi) \right]_{\xi_{\min}}^{\min(\xi_1(k_T^2), \xi_{\max})} \\
& + \frac{q}{\bar{p}_{\text{em}}} \theta(\xi_{\max} - \xi_1(k_T^2)) \log \frac{\xi_{\max}}{\xi_1(k_T^2)} \log \frac{1 - z_2}{1 - z_1},
\end{aligned}$$

where the function $G(a, b, \xi)$ is given by

$$G(a, b, \xi) = \log(a + b\xi) \log \left(1 - \frac{a + b\xi}{a} \right) + Li_2 \left(\frac{a + b\xi}{a} \right), \quad (31.16)$$

for $a < 0$ and by

$$G(a, b, \xi) = \log \left| \frac{b\xi}{a} \right| \log a - Li_2 \left(-\frac{b\xi}{a} \right) + \frac{\pi^2}{6}, \quad (31.17)$$

for $a > 0$.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
  procedure :: log_integrated_ubf => sudakov_massive_fsr_log_integrated_ubf

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_massive_fsr_log_integrated_ubf &
    (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_massive_fsr_log_integrated_ubf

<POWHEG matching: procedures>+≡
  pure module function sudakov_massive_fsr_log_integrated_ubf &
    (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: xi, xi_max, xi_1, xi_min
    real(default) :: q0, p_em, E_em, m2, mrec2, k0_rec_max
    type(vector4_t) :: p_emitter
    real(default) :: log_sudakov_up, log_sudakov_down, z1, z2
    logical :: within_boundaries
    within_boundaries = pt2 >= sudakov%powheg_settings%pt2_min &
      .and. pt2 <= sudakov%kt2_max ()
    if (within_boundaries) then

```

```

q0 = sqrt (sudakov%event_deps%s_hat)
p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
(1, sudakov%associated_emitter())
associate (p => p_emitter%p)
mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
E_em = p(0)
end associate
m2 = p_emitter**2
call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
p_em = space_part_norm (p_emitter)
xi_max = sudakov%xi_max_extended
xi_1 = (sqrt (pt2 * (pt2 * z1**2 + 8 * E_em * q0 * (one - z1))) - pt2 * z1) / &
(two * q0**2 * (one - z1))
xi_min = (sqrt (pt2 * (pt2 * z2**2 + 8 * E_em * q0 * (one - z2))) - pt2 * z2) / &
(two * q0**2 * (one - z2))
xi = min (xi_1, xi_max)
log_sudakov_up = log(xi) * log((one - z2) * q0 / pt2) + log(xi)**2 / two + &
G_FSR(-pt2, q0**2, xi) - G_FSR(two * E_em, -q0, xi)
xi = xi_min
log_sudakov_down = log(xi) * log((one - z2) * q0 / pt2) + log(xi)**2/two + &
G_FSR(-pt2, q0**2, xi) - G_FSR(two * E_em, -q0, xi)
log_sudakov = log_sudakov_up - log_sudakov_down
if (xi_max > xi_1) &
log_sudakov = log_sudakov + log(xi_max / xi_1) * log((one - z2) / (one - z1))
log_sudakov = twopi * q0 / p_em * log_sudakov
else
log_sudakov = 0
end if
end function sudakov_massive_fsr_log_integrated_ubf

```

For this UBF, we just overestimated α_s .

(POWHEG matching: sudakov massive fsr: TBP)+≡

```
procedure :: reweight_ubf => sudakov_massive_fsr_reweight_ubf
```

(POWHEG matching: sub interfaces)+≡

```

module function sudakov_massive_fsr_reweight_ubf &
(sudakov, pt2) result (accepted)
logical :: accepted
class(sudakov_massive_fsr_t), intent(inout) :: sudakov
real(default), intent(in) :: pt2
end function sudakov_massive_fsr_reweight_ubf

```

(POWHEG matching: procedures)+≡

```

module function sudakov_massive_fsr_reweight_ubf &
(sudakov, pt2) result (accepted)
logical :: accepted
class(sudakov_massive_fsr_t), intent(inout) :: sudakov
real(default), intent(in) :: pt2
real(default) :: alpha_s_true, alpha_s_rad
logical :: alpha_s_equal
if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_massive_fsr_reweight_ubf")
alpha_s_true = sudakov%alpha_s (pt2, use_correct = .true.)
alpha_s_rad = sudakov%alpha_s (pt2, use_correct = .false.)
call sudakov%rng%generate (sudakov%random)
alpha_s_equal = nearly_equal (alpha_s_true, alpha_s_rad)

```

```

accepted = alpha_s_equal .or. sudakov%random < alpha_s_true / alpha_s_rad
if (debug2_active (D_MATCHING)) then
  print *, ' sqrt(pt2) = ', sqrt(pt2)
  print *, ' alpha_s_true = ', alpha_s_true
  print *, ' sudakov%process_deps%lambda2_gen = ', &
    sudakov%process_deps%lambda2_gen
  print *, ' alpha_s_rad = ', alpha_s_rad
  print *, ' sudakov%random = ', sudakov%random
  print *, ' accepted = ', accepted
  if (alpha_s_rad < alpha_s_true .and. .not. alpha_s_equal) then
    call msg_fatal ("sudakov_massive_fsr_reweight_ubf: &
      &This should never happen. &
      &Have you chosen a running alpha_s?")
  end if
end if
end function sudakov_massive_fsr_reweight_ubf

```

In the massive case, we generated $0 < \xi < \xi_{\text{max_extended}}$ and thus we need to veto values of ξ larger than ξ_{max} in this extra veto step.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
  procedure :: reweight_xi_max => sudakov_massive_fsr_reweight_xi_max

<POWHEG matching: sub interfaces>+≡
  module function sudakov_massive_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    end function sudakov_massive_fsr_reweight_xi_max

<POWHEG matching: procedures>+≡
  module function sudakov_massive_fsr_reweight_xi_max &
    (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = xi < sqrt (sudakov%xi2_max)
    end function sudakov_massive_fsr_reweight_xi_max

```

Auxiliary functions

Implements the function $G(a, b, \xi)$ given in eq. (31.17) and eq. (31.16). Cannot be evaluated for $a = 0$.

```

<POWHEG matching: procedures>+≡
  elemental function G_FSR (a,b,xi)
    real(default) :: G_FSR
    real(default), intent(in) :: a, b, xi
    if (a > 0) then
      G_FSR = G_FSR_Plus (a,b,xi)
    else if (a < 0) then
      G_FSR = G_FSR_Minus (a,b,xi)
    end if
  end function G_FSR

```

```

elemental function G_FSR_Minus (a,b,xi)
  real(default) :: G_FSR_Minus
  real(default), intent(in) :: a, b, xi
  G_FSR_Minus = log(a+b*xi)*log(one - (a+b*xi)/a) + Li2((a+b*xi)/a)
end function G_FSR_Minus

elemental function G_FSR_Plus (a,b,xi)
  real(default) :: G_FSR_Plus
  real(default), intent(in) :: a, b, xi
  G_FSR_Plus = log(abs(b*xi/a))*log(a) - Li2(-b*xi/a) + pi**2/6
end function G_FSR_Plus

```

ISR

This is the Sudakov for ISR. This corresponds to 1002.2581, App. D. The `ubf_variant` determines which `log_integrated_ubf` is used.

```

<POWHEG matching: public>+≡
  public :: sudakov_isr_t

<POWHEG matching: types>+≡
  type, extends (sudakov_t) :: sudakov_isr_t
    real(default) :: xi_max_extended = 1._default
    integer :: ubf_variant = 2
  contains
    <POWHEG matching: sudakov_isr: TBP>
  end type sudakov_isr_t

```

This k_T measure differs by a factor of $\frac{1}{1-\xi}$ w.r.t. `sudakov_eeqq_fsr_kt2` to account for $s_{\text{born}} = s_{\text{real}} * (1 - \xi)$.

```

<POWHEG matching: sudakov_isr: TBP>≡
  procedure :: kt2 => sudakov_isr_kt2

<POWHEG matching: sub interfaces>+≡
  module function sudakov_isr_kt2 (sudakov, xi, y) result (kt2)
    real(default) :: kt2
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
  end function sudakov_isr_kt2

<POWHEG matching: procedures>+≡
  module function sudakov_isr_kt2 (sudakov, xi, y) result (kt2)
    real(default) :: kt2
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
    kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
      (sudakov%i_phs, sudakov%associated_emitter(), UBF_ISR, xi, y)
  end function sudakov_isr_kt2

```

The maximal transverse momentum is given by (D.4) in [1002.2581].

```

<POWHEG matching: sudakov_isr: TBP>+≡
  procedure :: kt2_max => sudakov_isr_kt2_max

```

```

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_isr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_isr_t), intent(in) :: sudakov
  end function sudakov_isr_kt2_max

<POWHEG matching: procedures>+≡
  pure module function sudakov_isr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default) :: s_hat, xb_plus, xb_minus
    s_hat = sudakov%event_deps%s_hat
    xb_plus = sudakov%event_deps%x_born(I_PLUS)
    xb_minus = sudakov%event_deps%x_born(I_MINUS)
    kt2_max = s_hat * (1 - xb_plus**2) * (1 - xb_minus**2) &
      / (xb_plus + xb_minus)**2
  end function sudakov_isr_kt2_max

```

This covers the soft singularity for $\xi \rightarrow 0$ and the collinear singularities to both beam axes $y \rightarrow \pm 1$.

```

<POWHEG matching: sudakov isr: TBP>+≡
  procedure :: upper_bound_func => sudakov_isr_upper_bound_func

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_isr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
  end function sudakov_isr_upper_bound_func

<POWHEG matching: procedures>+≡
  pure module function sudakov_isr_upper_bound_func &
    (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
    u = alpha_s / (xi * (1 - y**2))
  end function sudakov_isr_upper_bound_func

```

This is eq. (D.14) and (D.18) in [1002.2581]. It is similar to the eeqq case with the only difference being that the first log here includes both, $k_{T, \max}^2$ and s_b via q^2 .

```

<POWHEG matching: sudakov isr: TBP>+≡
  procedure :: log_integrated_ubf => sudakov_isr_log_integrated_ubf

<POWHEG matching: sub interfaces>+≡
  pure module function sudakov_isr_log_integrated_ubf &
    (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_isr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_isr_log_integrated_ubf

```

(POWHEG matching: procedures)+≡

```

pure module function sudakov_isr_log_integrated_ubf &
  (sudakov, pt2) result (log_sudakov)
  real(default) :: log_sudakov
  class(sudakov_isr_t), intent(in) :: sudakov
  real(default), intent(in) :: pt2
  real(default) :: kt2_max, Lambda2, s_hat, q2
  logical :: within_boundaries
  kt2_max = sudakov%kt2_max ()
  s_hat = sudakov%event_deps%s_hat
  q2 = kt2_max + s_hat
  Lambda2 = sudakov%process_deps%lambda2_gen
  within_boundaries = pt2 >= sudakov%powheg_settings%pt2_min &
    .and. pt2 <= kt2_max
  if (within_boundaries) then
    if (sudakov%ubf_variant == 1) then
      log_sudakov = pi / b0rad () * ( log (q2/Lambda2) * &
        log (log (kt2_max/Lambda2) / log (pt2/Lambda2)) - log (kt2_max/pt2) )
    elseif (sudakov%ubf_variant == 2) then
      if (pt2 < s_hat) then
        if (s_hat < kt2_max) then
          log_sudakov = pi / b0rad () * &
            ( log (two * s_hat / Lambda2) &
              * log (log (s_hat / Lambda2) / log (pt2 / Lambda2)) &
              - log (s_hat / pt2) &
              + log (two) * log ( log (kt2_max / Lambda2) / log (s_hat / Lambda2) ))
        else
          log_sudakov = pi / b0rad () * &
            (log (two * s_hat / Lambda2) &
              * log (log (kt2_max / Lambda2) / log (pt2 / Lambda2)) &
              - log (kt2_max / pt2) )
        end if
      else
        log_sudakov = pi / b0rad () * &
          (log (two) * log (log (kt2_max / Lambda2) / log (pt2 / Lambda2)))
      end if
    else
      log_sudakov = 0
    end if
  end if
end function sudakov_isr_log_integrated_ubf

```

In order to arrive at the log integrated Sudakov implemented in `sudakov_isr_log_integrated_ubf`, we overestimated

$$\log \left[\frac{\sqrt{x_+ - \rho} + \sqrt{x_- - \rho}}{\sqrt{x_+ - \rho} - \sqrt{x_- - \rho}} \right] \leq \log \left[\frac{\sqrt{x_+} + \sqrt{x_-}}{\sqrt{x_+} - \sqrt{x_-}} \right] = \frac{1}{2} \log \left[\frac{k_T^2 + s_b}{k_T^2} \right] \leq \frac{1}{2} \log \left[\frac{q^2}{k_T^2} \right] \quad (31.18)$$

with

$$x_{\pm} = \left(\sqrt{1 + \frac{k_T^2}{s_b}} \pm \frac{k_T}{\sqrt{s_b}} \right)^2, \quad \rho = \frac{s_b}{S} \quad \text{and} \quad q^2 = k_{T,\max}^2 + s_b. \quad (31.19)$$

We correct for this in this veto step. Additionally, we correct for overestimating α_s .

```

(POWHEG matching: sudakov_isr: TBP)+≡
  procedure :: reweight_ubf => sudakov_isr_reweight_ubf

(POWHEG matching: sub interfaces)+≡
  module function sudakov_isr_reweight_ubf (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_isr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_isr_reweight_ubf

(POWHEG matching: procedures)+≡
  module function sudakov_isr_reweight_ubf (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_isr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: log_bound, kT_max2, s_hat, s_had, rho, x_plus, x_minus, q2
    real(default) :: alpha_s_true, alpha_s_rad
    alpha_s_true = sudakov%alpha_s (pt2, use_correct = .true.)
    alpha_s_rad = sudakov%alpha_s (pt2, use_correct = .false.)
    s_hat = sudakov%event_deps%s_hat
    s_had = sudakov%event_deps%s_had
    rho = s_hat / s_had
    kT_max2 = sudakov%kt2_max ()
    q2 = kT_max2 + s_hat
    x_plus = ( sqrt( 1 + pt2 / s_hat ) + sqrt( pt2 / s_hat ) )**2
    x_minus = ( sqrt( 1 + pt2 / s_hat ) - sqrt( pt2 / s_hat ) )**2
    !!! These are not the ISR x values!
    call sudakov%rng%generate (sudakov%random)
    log_bound = log ((sqrt( x_plus - rho ) + sqrt( x_minus - rho )) &
      / (sqrt( x_plus - rho ) - sqrt( x_minus - rho )))
    if (sudakov%ubf_variant == 1) then
      accepted = sudakov%random * log( q2 / pt2 ) * alpha_s_rad &
        <= 2 * log_bound * alpha_s_true
    elseif (sudakov%ubf_variant == 2) then
      if (pt2 < s_hat) then
        accepted = sudakov%random * log( two * s_hat / pt2 ) * alpha_s_rad &
          <= 2 * log_bound * alpha_s_true
      else
        accepted = sudakov%random * log( two ) * alpha_s_rad &
          <= 2 * log_bound * alpha_s_true
      end if
    else
      accepted = .false.
      call msg_error("sudakov variant not implemented")
    end if
    if (debug2_active (D_MATCHING)) then
      print *, 'sudakov_isr_reweight_ubf:'
      print *, '  sqrt(pt2) = ', sqrt(pt2)
      print *, '  alpha_s_true = ', alpha_s_true
      print *, '  sudakov%process_deps%lambda2_gen = ', &
        sudakov%process_deps%lambda2_gen
      print *, '  alpha_s_rad = ', alpha_s_rad
      print *, '  sudakov%random = ', sudakov%random
    end if
  end function

```

```

    print *, ' accepted = ', accepted
    if (log( q2 / pt2 ) * alpha_s_rad < 2 * log_bound * alpha_s_true) then
        call msg_fatal ("sudakov_isr_reweight_ubf: This should never happen. &
            &Have you chosen a running alpha_s?")
    end if
end if
end if
end function sudakov_isr_reweight_ubf

```

In the ISR case, we overestimated ξ_{\max} with ξ_{\max}^{ext} . We veto too large ξ in this veto step.

```

<POWHEG matching: sudakov_isr: TBP>+≡
    procedure :: reweight_xi_max => sudakov_isr_reweight_xi_max

<POWHEG matching: sub interfaces>+≡
    module function sudakov_isr_reweight_xi_max (sudakov, xi) result (accepted)
        logical :: accepted
        class(sudakov_isr_t), intent(in) :: sudakov
        real(default), intent(in) :: xi
    end function sudakov_isr_reweight_xi_max

<POWHEG matching: procedures>+≡
    module function sudakov_isr_reweight_xi_max (sudakov, xi) result (accepted)
        logical :: accepted
        class(sudakov_isr_t), intent(in) :: sudakov
        real(default), intent(in) :: xi
        accepted = xi < sqrt (sudakov%xi2_max)
        if (debug2_active (D_MATCHING)) then
            print *, 'sudakov_isr_reweight_xi_max:'
            print *, ' xi = ', xi
            print *, ' xi_max = ', sqrt (sudakov%xi2_max)
            print *, ' xi accepted = ', accepted
        end if
    end function sudakov_isr_reweight_xi_max

```

The actual ξ_{\max} for ISR is given by eq. (27.39) and depends on y which will be known only after we generated ξ . We thus use an overestimated

$$\xi_{\max}^{\text{ext}} = 1 - \frac{s_b}{S_{\text{had}}}$$

to generate both and veto $\xi > \xi_{\max}$ later on in `sudakov_isr_reweight_xi_max`.

```

<POWHEG matching: sudakov_isr: TBP>+≡
    procedure :: compute_xi_max_extended &
        => sudakov_isr_compute_xi_max_extended

<POWHEG matching: sub interfaces>+≡
    module subroutine sudakov_isr_compute_xi_max_extended (sudakov)
        class(sudakov_isr_t), intent(inout) :: sudakov
        real(default) :: s_hat, s_had
    end subroutine sudakov_isr_compute_xi_max_extended

<POWHEG matching: procedures>+≡
    module subroutine sudakov_isr_compute_xi_max_extended (sudakov)
        class(sudakov_isr_t), intent(inout) :: sudakov
        real(default) :: s_hat, s_had

```

```

s_hat = sudakov%event_deps%s_hat
s_had = sudakov%event_deps%s_had
sudakov%xi_max_extended = one - s_hat / s_had
end subroutine sudakov_isr_compute_xi_max_extended

```

In the ISR case, we generate ξ from a random number and afterwards compute $y(p_T, \xi)$ as in the simple case.

```

(POWHEG matching: sudakov_isr: TBP)+≡
  procedure :: generate_xi_and_y_and_phi => &
    sudakov_isr_generate_xi_and_y_and_phi
(POWHEG matching: sub interfaces)+≡
  module subroutine sudakov_isr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    end subroutine sudakov_isr_generate_xi_and_y_and_phi
(POWHEG matching: procedures)+≡
  module subroutine sudakov_isr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    call sudakov%generate_xi (r)
    call sudakov%generate_y (r)
    call sudakov%generate_phi (r)
    call sudakov%compute_xi2_max (r)
    end subroutine sudakov_isr_generate_xi_and_y_and_phi

```

Inverting `real_kinematics_kt2`, we find

$$|y(k_T^2, \xi)| = \sqrt{1 - \frac{4(1-\xi)}{\xi^2} \frac{k_T^2}{s_b}}. \quad (31.20)$$

We then determine the sign randomly as there is no preferred direction.

```

(POWHEG matching: sudakov_isr: TBP)+≡
  procedure :: generate_y => sudakov_isr_generate_y
(POWHEG matching: sub interfaces)+≡
  module subroutine sudakov_isr_generate_y (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    end subroutine sudakov_isr_generate_y
(POWHEG matching: procedures)+≡
  module subroutine sudakov_isr_generate_y (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: s_hat
    s_hat = sudakov%event_deps%s_hat
    r%y = sqrt (1 - (4 * (1 - r%xi) * r%pt2 / (s_hat * r%xi**2)))
    call sudakov%rng%generate (sudakov%random)
    if (sudakov%random > 0.5_default) then
      r%y = - r%y
    end if
    end subroutine sudakov_isr_generate_y

```

We want to generate $x := 1 - \xi$ for the ISR UBF with probability density

$$f(x) = \frac{1}{\sqrt{(x_+ - x)(x_- - x)}}. \quad (31.21)$$

within the limits

$$\frac{s_b}{S} = x_{b,\oplus} x_{b,\ominus} = \rho \leq x \leq x_- = x_+ = \left(\sqrt{1 + \frac{k_T^2}{s_b}} - \frac{k_T}{\sqrt{s_b}} \right)^2. \quad (31.22)$$

To generate x according to the distribution

$$F(x) = \int f(x) dx = 2 \sinh^{-1} \left(\sqrt{\frac{x_- - x}{x_+ - x_-}} \right) \quad (31.23)$$

we use

$$x = x_- + (x_- - x_+) \sinh^2 \left(\frac{r_x}{2} \right) \quad (31.24)$$

with a random number $r_x \in \text{Unif}[F(x_-), F(\rho)] = \text{Unif} \left[0, 2 \sinh^{-1} \left(\sqrt{\frac{x_- - \rho}{x_+ - x_-}} \right) \right]$. Alternatively, an implementation making extended use of rejection sampling is available.

```

(POWHEG matching: sudakov isr: TBP)+≡
  procedure :: generate_xi => sudakov_isr_generate_xi

(POWHEG matching: sub interfaces)+≡
  module subroutine sudakov_isr_generate_xi (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_isr_generate_xi

(POWHEG matching: procedures)+≡
  module subroutine sudakov_isr_generate_xi (sudakov, r)
    class(sudakov_isr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: s_hat, s_had, r_x, x, x_minus, x_plus, rho
    integer, parameter :: variant = 1
    logical :: valid
    s_hat = sudakov%event_deps%s_hat
    s_had = sudakov%event_deps%s_had
    rho = s_hat / s_had
    x_plus = ( sqrt( 1 + r%pt2 / s_hat ) + sqrt( r%pt2 / s_hat ) )**2
    x_minus = ( sqrt( 1 + r%pt2 / s_hat ) - sqrt( r%pt2 / s_hat ) )**2
    if (variant == 1) then
      call sudakov%rng%generate (sudakov%random)
      r_x = sudakov%random
      r_x = r_x * 2 * asinh (sqrt ( (x_minus - rho) / (x_plus - x_minus) ) )
      x = x_minus + (x_minus - x_plus) * sinh (r_x / 2)**2
    elseif (variant == 2) then
      valid = .false.
      do while (.not. valid)
        if (signal_is_pending ()) return
        call sudakov%rng%generate (sudakov%random)
        r_x = sudakov%random
        x = x_minus - (sqrt (x_minus - rho) * r_x)**2
      end do
    end if
  end subroutine sudakov_isr_generate_xi

```

```

        call sudakov%rng%generate (sudakov%random)
        r_x = sudakov%random
        valid = r_x < sqrt ((x_plus - x_minus) / (x_plus - x))
    end do
end if
r%xi = 1 - x
end subroutine sudakov_isr_generate_xi

```

Computes the actual xi2_max for ISR. Can only be computed after y has been generated. Needs to be called before sudakov_isr_reweight_xi_max.

```

<POWHEG matching: sudakov_isr: TBP>+≡
    procedure :: compute_xi2_max => sudakov_isr_compute_xi2_max

<POWHEG matching: sub interfaces>+≡
    module subroutine sudakov_isr_compute_xi2_max (sudakov, r)
        class(sudakov_isr_t), intent(inout) :: sudakov
        type(radiation_t), intent(inout) :: r
    end subroutine sudakov_isr_compute_xi2_max

<POWHEG matching: procedures>+≡
    module subroutine sudakov_isr_compute_xi2_max (sudakov, r)
        class(sudakov_isr_t), intent(inout) :: sudakov
        type(radiation_t), intent(inout) :: r
        real(default) :: xi_max
        xi_max = get_xi_max_isr (sudakov%event_deps%x_born, r%y)
        sudakov%xi2_max = xi_max**2
    end subroutine sudakov_isr_compute_xi2_max

```

31.4.3 Main POWHEG class

```

<POWHEG matching: public>+≡
    public :: powheg_matching_t

<POWHEG matching: types>+≡
    type, extends(matching_t) :: powheg_matching_t
        type(grid_t) :: grid
        type(phs_fks_generator_t) :: phs_fks_generator
        type(powheg_settings_t) :: settings
        type(event_deps_t) :: event_deps
        type(process_deps_t) :: process_deps
        type(sudakov_wrapper_t), dimension(:), allocatable :: sudakov
        integer :: n_emissions = 0
        logical :: active = .true.
    contains
        <POWHEG matching: powheg matching: TBP>
    end type powheg_matching_t

<POWHEG matching: powheg matching: TBP>≡
    procedure :: get_method => powheg_matching_get_method

<POWHEG matching: sub interfaces>+≡
    module function powheg_matching_get_method (matching) result (method)
        type(string_t) :: method
    end function

```

```

        class(powheg_matching_t), intent(in) :: matching
        end function powheg_matching_get_method
<POWHEG matching: procedures>+≡
module function powheg_matching_get_method (matching) result (method)
    type(string_t) :: method
    class(powheg_matching_t), intent(in) :: matching
    method = matching_method (MATCH_POWHEG)
end function powheg_matching_get_method

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: before_shower => powheg_matching_before_shower
<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_matching_before_shower &
        (matching, particle_set, vetoed)
        class(powheg_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
    end subroutine powheg_matching_before_shower
<POWHEG matching: procedures>+≡
    module subroutine powheg_matching_before_shower &
        (matching, particle_set, vetoed)
        class(powheg_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
        if (debug_on) call msg_debug2 (D_MATCHING, "powheg_matching_before_shower")
        if (signal_is_pending ()) return
        if (.not. matching%active) return
        call matching%update (particle_set)
        if (matching%settings%test_sudakov) then
            call matching%test_sudakov ()
            stop
        end if
        if (.not. matching%settings%disable_sudakov) &
            call matching%generate_emission (particle_set = particle_set)
        vetoed = .false.
    end subroutine powheg_matching_before_shower

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: first_event => powheg_matching_first_event
<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_matching_first_event (matching)
        class(powheg_matching_t), intent(inout), target :: matching
    end subroutine powheg_matching_first_event
<POWHEG matching: procedures>+≡
    module subroutine powheg_matching_first_event (matching)
        class(powheg_matching_t), intent(inout), target :: matching
        associate (instance => matching%process_instance)
            matching%process_deps%lab_is_cm = instance%lab_is_cm (1)
        end associate
        call matching%setup_grids ()
    end subroutine powheg_matching_first_event

```

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: after_shower => powheg_matching_after_shower

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_after_shower &
    (matching, particle_set, vetoed)
    class(powheg_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
  end subroutine powheg_matching_after_shower

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_after_shower &
    (matching, particle_set, vetoed)
    class(powheg_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    vetoed = .false.
  end subroutine powheg_matching_after_shower

```

Output

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: write => powheg_write

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_write (matching, unit)
    class(powheg_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
  end subroutine powheg_write

<POWHEG matching: procedures>+≡
  module subroutine powheg_write (matching, unit)
    class(powheg_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
    integer :: u, alr
    u = given_output_unit (unit); if (u < 0) return
    call write_separator (u, 2)
    write (u, "(1X,A)") "POWHEG Emission Generator"
    write (u, "(1X,A)") "Process name: " // char (matching%process_name)
    if (allocated (matching%rng)) then
      call matching%rng%write (u)
    else
      write (u, "(1X,A)") "RNG not allocated"
    end if
    call matching%qcd%write (u)
    call matching%settings%write (u)
    call matching%event_deps%write (u)
    call matching%process_deps%write (u)
    do alr = 1, size (matching%sudakov)
      call write_separator (u)
      write (u, "(1X,A,I12,A)") "sudakov (alr = ", alr, ")"
      call matching%sudakov(alr)%s%write (u)
    end do
    call write_separator (u, 2)

```

```
end subroutine powheg_write
```

Finalization of the POWHEG matching. It creates a log file showing how many events failed at which stage of the POWHEG veto algorithm. It also issues a warning if too many POWHEG excess events occurred. If this is the case, the chosen upper-bounding function is unsuitable for the considered process.

```
(POWHEG matching: powheg matching: TBP)+≡
  procedure :: final => powheg_matching_final

(POWHEG matching: sub interfaces)+≡
  module subroutine powheg_matching_final (matching)
    class(powheg_matching_t), intent(in) :: matching
  end subroutine powheg_matching_final

(POWHEG matching: procedures)+≡
  module subroutine powheg_matching_final (matching)
    class(powheg_matching_t), intent(in) :: matching
    integer :: u, alr, n_fail_ubf_total, n_sqme_total
    real :: frac_ubf_fail
    type(string_t) :: filename
    n_fail_ubf_total = 0
    n_sqme_total = 0
    u = free_unit ()
    filename = matching%process_name // "_veto.log"
    open (file=char(filename), unit=u, action='write')
    write (u, '(A)') "Summary of POWHEG veto procedure"
    do alr = 1, matching%process_deps%n_alr
      write(u,'(A,I0)') 'alr: ', alr
      call matching%sudakov(alr)%s%veto_counter%write (u)
      call write_separator (u)
      n_fail_ubf_total = n_fail_ubf_total &
        + matching%sudakov(alr)%s%veto_counter%n_fail_ubf
      n_sqme_total = n_sqme_total &
        + matching%sudakov(alr)%s%veto_counter%n_sqme
    end do
    write (u,'(A,I0)') "Total number of events which radiate a gluon: ", &
      matching%n_emissions
    close (u)
    if (n_sqme_total > 0) then
      frac_ubf_fail = one * n_fail_ubf_total / n_sqme_total * 100
      if (frac_ubf_fail > 1) then
        write (msg_buffer, "(A16,I6,A2,F6.2,A24)") "There have been ", &
          n_fail_ubf_total,&
          " (", frac_ubf_fail, "%) POWHEG grid excesses."
        call msg_warning
      end if
    end if
  end subroutine powheg_matching_final
```

Initialization and Finalization

Setup the POWHEG grids. As they are filled during integration using the POWHEG hook, we can load them from file here.


```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: setup_grids => powheg_matching_setup_grids

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_setup_grids (matching)
    class(powheg_matching_t), intent(inout), target :: matching
  end subroutine powheg_matching_setup_grids

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_setup_grids (matching)
    class(powheg_matching_t), intent(inout), target :: matching
    call matching%prepare_for_events ()
    if (matching%check_grids ()) then
      call matching%load_grids ()
    else
      call msg_fatal ("POWHEG: POWHEG grids are invalid.")
    end if
    call matching%grid%compute_and_write_mean_and_max ()
    call matching%import_norms_from_grid ()
  end subroutine powheg_matching_setup_grids

```

Sets up the Sudakovs and chooses the correct UBF type. To determine the UBF type, we check for massive or initial state emitters for each ALR. For consistency, we thus also check the eeqq case for each ALR. Gfortran 7/8/9 bug, has to remain in the main module:

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: setup_sudakovs => powheg_matching_setup_sudakovs

<POWHEG matching: main procedures>≡
  subroutine powheg_matching_setup_sudakovs (powheg)
    class(powheg_matching_t), intent(inout), target :: powheg
    integer :: alr, ubf_type, n_in, emitter
    logical :: is_fsr, is_massive, is_eeqq
    allocate (powheg%sudakov (powheg%process_deps%n_alr))
    do alr = 1, powheg%process_deps%n_alr
      select type (pcm => powheg%process_instance%pcm)
      type is (pcm_nlo_t)
        associate(reg_data => pcm%region_data, &
          phs => powheg%phs_fks_generator)
          n_in = reg_data%get_n_in()
          emitter = reg_data%get_emitter (alr)
          is_fsr = emitter > n_in
          if (is_fsr) then
            is_massive = phs%is_massive (emitter)
          else
            if (emitter == 0) then
              is_massive = phs%is_massive (1) .or. phs%is_massive (2)
            else
              is_massive = phs%is_massive (emitter)
            end if
            if (is_massive) call msg_bug ("setup_sudakovs: ISR " // &
              "off massive emitters not implemented.")
          end if
        end associate
      end select
      is_eeqq = n_in == 2 .and. &
        reg_data%n_legs_born == 4 .and. &

```

```

        .not. phs%is_massive(3) .and. &
        .not. phs%is_massive(4)
        ! (PS 2021-05-28) This includes FSR regions of pp -> jj.
    end associate
end select
if (is_fsr) then
    if (is_eeqq) then
        ubf_type = UBF_FSR_MASSLESS_RECOIL
    else if (is_massive) then
        ubf_type = UBF_FSR_MASSIVE
    else
        ubf_type = powheg%settings%upper_bound_func_type
    end if
    select case (ubf_type)
    case (UBF_FSR_SIMPLE)
        allocate (sudakov_simple_fsr_t :: powheg%sudakov(alr)%s)
    case (UBF_FSR_MASSLESS_RECOIL)
        allocate (sudakov_eeqq_fsr_t :: powheg%sudakov(alr)%s)
    case (UBF_FSR_MASSIVE)
        allocate (sudakov_massive_fsr_t :: powheg%sudakov(alr)%s)
    case default
        call msg_fatal ("powheg_setup_sudakovs: Please choose " // &
            "upper bounding function!")
    end select
else
    allocate (sudakov_isr_t :: powheg%sudakov(alr)%s)
end if
if (allocated (powheg%rng)) then
    !!! generator mode
    call powheg%sudakov(alr)%s%init (powheg%process_deps, &
        powheg%event_deps, powheg%settings, &
        powheg%qcd, powheg%phs_fks_generator, powheg%rng)
else
    !!! lookup mode
    call powheg%sudakov(alr)%s%init (powheg%process_deps, &
        powheg%event_deps, powheg%settings, &
        powheg%qcd, powheg%phs_fks_generator)
end if
call powheg%sudakov(alr)%s%set_i_phs (alr)
end do
end subroutine powheg_matching_setup_sudakovs

```

(POWHEG matching: powheg matching: TBP)+≡

```
procedure :: init => powheg_matching_init
```

(POWHEG matching: sub interfaces)+≡

```

module subroutine powheg_matching_init (matching, var_list, process_name)
    class(powheg_matching_t), intent(out) :: matching
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_name
end subroutine powheg_matching_init

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_init (matching, var_list, process_name)
    class(powheg_matching_t), intent(out) :: matching

```

```

    <default matching init>
end subroutine powheg_matching_init

```

Updates the Born momenta and the Born matrix element stored in the event dependencies.

```

<POWHEG matching: powheg matching: TBP>+≡
    generic :: update => update_momenta, &
        update_particle_set
    procedure :: update_momenta => powheg_matching_update_momenta
    procedure :: update_particle_set => powheg_matching_update_particle_set

<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_matching_update_momenta (powheg, p_born)
        class(powheg_matching_t), intent(inout) :: powheg
        type(vector4_t), dimension(:), intent(in) :: p_born
    end subroutine powheg_matching_update_momenta
    module subroutine powheg_matching_update_particle_set (powheg, particle_set)
        class(powheg_matching_t), intent(inout) :: powheg
        type(particle_set_t), intent(in) :: particle_set
    end subroutine powheg_matching_update_particle_set

<POWHEG matching: procedures>+≡
    module subroutine powheg_matching_update_momenta (powheg, p_born)
        class(powheg_matching_t), intent(inout) :: powheg
        type(vector4_t), dimension(:), intent(in) :: p_born
        type(lorentz_transformation_t) :: lt_lab_to_cms
        real(default), dimension(:), allocatable :: sqme_born
        integer :: i_uborn, n_reg, alr
        real(default), dimension(2) :: x_born
        select type (pcm => powheg%process_instance%pcm)
        type is (pcm_nlo_t)
            associate (reg_data => pcm%region_data)
                n_reg = reg_data%n_regions
                allocate(sqme_born(n_reg))
                do alr = 1, n_reg
                    select type (pcm_work => powheg%process_instance%pcm_work)
                    class is (pcm_nlo_workspace_t)
                        i_uborn = reg_data%regions(alr)%uborn_index
                        sqme_born(alr) = pcm_work%real_sub%sqme_born(i_uborn)
                    end select
                end do
            end associate
        end select
        x_born = powheg%phs_fks_generator%isr_kinematics%x
        if (.not. powheg%process_deps%lab_is_cm) then
            lt_lab_to_cms = powheg%process_instance%get_boost_to_cms (1)
            call powheg%update_event_deps (sqme_born, p_born, x_born, lt_lab_to_cms)
        else
            call powheg%update_event_deps (sqme_born, p_born, x_born)
        end if
    end subroutine powheg_matching_update_momenta

    module subroutine powheg_matching_update_particle_set (powheg, particle_set)
        class(powheg_matching_t), intent(inout) :: powheg
        type(particle_set_t), intent(in) :: particle_set

```

```

integer, dimension(:), allocatable :: indices
logical, dimension(:), allocatable :: in_out_mask
integer :: i
allocate (in_out_mask (particle_set%get_n_tot()))
do i = 1, particle_set%get_n_tot()
    in_out_mask(i) = particle_set%prt(i)%get_status () == PRT_INCOMING &
        .or. particle_set%prt(i)%get_status () == PRT_OUTGOING
end do
allocate (indices (size (particle_set%get_indices (in_out_mask))))
indices = particle_set%get_indices (in_out_mask)
call powheg%update_momenta (particle_set%get_momenta (indices))
end subroutine powheg_matching_update_particle_set

```

(POWHEG matching: powheg matching: TBP)+≡

```

procedure :: update_event_deps => powheg_matching_update_event_deps

```

(POWHEG matching: sub interfaces)+≡

```

module subroutine powheg_matching_update_event_deps &
    (powheg, sqme_born, p_born, x_born, lt_lab_to_cms)
class(powheg_matching_t), intent(inout) :: powheg
real(default), dimension(:), intent(in) :: sqme_born
type(vector4_t), dimension(:), intent(in) :: p_born
real(default), dimension(2), intent(in) :: x_born
type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
end subroutine powheg_matching_update_event_deps

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_update_event_deps &
    (powheg, sqme_born, p_born, x_born, lt_lab_to_cms)
class(powheg_matching_t), intent(inout) :: powheg
real(default), dimension(:), intent(in) :: sqme_born
type(vector4_t), dimension(:), intent(in) :: p_born
real(default), dimension(2), intent(in) :: x_born
type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
call powheg%event_deps%update (sqme_born, p_born, x_born, lt_lab_to_cms)
end subroutine powheg_matching_update_event_deps

```

Boosts the real momenta to the LAB frame. We call this only for FSR so we can take the boost from the Born term.

(POWHEG matching: powheg matching: TBP)+≡

```

procedure :: boost_preal_to_lab_frame => &
    powheg_matching_boost_preal_to_lab_frame

```

(POWHEG matching: sub interfaces)+≡

```

module subroutine powheg_matching_boost_preal_to_lab_frame (powheg, i_phs)
class(powheg_matching_t), intent(inout) :: powheg
integer, intent(in) :: i_phs
end subroutine powheg_matching_boost_preal_to_lab_frame

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_boost_preal_to_lab_frame (powheg, i_phs)
class(powheg_matching_t), intent(inout) :: powheg
type(lorentz_transformation_t) :: lt_cms_to_lab
integer, intent(in) :: i_phs
associate (event_deps => powheg%event_deps)

```

```

    if (powheg%process_deps%lab_is_cm) then
        event_deps%p_real_lab%phs_point(i_phs) = &
        event_deps%p_real_cms%phs_point(i_phs)
    else
        lt_cms_to_lab = powheg%process_instance%get_boost_to_lab (1)
        event_deps%p_real_lab%phs_point(i_phs) = &
        lt_cms_to_lab * event_deps%p_real_cms%phs_point(i_phs)
    end if
end associate
end subroutine powheg_matching_boost_preal_to_lab_frame

```

Boosts the real momenta to the CM frame.

(POWHEG matching: powheg matching: TBP)+≡

```

    procedure :: boost_preal_to_cms => powheg_matching_boost_preal_to_cms

```

(POWHEG matching: sub interfaces)+≡

```

    module subroutine powheg_matching_boost_preal_to_cms (powheg, i_phs)
        class(powheg_matching_t), intent(inout) :: powheg
        integer, intent(in) :: i_phs
    end subroutine powheg_matching_boost_preal_to_cms

```

(POWHEG matching: procedures)+≡

```

    module subroutine powheg_matching_boost_preal_to_cms (powheg, i_phs)
        class(powheg_matching_t), intent(inout) :: powheg
        type(lorentz_transformation_t) :: lt
        type(vector4_t), dimension(:), allocatable :: p_real
        integer, intent(in) :: i_phs
        real(default) :: sqrts_real
        type(vector4_t) :: p0, p1
        associate (event_deps => powheg%event_deps)
            if (powheg%process_deps%lab_is_cm) then
                event_deps%p_real_cms%phs_point(i_phs) = event_deps%p_real_lab%phs_point(i_phs)
            else
                p_real = event_deps%p_real_lab%phs_point(i_phs)
                p0 = p_real(1) + p_real(2)
                sqrts_real = (p0)**1
                lt = boost (p0, sqrts_real)
                p1 = inverse(lt) * p_real(1)
                lt = lt * rotation_to_2nd (3, space_part (p1))
                p_real = inverse (lt) * p_real
                event_deps%p_real_cms%phs_point(i_phs) = p_real
            end if
        end associate
    end subroutine powheg_matching_boost_preal_to_cms

```

This is the last step of the Sudakov veto algorithm removing the dependence on the normalization factor $N(\xi_i, y_i)$ and the upper bounding function $U(\xi, y, \alpha_s)$ from the final result.

In cases where the Born kinematic failed the cuts, \mathcal{B} was artificially set to zero, so we cannot use it in a denominator. We assume that the generator cuts applied for parton showering are weak cuts to avoid divergent phase space regions, thus \mathcal{B} would have been large and the reweighting would have failed. Here, we can compute `sqme_real` directly with scale p_T but we still need to

correct sqme_born.

(POWHEG matching: powheg matching: TBP)+≡

```
procedure :: reweight_matrix_elements => &
  powheg_matching_reweight_matrix_elements
```

(POWHEG matching: sub interfaces)+≡

```
module function powheg_matching_reweight_matrix_elements &
  (powheg, r) result (accepted)
  logical :: accepted
  class(powheg_matching_t), intent(inout) :: powheg
  type(radiation_t), intent(in) :: r
end function powheg_matching_reweight_matrix_elements
```

(POWHEG matching: procedures)+≡

```
module function powheg_matching_reweight_matrix_elements &
  (powheg, r) result (accepted)
  logical :: accepted
  class(powheg_matching_t), intent(inout) :: powheg
  type(radiation_t), intent(in) :: r
  integer :: emitter, n_in, i_phs, i_term_born, alphas_power, em
  real(default) :: sqme_real_x_jac, sqme_born
  real(default) :: norm, ubf, ubound, random, weight
  real(default) :: alpha_s_kt, alpha_s_muren, alpha_s_kt_noNLL
  real(default) :: muren, mufac, pt2
  integer, dimension(2) :: flv_born
  real(double), dimension(-6:6) :: pdf_dbl
  real(double) :: x_dbl, q_dbl
  type(vector4_t), dimension(:), allocatable :: p_real_cms, p_real_lab
  real(default), dimension(2) :: pdf_born_mufac, pdf_born_kt
  logical :: cuts_passed
  if (debug_on) call msg_debug (D_MATCHING, "reweight_matrix_elements")
  cuts_passed = powheg%process_instance%get_sqme(powheg%process_deps%i_term_born) > 0
  if (cuts_passed) then
    sqme_born = powheg%event_deps%sqme_born(r%alr)
  else
    sqme_born = zero
  end if
  if (nearly_equal(sqme_born,zero)) then
    accepted = .false.
    return
  end if
  call powheg%rng%generate (random)
  i_phs = powheg%process_deps%alr_to_i_phs (r%alr)
  select type (pcm => powheg%process_instance%pcm)
  type is (pcm_nlo_t)
    emitter = pcm%region_data%get_emitter (r%alr)
    n_in = pcm%region_data%get_n_in()
    if (emitter <= n_in) then
      allocate(p_real_lab (pcm%region_data%get_n_legs_real()))
      call powheg%phs_fks_generator%generate_isr_from_xi_and_y (&
        r%xi, sqrt (powheg%sudakov(r%alr)%s%xi2_max), r%y, &
        r%phi, i_phs, powheg%event_deps%p_born_lab%get_momenta(1), &
        p_real_lab)
      powheg%event_deps%p_real_lab%phs_point(i_phs) = p_real_lab
      call powheg%boost_preal_to_cms (i_phs)
```

```

else
  allocate(p_real_cms (pcm%region_data%get_n_legs_real()))
  powheg%phs_fks_generator%m2 = invariant_mass_squared (powheg%event_deps%p_born_cms%get_m
  call powheg%phs_fks_generator%generate_fsr_from_xi_and_y (r%xi, r%y, &
    r%phi, emitter, i_phs, &
    powheg%event_deps%p_born_cms%get_momenta(1), &
    p_real_cms)
  powheg%event_deps%p_real_cms%phs_point(i_phs) = p_real_cms
  call powheg%boost_preal_to_lab_frame (i_phs)
end if
if (debug_active (D_MATCHING)) then
  if (emitter <= n_in) then
    pt2 = (transverse_part (p_real_lab (size(p_real_lab))))**2
  else
    pt2 = (transverse_part (p_real_cms (size(p_real_cms))))**2
  end if
  call assert_equal (OUTPUT_UNIT, r%pt2, pt2, &
    "reweight_matrix_elements: generated p_real does not fit to sudakovs pt2")
end if
call powheg%copy_momenta (i_phs)
norm = powheg%norm_from_xi_and_y (r)
associate (s => powheg%sudakov(r%alr)%s)
  alpha_s_kt = s%alpha_s (r%pt2, use_correct=.true.)
  alpha_s_kt_noNLL = s%alpha_s (r%pt2, use_correct=.true., improve_nll=.false.)
  i_term_born = powheg%process_deps%i_term_born
  muren = powheg%process_instance%term(i_term_born)%get_ren_scale ()
  mufac = powheg%process_instance%term(i_term_born)%get_fac_scale ()
  alpha_s_muren = s%alpha_s (muren**2, use_correct=.true., improve_nll=.false.)
  ubf = s%upper_bound_func (r%xi, r%y, alpha_s_kt)

  sqme_real_x_jac = powheg%compute_sqme_real (r%alr, sqrt(r%pt2))

  select type (pcm_work => powheg%process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    sqme_real_x_jac = pcm_work%powheg_kinematic_factors_real &
      (sqme_real_x_jac, r%alr)
  end select

  !!! Correct all factors of alphas to the NLL-corrected alphas(kt).
  alphas_power = powheg%process_deps%alphas_power
  sqme_born = (alpha_s_kt / alpha_s_muren)**alphas_power * sqme_born
  sqme_real_x_jac = (alpha_s_kt / alpha_s_kt_noNLL)**(alphas_power+1) * sqme_real_x_jac

  !!! Also correct the PDFs previously computed at mufac instead of kt
  select type (pcm => powheg%process_instance%pcm)
  type is (pcm_nlo_t)
    if (pcm%has_pdfs) then
      associate (reg_data => pcm%region_data)
        flv_born = reg_data%regions(r%alr)%flst_uborn%flst(1:2)
        where (flv_born == 21) flv_born = 0
      end associate
      associate (pdf_data => powheg%process_deps%pdf_data, &
        x_born => powheg%event_deps%x_born)
        do em = 1, 2

```

```

        x_dbl = x_born(em); q_dbl = mufac
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_born_mufac(em) = pdf_dbl(flv_born(em)) / x_born(em)
        x_dbl = x_born(em); q_dbl = sqrt(r%pt2)
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_born_kt(em) = pdf_dbl(flv_born(em)) / x_born(em)
    end do
    sqme_born = pdf_born_kt(1) * pdf_born_kt(2) / &
        (pdf_born_mufac(1) * pdf_born_mufac(2)) * sqme_born
    end associate
end if
end select

if (nearly_equal(sqme_born,zero) .or. sqme_born < 0) then
    accepted = .false.
    return
end if
ubound = sqme_born * ubf * norm
weight = sqme_real_x_jac / ubound
if (weight > 1) call s%veto_counter%record_ubf_fail()
if (debug_active (D_MATCHING)) then
    if (weight < 0) call msg_warning ("R/B < 0!")
end if
accepted = random < weight
end associate

if (debug_active (D_MATCHING)) then
    print *, ' r%alr = ', r%alr
    print *, ' r%xi = ', r%xi
    print *, ' r%y = ', r%y
    print *, ' r%phi = ', r%phi
    print *, ' r%pt = ', sqrt(r%pt2)
    print *, ' emitter = ', emitter
    print *, ' random = ', random
    print *, ' sqme_born = ', sqme_born
    print *, ' sqme_real_x_jac = ', sqme_real_x_jac
    print *, ' ubf = ', ubf
    print *, ' norm = ', norm
    print *, ' ubound = ', ubound
    print *, ' matrix element accepted = ', accepted
end if
end select
end function powheg_matching_reweight_matrix_elements

```

Generation algorithm and grid initialization

compute_sqme_real is the projected real matrix element $R_{\alpha_r} = S_{\alpha_r} R$ whereby the current α_r is implied by the emitter. Furthermore, it is multiplied by the real and the random number Jacobian.

(POWHEG matching: powheg matching: TBP) + \equiv

```
procedure :: compute_sqme_real => powheg_matching_compute_sqme_real
```



```

<POWHEG matching: sub interfaces>+≡
  module function powheg_matching_compute_sqme_real &
    (powheg, alr, scale) result (sqme)
    real(default) :: sqme
    class(powheg_matching_t), intent(inout) :: powheg
    integer, intent(in) :: alr
    real(default), intent(in), optional :: scale
  end function powheg_matching_compute_sqme_real

<POWHEG matching: procedures>+≡
  module function powheg_matching_compute_sqme_real &
    (powheg, alr, scale) result (sqme)
    real(default) :: sqme
    class(powheg_matching_t), intent(inout) :: powheg
    integer, intent(in) :: alr
    real(default), intent(in), optional :: scale
    real(default), allocatable :: q
    integer :: i_phs, i_term
    logical :: is_subtraction, cuts_passed
    is_subtraction = .false.
    select type (pcm_work => powheg%process_instance%pcm_work)
    class is (pcm_nlo_workspace_t)
      i_phs = powheg%process_deps%alr_to_i_phs (alr)
      i_term = powheg%process_deps%i_term_real (i_phs)
      associate (instance => powheg%process_instance)
        if (present(scale)) then
          if (.not. allocated (q)) then
            allocate (q, source = scale)
          else
            q = scale
          end if
          call instance%compute_sqme_rad &
            (i_term, i_phs, is_subtraction, scale_forced=q)
        else
          call instance%compute_sqme_rad (i_term, i_phs, is_subtraction)
        end if
        cuts_passed = instance%get_sqme(i_term) > 0
        if (cuts_passed) then
          sqme = pcm_work%real_sub%sqme_real_arr(alr)
        else
          sqme = zero
        end if
      end associate
    end select
  end function powheg_matching_compute_sqme_real

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: set_scale => powheg_matching_set_scale

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_set_scale (powheg, pT2)
    class(powheg_matching_t), intent(inout) :: powheg
    real(default), intent(in) :: pT2
  end subroutine powheg_matching_set_scale

```

```

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_set_scale (powheg, pT2)
    class(powheg_matching_t), intent(inout) :: powheg
    real(default), intent(in) :: pT2
    call powheg%process_instance%set_fac_scale (sqrt(pT2))
  end subroutine powheg_matching_set_scale

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: update_sudakovs => powheg_matching_update_sudakovs

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_update_sudakovs (powheg, alr, i_phs, y)
    class(powheg_matching_t), intent(inout) :: powheg
    integer, intent(in) :: alr, i_phs
    real(default), intent(in) :: y
  end subroutine powheg_matching_update_sudakovs

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_update_sudakovs (powheg, alr, i_phs, y)
    class(powheg_matching_t), intent(inout) :: powheg
    integer, intent(in) :: alr, i_phs
    real(default), intent(in) :: y
    real(default) :: q0, m2, mrec2, k0_rec_max
    type(vector4_t) :: p_emitter
    select type (s => powheg%sudakov(alr)%s)
    type is (sudakov_massive_fsr_t)
      q0 = sqrt (s%event_deps%s_hat)
      p_emitter = s%event_deps%p_born_lab%get_momentum (1, &
        s%associated_emitter ())
      associate (p => p_emitter%p)
        mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
      end associate
      m2 = p_emitter**2
      call compute_dalitz_bounds (q0, m2, mrec2, s%z1, s%z2, k0_rec_max)
      s%z = s%z2 - (s%z2 - s%z1) * (one + y) / two
    end select
  end subroutine powheg_matching_update_sudakovs

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: import_norms_from_grid => powheg_matching_import_norms_from_grid

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_import_norms_from_grid (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
  end subroutine powheg_matching_import_norms_from_grid

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_import_norms_from_grid (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    integer :: alr
    real(default) :: norm_max
    do alr = 1, powheg%process_deps%n_alr
      norm_max = powheg%grid%get_maximum_in_3d (alr)
      call powheg%sudakov(alr)%s%set_normalization (norm_max)
    end do
  end subroutine

```

```
end subroutine powheg_matching_import_norms_from_grid
```

We save the POWHEG grid to a file to be used for the event generation. If it has no non-zero entries, we assume that the integration was skipped because there were existing VAMP(2) and POWHEG grid files.

```
<POWHEG matching: powheg matching: TBP>+≡
  procedure :: save_grids => powheg_matching_save_grids

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_save_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
  end subroutine powheg_matching_save_grids

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_save_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    if (powheg%grid%has_non_zero_entries()) then
      call powheg%grid%save_to_file (char (filename))
    else
      call msg_warning("POWHEG grid not saved to file. An existing " // &
        & char(filename) // " will be used for the events.")
    end if
  end subroutine powheg_matching_save_grids

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: load_grids => powheg_matching_load_grids

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_load_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
  end subroutine powheg_matching_load_grids

<POWHEG matching: procedures>+≡
  module subroutine powheg_matching_load_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    call powheg%grid%load_from_file (char (filename))
    if (powheg%grid%has_non_zero_entries()) then
      write (msg_buffer, "(A,A,A)") "POWHEG: using grids from file '", &
        char (filename), "'"
    else
      call msg_fatal("POWHEG grid in " // char(filename) // &
        & " is zero and cannot be used for event generation.")
    end if
    call msg_message ()
  end subroutine powheg_matching_load_grids

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: check_grids => powheg_matching_check_grids
```

```

<POWHEG matching: sub interfaces>+=
  module function powheg_matching_check_grids (powheg) result (ok)
    logical :: ok
    class(powheg_matching_t), intent(in) :: powheg
  end function powheg_matching_check_grids

<POWHEG matching: procedures>+=
  module function powheg_matching_check_grids (powheg) result (ok)
    logical :: ok
    class(powheg_matching_t), intent(in) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    ok = os_file_exist (filename) .and. &
      verify_points_for_grid (char (filename), &
        [powheg%settings%size_grid_xi, &
        powheg%settings%size_grid_y, &
        powheg%process_deps%n_alr])
  end function powheg_matching_check_grids

```

This routine implements the Sudakov veto algorithm as explained in [1002.2581], Sec. 7.1 and Bijans thesis, Sec. 3.3 and B.2. Here, we veto in order to correct for

1. an overestimation of parts of the upper bounding function for complicated UBFs in `reweight_ubf` as well as the usage of α_s^{rad} instead of α_s^{true} .
2. the usage of `xi_max_extended` instead of `xi_max` in `reweight_xi_max` which is only non-trivial for massive FSR and ISR.
3. using the maximum of the entire POWHEG normalization grid N_{max} when generating p_T instead of the correct bin value $N(\xi_i, y_i)$ in `reweight_norm`.
4. the normalization grid and the upper bounding function in the first place in `reweight_matrix_elements` to retrieve the correct fraction $\frac{\mathcal{R}(\xi, y) \mathcal{J}(\xi, y)}{\mathcal{B}}$.

By looping over all ALRs and in the end choosing the ALR with the largest `pt2`, we are effectively implementing the highest bid procedure. To save some time generating equivalent phase spaces again and again, we could instead loop over all radiation regions `i_phs`, take the sum of all real matrix elements in the Sudakov and in the end pick the ALR with probability proportional to the corresponding \mathcal{R}_{α_r} . We might implement this optimization in the future.

We need to compute `xi2_max` before `kt2_max` here. In the simple case, it is given by $\xi_{\text{max}} = \frac{s - M_{\text{rec}}^2}{s}$ but we can also take the ξ_{max} from the phase space computed before; they coincide. This is possible already at this point because in the simple case, ξ_{max} only depends on the Born momentum of the emitter and not on the real kinematics. In the eeqq case, $M_{\text{rec}} = 0$, so $\xi_{\text{max}} = 1$ and in the massive case as well as in the ISR case, we compute an extended $\xi_{\text{max}}^{\text{ext}}$ because the actual ξ_{max} depends on the real kinematics.

```

<POWHEG matching: powheg matching: TBP>+=
  procedure :: generate_emission => powheg_matching_generate_emission

```

```

(POWHEG matching: sub interfaces)+≡
module subroutine powheg_matching_generate_emission &
  (powheg, particle_set, pt2_generated)
  class(powheg_matching_t), intent(inout) :: powheg
  type(particle_set_t), intent(inout), optional :: particle_set
  real(default), intent(out), optional :: pt2_generated
end subroutine powheg_matching_generate_emission

(POWHEG matching: procedures)+≡
module subroutine powheg_matching_generate_emission &
  (powheg, particle_set, pt2_generated)
  class(powheg_matching_t), intent(inout) :: powheg
  type(particle_set_t), intent(inout), optional :: particle_set
  real(default), intent(out), optional :: pt2_generated
  type(radiation_t) :: r, r_max
  real(default) :: xi2_max
  integer :: alr
  logical :: accepted
  logical, dimension(:), allocatable :: prt_status_mask
  type(vector4_t), dimension(:), allocatable :: p_real_max
  if (signal_is_pending ()) return
  if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_generate_emission")
  allocate(prt_status_mask(particle_set%get_n_tot()))
  prt_status_mask = .false.
  where (particle_set%prt%get_status () == PRT_INCOMING &
    .or. particle_set%prt%get_status () == PRT_OUTGOING) &
    prt_status_mask = .true.
  r_max%pt2 = zero
  r_max%alr = 0
  select type (pcm => powheg%process_instance%pcm)
  type is (pcm_nlo_t)
    allocate (p_real_max (pcm%region_data%n_legs_real))
  end select
  select type (pcm_work => powheg%process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    do alr = 1, powheg%process_deps%n_alr
      if (signal_is_pending ()) return
      if (present (particle_set)) then
        select type (pcm => powheg%process_instance%pcm)
        type is (pcm_nlo_t)
          if (any (pack(particle_set%prt%get_pdg (), prt_status_mask) /= &
            pcm%region_data%regions(alr)%flst_uborn%flst)) then
            cycle
          end if
        end select
      end select
    end if
  associate (sudakov => powheg%sudakov(alr)%s)
    select type (sudakov)
    type is (sudakov_simple_fsr_t)
      xi2_max = pcm_work%get_xi_max (alr)**2
      call sudakov%update_xi2_max (xi2_max)
      if (debug2_active (D_MATCHING)) then
        call check_xi2_max (sudakov)
      end if
    type is (sudakov_eeqq_fsr_t)

```

```

        call sudakov%update_xi2_max (one)
type is (sudakov_massive_fsr_t)
        call sudakov%compute_xi_max_extended ()
type is (sudakov_isr_t)
        call sudakov%compute_xi_max_extended ()
class default
        call msg_fatal ("powheg_matching_generate_emission: unknown Sudakov!")
end select
r%alr = alr
r%pt2 = sudakov%kt2_max ()
sudakov%sum_log_rands = 0
if (debug_on) call msg_debug (D_MATCHING, "Starting evolution at r%pt2", r%pt2)
PT_EVOLUTION: do
    if (signal_is_pending ()) return
    call sudakov%generate_emission (r, r_max)
    if (signal_is_pending ()) return
    if (r%valid) then
        accepted = powheg%reweight_norm (r)
        call sudakov%veto_counter%record_norm (.not. accepted)
        if (.not. accepted) cycle PT_EVOLUTION
        accepted = powheg%reweight_matrix_elements (r)
        call sudakov%veto_counter%record_sqme (.not. accepted)
        if (.not. accepted) cycle PT_EVOLUTION
    end if
    exit
end do PT_EVOLUTION
if (r%pt2 > r_max%pt2 .and. r%valid) then
    r_max = r
    p_real_max = powheg%event_deps%p_real_lab%get_momenta (sudakov%i_phs)
end if
end associate
end do
if (r_max%pt2 > powheg%settings%pt2_min) then
    powheg%n_emissions = powheg%n_emissions + 1
    call update_event_data (powheg, r_max%alr, r_max%pt2)
    if (present (particle_set)) then
        call powheg%build_particle_set (particle_set, &
            p_real_max, r_max%alr, r_max%y)
    end if
    if (present (pt2_generated)) pt2_generated = r_max%pt2
else
    call update_event_data (powheg, 1, powheg%settings%pt2_min)
    if (present (pt2_generated)) pt2_generated = powheg%settings%pt2_min
end if
end select
contains
subroutine check_xi2_max (sudakov)
    class(sudakov_t), intent(in) :: sudakov
    real(default) :: s_hat, mrec2, xi2_max
    type(vector4_t) :: p_emitter
    s_hat = sudakov%event_deps%s_hat
    p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
        (1, sudakov%associated_emitter())
    associate (p => p_emitter%p)

```

```

      mrec2 = (sqrt(s_hat) - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
    end associate
    xi2_max = (s_hat - mrec2) / s_hat
    xi2_max = xi2_max**2
    call assert_equal (OUTPUT_UNIT, sudakov%xi2_max, xi2_max, &
      "powheg_matching_generate_emission: xi_max inconsistent")
  end subroutine check_xi2_max
  !!! Force the scale pT and the value of alpha_s(p_T) into the event output.
  subroutine update_event_data (powheg, alr, pt2)
    class(powheg_matching_t), intent(inout) :: powheg
    integer, intent(in) :: alr
    real(default), intent(in) :: pt2
    real(default) :: alpha_s
    alpha_s = powheg%sudakov(alr)%s%alpha_s (pt2, use_correct = .true.)
    select type (core_state => powheg%process_instance%term(1)%core_state)
      class is (prc_external_state_t)
        core_state%alpha_qcd = alpha_s
      class is (omega_state_t)
        core_state%alpha_qcd = alpha_s
    end select
    call powheg%set_scale (pt2)
  end subroutine update_event_data
end subroutine powheg_matching_generate_emission

```

(POWHEG matching: powheg matching: TBP)+≡

```

  procedure :: build_particle_set => powheg_matching_build_particle_set

```

(POWHEG matching: sub interfaces)+≡

```

  module subroutine powheg_matching_build_particle_set &
    (powheg, particle_set, p_real, alr, y)
    class(powheg_matching_t), intent(inout) :: powheg
    type(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), dimension(:), intent(in) :: p_real
    integer, intent(in) :: alr
    real(default), intent(in) :: y
  end subroutine powheg_matching_build_particle_set

```

(POWHEG matching: procedures)+≡

```

  module subroutine powheg_matching_build_particle_set &
    (powheg, particle_set, p_real, alr, y)
    class(powheg_matching_t), intent(inout) :: powheg
    type(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), dimension(:), intent(in) :: p_real
    integer, intent(in) :: alr
    real(default), intent(in) :: y
    integer, dimension(:), allocatable :: i_flvs_real, flv_radiated
    real(default) :: r_col
    integer :: emitter, i_flv_real
    select type (pcm => powheg%process_instance%pcm)
      type is (pcm_nlo_t)
        i_flvs_real = pcm%region_data%get_flavor_indices (.false.)
        i_flv_real = i_flvs_real (alr)
        allocate (flv_radiated (size (pcm%region_data%get_flv_states_real (i_flv_real))))
        flv_radiated = pcm%region_data%get_flv_states_real (i_flv_real)
        emitter = pcm%region_data%get_emitter(alr)

```

```

      if (emitter == 0) then
        if (y > 0) then
          emitter = 1
        else
          emitter = 2
        end if
      end if
    end select
    call powheg%rng%generate (r_col)
    call particle_set%build_radiation (p_real, emitter, flv_radiated, &
      powheg%process_instance%process%get_model_ptr (), r_col)
  end subroutine powheg_matching_build_particle_set

```

When generating the transverse momentum in `sudakov_generate_pt2`, we used N^{\max} as normalization. In this veto step, we correct for this by keeping events with probability

$$\frac{N(\xi_i, y_i)}{N^{\max}}.$$

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: reweight_norm => powheg_matching_reweight_norm

<POWHEG matching: sub interfaces>+≡
  module function powheg_matching_reweight_norm (powheg, r) result (accepted)
    logical :: accepted
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
  end function powheg_matching_reweight_norm

<POWHEG matching: procedures>+≡
  module function powheg_matching_reweight_norm (powheg, r) result (accepted)
    logical :: accepted
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
    real(default) :: random, norm_max, norm_true
    if (debug_on) call msg_debug2 (D_MATCHING, "reweight_norm")
    call powheg%rng%generate (random)
    norm_true = powheg%norm_from_xi_and_y (r)
    norm_max = powheg%sudakov(r%alr)%s%norm_max
    accepted = random < norm_true / norm_max
    if (debug2_active (D_MATCHING)) then
      print *, ' r%alr = ', r%alr
      print *, ' random = ', random
      print *, ' norm_true = ', norm_true
      print *, ' norm_max = ', norm_max
      print *, ' norm accepted = ', accepted
    end if
    if (debug_active (D_MATCHING)) then
      if (.not. (zero < r%xi .and. &
        r%xi < sqrt(powheg%sudakov(r%alr)%s%xi2_max))) then
        call msg_bug ("powheg_matching_reweight_norm: xi is out of bounds")
      end if
      if (norm_true > norm_max) then
        call msg_bug ("powheg_matching_reweight_norm: norm shouldnt be larger than norm_max")
      end if
    end if
  end function

```



```

end if
end function powheg_matching_reweight_norm

```

Retrieves the value of the norm for given ξ and y from the pre-computed POWHEG grid. To find the correct bin we need to map (ξ, y) in some way to $[0, 1]^2$. This mapping is to the most extend arbitrary. We choose $y \mapsto |y|$ and $\xi \mapsto \log(1 - \xi) / \log(1 - \xi_{max})$. It may be possible to improve these mappings to tune the performance for processes with expensive matrix elements.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: norm_from_xi_and_y => powheg_matching_norm_from_xi_and_y

<POWHEG matching: sub interfaces>+≡
  module function powheg_matching_norm_from_xi_and_y &
    (powheg, r) result (norm_true)
    real(default) :: norm_true
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
    end function powheg_matching_norm_from_xi_and_y

<POWHEG matching: procedures>+≡
  module function powheg_matching_norm_from_xi_and_y &
    (powheg, r) result (norm_true)
    real(default) :: norm_true
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
    real(default) :: f_alr, xi_max
    real(default), dimension(2) :: rands
    f_alr = (one * r%alr) / powheg%process_deps%n_alr - tiny_07
    rands(I_Y) = abs(r%y)
    xi_max = min(sqrt(powheg%sudakov(r%alr)%s%xi2_max), 1 - tiny_07)
    if (r%xi > xi_max) then
      rands(I_XI) = 1
    else
      rands(I_XI) = log(1 - r%xi) / log(1 - xi_max)
    end if
    norm_true = powheg%grid%get_value ([rands, f_alr])
  end function powheg_matching_norm_from_xi_and_y

```

31.4.4 α_s and its reweighting

The main point to ensure here is that the simple fixed-flavor-1-loop expression α_s^{rad} is larger than the more accurate α_s such that we can use a reweighting veto and use α_s^{rad} for the generation of the emission. This can be done by setting

$$\alpha_s^{\text{rad}}(\mu_0) = \alpha_s(\mu_0) \quad (31.25)$$

whereby μ_0^2 is the `scale_to_relate2` that is taken to be $(2\Lambda_{\overline{MS}}^{(5)})^2$.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: prepare_for_events => powheg_matching_prepare_for_events

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_matching_prepare_for_events (matching)
    class(powheg_matching_t), intent(inout), target :: matching
    end subroutine powheg_matching_prepare_for_events

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_prepare_for_events (matching)
  class(powheg_matching_t), intent(inout), target :: matching
  if (debug_on) call msg_debug &
    (D_MATCHING, "powheg_matching_prepare_for_events")
  call matching%setup_nlo_environment ()
  call matching%grid%init ([matching%settings%size_grid_xi, &
    matching%settings%size_grid_y, matching%process_deps%n_alr])
  call matching%compute_lambda5MSB ()
  call matching%compute_lambda2_gen ()
  call matching%setup_sudakovs ()
end subroutine powheg_matching_prepare_for_events

```

Computes the scale Λ used for the (log integrated) UBFs. By construction, it is always $p_{T,\min} > \Lambda$.

(POWHEG matching: powheg matching: TBP)+≡

```

procedure :: compute_lambda2_gen => powheg_matching_compute_lambda2_gen

```

(POWHEG matching: sub interfaces)+≡

```

module subroutine powheg_matching_compute_lambda2_gen (matching)
  class(powheg_matching_t), intent(inout) :: matching
end subroutine powheg_matching_compute_lambda2_gen

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_compute_lambda2_gen (matching)
  class(powheg_matching_t), intent(inout) :: matching
  real(default) :: scale_to_relate2, alpha_s
  scale_to_relate2 = (2*matching%process_deps%lambda5MSB)**2
  alpha_s = get_alpha_s (matching%qcd, scale_to_relate2, 3)
  matching%process_deps%lambda2_gen = exp (- one / (b0rad () * alpha_s)) * &
    scale_to_relate2
end subroutine powheg_matching_compute_lambda2_gen

```

Computes the scale $\Lambda_{\overline{MS}}^{(5)}$ used to determine the scale at which we relate α_s^{rad} and α_s^{true} .

(POWHEG matching: powheg matching: TBP)+≡

```

procedure :: compute_lambda5MSB => powheg_matching_compute_lambda5MSB

```

(POWHEG matching: sub interfaces)+≡

```

module subroutine powheg_matching_compute_lambda5MSB (matching)
  class(powheg_matching_t), intent(inout) :: matching
end subroutine powheg_matching_compute_lambda5MSB

```

(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_compute_lambda5MSB (matching)
  class(powheg_matching_t), intent(inout) :: matching
  real(default) :: alpha_s
  integer :: nf, order
  logical :: print_once = .true.
  if (matching%settings%lambda == 0) then
    alpha_s = matching%qcd%alpha%get(MZ_REF)
    select type (alpha => matching%qcd%alpha)
    type is (alpha_qcd_from_scale_t)
      order = alpha%order
    type is (alpha_qcd_from_lambda_t)

```

```

        order = alpha%order
type is (alpha_qcd_lhapdf_t)
        order = alpha%get_order ()
class default
    if (print_once) then
        call msg_warning ("compute_lambda5MSB: alpha_qcd not running!" // &
            " Assuming LO (1-loop) running!")
        print_once = .false.
    end if
    order = 0
end select
nf = 5
matching%process_deps%lambda5MSB = lambda_qcd(alpha_s, MZ_REF, nf, order)
else if (matching%settings%lambda > 0) then
    matching%process_deps%lambda5MSB = matching%settings%lambda
else
    call msg_fatal ("compute_lambda5MSB: lambda5MSB < 0")
end if
end subroutine powheg_matching_compute_lambda5MSB

```

This is the setup of the process dependencies stored for the matching.

```

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: setup_nlo_environment => powheg_matching_setup_nlo_environment

<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_matching_setup_nlo_environment (matching)
        class(powheg_matching_t), intent(inout) :: matching
        end subroutine powheg_matching_setup_nlo_environment

<POWHEG matching: procedures>+≡
    module subroutine powheg_matching_setup_nlo_environment (matching)
        class(powheg_matching_t), intent(inout) :: matching
        integer :: n_tot_born, n_tot_real
        integer :: i_phs, i_term_real, i_term
        integer :: n_phs, nlo_type
        if (debug_on) call msg_debug &
            (D_MATCHING, "powheg_matching_setup_nlo_environment")
        select type (pcm_work => matching%process_instance%pcm_work)
        class is (pcm_nlo_workspace_t)
            matching%process_deps%sqrts = matching%process_instance%get_sqrts ()
            select type (pcm => matching%process_instance%pcm)
            type is (pcm_nlo_t)
                matching%process_deps%n_alr = pcm%region_data%n_regions
                n_tot_born = pcm%region_data%n_legs_born
                n_tot_real = pcm%region_data%n_legs_real
                call pcm%setup_phs_generator (pcm_work, &
                    matching%phs_fks_generator, matching%process_deps%sqrts, &
                    singular_jacobian = matching%settings%singular_jacobian)
            end select
        associate (instance => matching%process_instance)
            i_term_real = instance%process%get_first_real_component ()
            associate (process_deps => matching%process_deps)
                select type (phs => instance%kin(i_term_real)%phs)
                type is (phs_fks_t)
                    n_phs = size (phs%phs_identifiers)

```

```

        allocate (process_deps%phs_identifiers (n_phs))
        process_deps%phs_identifiers = phs%phs_identifiers
    end select
    call instance%process%get_coupling_powers(process_deps%alpha_power, &
        process_deps%alphas_power)
    allocate (matching%process_deps%alr_to_i_phs &
        (size (pcm_work%real_kinematics%alr_to_i_phs)))
    process_deps%alr_to_i_phs = pcm_work%real_kinematics%alr_to_i_phs
    allocate (process_deps%i_term_real (n_phs))
    i_phs = 1
    do i_term = 1, size (instance%term)
        nlo_type = instance%term(i_term)%nlo_type
        if (nlo_type == BORN) then
            process_deps%i_term_born = i_term
        else if (nlo_type == NLO_REAL) then
            if (instance%kin(i_term)%emitter >= 0) then
                process_deps%i_term_real(i_phs) = i_term
                i_phs = i_phs + 1
            end if
        end if
    end do
end associate
end associate
call matching%event_deps%p_born_lab%init (n_tot_born, 1)
call matching%event_deps%p_born_cms%init (n_tot_born, 1)
call matching%event_deps%p_real_lab%init (n_tot_real, n_phs)
call matching%event_deps%p_real_cms%init (n_tot_real, n_phs)
end select
end subroutine powheg_matching_setup_nlo_environment

```

Copy momenta from event_deps to real_kinematics for them to be available for the int_hard in compute_sqme_rad.

```

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: copy_momenta => powheg_matching_copy_momenta

<POWHEG matching: sub interfaces>+≡
    module subroutine powheg_matching_copy_momenta (matching, i_phs)
        class(powheg_matching_t), intent(inout) :: matching
        integer, intent(in) :: i_phs
    end subroutine powheg_matching_copy_momenta

<POWHEG matching: procedures>+≡
    module subroutine powheg_matching_copy_momenta (matching, i_phs)
        class(powheg_matching_t), intent(inout) :: matching
        integer, intent(in) :: i_phs
        select type (pcm_work => matching%process_instance%pcm_work)
        class is (pcm_nlo_workspace_t)
            call pcm_work%real_kinematics%p_real_cms%set_momenta &
                (i_phs, matching%event_deps%p_real_cms%get_momenta (i_phs))
            call pcm_work%real_kinematics%p_real_lab%set_momenta &
                (i_phs, matching%event_deps%p_real_lab%get_momenta (i_phs))
        end select
    end subroutine powheg_matching_copy_momenta

```

`qcd%alpha%get` should implement a variable-flavor result and optionally return `n_flavors` that are active at the scale. Optionally takes `nf` as input preceeding the PDFs value. We need this to compute α_s^{rad} always with `nf=3`.

(POWHEG matching: procedures)+≡

```
function get_alpha_s (qcd, scale2, nf_in, improve_nll_opt) result (alpha_s)
  real(default) :: alpha_s
  class(qcd_t), intent(in) :: qcd
  real(default), intent(in) :: scale2
  integer, optional, intent(in) :: nf_in
  logical, optional, intent(in) :: improve_nll_opt
  logical :: improve_nll
  real(default) :: mb, mc
  integer :: nf
  logical :: print_once = .true.
  ! TODO: (bcn 2015-01-30) implement variable flavor alpha_s for all types
  improve_nll = .true.; if (present(improve_nll_opt)) improve_nll = improve_nll_opt
  alpha_s = qcd%alpha%get (sqrt(scale2))
  select type (alpha => qcd%alpha)
    type is (alpha_qcd_from_scale_t)
      nf = alpha%nf
    type is (alpha_qcd_from_lambda_t)
      nf = alpha%nf
    type is (alpha_qcd_lhapdf_t)
      mc = alpha%get_qmass(4)
      mb = alpha%get_qmass(5)
      if (scale2 > mb**2) then
        nf = 5
      elseif (scale2 > mc**2) then
        nf = 4
      else
        nf = 3
      end if
  class default
    if (print_once) then
      call msg_warning ("get_alpha_s: QCD type is not running!" // &
        " Assuming 5-flavors and LO (1-loop) running!")
      print_once = .false.
    end if
    nf = 5
  end select
  if (present(nf_in)) then
    nf = nf_in
  end if
  if (improve_nll) then
    alpha_s = improve_nll_accuracy (alpha_s, nf)
  end if
end function get_alpha_s
```

See Eq. (4.31) in 0709.2092. Should be used everywhere in the Sudakov exponent.

(POWHEG matching: procedures)+≡

```
pure function improve_nll_accuracy (alpha_s, n_flavors) result (alpha_s_imp)
  real(default) :: alpha_s_imp
```

```

    real(default), intent(in) :: alpha_s
    integer, intent(in) :: n_flavors
    alpha_s_imp = alpha_s * (one + alpha_s / (two*pi) * &
        ((67.0_default/18 - pi**2/6) * CA - five/9 * n_flavors))
end function improve_nll_accuracy

```

Wrapper for $b_0(n_f = 5)$ from the `sm_physics` module. It is fixed to $n_f = 5$ for radiation generation and will be reweighted to the more precise α_s .

```

<POWHEG matching: procedures>+≡
    pure function b0rad () result (b0)
    real(default) :: b0
    b0 = coeff_b0(five)
end function b0rad

```

Computes the overestimated α_s for the sudakov before the α_s -Veto. We do not NLL-correct α_s again. We did so already when computing `lambda2_gen`.

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: alpha_s_rad => sudakov_alpha_s_rad

<POWHEG matching: sub interfaces>+≡
    elemental module function sudakov_alpha_s_rad (sudakov, scale2) result (alpha_s_rad)
    real(default) :: alpha_s_rad
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: scale2
    end function sudakov_alpha_s_rad

<POWHEG matching: procedures>+≡
    elemental module function sudakov_alpha_s_rad (sudakov, scale2) result (alpha_s_rad)
    real(default) :: alpha_s_rad
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: scale2
    alpha_s_rad = one / (b0rad () * log (scale2 / sudakov%process_deps%lambda2_gen))
end function sudakov_alpha_s_rad

```

31.4.5 POWHEG hook

We provide a POWHEG hook to be called by `process_instance_evaluate` to prefill the adaptation grid.

We store the actual `powheg` object, which does the computations.

```

<POWHEG matching: public>+≡
    public :: powheg_matching_hook_t

<POWHEG matching: types>+≡
    type, extends(process_instance_hook_t) :: powheg_matching_hook_t
    type(string_t) :: process_name
    type(powheg_matching_t) :: powheg
contains
    <POWHEG matching: powheg matching hook: TBP>
end type powheg_matching_hook_t

```

Init the hook. The init procedure will be called in `setup_process`, after everything is set up.

Additionally, we have to include `var_list` in order to retrieve the grid size in `xi` and `y`.

```

(POWHEG matching: powheg matching hook: TBP)≡
  procedure :: init => powheg_matching_hook_init

(POWHEG matching: sub interfaces)+≡
  module subroutine powheg_matching_hook_init (hook, var_list, &
    instance, pdf_data)
    class(powheg_matching_hook_t), intent(inout), target :: hook
    type(var_list_t), intent(in) :: var_list
    class(process_instance_t), intent(in), target :: instance
    type(pdf_data_t), intent(in), optional :: pdf_data
  end subroutine powheg_matching_hook_init

(POWHEG matching: procedures)+≡
  module subroutine powheg_matching_hook_init (hook, var_list, &
    instance, pdf_data)
    class(powheg_matching_hook_t), intent(inout), target :: hook
    type(var_list_t), intent(in) :: var_list
    class(process_instance_t), intent(in), target :: instance
    type(pdf_data_t), intent(in), optional :: pdf_data
    if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_hook_init")
    hook%process_name = instance%get_process_name ()
    call hook%powheg%init (var_list, hook%process_name)
    hook%powheg%qcd = instance%get_qcd ()
    call hook%powheg%connect (instance)
    hook%powheg%process_deps%lab_is_cm = &
      hook%powheg%process_instance%lab_is_cm (1)
    if (present(pdf_data)) then
      hook%powheg%process_deps%pdf_data = pdf_data
    end if
    call hook%powheg%prepare_for_events ()
  end subroutine powheg_matching_hook_init

```

We save the filled grid to file, such that it can be retrieved later on. The hook object will be deallocated when the instance gets deallocated.

```

(POWHEG matching: powheg matching hook: TBP)+≡
  procedure :: final => powheg_matching_hook_final

(POWHEG matching: sub interfaces)+≡
  module subroutine powheg_matching_hook_final (hook)
    class(powheg_matching_hook_t), intent(inout) :: hook
  end subroutine powheg_matching_hook_final

(POWHEG matching: procedures)+≡
  module subroutine powheg_matching_hook_final (hook)
    class(powheg_matching_hook_t), intent(inout) :: hook
    type(string_t) :: filename
    if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_hook_final")
    (POWHEG matching: powheg matching hook final: reduce)
    call hook%powheg%save_grids ()
  end subroutine powheg_matching_hook_final

```

(POWHEG matching: powheg matching hook final: reduce)≡

Reduce all grids to a single grid by using MPI_MAX on each element.

(MPI: POWHEG matching: powheg matching hook final: reduce)≡

call hook%powheg%grid%mpi_reduce (MPI_MAX)

This routine fills each bin of the POWHEG normalization grid $\{\tilde{\xi}, \tilde{y}\}$ such that

$$N(\{\tilde{\xi}, \tilde{y}\}) = \max_{\forall \xi, y \in \{\tilde{\xi}, \tilde{y}\}} \frac{\mathcal{R}(\xi, y) \mathcal{J}(\xi, y)}{\mathcal{B} U(\xi, y, \alpha_s^{\text{true}})} \quad (31.26)$$

where $\mathcal{R}(\xi, y)$ is the real cross section `sqme_real`, \mathcal{B} is the Born cross section `sqme_born`, \mathcal{J} is the Jacobian and U the upper bounding function `ubf`.

For each underlying Born f_b , there is a number of radiation regions. A radiation region `rr` may correspond to multiple α_r s. The phase space only depends upon the radiation region kinematics `rr` and not on the specific α_r . α_r can be picked in the set $\{\alpha_r | f_b, rr\}$ proportional to their R_{α_r} . For now, we simplify things though and just work with the α_r .

References:

- [1002.2581], Sec. 7.1
- Bijans Thesis, Sec. 3.3 and B.2

In cases where just the Born kinematic failed the cuts, \mathcal{B} was artificially set to zero. Unfortunately, we lost information about the value of `sqme_born` in these cases but we assume that the generator cuts applied for parton showering are weak cuts to avoid divergent phase space regions, thus \mathcal{B} is large and does not influence N so we can skip these phase space points.

A more appropriate way to solve this problem of Born zeroes is given by the real partition. With real partition, there are two possible cases if $\mathcal{B} = 0$: if the real phase space point belongs to the real singular, the real kinematic is Born-like and very likely also fails the cuts. If the real kinematic is not Born-like, it belongs to the real finite. In both cases, it is $\mathcal{R} = \mathcal{B} = 0$ and we can safely skip the phase space point.

In cases where just the real kinematic failed the cuts, \mathcal{R} was artificially set to zero and we have no way to recover it. We skip these phase space points too. If we apply the same cuts during integration and event generation, these points are not relevant. We also skip points where either matrix element is negative. If just one of both is negative, their ratio is negative and thus cannot possibly be relevant for the grid. If both are negative, we are in an unphysical region for the PDFs. We also need to correct all scale dependences of `sqme_born` and `sqme_real` from the process' scale to p_T as this is the scale of the entire Sudakov. This affects the PDFs and also α_s .

(POWHEG matching: powheg matching hook: TBP)+≡

procedure :: evaluate => powheg_matching_hook_evaluate

(POWHEG matching: sub interfaces)+≡

```
module subroutine powheg_matching_hook_evaluate (hook, instance)
  class(powheg_matching_hook_t), intent(inout) :: hook
  class(process_instance_t), intent(in), target :: instance
end subroutine powheg_matching_hook_evaluate
```


(POWHEG matching: procedures)+≡

```

module subroutine powheg_matching_hook_evaluate (hook, instance)
  class(powheg_matching_hook_t), intent(inout) :: hook
  class(process_instance_t), intent(in), target :: instance
  type(vector4_t), dimension(:), allocatable :: p_hard_born
  real(default), dimension(:), allocatable :: x
  real(default) :: kt2, xi, y, xi_max, onepy, onemy
  real(default), dimension(2) :: x_real
  real(default) :: sqme_born, sqme_real_x_jac
  real(default) :: muren_born, mufac_born, muren_real, mufac_real
  real(default) :: alpha_s_kt, alpha_s_muren_born, alpha_s_muren_real
  real(default) :: f_alr, norm, ubf
  real(default) :: r_xi, r_y
  real(double), dimension(-6:6) :: pdf_dbl
  real(default), dimension(2) :: pdf_born_mufac, pdf_born_kt, &
    pdf_real_mufac, pdf_real_kt
  real(double) :: x_dbl, q_dbl
  integer, dimension(2) :: flv_born, flv_real
  integer :: alr, i_phs, n_x, i_term_born, i_term_real, em
  integer :: alphas_power, i_uborn
  logical :: is_isr
  if (instance%get_active_component_type () == COMP_REAL_FIN) return
  associate (powheg => hook%powheg)
    i_term_born = powheg%process_deps%i_term_born
    allocate (p_hard_born (size (instance%get_p_hard (i_term_born))))
    p_hard_born = instance%get_p_hard (i_term_born)
    call powheg%update (p_hard_born)
    do alr = 1, powheg%process_deps%n_alr
      i_phs = powheg%process_deps%alr_to_i_phs (alr)
      i_term_real = powheg%process_deps%i_term_real(i_phs)
      select type (phs => instance%kin(i_term_real)%phs)
        type is (phs_fks_t)
          call phs%generator%get_radiation_variables (i_phs, xi, y)
        end select
      call powheg%update_sudakovs (alr, i_phs, y)
      kt2 = powheg%sudakov(alr)%s%kt2 (xi, y)
      if (kt2 >= powheg%settings%pt2_min) then
        select type (pcm => instance%pcm)
          type is (pcm_nlo_t)
            associate (reg_data => pcm%region_data)
              i_uborn = reg_data%regions(alr)%uborn_index
            end associate
          end select
          is_isr = instance%kin(i_term_real)%emitter <= instance%kin(i_term_real)%n_in
          select type (pcm_work => instance%pcm_work)
            class is (pcm_nlo_workspace_t)
              sqme_born = pcm_work%real_sub%sqme_born(i_uborn)
              sqme_real_x_jac = pcm_work%real_sub%sqme_real_arr(alr)
              sqme_real_x_jac = pcm_work%powheg_kinematic_factors_real &
                (sqme_real_x_jac, alr)
            end select
          if (sqme_born == 0 .or. sqme_real_x_jac == 0) then
            cycle
          end if
        end if
      end if
    end do
  end associate
end subroutine

```

```

associate (s => powheg%/sudakov(alr)%s)
  alpha_s_kt = s%alpha_s (kt2, use_correct=.true.)
  muren_born = instance%term(i_term_born)%get_ren_scale ()
  mufac_born = instance%term(i_term_born)%get_fac_scale ()
  muren_real = instance%term(i_term_real)%get_ren_scale ()
  mufac_real = instance%term(i_term_real)%get_fac_scale ()
  alpha_s_muren_born = s%alpha_s (muren_born**2, use_correct=.true., improve_nll=.fa
  alpha_s_muren_real = s%alpha_s (muren_real**2, use_correct=.true., improve_nll=.fa
  ubf = s%upper_bound_func (xi, y, alpha_s_kt)
end associate

!!! Correct all factors of alphas(muren) to alphas(kt).
alphas_power = powheg%/process_deps%alphas_power
sqme_born = (alpha_s_kt / alpha_s_muren_born)**alphas_power * sqme_born
sqme_real_x_jac = (alpha_s_kt / alpha_s_muren_real)**(alphas_power+1) * sqme_real_x_j

!!! Also correct the PDFs previously computed at mufac instead of kt
select type (pcm => instance%pcm)
type is (pcm_nlo_t)
  if (pcm%has_pdfs) then
    associate (reg_data => pcm%region_data)
      flv_born = reg_data%regions(alr)%flst_uborn%flst(1:2)
      where (flv_born == 21) flv_born = 0
      flv_real = reg_data%regions(alr)%flst_real%flst(1:2)
      where (flv_real == 21) flv_real = 0
    end associate
    associate (pdf_data => powheg%/process_deps%pdf_data, &
      x_born => powheg%/event_deps%x_born)
      if (.not. pdfs_valid(instance, pdf_data, alr, &
        sqrt(kt2), x_born, is_isr)) cycle
      do em = 1, 2
        x_dbl = x_born(em) ; q_dbl = mufac_born
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_born_mufac(em) = pdf_dbl(flv_born(em)) / x_born(em)
        x_dbl = x_born(em) ; q_dbl = sqrt(kt2)
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_born_kt(em) = pdf_dbl(flv_born(em)) / x_born(em)
      end do
      if (is_isr) then
        onepy = one + y; onemy = one - y
        x_real(1) = x_born(1) * sqrt ((two - xi * onemy) / (two - xi * onepy))
        x_real(2) = x_born(2) * sqrt ((two - xi * onemy) / (two - xi * onepy))
        x_real = x_real / sqrt (one - xi)
      else
        x_real = x_born
      end if
      do em = 1, 2
        x_dbl = x_real(em) ; q_dbl = mufac_real
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_real_mufac(em) = pdf_dbl(flv_real(em)) / x_real(em)
        x_dbl = x_real(em) ; q_dbl = sqrt(kt2)
        call pdf_data%evolve(x_dbl, q_dbl, pdf_dbl)
        pdf_real_kt(em) = pdf_dbl(flv_real(em)) / x_real(em)

```

```

        end do
        sqme_born = pdf_born_kt(1) * pdf_born_kt(2) / &
            (pdf_born_mufac(1) * pdf_born_mufac(2)) * sqme_born
        sqme_real_x_jac = pdf_real_kt(1) * pdf_real_kt(2) / &
            (pdf_real_mufac(1) * pdf_real_mufac(2)) * sqme_real_x_jac
        end associate
    end if
end select

if (sqme_born <= 0 .or. sqme_real_x_jac <= 0) then
    cycle
end if

norm = sqme_real_x_jac / (sqme_born * ubf)
f_alr = (one * alr) / powheg%process_deps%n_alr - tiny_07

r_y = abs(y)
select type (pcm_work => instance%pcm_work)
class is (pcm_nlo_workspace_t)
    xi_max = min(pcm_work%get_xi_max (alr), 1 - tiny_07)
end select
if (xi > xi_max) then
    r_xi = 1
else
    r_xi = log(1 - xi) / log(1 - xi_max)
end if
call powheg%grid%update_maxima ([r_xi, r_y, f_alr], norm)
end if
end do
end associate
contains
<POWHEG matching: powheg matching hook: evaluate: contained>
end subroutine powheg_matching_hook_evaluate

```

In some phase space point, the quark PDF may vanish although the gluon PDF does not. This may lead to very large ratios \mathcal{R}/\mathcal{B} which may spoil the reweighting performance of the POWHEG grid. Excluding these values when filling the grid is a minor approximation with a huge performance gain. The PDF veto we perform is independent on the actual emitter to not artificially favor specific ALRs.

```

<POWHEG matching: powheg matching hook: evaluate: contained>≡
function pdfs_valid (instance, pdf_data, alr, q, x, is_isr) result (valid)
    logical :: valid
    class(process_instance_t), intent(in), target :: instance
    type(pdf_data_t), intent(inout) :: pdf_data
    integer, intent(in) :: alr
    real(default), intent(in) :: q
    real(default), dimension(2), intent(in) :: x
    real(double) :: q_dbl
    real(double), dimension(2) :: x_dbl
    logical, intent(in) :: is_isr
    real(default) :: sum_pdf_q
    real(default), dimension(-6:6) :: pdf

```

```

real(double), dimension(-6:6) :: pdf_dbl
integer :: flv_born_em, em, i_q
logical :: warned_once = .false.
valid = .true.
if (is_isr) then
  if (q**2 < two .or. any(x > 0.9_default)) then
    valid = .false.
    return
  end if
  x_dbl = x
  q_dbl = q
  do em = 1, 2
    call pdf_data%evolve(x_dbl(em), q_dbl, pdf_dbl)
    pdf = pdf_dbl / x(em)
    select type (pcm => instance%pcm)
    type is (pcm_nlo_t)
      flv_born_em = pcm%region_data%regions(alr)%flst_uborn%flst(em)
    end select
    if (is_gluon(flv_born_em)) then
      sum_pdf_q = 0
      do i_q = 1, 6
        sum_pdf_q = sum_pdf_q + pdf(-i_q) + pdf(i_q)
      end do
      if (sum_pdf_q * x(em) * (1-x(em)) > 30._default * pdf(0)) then
        valid = .false.
        return
      end if
    elseif (is_quark(flv_born_em)) then
      if (pdf(0) * x(em) * (1-x(em)) > 30._default * pdf(flv_born_em)) then
        valid = .false.
        return
      end if
    else
      if (.not. warned_once) then
        call msg_warning ("powheg_matching_hook_evaluate: unexpected emitter flavor")
        warned_once = .true.
      end if
    end if
  end do
end if
end function pdfs_valid

```

31.4.6 Unit tests

Test module, followed by the corresponding implementation module.

`<powheg_matching_ut.f90>`≡

<File header>

```

module powheg_matching_ut
  use unit_tests
  use powheg_matching_ut

```

```

    <Standard module head>

    <POWHEG matching: public test>

contains

    <POWHEG matching: test driver>

end module powheg_matching_ut

<powheg_matching_uti.f90>≡
    <File header>

module powheg_matching_uti

    <Use kinds>
    <Use strings>
    use constants, only: zero, one
    use lorentz
    use physics_defs, only: LAMBDA_QCD_REF
    use sm_qcd
    use subevents, only: PRT_INCOMING, PRT_OUTGOING
    use model_data
    use particles
    use rng_base
    use variables
    use shower_base
    use shower_core

    use powheg_matching

    use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <POWHEG matching: test declarations>

contains

    <POWHEG matching: tests>

end module powheg_matching_uti
API: driver for the unit tests below.
<POWHEG matching: public test>≡
    public :: powheg_test
<POWHEG matching: test driver>≡
    subroutine powheg_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <POWHEG matching: execute tests>
    end subroutine powheg_test

```

Initialization

There are no Powheg unit tests so far.

Compare generated emission with Sudakov form factor

This is a nontrivial test of the generation algorithm and should be independent of the used upper bounding function (as long as all singularities are included).

It runs for an extensive amount of time generating a file `sudakov.dat` containing a histogram for the Sudakov factor in bins of the radiation's transverse momentum p_T^2 .

So far, it is only designed to work for lepton collisions without beam spectra and cuts. In its current state however, it fills the histogram with either 1 or NaN as the `p_hard` received in `term_instance_evaluate_interaction` is identically zero.

```
<POWHEG matching: powheg matching: TBP>+≡
  procedure :: test_sudakov => powheg_test_sudakov

<POWHEG matching: sub interfaces>+≡
  module subroutine powheg_test_sudakov (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
  end subroutine powheg_test_sudakov

<POWHEG matching: procedures>+≡
  module subroutine powheg_test_sudakov (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    integer :: n_calls1, n_calls2
    integer, parameter :: n_bins = 20
    real(default) :: sqme_real_x_jac, sqme_born
    type(vector4_t), dimension(:), allocatable :: p_born
    real(default), dimension(3) :: random
    real(default) :: xi, y
    integer :: i_call, i_bin, alr, emitter, i_phs
    real(default) :: alpha_s, kT2, weight
    real(default) :: pt2_min, s, random_jacobian
    real(default), dimension(n_bins) :: histo1, histo2, histo1sq, histo2sq
    real(default), dimension(n_bins) :: tmp
    integer :: i_strip, n_in_strip, n_strips
    real(default), dimension(n_bins) :: average, average_sq, error
    real(default), dimension(n_bins) :: &
      sudakov_0, sudakov_p, sudakov_m, rel_error
    integer :: u

    p_born = powheg%event_deps%p_born_lab%get_momenta (1)
    s = powheg%event_deps%s_hat
    pt2_min = powheg%settings%pt2_min
    n_calls1 = 100000; n_calls2 = 1000000
    histo1 = zero; histo2 = zero; histo1sq = zero; histo2sq = zero
    n_strips = 10

    call compute_integrals ()
    call generate_emissions ()
    call write_to_screen_and_file ()

contains
```

<POWHEG matching: powheg test sudakov: procedures>

```
end subroutine powheg_test_sudakov
```

This determines the binning of the Sudakov histogram. Linear and logarithmic binning are available.

<POWHEG matching: powheg test sudakov: procedures>≡

```
pure function binning (i) result (pt2)
  real(default) :: pt2
  integer, intent(in) :: i
  !pt2 = pt2_min + (s-pt2_min) * (i-1) / (n_bins-1)
  pt2 = pt2_min * exp (log (s / pt2_min) * (i-1) / (n_bins-1))
end function
```

<POWHEG matching: powheg test sudakov: procedures>+≡

```
subroutine compute_integrals ()
  write (msg_buffer, "(A)") "POWHEG: test_sudakov: Computing integrals"
  call msg_message ()
  select type (pcm_work => powheg%process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    associate (fks => powheg%phs_fks_generator)
      do i_call = 1, n_calls1
        do alr = 1, powheg%process_deps%n_alr
          call powheg%rng%generate (random)
          select type (pcm => powheg%process_instance%pcm)
          type is (pcm_nlo_t)
            emitter = pcm%region_data%get_emitter (alr)
            i_phs = powheg%process_deps%alr_to_i_phs(alr)
          end select
          !!! The sudakov test works only with lepton collisions without beam spectra
          !!! so we can identify the cms and lab momenta.
          powheg%event_deps%p_real_lab = powheg%event_deps%p_real_cms
          call powheg%copy_momenta (i_phs)
          call fks%get_radiation_variables (i_phs, xi, y)
          kT2 = powheg%sudakov(alr)%s%kt2(xi, y)
          if (kT2 >= pt2_min .and. xi < one - tiny_07) then
            alpha_s = get_alpha_s (powheg%qcd, kT2)
            sqme_born = powheg%event_deps%sqme_born(alr)
            sqme_real_x_jac = powheg%compute_sqme_real (alr, sqrt(kT2))
            random_jacobian = pcm_work%real_kinematics%jac_rand (emitter)
            weight = sqme_real_x_jac * random_jacobian / sqme_born
            do i_bin = 1, n_bins
              if (kT2 > binning(i_bin)) then
                histo1(i_bin) = histo1(i_bin) + weight
                histo1sq(i_bin) = histo1sq(i_bin) + weight**2
              end if
            end do
          end if
        end do
      end do
      ! Do not cycle since there is a Heaviside in the exponent
    end do
  call msg_show_progress (i_call, n_calls1)
end do
```

```

        end associate
    end select
    average = histo1 / n_calls1
    average_sq = histo1sq / n_calls1
    error = sqrt ((average_sq - average**2) / n_calls1)
    sudakov_0 = exp(-average)
    sudakov_p = exp(-(average + error))
    sudakov_m = exp(-(average - error))
    rel_error = (sudakov_m - sudakov_p) / (2 * sudakov_0) * 100
end subroutine compute_integrals

```

(*POWHEG matching: powheg test sudakov: procedures*)+=

```

subroutine generate_emissions ()
    write (msg_buffer, "(A)") "POWHEG: test_sudakov: Generating emissions"
    call msg_message ()
    do i_strip = 1, n_strips
        tmp = 0
        n_in_strip = n_calls2 / n_strips
        do i_call = 1, n_in_strip
            if (signal_is_pending ()) return
            call powheg%generate_emission (pt2_generated = kT2)
            do i_bin = 1, n_bins
                if (kT2 > binning(i_bin)) then
                    tmp(i_bin) = tmp(i_bin) + 1
                end if
            end do
        end do
        tmp = one - (one * tmp) / n_in_strip
        histo2 = histo2 + tmp
        histo2sq = histo2sq + tmp**2
        call msg_show_progress (i_strip, n_strips)
    end do
    average = histo2 / n_strips
    average_sq = histo2sq / n_strips
    error = sqrt ((average_sq - average**2) / n_strips)
end subroutine generate_emissions

```

(*POWHEG matching: powheg test sudakov: procedures*)+=

```

subroutine write_to_screen_and_file ()
    u = free_unit ()
    open (file='sudakov.dat', unit=u, action='write')
    print *, 'exp(-Integrated R/B)-distribution: '
    print *, 'pT2  sudakov+  sudakov_0  sudakov_-  rel_err[%]: '
    do i_bin = 1, n_bins
        print *, binning(i_bin), &
            sudakov_p(i_bin), sudakov_0(i_bin), sudakov_m(i_bin), &
            rel_error(i_bin)
        write (u, "(6(" // FMT_16 // ",2X))") binning(i_bin), &
            sudakov_p(i_bin), sudakov_0(i_bin), sudakov_m(i_bin), &
            average(i_bin), error(i_bin)
    end do
    close (u)
    print *, '*****'

```



```
print *, 'Noemission probability: '  
do i_bin = 1, n_bins  
  print *, binning (i_bin), average (i_bin), error(i_bin)  
end do  
end subroutine write_to_screen_and_file
```

Chapter 32

Event Implementation

With a process object and the associated methods at hand, we can generate events for elementary processes and, by subsequent transformation, for complete physical processes.

We have the following modules:

event_transforms Abstract base type for transforming a physical process with process instance and included evaluators, etc., into a new object. The following modules extend this base type.

resonance_insertion Insert a resonance history into an event record, based on kinematical and matrix-element information.

recoil_kinematics Common kinematics routines for the ISR and EPA handlers.

isr_photon_handler Transform collinear kinematics, as it results from applying ISR radiation, to non-collinear kinematics with a reasonable transverse-momentum distribution of the radiated photons, and also of the recoiling partonic event.

epa_beam_handler For photon-initiated processes where the effective photon approximation is used in integration, to add in beam-particle recoil. Analogous to the ISR handler.

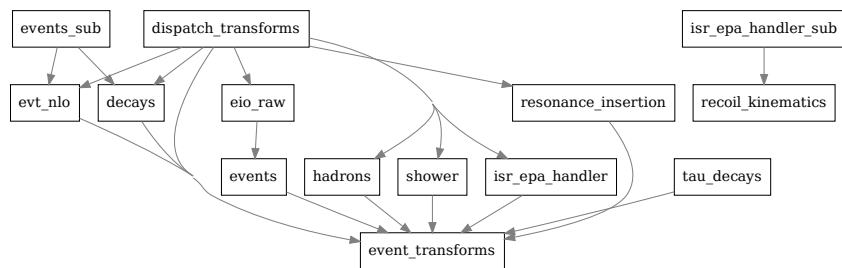


Figure 32.1: Module dependencies in `src/transforms`.

decays Combine the elementary process with elementary decay processes and thus transform the elementary event into a decayed event, still at the parton level.

showers Create QED/QCD showers out of the partons that are emitted by elementary processes. This should be interleaved with showering of radiated particles (structure functions) and multiple interactions.

hadrons (not implemented yet) Apply hadronization to the partonic events, interleaved with hadron decays. (The current setup relies on hadronizing partonic events externally.)

tau_decays (not implemented yet) Let τ leptons decay taking full spin correlations into account.

evt_nlo Handler for fixed-order NLO events.

events Combine all pieces to generate full events.

eio_raw Raw I/O for complete events.

32.1 Abstract Event Transforms

```

(event_transforms.f90)≡
  <File header>

  module event_transforms

    <Use kinds>
    <Use strings>
    use quantum_numbers, only: quantum_numbers_t
    use interactions
    use particles
    use model_data
    use rng_base
    use process, only: process_t
    use instances, only: process_instance_t
    use process_stacks

    <Standard module head>

    <Event transforms: public>

    <Event transforms: types>

    <Event transforms: interfaces>

    interface
    <Event transforms: sub interfaces>
    end interface

  end module event_transforms

```

```

<event_transforms_sub.f90>≡
  <File header>

  submodule (event_transforms) event_transforms_s

    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use subevents

    implicit none

  contains

  <Event transforms: procedures>

  end submodule event_transforms_s

```

32.1.1 Abstract base type

Essentially, all methods are abstract, but some get minimal base versions. We know that there will be a random-number generator at top level, and that we will relate to an elementary process.

The model is stored separately. It may contain modified settings that differ from the model instance stored in the process object.

Each event transform contains a particle set that it can fill for further use. There is a flag that indicates this.

We will collect event transforms in a list, therefore we include `previous` and `next` pointers.

```

<Event transforms: public>≡
  public :: evt_t

<Event transforms: types>≡
  type, abstract :: evt_t
    type(process_t), pointer :: process => null ()
    type(process_instance_t), pointer :: process_instance => null ()
    class(model_data_t), pointer :: model => null ()
    class(rng_t), allocatable :: rng
    integer :: rejection_count = 0
    logical :: particle_set_exists = .false.
    type(particle_set_t) :: particle_set
    class(evt_t), pointer :: previous => null ()
    class(evt_t), pointer :: next => null ()
    logical :: only_weighted_events = .false.
  contains
  <Event transforms: evt: TBP>
  end type evt_t

```

Finalizer. In any case, we finalize the r.n.g. The process instance is a pointer and should not be finalized here.

```

<Event transforms: evt: TBP>≡

```

```

    procedure :: final => evt_final
    procedure :: base_final => evt_final
  <Event transforms: sub interfaces>≡
    module subroutine evt_final (evt)
      class(evt_t), intent(inout) :: evt
    end subroutine evt_final
  <Event transforms: procedures>≡
    module subroutine evt_final (evt)
      class(evt_t), intent(inout) :: evt
      if (allocated (evt%rng)) call evt%rng%final ()
      if (evt%particle_set_exists) &
        call evt%particle_set%final ()
    end subroutine evt_final

```

Print out the type of the evt.

```

  <Event transforms: evt: TBP>+≡
    procedure (evt_write_name), deferred :: write_name
  <Event transforms: interfaces>≡
    abstract interface
      subroutine evt_write_name (evt, unit)
        import
        class(evt_t), intent(in) :: evt
        integer, intent(in), optional :: unit
      end subroutine evt_write_name
    end interface
  <Event transforms: evt: TBP>+≡
    procedure (evt_write), deferred :: write
  <Event transforms: interfaces>+≡
    abstract interface
      subroutine evt_write (evt, unit, verbose, more_verbose, testflag)
        import
        class(evt_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
      end subroutine evt_write
    end interface

```

Output. We can print r.n.g. info.

```

  <Event transforms: evt: TBP>+≡
    procedure :: base_write => evt_base_write
  <Event transforms: sub interfaces>+≡
    module subroutine evt_base_write (evt, unit, testflag, show_set)
      class(evt_t), intent(in) :: evt
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: testflag, show_set
    end subroutine evt_base_write

```

<Event transforms: procedures>+≡

```

module subroutine evt_base_write (evt, unit, testflag, show_set)
  class(evt_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag, show_set
  integer :: u
  logical :: show
  u = given_output_unit (unit)
  show = .true.; if (present (show_set)) show = show_set
  if (associated (evt%process)) then
    write (u, "(3x,A,A,A)") "Associated process: '", &
      char (evt%process%get_id ()), "'"
  end if
  if (allocated (evt%rng)) then
    call evt%rng%write (u, 1)
    write (u, "(3x,A,I0)") "Number of tries = ", evt%rejection_count
  end if
  if (show) then
    if (evt%particle_set_exists) then
      call write_separator (u)
      call evt%particle_set%write (u, testflag = testflag)
    end if
  end if
end subroutine evt_base_write

```

Connect the transform with a process instance (and thus with the associated process). Use this to allocate the master random-number generator.

This is not an initializer; we may initialize the transform by implementation-specific methods.

<Event transforms: evt: TBP>+≡

```

procedure :: connect => evt_connect
procedure :: base_connect => evt_connect

```

<Event transforms: sub interfaces>+≡

```

module subroutine evt_connect (evt, process_instance, model, process_stack)
  class(evt_t), intent(inout), target :: evt
  type(process_instance_t), intent(in), target :: process_instance
  class(model_data_t), intent(in), target :: model
  type(process_stack_t), intent(in), optional :: process_stack
end subroutine evt_connect

```

<Event transforms: procedures>+≡

```

module subroutine evt_connect (evt, process_instance, model, process_stack)
  class(evt_t), intent(inout), target :: evt
  type(process_instance_t), intent(in), target :: process_instance
  class(model_data_t), intent(in), target :: model
  type(process_stack_t), intent(in), optional :: process_stack
  evt%process => process_instance%process
  evt%process_instance => process_instance
  evt%model => model
  call evt%process%make_rng (evt%rng)
end subroutine evt_connect

```

Reset internal state.

```

(Event transforms: evt: TBP)+≡
  procedure :: reset => evt_reset
  procedure :: base_reset => evt_reset

(Event transforms: sub interfaces)+≡
  module subroutine evt_reset (evt)
    class(evt_t), intent(inout) :: evt
  end subroutine evt_reset

(Event transforms: procedures)+≡
  module subroutine evt_reset (evt)
    class(evt_t), intent(inout) :: evt
    evt%rejection_count = 0
    call evt%particle_set%final ()
    evt%particle_set_exists = .false.
  end subroutine evt_reset

```

Prepare for a new event: reset internal state, if necessary. We provide MCI and term index of the parent process.

```

(Event transforms: evt: TBP)+≡
  procedure (evt_prepare_new_event), deferred :: prepare_new_event

(Event transforms: interfaces)+≡
  interface
    subroutine evt_prepare_new_event (evt, i_mci, i_term)
      import
      class(evt_t), intent(inout) :: evt
      integer, intent(in) :: i_mci, i_term
    end subroutine evt_prepare_new_event
  end interface

```

Generate a weighted event, using a valid initiator event in the process instance, and the random-number generator. The returned event probability should be a number between zero and one that we can use for rejection.

```

(Event transforms: evt: TBP)+≡
  procedure (evt_generate_weighted), deferred :: generate_weighted

(Event transforms: interfaces)+≡
  abstract interface
    subroutine evt_generate_weighted (evt, probability)
      import
      class(evt_t), intent(inout) :: evt
      real(default), intent(inout) :: probability
    end subroutine evt_generate_weighted
  end interface

```

The unweighted event generation routine is actually implemented. It uses the random-number generator for simple rejection. Of course, the implementation may override this and implement a different way of generating an unweighted event.

```

(Event transforms: evt: TBP)+≡
  procedure :: generate_unweighted => evt_generate_unweighted
  procedure :: base_generate_unweighted => evt_generate_unweighted

```

```

(Event transforms: sub interfaces)+≡
  module subroutine evt_generate_unweighted (evt)
    class(evt_t), intent(inout) :: evt
  end subroutine evt_generate_unweighted

```

```

(Event transforms: procedures)+≡
  module subroutine evt_generate_unweighted (evt)
    class(evt_t), intent(inout) :: evt
    real(default) :: p, x
    evt%rejection_count = 0
    REJECTION: do
      evt%rejection_count = evt%rejection_count + 1
      call evt%generate_weighted (p)
      if (signal_is_pending ()) return
      call evt%rng%generate (x)
      if (x < p) exit REJECTION
    end do REJECTION
  end subroutine evt_generate_unweighted

```

Make a particle set. This should take the most recent evaluator (or whatever stores the event), factorize the density matrix if necessary, and store as a particle set.

If applicable, the factorization should make use of the `factorization_mode` and `keep_correlations` settings.

The values `r`, if set, should control the factorization in more detail, e.g., bypassing the random-number generator.

```

(Event transforms: evt: TBP)+≡
  procedure (evt_make_particle_set), deferred :: make_particle_set

```

```

(Event transforms: interfaces)+≡
  interface
    subroutine evt_make_particle_set &
      (evt, factorization_mode, keep_correlations, r)
    import
    class(evt_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_make_particle_set
  end interface

```

Copy an existing particle set into the event record. This bypasses all methods to evaluate the internal state, but may be sufficient for further processing.

```

(Event transforms: evt: TBP)+≡
  procedure :: set_particle_set => evt_set_particle_set

```

```

(Event transforms: sub interfaces)+≡
  module subroutine evt_set_particle_set (evt, particle_set, i_mci, i_term)
    class(evt_t), intent(inout) :: evt
    type(particle_set_t), intent(in) :: particle_set
    integer, intent(in) :: i_term, i_mci
  end subroutine evt_set_particle_set

```


(Event transforms: procedures)+≡

```

module subroutine evt_set_particle_set (evt, particle_set, i_mci, i_term)
  class(evt_t), intent(inout) :: evt
  type(particle_set_t), intent(in) :: particle_set
  integer, intent(in) :: i_term, i_mci
  call evt%prepare_new_event (i_mci, i_term)
  evt%particle_set = particle_set
  evt%particle_set_exists = .true.
end subroutine evt_set_particle_set

```

This procedure can help in the previous task, if the particles are available in the form of an interaction object. We need two interactions, one with color summed over, the `int_matrix`, and one with the probability distributed among flows, the `int_flows`.

We use the two values from the random number generator saved in `r` for factorizing the state. For testing purposes, we can provide those numbers explicitly.

The optional `qn_select` allows to limit the number of quantum numbers to choose from when factorizing. If only a single set of quantum numbers is given, it effectively dictates the quantum numbers chosen for the event.

(Event transforms: evt: TBP)+≡

```

procedure :: factorize_interactions => evt_factorize_interactions

```

(Event transforms: sub interfaces)+≡

```

module subroutine evt_factorize_interactions &
  (evt, int_matrix, int_flows, factorization_mode, &
   keep_correlations, r, qn_select)
  class(evt_t), intent(inout) :: evt
  type(interaction_t), intent(in), target :: int_matrix, int_flows
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
  type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
end subroutine evt_factorize_interactions

```

(Event transforms: procedures)+≡

```

module subroutine evt_factorize_interactions &
  (evt, int_matrix, int_flows, factorization_mode, &
   keep_correlations, r, qn_select)
  class(evt_t), intent(inout) :: evt
  type(interaction_t), intent(in), target :: int_matrix, int_flows
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
  type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
  real(default), dimension(2) :: x
  if (present (r)) then
    if (size (r) == 2) then
      x = r
    else
      call msg_bug ("event factorization: size of r array must be 2")
    end if
  else
    call evt%rng%generate (x)
  end if
end subroutine evt_factorize_interactions

```

```

end if
call evt%particle_set%init (evt%particle_set_exists, &
    int_matrix, int_flows, factorization_mode, x, &
    keep_correlations, keep_virtual=.true., qn_select = qn_select)
evt%particle_set_exists = .true.
end subroutine evt_factorize_interactions

<Event transforms: public>+≡
public :: make_factorized_particle_set

<Event transforms: sub interfaces>+≡
module subroutine make_factorized_particle_set (evt, factorization_mode, &
    keep_correlations, r, ii_term, qn_select)
class(evt_t), intent(inout) :: evt
integer, intent(in) :: factorization_mode
logical, intent(in) :: keep_correlations
real(default), dimension(:), intent(in), optional :: r
integer, intent(in), optional :: ii_term
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
end subroutine make_factorized_particle_set

<Event transforms: procedures>+≡
module subroutine make_factorized_particle_set (evt, factorization_mode, &
    keep_correlations, r, ii_term, qn_select)
class(evt_t), intent(inout) :: evt
integer, intent(in) :: factorization_mode
logical, intent(in) :: keep_correlations
real(default), dimension(:), intent(in), optional :: r
integer, intent(in), optional :: ii_term
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
integer :: i_term
type(interaction_t), pointer :: int_matrix, int_flows
if (evt%process_instance%is_complete_event ()) then
    if (present (ii_term)) then
        i_term = ii_term
    else
        i_term = evt%process_instance%select_i_term ()
    end if
    int_matrix => evt%process_instance%get_matrix_int_ptr (i_term)
    int_flows => evt%process_instance%get_flows_int_ptr (i_term)
    call evt%factorize_interactions (int_matrix, int_flows, &
        factorization_mode, keep_correlations, r, qn_select)
    call evt%tag_incoming ()
else
    call msg_bug ("Event factorization: event is incomplete")
end if
end subroutine make_factorized_particle_set

```

Mark the incoming particles as incoming in the particle set. This is necessary because in the interaction objects they are usually marked as virtual.

In the inquiry functions we set the term index to one; the indices of beams and incoming particles should be identical for all process terms.

We use the initial elementary process for obtaining the indices. Thus, we implicitly assume that the beam and incoming indices stay the same across event

transforms. If this is not true for a transform (say, MPI), it should override this method.

```

<Event transforms: evt: TBP>+≡
    procedure :: tag_incoming => evt_tag_incoming

<Event transforms: sub interfaces>+≡
    module subroutine evt_tag_incoming (evt)
        class(evt_t), intent(inout) :: evt
    end subroutine evt_tag_incoming

<Event transforms: procedures>+≡
    module subroutine evt_tag_incoming (evt)
        class(evt_t), intent(inout) :: evt
        integer :: i_term, n_in
        integer, dimension(:), allocatable :: beam_index, in_index
        n_in = evt%process%get_n_in ()
        i_term = 1
        allocate (beam_index (n_in))
        call evt%process_instance%get_beam_index (i_term, beam_index)
        call evt%particle_set%reset_status (beam_index, PRT_BEAM)
        allocate (in_index (n_in))
        call evt%process_instance%get_in_index (i_term, in_index)
        call evt%particle_set%reset_status (in_index, PRT_INCOMING)
    end subroutine evt_tag_incoming

```

32.1.2 Implementation: Trivial transform

This transform contains just a pointer to process and process instance. The **generate** methods do nothing.

```

<Event transforms: public>+≡
    public :: evt_trivial_t

<Event transforms: types>+≡
    type, extends (evt_t) :: evt_trivial_t
    contains
    <Event transforms: evt trivial: TBP>
    end type evt_trivial_t

<Event transforms: evt trivial: TBP>≡
    procedure :: write_name => evt_trivial_write_name

<Event transforms: sub interfaces>+≡
    module subroutine evt_trivial_write_name (evt, unit)
        class(evt_trivial_t), intent(in) :: evt
        integer, intent(in), optional :: unit
    end subroutine evt_trivial_write_name

<Event transforms: procedures>+≡
    module subroutine evt_trivial_write_name (evt, unit)
        class(evt_trivial_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: trivial (hard process)"
    end subroutine evt_trivial_write_name

```

```
end subroutine evt_trivial_write_name
```

The finalizer is trivial. Some output:

```
<Event transforms: evt trivial: TBP>+≡
  procedure :: write => evt_trivial_write

<Event transforms: sub interfaces>+≡
  module subroutine evt_trivial_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_trivial_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
  end subroutine evt_trivial_write

<Event transforms: procedures>+≡
  module subroutine evt_trivial_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_trivial_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag)
    !!! More readable but wider output; in line with evt_resonance_write
    !   if (verbose .and. evt%particle_set_exists) then
    !     call evt%particle_set%write &
    !       (u, summary = .true., compressed = .true., testflag = testflag)
    !     call write_separator (u)
    !   end if
  end subroutine evt_trivial_write
```

Nothing to do here:

```
<Event transforms: evt trivial: TBP>+≡
  procedure :: prepare_new_event => evt_trivial_prepare_new_event

<Event transforms: sub interfaces>+≡
  module subroutine evt_trivial_prepare_new_event (evt, i_mci, i_term)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_trivial_prepare_new_event

<Event transforms: procedures>+≡
  module subroutine evt_trivial_prepare_new_event (evt, i_mci, i_term)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_trivial_prepare_new_event
```

The weighted generator is, surprisingly, trivial.

```
<Event transforms: evt trivial: TBP>+≡
  procedure :: generate_weighted => evt_trivial_generate_weighted
```

```

<Event transforms: sub interfaces>+≡
  module subroutine evt_trivial_generate_weighted (evt, probability)
    class(evt_trivial_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
  end subroutine evt_trivial_generate_weighted

```

```

<Event transforms: procedures>+≡
  module subroutine evt_trivial_generate_weighted (evt, probability)
    class(evt_trivial_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    probability = 1
  end subroutine evt_trivial_generate_weighted

```

This routine makes a particle set, using the associated process instance as-is. Note that it is a potential risk to tolerate a non-existent particle set at this point. We should remove it once the flavors are determined correctly in all cases. It is currently necessary if we are keeping failed events `?keep_failed_events = .true.` For these events, we do not compute the matrix elements, so the factorization fails trying to determine the quantum numbers. Additionally, it is necessary for the trivial event transformation preceding the event transformations required for POWHEG matching.

```

<Event transforms: evt trivial: TBP>+≡
  procedure :: make_particle_set => evt_trivial_make_particle_set

```

```

<Event transforms: sub interfaces>+≡
  module subroutine evt_trivial_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_trivial_make_particle_set

```

```

<Event transforms: procedures>+≡
  module subroutine evt_trivial_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    call make_factorized_particle_set (evt, factorization_mode, &
      keep_correlations, r)
    evt%particle_set_exists = .true.
  end subroutine evt_trivial_make_particle_set

```

32.1.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<event_transforms_ut.f90>≡
  <File header>

```

```

  module event_transforms_ut
    use unit_tests

```

```

    use event_transforms_uti

    <Standard module head>

    <Event transforms: public test>

contains

    <Event transforms: test driver>

end module event_transforms_ut
(event_transforms_uti.f90)≡
    <File header>

module event_transforms_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use sm_qcd
    use models
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions, only: reset_interaction_counter
    use process_libraries
    use rng_base
    use mci_base
    use mci_midpoint
    use phs_base
    use phs_single
    use prc_core
    use prc_test, only: prc_test_create_library

    use process, only: process_t
    use instances, only: process_instance_t

    use event_transforms

    use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <Event transforms: test declarations>

contains

    <Event transforms: tests>

    <Event transforms: test auxiliary>

end module event_transforms_uti

```

API: driver for the unit tests below.

```

<Event transforms: public test>≡
    public :: event_transforms_test

<Event transforms: test driver>≡
    subroutine event_transforms_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Event transforms: execute tests>
    end subroutine event_transforms_test

```

Test trivial event transform

The trivial transform, as an instance of the abstract transform, does nothing but to trigger event generation for an elementary process.

```

<Event transforms: execute tests>≡
    call test (event_transforms_1, "event_transforms_1", &
        "trivial event transform", &
        u, results)

<Event transforms: test declarations>≡
    public :: event_transforms_1

<Event transforms: tests>≡
    subroutine event_transforms_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_library_t), target :: lib
        type(string_t) :: libname, procname1
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(process_t), allocatable, target :: process
        type(process_instance_t), allocatable, target :: process_instance
        class(evt_t), allocatable :: evt
        integer :: factorization_mode
        logical :: keep_correlations

        write (u, "(A)")  "* Test output: event_transforms_1"
        write (u, "(A)")  "*   Purpose: handle trivial transform"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment and parent process"
        write (u, "(A)")

        call os_data%init ()

        libname = "event_transforms_1_lib"
        procname1 = "event_transforms_1_p"

        call prc_test_create_library (libname, lib, &
            scattering = .true., procname1 = procname1)
        call reset_interaction_counter ()

        call model%init_test ()
    end subroutine event_transforms_1

```

```

allocate (process)
call process%init (procname1, lib, os_data, model)
call process%setup_test_cores ()

allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_test_midpoint)
call process%setup_terms ()

allocate (process_instance)
call process_instance%init (process)
call process_instance%integrate (1, n_it=1, n_calls=100)
call process_instance%final_integration (1)
call process_instance%final ()
deallocate (process_instance)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")  "* Initialize trivial event transform"
write (u, "(A)")

allocate (evt_trivial_t :: evt)
call evt%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")  "* Generate event and subsequent transform"
write (u, "(A)")

call process_instance%generate_unweighted_event (1)
call process_instance%evaluate_event_data ()

call evt%prepare_new_event (1, 1)
call evt%generate_unweighted ()

call write_separator (u, 2)
call evt%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Obtain particle set"
write (u, "(A)")

factorization_mode = FM_IGNORE_HELICITY
keep_correlations = .false.

call evt%make_particle_set (factorization_mode, keep_correlations)

```



```

call write_separator (u, 2)
call evt%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt%final ()
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Test output end: event_transforms_1"

end subroutine event_transforms_1

```

MCI record prepared for midpoint integrator.

```

<Event transforms: test auxiliary>≡
subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
  use variables, only: var_list_t
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

32.2 Hadronization interface

```

<hadrons.f90>≡
<File header>

module hadrons

  <Use kinds with double>
  <Use strings>
  use event_transforms
  use lorentz
  use model_data
  use models
  use particles
  use physics_defs
  use process, only: process_t
  use instances, only: process_instance_t
  use process_stacks
  use whizard_lha
  use pythia8
  use rng_base, only: rng_t
  use shower_base
  use shower_pythia6
  use sm_qcd

```

```

        use variables

        <Standard module head>

        <Hadrons: public>

        <Hadrons: parameters>

        <Hadrons: types>

        <Hadrons: interfaces>

        interface
        <Hadrons: sub interfaces>
        end interface

    end module hadrons

    <hadrons_sub.f90>≡
    <File header>

    submodule (hadrons) hadrons_s

    <Use debug>
        use constants
        use diagnostics
        use format_utils, only: write_separator
        use helicities
        use hep_common
        use io_units
        use numeric_utils, only: vanishes
        use subevents

        implicit none

    contains

    <Hadrons: procedures>

    end submodule hadrons_s

```

32.2.1 Hadronization implementations

```

    <Hadrons: public>≡
        public :: HADRONS_UNDEFINED, HADRONS_WHIZARD, HADRONS_PYTHIA6, HADRONS_PYTHIA8

    <Hadrons: parameters>≡
        integer, parameter :: HADRONS_UNDEFINED = 0
        integer, parameter :: HADRONS_WHIZARD = 1
        integer, parameter :: HADRONS_PYTHIA6 = 2
        integer, parameter :: HADRONS_PYTHIA8 = 3

    A dictionary
    <Hadrons: public>+≡

```

```

    public :: hadrons_method
<Hadrons: interfaces>≡
    interface hadrons_method
        module procedure hadrons_method_of_string
        module procedure hadrons_method_to_string
    end interface
<Hadrons: sub interfaces>≡
    elemental module function hadrons_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
    end function hadrons_method_of_string
    elemental module function hadrons_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
    end function hadrons_method_to_string
<Hadrons: procedures>≡
    elemental module function hadrons_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
        select case (char(string))
        case ("WHIZARD")
            i = HADRONS_WHIZARD
        case ("PYTHIA6")
            i = HADRONS_PYTHIA6
        case ("PYTHIA8")
            i = HADRONS_PYTHIA8
        case default
            i = HADRONS_UNDEFINED
        end select
    end function hadrons_method_of_string

    elemental module function hadrons_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
        case (HADRONS_WHIZARD)
            string = "WHIZARD"
        case (HADRONS_PYTHIA6)
            string = "PYTHIA6"
        case (HADRONS_PYTHIA8)
            string = "PYTHIA8"
        case default
            string = "UNDEFINED"
        end select
    end function hadrons_method_to_string

```

32.2.2 Hadronization settings

These are the general settings and parameters for the different shower methods.

```

<Hadrons: public>+≡
    public :: hadron_settings_t

```

```

<Hadrons: types>≡
  type :: hadron_settings_t
    logical :: active = .false.
    integer :: method = HADRONS_UNDEFINED
    real(default) :: enhanced_fraction = 0
    real(default) :: enhanced_width = 0
  contains
    <Hadrons: hadron settings: TBP>
  end type hadron_settings_t

```

Read in the hadronization settings.

```

<Hadrons: hadron settings: TBP>≡
  procedure :: init => hadron_settings_init

<Hadrons: sub interfaces>+≡
  module subroutine hadron_settings_init (hadron_settings, var_list)
    class(hadron_settings_t), intent(out) :: hadron_settings
    type(var_list_t), intent(in) :: var_list
  end subroutine hadron_settings_init

<Hadrons: procedures>+≡
  module subroutine hadron_settings_init (hadron_settings, var_list)
    class(hadron_settings_t), intent(out) :: hadron_settings
    type(var_list_t), intent(in) :: var_list
    hadron_settings%active = &
      var_list%get_lval (var_str ("?hadronization_active"))
    hadron_settings%method = hadrons_method_of_string ( &
      var_list%get_sval (var_str ("$hadronization_method")))
    hadron_settings%enhanced_fraction = &
      var_list%get_rval (var_str ("hadron_enhanced_fraction"))
    hadron_settings%enhanced_width = &
      var_list%get_rval (var_str ("hadron_enhanced_width"))
  end subroutine hadron_settings_init

<Hadrons: hadron settings: TBP>+≡
  procedure :: write => hadron_settings_write

<Hadrons: sub interfaces>+≡
  module subroutine hadron_settings_write (settings, unit)
    class(hadron_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
  end subroutine hadron_settings_write

<Hadrons: procedures>+≡
  module subroutine hadron_settings_write (settings, unit)
    class(hadron_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Hadronization settings:"
    call write_separator (u)
    write (u, "(1x,A)") "Master switches:"
    write (u, "(3x,A,1x,L1)") &
      "active          = ", settings%active
    write (u, "(1x,A)") "General settings:"

```

```

if (settings%active) then
  write (u, "(3x,A)" &
    "hadron_method          = " // &
    char (hadrons_method_to_string (settings%method))
else
  write (u, "(3x,A)" " [Hadronization off]"
end if
write (u, "(1x,A)" " pT generation parameters"
write (u, "(3x,A,1x,ES19.12)" &
  "enhanced_fraction      = ", settings%enhanced_fraction
write (u, "(3x,A,1x,ES19.12)" &
  "enhanced_width         = ", settings%enhanced_width
end subroutine hadron_settings_write

```

32.2.3 Abstract Hadronization Type

The model is the fallback model including all hadrons

```

<Hadrons: types>+≡
  type, abstract :: hadrons_t
    class(rng_t), allocatable :: rng
    type(shower_settings_t) :: shower_settings
    type(hadron_settings_t) :: hadron_settings
    type(model_t), pointer :: model => null()
  contains
    <Hadrons: hadrons: TBP>
  end type hadrons_t

<Hadrons: hadrons: TBP>≡
  procedure (hadrons_init), deferred :: init

<Hadrons: interfaces>+≡
  abstract interface
    subroutine hadrons_init &
      (hadrons, shower_settings, hadron_settings, model_hadrons)
    import
    class(hadrons_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), target, intent(in) :: model_hadrons
  end subroutine hadrons_init
  end interface

<Hadrons: hadrons: TBP>+≡
  procedure (hadrons_hadronize), deferred :: hadronize

<Hadrons: interfaces>+≡
  abstract interface
    subroutine hadrons_hadronize (hadrons, particle_set, valid)
    import
    class(hadrons_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
  end subroutine hadrons_hadronize
  end interface

```

```

        end subroutine hadrons_hadronize
    end interface

    <Hadrons: hadrons: TBP>+≡
        procedure (hadrons_make_particle_set), deferred :: make_particle_set

    <Hadrons: interfaces>+≡
        abstract interface
            subroutine hadrons_make_particle_set (hadrons, particle_set, &
                model, valid)
            import
            class(hadrons_t), intent(in) :: hadrons
            type(particle_set_t), intent(inout) :: particle_set
            class(model_data_t), intent(in), target :: model
            logical, intent(out) :: valid
        end subroutine hadrons_make_particle_set
    end interface

    <Hadrons: hadrons: TBP>+≡
        procedure :: import_rng => hadrons_import_rng

    <Hadrons: sub interfaces>+≡
        pure module subroutine hadrons_import_rng (hadrons, rng)
            class(hadrons_t), intent(inout) :: hadrons
            class(rng_t), intent(inout), allocatable :: rng
        end subroutine hadrons_import_rng

    <Hadrons: procedures>+≡
        pure module subroutine hadrons_import_rng (hadrons, rng)
            class(hadrons_t), intent(inout) :: hadrons
            class(rng_t), intent(inout), allocatable :: rng
            call move_alloc (from = rng, to = hadrons%rng)
        end subroutine hadrons_import_rng

```

32.2.4 WHIZARD Hadronization Type

Hadronization can be (incompletely) performed through WHIZARD's internal routine.

```

    <Hadrons: public>+≡
        public :: hadrons_hadrons_t

    <Hadrons: types>+≡
        type, extends (hadrons_t) :: hadrons_hadrons_t
            contains
                <Hadrons: hadrons hadrons: TBP>
            end type hadrons_hadrons_t

    <Hadrons: hadrons hadrons: TBP>≡
        procedure :: init => hadrons_hadrons_init

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_hadrons_init &
    (hadrons, shower_settings, hadron_settings, model_hadrons)
    class(hadrons_hadrons_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), intent(in), target :: model_hadrons
end subroutine hadrons_hadrons_init

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_hadrons_init &
    (hadrons, shower_settings, hadron_settings, model_hadrons)
    class(hadrons_hadrons_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), intent(in), target :: model_hadrons
    hadrons%model => model_hadrons
    hadrons%shower_settings = shower_settings
    hadrons%hadron_settings = hadron_settings
    call msg_message &
        ("Hadronization: WHIZARD model for hadronization and decays")
end subroutine hadrons_hadrons_init

```

<Hadrons: hadrons hadrons: TBP>+≡

```

procedure :: hadronize => hadrons_hadrons_hadronize

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_hadrons_hadronize (hadrons, particle_set, valid)
    class(hadrons_hadrons_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
end subroutine hadrons_hadrons_hadronize

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_hadrons_hadronize (hadrons, particle_set, valid)
    class(hadrons_hadrons_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
    integer, dimension(:), allocatable :: cols, acol, octs
    integer :: n
    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_hadrons_hadronize")
    call particle_set%write (6, compressed=.true.)
    n = particle_set%get_n_tot ()
    allocate (cols (n), acol (n), octs (n))
    call extract_color_systems (particle_set, cols, acol, octs)
    print *, "size(cols) = ", size (cols)
    if (size(cols) > 0) then
        print *, "cols = ", cols
    end if
    print *, "size(acol) = ", size(acol)
    if (size(acol) > 0) then
        print *, "acol = ", acol
    end if
    print *, "size(octs) = ", size(octs)

```

```

    if (size (octs) > 0) then
        print *, "octs  = ", octs
    end if
    !!! if all arrays are empty, i.e. zero particles found, nothing to do
end subroutine hadrons_hadrons_hadronize

```

This type contains a flavor selector for the creation of hadrons, including parameters for the special handling of baryons.

```

<Hadrons: public>+≡
    public :: had_flav_t

<Hadrons: types>+≡
    type had_flav_t
end type had_flav_t

```

This is the type for the ends of Lund strings.

```

<Hadrons: public>+≡
    public :: lund_end

<Hadrons: types>+≡
    type lund_end
        logical :: from_pos
        integer :: i_end
        integer :: i_max
        integer :: id_had
        integer :: i_pos_old
        integer :: i_neg_old
        integer :: i_pos_new
        integer :: i_neg_new
        real(default) :: px_old
        real(default) :: py_old
        real(default) :: px_new
        real(default) :: py_new
        real(default) :: px_had
        real(default) :: py_had
        real(default) :: m_had
        real(default) :: mT2_had
        real(default) :: z_had
        real(default) :: gamma_old
        real(default) :: gamma_new
        real(default) :: x_pos_old
        real(default) :: x_pos_new
        real(default) :: x_pos_had
        real(default) :: x_neg_old
        real(default) :: x_neg_new
        real(default) :: x_neg_had
        type(had_flav_t) :: old_flav
        type(had_flav_t) :: new_flav
        type(vector4_t) :: p_had
        type(vector4_t) :: p_pre
    end type lund_end

```


Generator for transverse momentum for the fragmentation.

```

<Hadrons: public>+≡
    public :: lund_pt_t

<Hadrons: types>+≡
    type lund_pt_t
        real(default) :: sigma_min
        real(default) :: sigma_q
        real(default) :: enhanced_frac
        real(default) :: enhanced_width
        real(default) :: sigma_to_had
        class(rng_t), allocatable :: rng
    contains
        <Hadrons: lund pT: TBP>
    end type lund_pt_t

<Hadrons: lund pT: TBP>≡
    procedure :: init => lund_pt_init

<Hadrons: sub interfaces>+≡
    module subroutine lund_pt_init (lund_pt, settings)
        class (lund_pt_t), intent(out) :: lund_pt
        type(hadron_settings_t), intent(in) :: settings
    end subroutine lund_pt_init

<Hadrons: procedures>+≡
    module subroutine lund_pt_init (lund_pt, settings)
        class (lund_pt_t), intent(out) :: lund_pt
        type(hadron_settings_t), intent(in) :: settings
    end subroutine lund_pt_init

<Hadrons: hadrons hadrons: TBP>+≡
    procedure :: make_particle_set => hadrons_hadrons_make_particle_set

<Hadrons: sub interfaces>+≡
    module subroutine hadrons_hadrons_make_particle_set &
        (hadrons, particle_set, model, valid)
        class(hadrons_hadrons_t), intent(in) :: hadrons
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        logical, intent(out) :: valid
    end subroutine hadrons_hadrons_make_particle_set

<Hadrons: procedures>+≡
    module subroutine hadrons_hadrons_make_particle_set &
        (hadrons, particle_set, model, valid)
        class(hadrons_hadrons_t), intent(in) :: hadrons
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        logical, intent(out) :: valid
        if (signal_is_pending ()) return
        valid = .false.
        if (valid) then
        else
            call msg_fatal ("WHIZARD hadronization not yet implemented")
        end if
    end subroutine

```

```
end subroutine hadrons_hadrons_make_particle_set
```

<Hadrons: procedures>+≡

```
subroutine extract_color_systems (p_set, cols, acols, octs)
  type(particle_set_t), intent(in) :: p_set
  integer, dimension(:), allocatable, intent(out) :: cols, acols, octs
  logical, dimension(:), allocatable :: mask
  integer :: i, n, n_cols, n_acols, n_octs
  n = p_set%get_n_tot ()
  allocate (mask (n))
  do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () /= 0 .and. &
      p_set%prt(i)%col%get_acl () == 0 .and. &
      p_set%prt(i)%get_status () == PRT_OUTGOING
  end do
  n_cols = count (mask)
  allocate (cols (n_cols))
  cols = p_set%get_indices (mask)
  do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () == 0 .and. &
      p_set%prt(i)%col%get_acl () /= 0 .and. &
      p_set%prt(i)%get_status () == PRT_OUTGOING
  end do
  n_acols = count (mask)
  allocate (acols (n_acols))
  acols = p_set%get_indices (mask)
  do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () /= 0 .and. &
      p_set%prt(i)%col%get_acl () /= 0 .and. &
      p_set%prt(i)%get_status () == PRT_OUTGOING
  end do
  n_octs = count (mask)
  allocate (octs (n_octs))
  octs = p_set%get_indices (mask)
end subroutine extract_color_systems
```

32.2.5 PYTHIA6 Hadronization Type

Hadronization via PYTHIA6 is at another option for hadronization within WHIZARD.

<Hadrons: public>+≡

```
public :: hadrons_pythia6_t
```

<Hadrons: types>+≡

```
type, extends (hadrons_t) :: hadrons_pythia6_t
contains
  <Hadrons: hadrons pythia6: TBP>
end type hadrons_pythia6_t
```

<Hadrons: hadrons pythia6: TBP>≡

```
procedure :: init => hadrons_pythia6_init
```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_pythia6_init &
  (hadrons, shower_settings, hadron_settings, model_hadrons)
  class(hadrons_pythia6_t), intent(out) :: hadrons
  type(shower_settings_t), intent(in) :: shower_settings
  type(hadron_settings_t), intent(in) :: hadron_settings
  type(model_t), intent(in), target :: model_hadrons
end subroutine hadrons_pythia6_init

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_pythia6_init &
  (hadrons, shower_settings, hadron_settings, model_hadrons)
  class(hadrons_pythia6_t), intent(out) :: hadrons
  type(shower_settings_t), intent(in) :: shower_settings
  type(hadron_settings_t), intent(in) :: hadron_settings
  type(model_t), intent(in), target :: model_hadrons
  logical :: pygive_not_set_by_shower
  hadrons%model => model_hadrons
  hadrons%shower_settings = shower_settings
  hadrons%hadron_settings = hadron_settings
  pygive_not_set_by_shower = .not. (shower_settings%method == PS_PYTHIA6 &
    .and. (shower_settings%isr_active .or. shower_settings%fsr_active))
  if (pygive_not_set_by_shower) then
    call pythia6_set_verbose (shower_settings%verbose)
    call pythia6_set_config (shower_settings%pythia6_pygive)
  end if
  call msg_message &
    ("Hadronization: Using PYTHIA6 interface for hadronization and decays")
end subroutine hadrons_pythia6_init

```

Assume that the event record is still in the PYTHIA COMMON BLOCKS transferred there by the WHIZARD or PYTHIA6 shower routines.

<Hadrons: hadrons pythia6: TBP>+≡

```

procedure :: hadronize => hadrons_pythia6_hadronize

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_pythia6_hadronize (hadrons, particle_set, valid)
  class(hadrons_pythia6_t), intent(inout) :: hadrons
  type(particle_set_t), intent(in) :: particle_set
  logical, intent(out) :: valid
end subroutine hadrons_pythia6_hadronize

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_pythia6_hadronize (hadrons, particle_set, valid)
  class(hadrons_pythia6_t), intent(inout) :: hadrons
  type(particle_set_t), intent(in) :: particle_set
  logical, intent(out) :: valid
  integer :: N, NPAD, K
  real(double) :: P, V
  common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
  save /PYJETS/
  if (signal_is_pending ()) return
  if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia6_hadronize")
  call pygive ("MSTP(111)=1")    !!! Switch on hadronization and decays
  call pygive ("MSTJ(1)=1")     !!! String fragmentation

```

```

call pygive ("MSTJ(21)=2")      !!! String fragmentation keeping resonance momentum
call pygive ("MSTJ(28)=0")      !!! Switch off tau decays
if (debug_active (D_TRANSFORMS)) then
  call msg_debug (D_TRANSFORMS, "N", N)
  call pylist(2)
  print *, ' line 7 : ', k(7,1:5), p(7,1:5)
end if
call pyedit (12)
call pythia6_set_last_treated_line (N)
call pyexec ()
call pyedit (12)
valid = .true.
end subroutine hadrons_pythia6_hadronize

```

<Hadrons: hadrons pythia6: TBP>+≡

```

procedure :: make_particle_set => hadrons_pythia6_make_particle_set

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_pythia6_make_particle_set &
  (hadrons, particle_set, model, valid)
  class(hadrons_pythia6_t), intent(in) :: hadrons
  type(particle_set_t), intent(inout) :: particle_set
  class(model_data_t), intent(in), target :: model
  logical, intent(out) :: valid
end subroutine hadrons_pythia6_make_particle_set

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_pythia6_make_particle_set &
  (hadrons, particle_set, model, valid)
  class(hadrons_pythia6_t), intent(in) :: hadrons
  type(particle_set_t), intent(inout) :: particle_set
  class(model_data_t), intent(in), target :: model
  logical, intent(out) :: valid
  if (signal_is_pending ()) return
  valid = pythia6_handle_errors ()
  if (valid) then
    call pythia6_combine_with_particle_set &
      (particle_set, model, hadrons%model, hadrons%shower_settings)
  end if
end subroutine hadrons_pythia6_make_particle_set

```

32.2.6 PYTHIA8 Hadronization

<Hadrons: public>+≡

```

public :: hadrons_pythia8_t

```

<Hadrons: types>+≡

```

type, extends (hadrons_t) :: hadrons_pythia8_t
  type(pythia8_t) :: pythia
  type(whizard_lha_t) :: lhaup
  logical :: user_process_set = .false.
  logical :: pythia_initialized = .false., &
    lhaup_initialized = .false.

```

```
contains
  <Hadrons: hadrons pythia8: TBP>
end type hadrons_pythia8_t
```

```
<Hadrons: hadrons pythia8: TBP>≡
  procedure :: init => hadrons_pythia8_init

<Hadrons: sub interfaces>+≡
  module subroutine hadrons_pythia8_init &
    (hadrons, shower_settings, hadron_settings, model_hadrons)
    class(hadrons_pythia8_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), intent(in), target :: model_hadrons
  end subroutine hadrons_pythia8_init

<Hadrons: procedures>+≡
  module subroutine hadrons_pythia8_init &
    (hadrons, shower_settings, hadron_settings, model_hadrons)
    class(hadrons_pythia8_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), intent(in), target :: model_hadrons
    hadrons%model => model_hadrons
    hadrons%shower_settings = shower_settings
    hadrons%hadron_settings = hadron_settings
    call msg_message ("Hadronization: Using PYTHIA8 interface " // &
      "for hadronization and decays.")
    ! TODO sbrass which verbose?
    call hadrons%pythia%init (verbose = shower_settings%verbose)
    call hadrons%lhaupt%init ()
  end subroutine hadrons_pythia8_init
```

Transfer hadron settings to PYTHIA8.

```
<Hadrons: hadrons pythia8: TBP>+≡
  procedure, private :: transfer_settings => hadrons_pythia8_transfer_settings

<Hadrons: sub interfaces>+≡
  module subroutine hadrons_pythia8_transfer_settings (hadrons)
    class(hadrons_pythia8_t), intent(inout), target :: hadrons
  end subroutine hadrons_pythia8_transfer_settings

<Hadrons: procedures>+≡
  module subroutine hadrons_pythia8_transfer_settings (hadrons)
    class(hadrons_pythia8_t), intent(inout), target :: hadrons
    real(default) :: r
    if (debug_on) call msg_debug &
      (D_TRANSFORMS, "hadrons_pythia8_transfer_settings")
    if (debug_on) call msg_debug2 &
      (D_TRANSFORMS, "pythia_initialized", hadrons%pythia_initialized)
    if (hadrons%pythia_initialized) return
    call hadrons%pythia%import_rng (hadrons%rng)
    call hadrons%pythia%parse_and_set_config &
      (hadrons%shower_settings%pythia8_config)
    if (len (hadrons%shower_settings%pythia8_config_file) > 0) &
```

```

        call hadrons%pythia%read_file &
            (hadrons%shower_settings%pythia8_config_file)
    call hadrons%pythia%read_string (var_str ("Beams:frameType = 5"))
    call hadrons%pythia%read_string (var_str ("ProcessLevel:all = off"))
    if (.not. hadrons%shower_settings%verbose) then
        call hadrons%pythia%read_string (var_str ("Print:quiet = on"))
    end if
    call hadrons%pythia%set_lhaup_ptr (hadrons%lhaup)
    call hadrons%pythia%init_pythia ()
    hadrons%pythia_initialized = .true.
end subroutine hadrons_pythia8_transfer_settings

```

Set user process for the LHA interface.

```

<Hadrons: hadrons pythia8: TBP>+≡
    procedure, private :: set_user_process => hadrons_pythia8_set_user_process

<Hadrons: sub interfaces>+≡
    module subroutine hadrons_pythia8_set_user_process (hadrons, pset)
        class(hadrons_pythia8_t), intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: pset
    end subroutine hadrons_pythia8_set_user_process

<Hadrons: procedures>+≡
    module subroutine hadrons_pythia8_set_user_process (hadrons, pset)
        class(hadrons_pythia8_t), intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: pset
        integer, dimension(2) :: beam_pdg
        real(default), dimension(2) :: beam_energy
        integer, parameter :: process_id = 0, n_processes = 0
        if (debug_on) call msg_debug &
            (D_TRANSFORMS, "hadrons_pythia8_set_user_process")
        beam_pdg = [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()]
        beam_energy = [energy(pset%prt(1)%p), energy(pset%prt(2)%p)]
        call hadrons%lhaup%set_init (beam_pdg, beam_energy, &
            n_processes, unweighted = .false., negative_weights = .false.)
        call hadrons%lhaup%set_process_parameters (process_id = process_id, &
            cross_section = one, error = one)
    end subroutine hadrons_pythia8_set_user_process

```

Import particle set.

```

<Hadrons: hadrons pythia8: TBP>+≡
    procedure, private :: import_particle_set => &
        hadrons_pythia8_import_particle_set

<Hadrons: sub interfaces>+≡
    module subroutine hadrons_pythia8_import_particle_set &
        (hadrons, particle_set)
        class(hadrons_pythia8_t), target, intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: particle_set
    end subroutine hadrons_pythia8_import_particle_set

<Hadrons: procedures>+≡
    module subroutine hadrons_pythia8_import_particle_set (hadrons, particle_set)
        class(hadrons_pythia8_t), target, intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: particle_set

```

```

integer, parameter :: PROCESS_ID = 1
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "hadrons_pythia8_import_particle_set")
if (.not. hadrons%user_process_set) then
    call hadrons%set_user_process (particle_set)
    hadrons%user_process_set = .true.
end if
call hadrons%lhaup%set_event_process (process_id = PROCESS_ID, &
    scale = -one, alpha_qcd = -one, alpha_qed = -one, weight = -one)
call hadrons%lhaup%set_event (process_id = PROCESS_ID, &
    particle_set = particle_set, polarization = .true.)
if (debug_active (D_TRANSFORMS)) then
    call hadrons%lhaup%list_init ()
end if
end subroutine hadrons_pythia8_import_particle_set

```

<Hadrons: hadrons pythia8: TBP>+≡

```

procedure :: hadronize => hadrons_pythia8_hadronize

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_pythia8_hadronize (hadrons, particle_set, valid)
    class(hadrons_pythia8_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
end subroutine hadrons_pythia8_hadronize

```

<Hadrons: procedures>+≡

```

module subroutine hadrons_pythia8_hadronize (hadrons, particle_set, valid)
    class(hadrons_pythia8_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
    if (signal_is_pending ()) return
    call hadrons%import_particle_set (particle_set)
    if (.not. hadrons%pythia_initialized) &
        call hadrons%transfer_settings ()
    call hadrons%pythia%next (valid)
    if (debug_active (D_TRANSFORMS)) then
        call hadrons%pythia%list_event ()
        call particle_set%write (summary=.true., compressed=.true.)
    end if
end subroutine hadrons_pythia8_hadronize

```

<Hadrons: hadrons pythia8: TBP>+≡

```

procedure :: make_particle_set => hadrons_pythia8_make_particle_set

```

<Hadrons: sub interfaces>+≡

```

module subroutine hadrons_pythia8_make_particle_set &
    (hadrons, particle_set, model, valid)
    class(hadrons_pythia8_t), intent(in) :: hadrons
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: valid
end subroutine hadrons_pythia8_make_particle_set

```

```

<Hadrons: procedures>+≡
module subroutine hadrons_pythia8_make_particle_set &
    (hadrons, particle_set, model, valid)
    class(hadrons_pythia8_t), intent(in) :: hadrons
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: valid
    type(particle_t), dimension(:), allocatable :: beam
    if (debug_on) call msg_debug &
        (D_TRANSFORMS, "hadrons_pythia8_make_particle_set")
    if (signal_is_pending ()) return
    associate (settings => hadrons%shower_settings)
        if (debug_active (D_TRANSFORMS)) then
            call msg_debug (D_TRANSFORMS, 'Combine PYTHIA8 with particle set')
            call msg_debug (D_TRANSFORMS, 'Particle set before replacing')
            call particle_set%write (summary=.true., compressed=.true.)
            call hadrons%pythia%list_event ()
            call msg_debug (D_TRANSFORMS, string = "settings%hadron_collision", &
                value = settings%hadron_collision)
        end if
        call hadrons%pythia%get_hadron_particles (&
            model, hadrons%model, particle_set, &
            helicity = PRT_DEFINITE_HELICITY)
    end associate
    if (debug_active (D_TRANSFORMS)) then
        print *, 'Particle set after replacing'
        call particle_set%write (summary=.true., compressed=.true.)
    end if
    valid = .true.
end subroutine hadrons_pythia8_make_particle_set

```

32.2.7 Hadronization Event Transform

This is the type for the hadronization event transform. It does not depend on the specific hadronization implementation of `hadrons_t`.

```

<Hadrons: public>+≡
public :: evt_hadrons_t

<Hadrons: types>+≡
type, extends (evt_t) :: evt_hadrons_t
    class(hadrons_t), allocatable :: hadrons
    type(model_t), pointer :: model_hadrons => null()
    type(qcd_t) :: qcd
    logical :: is_first_event
contains
    <Hadrons: evt hadrons: TBP>
end type evt_hadrons_t

```

Initialize the parameters. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that may be generated in the shower.

```

<Hadrons: evt hadrons: TBP>≡
procedure :: init => evt_hadrons_init

```



```

<Hadrons: sub interfaces>+≡
    module subroutine evt_hadrons_init (evt, model_hadrons)
        class(evt_hadrons_t), intent(out) :: evt
        type(model_t), intent(in), target :: model_hadrons
    end subroutine evt_hadrons_init

```

```

<Hadrons: procedures>+≡
    module subroutine evt_hadrons_init (evt, model_hadrons)
        class(evt_hadrons_t), intent(out) :: evt
        type(model_t), intent(in), target :: model_hadrons
        evt%model_hadrons => model_hadrons
        evt%is_first_event = .true.
    end subroutine evt_hadrons_init

```

```

<Hadrons: evt hadrons: TBP>+≡
    procedure :: write_name => evt_hadrons_write_name

```

```

<Hadrons: sub interfaces>+≡
    module subroutine evt_hadrons_write_name (evt, unit)
        class(evt_hadrons_t), intent(in) :: evt
        integer, intent(in), optional :: unit
    end subroutine evt_hadrons_write_name

```

```

<Hadrons: procedures>+≡
    module subroutine evt_hadrons_write_name (evt, unit)
        class(evt_hadrons_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: hadronization"
    end subroutine evt_hadrons_write_name

```

Output.

```

<Hadrons: evt hadrons: TBP>+≡
    procedure :: write => evt_hadrons_write

```

```

<Hadrons: sub interfaces>+≡
    module subroutine evt_hadrons_write &
        (evt, unit, verbose, more_verbose, testflag)
        class(evt_hadrons_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
    end subroutine evt_hadrons_write

```

```

<Hadrons: procedures>+≡
    module subroutine evt_hadrons_write &
        (evt, unit, verbose, more_verbose, testflag)
        class(evt_hadrons_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        call evt%write_name (u)
        call write_separator (u)
        call evt%base_write (u, testflag = testflag, show_set = .false.)
    end subroutine evt_hadrons_write

```

```

    if (evt%particle_set_exists) &
        call evt%particle_set%write &
            (u, summary = .true., compressed = .true., testflag = testflag)
    call write_separator (u)
    call evt%hadrons%shower_settings%write (u)
    call write_separator (u)
    call evt%hadrons%hadron_settings%write (u)
end subroutine evt_hadrons_write

```

<Hadrons: evt hadrons: TBP>+≡

```

    procedure :: first_event => evt_hadrons_first_event

```

<Hadrons: sub interfaces>+≡

```

    module subroutine evt_hadrons_first_event (evt)
        class(evt_hadrons_t), intent(inout) :: evt
    end subroutine evt_hadrons_first_event

```

<Hadrons: procedures>+≡

```

    module subroutine evt_hadrons_first_event (evt)
        class(evt_hadrons_t), intent(inout) :: evt
        if (debug_on) call msg_debug (D_TRANSFORMS, "evt_hadrons_first_event")
        associate (settings => evt%hadrons%shower_settings)
            settings%hadron_collision = .false.
            if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () <= 39)) then
                settings%hadron_collision = .false.
            else if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () >= 100)) then
                settings%hadron_collision = .true.
            else
                call msg_fatal ("evt_hadrons didn't recognize beams setup")
            end if
            if (debug_on) call msg_debug &
                (D_TRANSFORMS, "hadron_collision", settings%hadron_collision)
            if (.not. (settings%isr_active .or. settings%fsr_active)) then
                call msg_fatal ("Hadronization without shower is not supported")
            end if
        end associate
        evt%is_first_event = .false.
    end subroutine evt_hadrons_first_event

```

Here we take the particle set from the previous event transform and apply the hadronization. The result is stored in the `evt%hadrons` object. We always return a probability of unity as we don't have the analytic weight of the hadronization. Invalid events have to be discarded by the caller which is why we mark the particle set as invalid.

<Hadrons: evt hadrons: TBP>+≡

```

    procedure :: generate_weighted => evt_hadrons_generate_weighted

```

<Hadrons: sub interfaces>+≡

```

    module subroutine evt_hadrons_generate_weighted (evt, probability)
        class(evt_hadrons_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
    end subroutine evt_hadrons_generate_weighted

```

```

<Hadrons: procedures>+≡
module subroutine evt_hadrons_generate_weighted (evt, probability)
  class(evt_hadrons_t), intent(inout) :: evt
  real(default), intent(inout) :: probability
  logical :: valid
  if (signal_is_pending ()) return
  evt%particle_set = evt%previous%particle_set
  if (evt%is_first_event) then
    call evt%first_event ()
  end if
  call evt%hadrons%hadronize (evt%particle_set, valid)
  probability = 1
  evt%particle_set_exists = valid
end subroutine evt_hadrons_generate_weighted

```

The factorization parameters are irrelevant.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: make_particle_set => evt_hadrons_make_particle_set

<Hadrons: sub interfaces>+≡
  module subroutine evt_hadrons_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_hadrons_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_hadrons_make_particle_set

<Hadrons: procedures>+≡
module subroutine evt_hadrons_make_particle_set &
  (evt, factorization_mode, keep_correlations, r)
  class(evt_hadrons_t), intent(inout) :: evt
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
  logical :: valid
  call evt%hadrons%make_particle_set (evt%particle_set, evt%model, valid)
  evt%particle_set_exists = evt%particle_set_exists .and. valid
end subroutine evt_hadrons_make_particle_set

```

Connect the process with the hadrons object.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: connect => evt_hadrons_connect

<Hadrons: sub interfaces>+≡
  module subroutine evt_hadrons_connect &
    (evt, process_instance, model, process_stack)
    class(evt_hadrons_t), intent(inout), target :: evt
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
  end subroutine evt_hadrons_connect

```

```

<Hadrons: procedures>+≡
  module subroutine evt_hadrons_connect &
    (evt, process_instance, model, process_stack)
    class(evt_hadrons_t), intent(inout), target :: evt
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    call evt%base_connect (process_instance, model, process_stack)
    call evt%make_rng (evt%process)
  end subroutine evt_hadrons_connect

```

Create RNG instances, spawned by the process object.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: make_rng => evt_hadrons_make_rng

<Hadrons: sub interfaces>+≡
  module subroutine evt_hadrons_make_rng (evt, process)
    class(evt_hadrons_t), intent(inout) :: evt
    type(process_t), intent(inout) :: process
    class(rng_t), allocatable :: rng
  end subroutine evt_hadrons_make_rng

<Hadrons: procedures>+≡
  module subroutine evt_hadrons_make_rng (evt, process)
    class(evt_hadrons_t), intent(inout) :: evt
    type(process_t), intent(inout) :: process
    class(rng_t), allocatable :: rng
    call process%make_rng (rng)
    call evt%hadrons%import_rng (rng)
  end subroutine evt_hadrons_make_rng

<Hadrons: evt hadrons: TBP>+≡
  procedure :: prepare_new_event => evt_hadrons_prepare_new_event

<Hadrons: sub interfaces>+≡
  module subroutine evt_hadrons_prepare_new_event (evt, i_mci, i_term)
    class(evt_hadrons_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_hadrons_prepare_new_event

<Hadrons: procedures>+≡
  module subroutine evt_hadrons_prepare_new_event (evt, i_mci, i_term)
    class(evt_hadrons_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_hadrons_prepare_new_event

```

32.3 Resonance Insertion

```

<resonance_insertion.f90>≡
  <File header>

  module resonance_insertion

```

```

    <Use kinds>
    <Use strings>
    use rng_base, only: rng_t
    use selectors, only: selector_t
    use particles, only: particle_t, particle_set_t
    use resonances, only: resonance_history_set_t
    use resonances, only: resonance_tree_t
    use instances, only: process_instance_ptr_t
    use event_transforms

    <Standard module head>

    <Resonance insertion: public>

    <Resonance insertion: types>

    interface
    <Resonance insertion: sub interfaces>
    end interface

    end module resonance_insertion

    <resonance_insertion_sub.f90>≡
    <File header>

    submodule (resonance_insertion) resonance_insertion_s

    use io_units
    use format_utils, only: write_separator
    use format_defs, only: FMT_12
    use interactions, only: interaction_t
    use subevents, only: PRT_RESONANT

    implicit none

    contains

    <Resonance insertion: procedures>

    end submodule resonance_insertion_s

```

32.3.1 Resonance-Insertion Event Transform

This is the type for the event transform that applies resonance insertion. The resonance history set describe the resonance histories that we may consider. There is a process library with process objects that correspond to the resonance histories. Library creation, compilation etc. is done outside the scope of this module.

```

    <Resonance insertion: public>≡
    public :: evt_resonance_t

```

```

<Resonance insertion: types>≡
  type, extends (evt_t) :: evt_resonance_t
    type(resonance_history_set_t), dimension(:), allocatable :: res_history_set
    integer, dimension(:), allocatable :: index_offset
    integer :: selected_component = 0
    type(string_t) :: libname
    type(string_t), dimension(:), allocatable :: proc_id
    real(default) :: on_shell_limit = 0
    real(default) :: on_shell_turnoff = 0
    real(default) :: background_factor = 1
    logical :: selector_active = .false.
    type(selector_t) :: selector
    integer :: selected_history = 0
    type(process_instance_ptr_t), dimension(:), allocatable :: instance
  contains
    <Resonance insertion: evt resonance: TBP>
  end type evt_resonance_t

```

```

<Resonance insertion: evt resonance: TBP>≡
  procedure :: write_name => evt_resonance_write_name

```

```

<Resonance insertion: sub interfaces>≡
  module subroutine evt_resonance_write_name (evt, unit)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
  end subroutine evt_resonance_write_name

```

```

<Resonance insertion: procedures>≡
  module subroutine evt_resonance_write_name (evt, unit)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: resonance insertion"
  end subroutine evt_resonance_write_name

```

Output.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: write => evt_resonance_write

```

```

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
  end subroutine evt_resonance_write

```

```

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u, i

```

```

u = given_output_unit (unit)
call write_separator (u, 2)
call evt%write_name (u)
call write_separator (u, 2)
write (u, "(1x,A,A,A)") "Process library = '", char (evt%libname), "'"
if (allocated (evt%res_history_set)) then
  do i = 1, size (evt%res_history_set)
    if (i == evt%selected_component) then
      write (u, "(1x,A,I0,A)") "Component #", i, ":"
    else
      write (u, "(1x,A,I0,A)") "Component #", i, ":"
    end if
    call evt%res_history_set(i)%write (u, indent=1)
  end do
end if
call write_separator (u)
if (allocated (evt%instance)) then
  write (u, "(1x,A)") "Subprocess instances: allocated"
else
  write (u, "(1x,A)") "Subprocess instances: not allocated"
end if
if (evt%particle_set_exists) then
  if (evt%selected_history > 0) then
    write (u, "(1x,A,I0)") "Selected: resonance history #", &
      evt%selected_history
  else
    write (u, "(1x,A)") "Selected: no resonance history"
  end if
else
  write (u, "(1x,A)") "Selected: [none]"
end if
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "On-shell limit    =", evt%on_shell_limit
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "On-shell turnoff =", evt%on_shell_turnoff
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "Background factor =", evt%background_factor
call write_separator (u)
if (evt%selector_active) then
  write (u, "(2x)", advance="no")
  call evt%selector%write (u, testflag=testflag)
  call write_separator (u)
end if
call evt%base_write (u, testflag = testflag, show_set = .false.)
call write_separator (u)
if (evt%particle_set_exists) then
  call evt%particle_set%write &
    (u, summary = .true., compressed = .true., testflag = testflag)
  call write_separator (u)
end if
end subroutine evt_resonance_write

```

32.3.2 Set contained data

Insert the resonance data, in form of a pre-generated resonance history set. Accumulate the number of histories for each set, to initialize an array of index offsets for lookup.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: set_resonance_data => evt_resonance_set_resonance_data

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_set_resonance_data (evt, res_history_set)
        class(evt_resonance_t), intent(inout) :: evt
        type(resonance_history_set_t), dimension(:), intent(in) :: res_history_set
    end subroutine evt_resonance_set_resonance_data

<Resonance insertion: procedures>+≡
    module subroutine evt_resonance_set_resonance_data (evt, res_history_set)
        class(evt_resonance_t), intent(inout) :: evt
        type(resonance_history_set_t), dimension(:), intent(in) :: res_history_set
        integer :: i
        evt%res_history_set = res_history_set
        allocate (evt%index_offset (size (evt%res_history_set)), source = 0)
        do i = 2, size (evt%res_history_set)
            evt%index_offset(i) = &
                evt%index_offset(i-1) + evt%res_history_set(i-1)%get_n_history ()
        end do
    end subroutine evt_resonance_set_resonance_data

```

Set the library that contains the resonant subprocesses.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: set_library => evt_resonance_set_library

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_set_library (evt, libname)
        class(evt_resonance_t), intent(inout) :: evt
        type(string_t), intent(in) :: libname
    end subroutine evt_resonance_set_library

<Resonance insertion: procedures>+≡
    module subroutine evt_resonance_set_library (evt, libname)
        class(evt_resonance_t), intent(inout) :: evt
        type(string_t), intent(in) :: libname
        evt%libname = libname
    end subroutine evt_resonance_set_library

```

Assign pointers to subprocess instances. Once a subprocess has been selected, the instance is used for generating the particle set with valid quantum-number assignments, ready for resonance insertion.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: set_subprocess_instances &
        => evt_resonance_set_subprocess_instances

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_set_subprocess_instances (evt, instance)
        class(evt_resonance_t), intent(inout) :: evt
        type(process_instance_ptr_t), dimension(:), intent(in) :: instance
    end subroutine evt_resonance_set_subprocess_instances

```



```

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_set_subprocess_instances (evt, instance)
    class(evt_resonance_t), intent(inout) :: evt
    type(process_instance_ptr_t), dimension(:), intent(in) :: instance
    evt%instance = instance
  end subroutine evt_resonance_set_subprocess_instances

```

Set the on-shell limit, the relative distance from a resonance that is still considered to be on-shell. The probability for being considered on-shell can be reduced by the turnoff parameter below. For details, see the `resonances` module.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: set_on_shell_limit => evt_resonance_set_on_shell_limit

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_set_on_shell_limit (evt, on_shell_limit)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_limit
  end subroutine evt_resonance_set_on_shell_limit

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_set_on_shell_limit (evt, on_shell_limit)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_limit
    evt%on_shell_limit = on_shell_limit
  end subroutine evt_resonance_set_on_shell_limit

```

Set the Gaussian on-shell turnoff parameter, the width of the weighting factor for the resonance squared matrix element. If the resonance is off shell, this factor reduces the weight of the matrix element in the selector, such that the probability for considered resonant is reduced. The factor is applied only if the offshellness is less than the `on_shell_limit` above. For details, see the `resonances` module.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: set_on_shell_turnoff => evt_resonance_set_on_shell_turnoff

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_set_on_shell_turnoff (evt, on_shell_turnoff)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_turnoff
  end subroutine evt_resonance_set_on_shell_turnoff

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_set_on_shell_turnoff (evt, on_shell_turnoff)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_turnoff
    evt%on_shell_turnoff = on_shell_turnoff
  end subroutine evt_resonance_set_on_shell_turnoff

```

Reweight (suppress) the background contribution if there is a resonance history that applies. The event will be registered as background if there is no applicable resonance history, or if the background configuration has been selected based on (reweighted) squared matrix elements.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: set_background_factor => evt_resonance_set_background_factor

```

```

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_set_background_factor &
    (evt, background_factor)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: background_factor
  end subroutine evt_resonance_set_background_factor

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_set_background_factor (evt, background_factor)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: background_factor
    evt%background_factor = background_factor
  end subroutine evt_resonance_set_background_factor

```

32.3.3 Selector

Manually import a random-number generator object. This should be done only for testing purposes. The standard procedure is to `connect` a process to an event transform; this will create an appropriate `rng` from the RNG factory in the process object.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: import_rng => evt_resonance_import_rng

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_import_rng (evt, rng)
    class(evt_resonance_t), intent(inout) :: evt
    class(rng_t), allocatable, intent(inout) :: rng
  end subroutine evt_resonance_import_rng

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_import_rng (evt, rng)
    class(evt_resonance_t), intent(inout) :: evt
    class(rng_t), allocatable, intent(inout) :: rng
    call move_alloc (from = rng, to = evt%rng)
  end subroutine evt_resonance_import_rng

We use a standard selector object to choose from the available resonance histories. If the selector is inactive, we do not insert resonances.

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: write_selector => evt_resonance_write_selector

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_write_selector (evt, unit, testflag)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine evt_resonance_write_selector

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_write_selector (evt, unit, testflag)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u

```

```

u = given_output_unit (unit)
if (evt%selector_active) then
    call evt%selector%write (u, testflag)
else
    write (u, "(1x,A)") "Selector: [inactive]"
end if
end subroutine evt_resonance_write_selector

```

The selector is initialized with relative weights of histories which need not be normalized. Channels with weight zero are ignored.

The `offset` will normally be -1 , so we count from zero, and zero is a valid result from the selector. Selecting the zero entry implies no resonance insertion. However, this behavior is not hard-coded here (without offset, no resonance is not possible as a result).

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: init_selector => evt_resonance_init_selector

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_init_selector (evt, weight, offset)
        class(evt_resonance_t), intent(inout) :: evt
        real(default), dimension(:), intent(in) :: weight
        integer, intent(in), optional :: offset
    end subroutine evt_resonance_init_selector

<Resonance insertion: procedures>+≡
    module subroutine evt_resonance_init_selector (evt, weight, offset)
        class(evt_resonance_t), intent(inout) :: evt
        real(default), dimension(:), intent(in) :: weight
        integer, intent(in), optional :: offset
        if (any (weight > 0)) then
            call evt%selector%init (weight, offset = offset)
            evt%selector_active = .true.
        else
            evt%selector_active = .false.
        end if
    end subroutine evt_resonance_init_selector

```

Return all selector weights, for inspection. Note that the index counts from zero.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: get_selector_weights => evt_resonance_get_selector_weights

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_get_selector_weights (evt, weight)
        class(evt_resonance_t), intent(in) :: evt
        real(default), dimension(0:), intent(out) :: weight
    end subroutine evt_resonance_get_selector_weights

<Resonance insertion: procedures>+≡
    module subroutine evt_resonance_get_selector_weights (evt, weight)
        class(evt_resonance_t), intent(in) :: evt
        real(default), dimension(0:), intent(out) :: weight
        integer :: i
        do i = 0, ubound (weight,1)

```

```

        weight(i) = evt%selector%get_weight (i)
    end do
end subroutine evt_resonance_get_selector_weights

```

32.3.4 Runtime calculations

Use the associated master process instance and the subprocess instances to distribute the current momentum set, then compute the squared matrix elements weights for all subprocesses.

NOTE: Procedures in this subsection are not covered by unit tests in this module, but by unit tests of the `restricted_subprocesses` module.

Fill the particle set, so the momentum configuration can be used by the subprocess instances. The standard workflow is to copy from the previous particle set.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: fill_momenta => evt_resonance_fill_momenta

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_fill_momenta (evt)
        class(evt_resonance_t), intent(inout) :: evt
    end subroutine evt_resonance_fill_momenta

<Resonance insertion: procedures>+≡
    module subroutine evt_resonance_fill_momenta (evt)
        class(evt_resonance_t), intent(inout) :: evt
        integer :: i, n
        if (associated (evt%previous)) then
            evt%particle_set = evt%previous%particle_set
        else if (associated (evt%process_instance)) then
            ! this branch only for unit test
            call evt%process_instance%get_trace &
                (evt%particle_set, i_term=1, n_incoming=evt%process%get_n_in ())
        end if
    end subroutine evt_resonance_fill_momenta

```

Return the indices of those subprocesses which can be considered on-shell. The result depends on the stored particle set (outgoing momenta) and on the on-shell limit value.

The index `evt%selected_component` identifies the particular history set that corresponds to the given process component. Recall that process components may have different external particles, so they have distinct history sets.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: determine_on_shell_histories &
        => evt_resonance_determine_on_shell_histories

<Resonance insertion: sub interfaces>+≡
    module subroutine evt_resonance_determine_on_shell_histories &
        (evt, index_array)
        class(evt_resonance_t), intent(in) :: evt
        integer, dimension(:), allocatable, intent(out) :: index_array
    end subroutine evt_resonance_determine_on_shell_histories

```

```

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_determine_on_shell_histories &
    (evt, index_array)
    class(evt_resonance_t), intent(in) :: evt
    integer, dimension(:), allocatable, intent(out) :: index_array
    integer :: i
    i = evt%selected_component
    call evt%res_history_set(i)%determine_on_shell_histories &
      (evt%particle_set%get_outgoing_momenta (), &
       evt%on_shell_limit, &
       index_array)
  end subroutine evt_resonance_determine_on_shell_histories

```

Evaluate selected subprocesses. (In actual operation, the ones that have been tagged as on-shell.)

We assume that the MCI, term, and channel indices for the subprocesses can all be set to 1.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: evaluate_subprocess => evt_resonance_evaluate_subprocess

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_evaluate_subprocess (evt, index_array)
    class(evt_resonance_t), intent(inout) :: evt
    integer, dimension(:), intent(in) :: index_array
  end subroutine evt_resonance_evaluate_subprocess

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_evaluate_subprocess (evt, index_array)
    class(evt_resonance_t), intent(inout) :: evt
    integer, dimension(:), intent(in) :: index_array
    integer :: k, i
    if (allocated (evt%instance)) then
      do k = 1, size (index_array)
        i = index_array(k)
        associate (instance => evt%instance(i)%p)
          call instance%choose_mci (1)
          call instance%set_trace (evt%particle_set, 1, check_match=.false.)
          call instance%recover (channel = 1, i_term = 1, &
                                update_sqme = .true., recover_phs = .false.)
        end associate
      end do
    end if
  end subroutine evt_resonance_evaluate_subprocess

```

Return the current squared matrix-element value of the master process, and of the selected resonant subprocesses, respectively.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: get_master_sqme => evt_resonance_get_master_sqme
  procedure :: get_subprocess_sqme => evt_resonance_get_subprocess_sqme

<Resonance insertion: sub interfaces>+≡
  module function evt_resonance_get_master_sqme (evt) result (sqme)
    class(evt_resonance_t), intent(in) :: evt
    real(default) :: sqme

```

```

end function evt_resonance_get_master_sqme
module subroutine evt_resonance_get_subprocess_sqme (evt, sqme, index_array)
  class(evt_resonance_t), intent(in) :: evt
  real(default), dimension(:), intent(out) :: sqme
  integer, dimension(:), intent(in), optional :: index_array
end subroutine evt_resonance_get_subprocess_sqme

<Resonance insertion: procedures>+≡
module function evt_resonance_get_master_sqme (evt) result (sqme)
  class(evt_resonance_t), intent(in) :: evt
  real(default) :: sqme
  sqme = evt%process_instance%get_sqme ()
end function evt_resonance_get_master_sqme

module subroutine evt_resonance_get_subprocess_sqme (evt, sqme, index_array)
  class(evt_resonance_t), intent(in) :: evt
  real(default), dimension(:), intent(out) :: sqme
  integer, dimension(:), intent(in), optional :: index_array
  integer :: k, i
  if (present (index_array)) then
    sqme = 0
    do k = 1, size (index_array)
      call get_sqme (index_array(k))
    end do
  else
    do i = 1, size (evt%instance)
      call get_sqme (i)
    end do
  end if
contains
  subroutine get_sqme (i)
    integer, intent(in) :: i
    associate (instance => evt%instance(i)%p)
      sqme(i) = instance%get_sqme ()
    end associate
  end subroutine get_sqme
end subroutine evt_resonance_get_subprocess_sqme

```

Apply a turnoff factor for off-shell kinematics to the sqme values. The sqme array indices are offset from the resonance history set entries.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: apply_turnoff_factor => evt_resonance_apply_turnoff_factor

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_apply_turnoff_factor &
    (evt, sqme, index_array)
    class(evt_resonance_t), intent(in) :: evt
    real(default), dimension(:), intent(inout) :: sqme
    integer, dimension(:), intent(in) :: index_array
  end subroutine evt_resonance_apply_turnoff_factor

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_apply_turnoff_factor (evt, sqme, index_array)
    class(evt_resonance_t), intent(in) :: evt
    real(default), dimension(:), intent(inout) :: sqme

```

```

integer, dimension(:), intent(in) :: index_array
integer :: k, i_res, i_prc
do k = 1, size (index_array)
  i_res = evt%selected_component
  i_prc = index_array(k) + evt%index_offset(i_res)
  sqme(i_prc) = sqme(i_prc) &
    * evt%res_history_set(i_res)%evaluate_gaussian &
    & (evt%particle_set%get_outgoing_momenta (), &
    & evt%on_shell_turnoff, index_array(k))
end do
end subroutine evt_resonance_apply_turnoff_factor

```

We use the calculations of resonant matrix elements to determine probabilities for all applicable resonance configurations. This method combines the steps implemented above.

First, we determine the selected process component.

TODO: the version below selects the first component which is found active. This make sense only for standard LO process components, where exactly one component corresponds to a MCI set.

For the selected process component, we query the kinematics and determine the applicable resonance histories. We collect squared matrix elements for those resonance histories and compare them to the master-process squared matrix element.

The result is the probability for each resonance history together with the probability for non-resonant background (zeroth entry). The latter is defined as the difference between the complete process result and the sum of the resonances, ignoring the possibility for interference. If the complete process result is actually undershooting the sum of resonances, we nevertheless count the background with positive probability.

When looking up the subprocess sqme, we must add the `index_offset` to the resulting array, since the indices returned by the individual history set all count from one, while the subprocess instances that belong to process components are collected in one flat array.

After determining matrix elements and background, we may reduce the weight of the matrix elements in the selector by applying a turnoff factor.

The factor `background_factor` indicates whether to include the background contribution at all, as long as there is a nonvanishing resonance contribution. Note that instead of setting background to zero, we just multiply it by a very small number. This ensures that indices are assigned correctly, and that background will eventually be selected if smooth turnoff is chosen.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: compute_probabilities => evt_resonance_compute_probabilities

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_compute_probabilities (evt)
    class(evt_resonance_t), intent(inout) :: evt
  end subroutine evt_resonance_compute_probabilities

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_compute_probabilities (evt)
    class(evt_resonance_t), intent(inout) :: evt
    integer, dimension(:), allocatable :: index_array

```

```

real(default) :: sqme_master, sqme_sum, sqme_bg
real(default), dimension(:), allocatable :: sqme_res
integer :: n, ic
if (.not. associated (evt%process_instance)) return
n = size (evt%instance)
call evt%select_component (0)
FIND_ACTIVE_COMPONENT: do ic = 1, evt%process%get_n_components ()
    if (evt%process%component_is_selected (ic)) then
        call evt%select_component (ic)
        exit FIND_ACTIVE_COMPONENT
    end if
end do FIND_ACTIVE_COMPONENT
if (evt%selected_component > 0) then
    call evt%determine_on_shell_histories (index_array)
else
    allocate (index_array (0))
end if
call evt%evaluate_subprocess &
    (index_array + evt%index_offset(evt%selected_component))
allocate (sqme_res (n), source = 0._default)
call evt%get_subprocess_sqme &
    (sqme_res, index_array + evt%index_offset(evt%selected_component))
sqme_master = evt%get_master_sqme ()
sqme_sum = sum (sqme_res)
sqme_bg = abs (sqme_master - sqme_sum)
if (evt%on_shell_turnoff > 0) then
    call evt%apply_turnoff_factor (sqme_res, index_array)
end if
if (any (sqme_res > 0)) then
    sqme_bg = sqme_bg * evt%background_factor
end if
call evt%init_selector ([sqme_bg, sqme_res], offset = -1)
end subroutine evt_resonance_compute_probabilities

```

Set the selected component (unit tests).

(Resonance insertion: evt_resonance: TBP)+≡

```

procedure :: select_component => evt_resonance_select_component

```

(Resonance insertion: sub interfaces)+≡

```

module subroutine evt_resonance_select_component (evt, i_component)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_component
end subroutine evt_resonance_select_component

```

(Resonance insertion: procedures)+≡

```

module subroutine evt_resonance_select_component (evt, i_component)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_component
    evt%selected_component = i_component
end subroutine evt_resonance_select_component

```


32.3.5 Sanity check

Check the color assignment, which may be wrong for the inserted resonances. Delegated to the particle-set component. Return offending particle indices and, optionally, particles as arrays.

This is done in a unit test. The current algorithm, i.e., selecting the color assignment from the resonant-subprocess instance, should not generate invalid color assignments.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: find_prt_invalid_color => evt_resonance_find_prt_invalid_color

(Resonance insertion: sub interfaces)+≡
  module subroutine evt_resonance_find_prt_invalid_color (evt, index, prt)
    class(evt_resonance_t), intent(in) :: evt
    integer, dimension(:), allocatable, intent(out) :: index
    type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
  end subroutine evt_resonance_find_prt_invalid_color

(Resonance insertion: procedures)+≡
  module subroutine evt_resonance_find_prt_invalid_color (evt, index, prt)
    class(evt_resonance_t), intent(in) :: evt
    integer, dimension(:), allocatable, intent(out) :: index
    type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
    if (evt%particle_set_exists) then
      call evt%particle_set%find_prt_invalid_color (index, prt)
    else
      allocate (prt (0))
    end if
  end subroutine evt_resonance_find_prt_invalid_color
```

32.3.6 API implementation

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: prepare_new_event => evt_resonance_prepare_new_event

(Resonance insertion: sub interfaces)+≡
  module subroutine evt_resonance_prepare_new_event (evt, i_mci, i_term)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_resonance_prepare_new_event

(Resonance insertion: procedures)+≡
  module subroutine evt_resonance_prepare_new_event (evt, i_mci, i_term)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_resonance_prepare_new_event
```

Select one of the histories, based on the momentum array from the current particle set. Compute the probabilities for all resonant subprocesses and initialize the selector accordingly. Then select one resonance history, or none.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: generate_weighted => evt_resonance_generate_weighted
```

```

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_generate_weighted (evt, probability)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
  end subroutine evt_resonance_generate_weighted

<Resonance insertion: procedures>+≡
  module subroutine evt_resonance_generate_weighted (evt, probability)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    integer :: i_term
    call evt%fill_momenta ()
    call evt%compute_probabilities ()
    if (associated (evt%process_instance)) then
      i_term = evt%process_instance%get_first_active_i_term ()
      if (evt%process_instance%term(i_term)%passed) then
        call evt%selector%generate (evt%rng, evt%selected_history)
      end if
    else
      call evt%selector%generate (evt%rng, evt%selected_history)
    end if
    probability = 1
  end subroutine evt_resonance_generate_weighted

```

Here take the current particle set and insert resonance intermediate states if applicable. The resonance history has already been chosen by the generator above. If no resonance history applies, just retain the particle set.

If a resonance history applies, we factorize the exclusive interaction of the selected (resonance-process) process instance. With a temporary particle set `pvt_set` as workspace, we then insert the resonances, reinstate parent-child relations and set colors and momenta for the resonances. The temporary is then copied back.

Taking the event data from the resonant subprocess instead of the master process, guarantees that all flavor, helicity, and color assignments are valid for the selected resonance history. Note that the transform may thus choose a quantum-number combination that is different from the one chosen by the master process.

The `i_term` value for the selected subprocess instance is always 1. We support only LO process. For those, the master process may have several terms (= components) that correspond to different external states. The subprocesses are distinct, each one corresponds to a definite master component, and by itself it consists of a single component/term.

However, if the selector chooses resonance history #0, i.e., no resonance, we just copy the particle set from the previous (i.e., trivial) event transform and ignore all subprocess data.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: make_particle_set => evt_resonance_make_particle_set

<Resonance insertion: sub interfaces>+≡
  module subroutine evt_resonance_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode

```

```

        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
    end subroutine evt_resonance_make_particle_set

    (Resonance insertion: procedures)+≡
    module subroutine evt_resonance_make_particle_set &
        (evt, factorization_mode, keep_correlations, r)
        class(evt_resonance_t), intent(inout) :: evt
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
        type(particle_set_t), target :: prt_set
        type(particle_t), dimension(:), allocatable :: prt
        integer :: n_beam, n_in, n_vir, n_res, n_out, i, i_res, i_term, i_tree
        type(interaction_t), pointer :: int_matrix, int_flows
        integer, dimension(:), allocatable :: map
        type(resonance_tree_t) :: res_tree
        if (associated (evt%previous)) then
            if (evt%previous%particle_set_exists) then
                if (evt%selected_history > 0) then
                    if (allocated (evt%instance)) then
                        associate (instance => evt%instance(evt%selected_history)%p)
                            call instance%evaluate_event_data (weight = 1._default)
                            i_term = 1
                            int_matrix => instance%get_matrix_int_ptr (i_term)
                            int_flows => instance%get_flows_int_ptr (i_term)
                            call evt%factorize_interactions (int_matrix, int_flows, &
                                factorization_mode, keep_correlations, r)
                            call evt%tag_incoming ()
                        end associate
                    else ! this branch only for unit test
                        evt%particle_set = evt%previous%particle_set
                    end if
                    i_tree = evt%selected_history &
                        - evt%index_offset(evt%selected_component)
                    call evt%res_history_set(evt%selected_component)%get_tree &
                        (i_tree, res_tree)
                    n_beam = evt%particle_set%get_n_beam ()
                    n_in = evt%particle_set%get_n_in ()
                    n_vir = evt%particle_set%get_n_vir ()
                    n_out = evt%particle_set%get_n_out ()
                    n_res = res_tree%get_n_resonances ()
                    allocate (map (n_beam + n_in + n_vir + n_out))
                    map(1:n_beam+n_in+n_vir) &
                        = [(i, i = 1, n_beam+n_in+n_vir)]
                    map(n_beam+n_in+n_vir+1:n_beam+n_in+n_vir+n_out) &
                        = [(i + n_res, &
                            & i = n_beam+n_in+n_vir+1, &
                            & n_beam+n_in+n_vir+n_out)]
                    call prt_set%transfer (evt%particle_set, n_res, map)
                    do i = 1, n_res
                        i_res = n_beam + n_in + n_vir + i
                        call prt_set%insert (i_res, &
                            PRT_RESONANT, &
                            res_tree%get_flv (i), &

```

```

        res_tree%get_children (i, &
            & n_beam+n_in+n_vir, n_beam+n_in+n_vir+n_res))
    end do
    do i = n_res, 1, -1
        i_res = n_beam + n_in + n_vir + i
        call prt_set%recover_color (i_res)
    end do
    call prt_set%set_momentum &
        (map(:), evt%particle_set%get_momenta (), on_shell = .true.)
    do i = n_res, 1, -1
        i_res = n_beam + n_in + n_vir + i
        call prt_set%recover_momentum (i_res)
    end do
    call evt%particle_set%final ()
    evt%particle_set = prt_set
    call prt_set%final ()
    evt%particle_set_exists = .true.
else ! retain particle set, as copied from previous evt
    evt%particle_set_exists = .true.
end if
else
    evt%particle_set_exists = .false.
end if
else
    evt%particle_set_exists = .false.
end if
end subroutine evt_resonance_make_particle_set

```

32.3.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<resonance_insertion_ut.f90>≡
  <File header>

  module resonance_insertion_ut
    use unit_tests
    use resonance_insertion_uti

    <Standard module head>

    <Resonance insertion: public test>

    contains

    <Resonance insertion: test driver>

  end module resonance_insertion_ut
<resonance_insertion_uti.f90>≡
  <File header>

  module resonance_insertion_uti

```

```

<Use kinds>
<Use strings>
  use format_utils, only: write_separator
  use os_interface
  use lorentz
  use rng_base, only: rng_t
  use flavors, only: flavor_t
  use colors, only: color_t
  use models, only: syntax_model_file_init, syntax_model_file_final
  use models, only: model_list_t, model_t
  use particles, only: particle_t, particle_set_t

  use resonances, only: resonance_info_t
  use resonances, only: resonance_history_t
  use resonances, only: resonance_history_set_t

  use event_transforms
  use resonance_insertion

  use rng_base_ut, only: rng_test_t

<Standard module head>

<Resonance insertion: test declarations>

contains

<Resonance insertion: tests>

end module resonance_insertion_util

```

API: driver for the unit tests below.

```

<Resonance insertion: public test>≡
  public :: resonance_insertion_test

<Resonance insertion: test driver>≡
  subroutine resonance_insertion_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Resonance insertion: execute tests>
  end subroutine resonance_insertion_test

```

Test resonance insertion as event transform

Insert a resonance (W boson) into an event with momentum assignment.

```

<Resonance insertion: execute tests>≡
  call test (resonance_insertion_1, "resonance_insertion_1", &
    "simple resonance insertion", &
    u, results)

<Resonance insertion: test declarations>≡
  public :: resonance_insertion_1

```

<Resonance insertion: tests>≡

```

subroutine resonance_insertion_1 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(particle_set_t) :: pset
  type(model_list_t) :: model_list
  type(model_t), pointer :: model
  type(resonance_info_t) :: res_info
  type(resonance_history_t) :: res_history
  type(resonance_history_set_t), dimension(1) :: res_history_set
  type(evt_trivial_t), target :: evt_trivial
  type(evt_resonance_t), target :: evt_resonance
  type(flavor_t) :: fw
  type(color_t) :: col
  real(default) :: mw, ew, pw
  type(vector4_t), dimension(5) :: p
  class(rng_t), allocatable :: rng
  real(default) :: probability
  integer, dimension(:), allocatable :: i_invalid
  type(particle_t), dimension(:), allocatable :: prt_invalid
  integer :: i

  write (u, "(A)")  "* Test output: resonance_insertion_1"
  write (u, "(A)")  "* Purpose: apply simple resonance insertion"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize environment"
  write (u, "(A)")

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
     os_data, model)
  ! reset slightly in order to avoid a rounding ambiguity
  call model%set_real (var_str ("mW"), 80.418_default)

  write (u, "(A)")  "* Initialize particle set"
  write (u, "(A)")

  call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
    pdg = [1, -1, 1, -2, 24], model = model)

  call fw%init (24, model)

  mw = fw%get_mass ()
  ew = 200._default
  pw = sqrt (ew**2 - mw**2)

  p(1) = vector4_moving (ew, ew, 3)
  p(2) = vector4_moving (ew,-ew, 3)
  p(3) = vector4_moving (ew/2, vector3_moving ([pw/2, mw/2, 0._default]))
  p(4) = vector4_moving (ew/2, vector3_moving ([pw/2,-mw/2, 0._default]))
  p(5) = vector4_moving (ew, vector3_moving ([-pw, 0._default, 0._default]))

```

```

call pset%set_momentum (p, on_shell = .true.)

call col%init_col_acl (1,0)
call pset%set_color (1, col)

call col%init_col_acl (0,1)
call pset%set_color (2, col)

call col%init_col_acl (2,0)
call pset%set_color (3, col)

call col%init_col_acl (0,2)
call pset%set_color (4, col)

call col%init_col_acl (0,0)
call pset%set_color (5, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 2)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"

```

```

write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)") "Event probability =", probability

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)") "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
  write (u, "(2x,A)") "[none]"
case default
  do i = 1, size (prt_invalid)
    write (u, "(1x,A,1x,I0)", advance="no") "Particle", i_invalid(i)
    call prt_invalid(i)%write (u)
  end do
end select

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: resonance_insertion_1"

end subroutine resonance_insertion_1

```

Resonance insertion with color mismatch

Same as previous test (but no momenta); resonance insertion should fail because of color mismatch: W boson is color-neutral.

```

<Resonance insertion: execute tests>+≡
  call test (resonance_insertion_2, "resonance_insertion_2", &
    "resonance color mismatch", &
    u, results)

<Resonance insertion: test declarations>+≡
  public :: resonance_insertion_2

<Resonance insertion: tests>+≡
  subroutine resonance_insertion_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data

```



```

type(particle_set_t) :: pset
type(model_list_t) :: model_list
type(model_t), pointer :: model
type(resonance_info_t) :: res_info
type(resonance_history_t) :: res_history
type(resonance_history_set_t), dimension(1) :: res_history_set
type(evt_trivial_t), target :: evt_trivial
type(evt_resonance_t), target :: evt_resonance
type(color_t) :: col
class(rng_t), allocatable :: rng
real(default) :: probability
type(particle_t), dimension(:), allocatable :: prt_invalid
integer, dimension(:), allocatable :: i_invalid
integer :: i

write (u, "(A)")  "* Test output: resonance_insertion_2"
write (u, "(A)")  "* Purpose: resonance insertion with color mismatch"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
    pdg = [1, -1, 1, -2, 24], model = model)

call col%init_col_acl (1,0)
call pset%set_color (1, col)

call col%init_col_acl (0,2)
call pset%set_color (2, col)

call col%init_col_acl (1,0)
call pset%set_color (3, col)

call col%init_col_acl (0,2)
call pset%set_color (4, col)

call col%init_col_acl (0,0)
call pset%set_color (5, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)

```

```

call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 2)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)")  "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
    write (u, "(2x,A)")  "[none]"
case default
    do i = 1, size (prt_invalid)
        write (u, "(1x,A,1x,I0)", advance="no")  "Particle", i_invalid(i)
        call prt_invalid(i)%write (u)
    end do

```

```

end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_2"

end subroutine resonance_insertion_2

```

Complex resonance history

This is the resonance history $u\bar{u} \rightarrow (t \rightarrow W^+b) + (\bar{t} \rightarrow (h \rightarrow b\bar{b}) + (\bar{t}^* \rightarrow W^- \bar{b}))$.

```

<Resonance insertion: execute tests>+≡
  call test (resonance_insertion_3, "resonance_insertion_3", &
    "complex resonance history", &
    u, results)

<Resonance insertion: test declarations>+≡
  public :: resonance_insertion_3

<Resonance insertion: tests>+≡
  subroutine resonance_insertion_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(evt_trivial_t), target :: evt_trivial
    type(evt_resonance_t), target :: evt_resonance
    type(color_t) :: col
    class(rng_t), allocatable :: rng
    real(default) :: probability
    type(particle_t), dimension(:), allocatable :: prt_invalid
    integer, dimension(:), allocatable :: i_invalid
    integer :: i

    write (u, "(A)")  "* Test output: resonance_insertion_3"
    write (u, "(A)")  "* Purpose: resonance insertion with color mismatch"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &

```

```

        (var_str ("SM"), var_str ("SM.mdl"), &
        os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 6, &
        pdg = [2, -2, 24, 5, 5, -5, -24, -5], model = model)

call col%init_col_acl (1,0)
call pset%set_color (1, col)

call col%init_col_acl (0,2)
call pset%set_color (2, col)

call col%init_col_acl (0,0)
call pset%set_color (3, col)

call col%init_col_acl (1,0)
call pset%set_color (4, col)

call col%init_col_acl (3,0)
call pset%set_color (5, col)

call col%init_col_acl (0,3)
call pset%set_color (6, col)

call col%init_col_acl (0,0)
call pset%set_color (7, col)

call col%init_col_acl (0,2)
call pset%set_color (8, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, 6, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (12, 25, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (60, -6, model, 6)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)

```

```

call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)")  "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
    write (u, "(2x,A)")  "[none]"
case default
    do i = 1, size (prt_invalid)
        write (u, "(1x,A,1x,I0)", advance="no")  "Particle", i_invalid(i)
        call prt_invalid(i)%write (u)
    end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_3"

end subroutine resonance_insertion_3

```

Resonance history selection

Another test with zero momenta: select one of several resonant channels using the selector component.

```
(Resonance insertion: execute tests)+≡
    call test (resonance_insertion_4, "resonance_insertion_4", &
        "resonance history selection", &
        u, results)

(Resonance insertion: test declarations)+≡
    public :: resonance_insertion_4

(Resonance insertion: tests)+≡
    subroutine resonance_insertion_4 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        type(color_t) :: col
        class(rng_t), allocatable :: rng
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: resonance_insertion_4"
        write (u, "(A)")  "* Purpose: resonance history selection"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM"), var_str ("SM.mdl"), &
            os_data, model)

        write (u, "(A)")  "* Initialize particle set"
        write (u, "(A)")

        call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 4, &
            pdg = [1, -1, 1, -2, -3, 4], model = model)

        write (u, "(A)")  "* Fill trivial event transform"
        write (u, "(A)")

        call evt_trivial%reset ()
        call evt_trivial%set_particle_set (pset, 1, 1)
        call evt_trivial%write (u)
        call write_separator (u, 2)
```

```

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 4)
call res_history%add_resonance (res_info)
call res_info%init (15, 25, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

do i = 1, 6
  write (u, "(A,1x,I0)")  "* Event #", i
  write (u, "(A)")

  call evt_resonance%prepare_new_event (1, 1)
  call evt_resonance%init_selector ([1._default, 2._default, 1._default])
  call evt_resonance%generate_weighted (probability)
  call evt_resonance%make_particle_set (0, .false.)

  call evt_resonance%write (u)
  write (u, "(A)")

```

```

end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_4"

end subroutine resonance_insertion_4

```

Resonance history selection

Another test with zero momenta: select either a resonant channel or no resonance.

```

<Resonance insertion: execute tests>+≡
  call test (resonance_insertion_5, "resonance_insertion_5", &
    "resonance history on/off", &
    u, results)

<Resonance insertion: test declarations>+≡
  public :: resonance_insertion_5

<Resonance insertion: tests>+≡
  subroutine resonance_insertion_5 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(evt_trivial_t), target :: evt_trivial
    type(evt_resonance_t), target :: evt_resonance
    type(color_t) :: col
    class(rng_t), allocatable :: rng
    real(default) :: probability
    integer :: i

    write (u, "(A)")  "* Test output: resonance_insertion_5"
    write (u, "(A)")  "* Purpose: resonance history selection including no resonance"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &

```



```

        (var_str ("SM"), var_str ("SM.mdl"), &
        os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 4, &
        pdg = [1, -1, 1, -2, -3, 4], model = model)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)

write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)

write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

do i = 1, 2
    write (u, "(A,1x,I0)")  "* Event #", i
    write (u, "(A)")

    call evt_resonance%prepare_new_event (1, 1)
    call evt_resonance%init_selector ([1._default, 3._default], offset = -1)
    call evt_resonance%generate_weighted (probability)
    call evt_resonance%make_particle_set (0, .false.)

    call evt_resonance%write (u)
    write (u, "(A)")
end do

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_5"

end subroutine resonance_insertion_5

```

Resonance insertion with structured beams

Insert a resonance (W boson) into an event with beam and virtual particles.

```

<Resonance insertion: execute tests>+≡
  call test (resonance_insertion_6, "resonance_insertion_6", &
    "resonance insertion with beam structure", &
    u, results)

<Resonance insertion: test declarations>+≡
  public :: resonance_insertion_6

<Resonance insertion: tests>+≡
  subroutine resonance_insertion_6 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(particle_set_t) :: pset
    type(model_t), pointer :: model
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(evt_trivial_t), target :: evt_trivial
    type(evt_resonance_t), target :: evt_resonance
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: resonance_insertion_6"
    write (u, "(A)")  "* Purpose: resonance insertion with structured beams"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

```

```

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
    pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, 23, model, 2)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_inseersion_6"

end subroutine resonance_inseersion_6

```

32.4 Recoil kinematics

```

⟨recoil_kinematics.f90⟩≡
  ⟨File header⟩

  module recoil_kinematics

    ⟨Use kinds⟩
    use lorentz, only: vector4_t
    use lorentz, only: vector4_null
    use lorentz, only: vector4_moving
    use lorentz, only: vector3_moving
    use lorentz, only: transverse_part
    use lorentz, only: lorentz_transformation_t
    use lorentz, only: inverse
    use lorentz, only: boost
    use lorentz, only: transformation
    use lorentz, only: operator(+)
    use lorentz, only: operator(-)
    use lorentz, only: operator(*)
    use lorentz, only: operator(**)
    use lorentz, only: lambda

    ⟨Standard module head⟩

    ⟨Recoil kinematics: public⟩

    ⟨Recoil kinematics: parameters⟩

    ⟨Recoil kinematics: types⟩

    interface
    ⟨Recoil kinematics: sub interfaces⟩
    end interface

  end module recoil_kinematics

⟨recoil_kinematics_sub.f90⟩≡
  ⟨File header⟩

  submodule (recoil_kinematics) recoil_kinematics_s

```

```

    use constants, only: twopi

    implicit none

contains

    <Recoil kinematics: procedures>

end submodule recoil_kinematics_s

```

32.4.1 ϕ sampler

This is trivial. Generate an azimuthal angle, given a $(0,1)$ RNG parameter.

```

    <Recoil kinematics: procedures>≡
    elemental subroutine generate_phi_recoil (r, phi)
        real(default), intent(in) :: r
        real(default), intent(out) :: phi

        phi = r * twopi

    end subroutine generate_phi_recoil

```

32.4.2 Q^2 sampler

The dynamics of factorization suggests to generate a flat Q^2 distribution from a (random) number, event by event.

At the lowest momentum transfer values, the particle (electron) mass sets a smooth cutoff. The formula can produce Q values below the electron mass, down to zero, but with a power distribution that eventually evolves into the expected logarithmic distribution for $Q^2 > m^2$.

We are talking about the absolute value here, so all Q^2 values are positive. For the actual momentum transfer, $q^2 = -Q^2$.

```

    <Recoil kinematics: public>≡
    public :: generate_q2_recoil

    <Recoil kinematics: sub interfaces>≡
    elemental module subroutine generate_q2_recoil (s, x_bar, q2_max, m2, r, q2)
        real(default), intent(in) :: s
        real(default), intent(in) :: q2_max
        real(default), intent(in) :: x_bar
        real(default), intent(in) :: m2
        real(default), intent(in) :: r
        real(default), intent(out) :: q2
    end subroutine generate_q2_recoil

    <Recoil kinematics: procedures>+≡
    elemental module subroutine generate_q2_recoil (s, x_bar, q2_max, m2, r, q2)
        real(default), intent(in) :: s
        real(default), intent(in) :: q2_max
        real(default), intent(in) :: x_bar
        real(default), intent(in) :: m2

```

```

real(default), intent(in) :: r
real(default), intent(out) :: q2

real(default) :: q2_max_evt

q2_max_evt = q2_max_event (s, x_bar, q2_max)

q2 = m2 * (exp (r * log (1 + (q2_max_evt / m2))) - 1)

end subroutine generate_q2_recoil

```

The Q distribution is cut off from above by the kinematic limit, which depends on the energy that is available for the radiated photon, or by a user-defined cutoff – whichever is less. The kinematic limit fits the formulas for recoil momenta (see below), and it also implicitly enters the ISR collinear structure function, so the normalization of the distribution should be correct.

(Recoil kinematics: procedures)+≡

```

elemental function q2_max_event (s, x_bar, q2_max) result (q2)
  real(default), intent(in) :: s
  real(default), intent(in) :: x_bar
  real(default), intent(in) :: q2_max
  real(default) :: q2

  q2 = min (x_bar * s, q2_max)

end function q2_max_event

```

32.4.3 Kinematics functions

Given values for energies, $Q_{1,2}^2$, azimuthal angle, compute the matching polar angle of the radiating particle. The subroutine returns $\sin\theta$ and $\cos\theta$.

(Recoil kinematics: procedures)+≡

```

subroutine polar_angles (s, xb, rho, ee, q2, sin_th, cos_th, ok)
  real(default), intent(in) :: s
  real(default), intent(in) :: xb
  real(default), intent(in) :: rho
  real(default), dimension(2), intent(in) :: ee
  real(default), dimension(2), intent(in) :: q2
  real(default), dimension(2), intent(out) :: sin_th
  real(default), dimension(2), intent(out) :: cos_th
  logical, intent(out) :: ok

  real(default), dimension(2) :: sin2_th_2

  sin2_th_2 = q2 / (ee * rho * xb * s)

  if (all (sin2_th_2 <= 1)) then
    sin_th = 2 * sqrt (sin2_th_2 * (1 - sin2_th_2))
    cos_th = 1 - 2 * sin2_th_2
    ok = .true.
  else

```

```

        sin_th = 0
        cos_th = 1
        ok = .false.
    end if

end subroutine polar_angles

```

Compute the acollinearity parameter λ from azimuthal and polar angles. The result is a number between 0 and 1.

(Recoil kinematics: procedures)+≡

```

function lambda_factor (sin_th, cos_th, cphi) result (lambda)
    real(default), dimension(2), intent(in) :: sin_th
    real(default), dimension(2), intent(in) :: cos_th
    real(default), intent(in) :: cphi
    real(default) :: lambda

    lambda = (1 - cos_th(1) * cos_th(2) - cphi * sin_th(1) * sin_th(2)) / 2

end function lambda_factor

```

Compute the factor that rescales photon energies, such that the radiation angles match the kinematics parameters.

For small values of $\bar{x}/\cosh\eta$, we have to use the Taylor expansion if we do not want to lose precision. The optional argument allows for a unit test that compares exact and approximate.

(Recoil kinematics: procedures)+≡

```

function scale_factor (che, lambda, xb0, approximate) result (rho)
    real(default), intent(in) :: che
    real(default), intent(in) :: lambda
    real(default), intent(in) :: xb0
    logical, intent(in), optional :: approximate
    real(default) :: rho

    real(default), parameter :: &
        e0 = (100 * epsilon (1._default)) ** (0.3_default)
    logical :: approx

    if (present (approximate)) then
        approx = approximate
    else
        approx = (xb0/che) < e0
    end if

    if (approx) then
        rho = 1 - lambda * (xb0/(2*che)) * (1 + (1-lambda) * (xb0/che))
    else
        rho = (che / ((1-lambda)*xb0)) &
            * (1 - sqrt (1 - 2 * (1-lambda) * (xb0/che) &
                & + (1-lambda) * (xb0 / che)**2))
    end if

end function scale_factor

```

The code snippet below is not used anywhere, but may be manually inserted in a unit test to numerically verify the approximation above.

```

<Recoil kinematics: extra test code>≡
    write (u, "(A)")
    write (u, "(A)") "*** Table: scale factor calculation"
    write (u, "(A)")

    lambda = 0.25_default
    write (u, FMT1) "lambda =", lambda

    che = 4._default
    write (u, FMT1) "che   =", che

    write (u, "(A)") "   x0    rho(exact)    rho(approx)    rho(chosen)"
    xb0 = 1._default
    do i = 1, 30
        xb0 = xb0 / 10
        write (u, FMT4)  xb0, &
            scale_factor (che, lambda, xb0, approximate=.false.), &
            scale_factor (che, lambda, xb0, approximate=.true.), &
            scale_factor (che, lambda, xb0)
    end do

```

Compute the current values for the $x_{1,2}$ parameters, given the updated scale factor ρ and the collinear parameters.

```

<Recoil kinematics: procedures>+≡
    subroutine scaled_x (rho, ee, xb0, x, xb)
        real(default), intent(in) :: rho
        real(default), dimension(2), intent(in) :: ee
        real(default), intent(in) :: xb0
        real(default), dimension(2), intent(out) :: x
        real(default), dimension(2), intent(out) :: xb

        xb = rho * ee * xb0
        x = 1 - xb

    end subroutine scaled_x

```

32.4.4 Iterative solution of kinematics constraints

Find a solution of the kinematics constraints. We know the parameters appropriate for collinear kinematics \sqrt{s} , $x_{1,2}^c$. We have picked values vor the momentum transfer $Q_{1,2}$ and the azimuthal angles $\phi_{1,2}$. The solution consists of modified energy fractions $x_{1,2}$ and polar angles $\theta_{1,2}$.

If the computation fails, which can happen for large momentum transfer, the flag `ok` will indicate this.

```

<Recoil kinematics: public>+≡
    public :: solve_recoil

<Recoil kinematics: sub interfaces>+≡
    module subroutine solve_recoil &
        (sqrts, xc, xcb, phi, q2, x, xb, cos_th, sin_th, ok)

```



```

    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xcb
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: q2
    real(default), dimension(2), intent(out) :: x
    real(default), dimension(2), intent(out) :: xb
    real(default), dimension(2), intent(out) :: cos_th
    real(default), dimension(2), intent(out) :: sin_th
    logical, intent(out) :: ok
end subroutine solve_recoil

```

(Recoil kinematics: procedures)+≡

```

module subroutine solve_recoil &
    (sqrts, xc, xcb, phi, q2, x, xb, cos_th, sin_th, ok)
    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xcb
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: q2
    real(default), dimension(2), intent(out) :: x
    real(default), dimension(2), intent(out) :: xb
    real(default), dimension(2), intent(out) :: cos_th
    real(default), dimension(2), intent(out) :: sin_th
    logical, intent(out) :: ok

    real(default) :: s
    real(default), dimension(2) :: ee
    real(default), dimension(2) :: th
    real(default) :: xb0, cphi
    real(default) :: che, lambda
    real(default) :: rho_new, rho, rho_old
    real(default) :: dr_old, dr_new
    real(default), parameter :: dr_limit = 100 * epsilon (1._default)
    integer, parameter :: n_it_max = 20
    integer :: i

    ok = .true.

    s = sqrts**2
    ee = sqrt ([xcb(1)/xcb(2), xcb(2)/xcb(1)])
    che = sum (ee) / 2
    xb0 = sqrt (xcb(1) * xcb(2))
    cphi = cos (phi(1) - phi(2))

    rho_old = 10
    rho = 1
    th = 0
    sin_th = sin (th)
    cos_th = cos (th)
    lambda = lambda_factor (sin_th, cos_th, cphi)
    call scaled_x (rho, ee, xb0, x, xb)

    iterate_loop: do i = 1, n_it_max

```

```

    call polar_angles (s, xb0, rho, ee, q2, sin_th, cos_th, ok)
    if (.not. ok) return
    th = atan2 (sin_th, cos_th)

    lambda = lambda_factor (sin_th, cos_th, cphi)
    rho_new = scale_factor (che, lambda, xb0)
    call scaled_x (rho_new, ee, xb0, x, xb)

    dr_old = abs (rho - rho_old)
    dr_new = abs (rho_new - rho)

    rho_old = rho
    rho = rho_new

    if (dr_new < dr_limit .or. dr_new >= dr_old) exit iterate_loop

end do iterate_loop

end subroutine solve_recoil

```

With all kinematics parameters known, construct actual four-vectors for the recoil momenta, the off-shell (spacelike) parton momenta, and on-shell projected parton momenta.

```

<Recoil kinematics: public>+≡
  public :: recoil_momenta

<Recoil kinematics: sub interfaces>+≡
  module subroutine recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, &
    km, qm, qo, ok)
    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xb
    real(default), dimension(2), intent(in) :: cos_th
    real(default), dimension(2), intent(in) :: sin_th
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: mo
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm
    type(vector4_t), dimension(2), intent(out) :: qo
    logical, intent(out) :: ok
  end subroutine recoil_momenta

<Recoil kinematics: procedures>+≡
  module subroutine recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, &
    km, qm, qo, ok)
    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xb
    real(default), dimension(2), intent(in) :: cos_th
    real(default), dimension(2), intent(in) :: sin_th
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: mo
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm

```

```

type(vector4_t), dimension(2), intent(out) :: qo
logical, intent(out) :: ok

type(vector4_t), dimension(2) :: pm
type(lorentz_transformation_t) :: lt
real(default) :: sqsh
real(default) :: po4, po2
real(default), dimension(2) :: p0, p3

pm(1) = &
    vector4_moving (sqrts/2, &
    vector3_moving ([0._default, 0._default, sqrts/2]))
pm(2) = &
    vector4_moving (sqrts/2, &
    vector3_moving ([0._default, 0._default, -sqrts/2]))

km(1) = xb(1) * (sqrts/2) * vector4_moving ( &
    1._default, &
    vector3_moving ([ &
    &    sin_th(1) * cos (phi(1)), &
    &    sin_th(1) * sin (phi(1)), &
    &    cos_th(1)]) &
    )
km(2) = xb(2) * (sqrts/2) * vector4_moving ( &
    1._default, &
    vector3_moving ([ &
    &    -sin_th(2) * cos (phi(2)), &
    &    -sin_th(2) * sin (phi(2)), &
    &    -cos_th(2)]) &
    )

qm(1) = pm(1) - km(1)
qm(2) = pm(2) - km(2)

sqsh = sqrt (xc(1)*xc(2)) * sqrts
lt = transformation (3, qm(1), qm(2), sqsh)

po4 = lambda (sqsh**2, mo(1)**2, mo(2)**2)
ok = po4 > 0
if (ok) then
    po2 = sqrt (po4)/4
    p0 = sqrt (po2 + mo**2)
    p3 = [sqrt (po2), -sqrt (po2)]
    qo = lt * vector4_moving (p0, p3, 3)
else
    qo = vector4_null
end if

end subroutine recoil_momenta

```

Compute the Lorentz transformation that we can use to transform any outgoing momenta into the new c.m. system of the incoming partons. Not relying on the previous calculations, we determine the transformation that transforms the

original collinear partons into their c.m. system, and then transform this to the new c.m. system.

```

<Recoil kinematics: public>+≡
    public :: recoil_transformation

<Recoil kinematics: sub interfaces>+≡
    module subroutine recoil_transformation (sqrts, xc, qo, lt)
        real(default), intent(in) :: sqrts
        real(default), dimension(2), intent(in) :: xc
        type(vector4_t), dimension(2), intent(in) :: qo
        type(lorentz_transformation_t), intent(out) :: lt
    end subroutine recoil_transformation

<Recoil kinematics: procedures>+≡
    module subroutine recoil_transformation (sqrts, xc, qo, lt)
        real(default), intent(in) :: sqrts
        real(default), dimension(2), intent(in) :: xc
        type(vector4_t), dimension(2), intent(in) :: qo
        type(lorentz_transformation_t), intent(out) :: lt

        real(default) :: sqsh
        type(vector4_t), dimension(2) :: qc
        type(lorentz_transformation_t) :: ltc, lto

        qc(1) = xc(1) * vector4_moving (sqrts/2, sqrts/2, 3)
        qc(2) = xc(2) * vector4_moving (sqrts/2, -sqrts/2, 3)

        sqsh = sqrt (xc(1) * xc(2)) * sqrts
        ltc = transformation (3, qc(1), qc(2), sqsh)
        lto = transformation (3, qo(1), qo(2), sqsh)
        lt = lto * inverse (ltc)

    end subroutine recoil_transformation

```

Compute the Lorentz boost that transforms the c.m. frame of the momenta into the lab frame where they are given. Also return their common invariant mass, \sqrt{s} .

If the initial momenta are not collinear, `ok` is set false.

```

<Recoil kinematics: public>+≡
    public :: initial_transformation

<Recoil kinematics: sub interfaces>+≡
    module subroutine initial_transformation (p, sqrts, lt, ok)
        type(vector4_t), dimension(2), intent(in) :: p
        real(default), intent(out) :: sqrts
        type(lorentz_transformation_t), intent(out) :: lt
        logical, intent(out) :: ok
    end subroutine initial_transformation

<Recoil kinematics: procedures>+≡
    module subroutine initial_transformation (p, sqrts, lt, ok)
        type(vector4_t), dimension(2), intent(in) :: p
        real(default), intent(out) :: sqrts
        type(lorentz_transformation_t), intent(out) :: lt
        logical, intent(out) :: ok

```

```

ok = all (transverse_part (p) == 0)

sqrtts = (p(1) + p(2)) ** 1
lt = boost (p(1) + p(2), sqrtts)

end subroutine initial_transformation

```

32.4.5 Generate recoil event

Combine the above kinematics calculations. First generate azimuthal angles and momentum transfer, solve kinematics and compute momenta for the radiated photons and the on-shell projected, recoiling partons.

The `mo` masses are used for the on-shell projection of the partons after radiation. They may be equal to `m`, or set to zero.

If `ok` is false, the data point has failed and we should repeat the procedure for a new set of RNG parameters `r`.

```

<Recoil kinematics: public>+≡
  public :: generate_recoil

<Recoil kinematics: sub interfaces>+≡
  module subroutine generate_recoil &
    (sqrtts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
    real(default), intent(in) :: sqrtts
    real(default), intent(in), dimension(2) :: q_max
    real(default), intent(in), dimension(2) :: m
    real(default), intent(in), dimension(2) :: mo
    real(default), intent(in), dimension(2) :: xc
    real(default), intent(in), dimension(2) :: xcb
    real(default), intent(in), dimension(4) :: r
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm
    type(vector4_t), dimension(2), intent(out) :: qo
    logical, intent(out) :: ok
  end subroutine generate_recoil

<Recoil kinematics: procedures>+≡
  module subroutine generate_recoil &
    (sqrtts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
    real(default), intent(in) :: sqrtts
    real(default), intent(in), dimension(2) :: q_max
    real(default), intent(in), dimension(2) :: m
    real(default), intent(in), dimension(2) :: mo
    real(default), intent(in), dimension(2) :: xc
    real(default), intent(in), dimension(2) :: xcb
    real(default), intent(in), dimension(4) :: r
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm
    type(vector4_t), dimension(2), intent(out) :: qo
    logical, intent(out) :: ok

    real(default), dimension(2) :: q2
    real(default), dimension(2) :: phi

```

```

real(default), dimension(2) :: x
real(default), dimension(2) :: xb
real(default), dimension(2) :: cos_th
real(default), dimension(2) :: sin_th

call generate_q2_recoil (sqrt2, xcb, q_max2, m2, r(1:2), q2)
call generate_phi_recoil (r(3:4), phi)

call solve_recoil (sqrt2, xc, xcb, phi, q2, x, xb, cos_th, sin_th, ok)
if (ok) then
    call recoil_momenta &
        (sqrt2, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
end if

end subroutine generate_recoil

```

32.4.6 Unit tests

Test module, followed by the corresponding implementation module.

`<recoil_kinematics_ut.f90>`≡

<File header>

```

module recoil_kinematics_ut
    use unit_tests
    use recoil_kinematics_util

```

<Standard module head>

<Recoil kinematics: public test>

`contains`

<Recoil kinematics: test driver>

`end module recoil_kinematics_ut`

`<recoil_kinematics_util.f90>`≡

<File header>

```

module recoil_kinematics_util

```

<Use kinds>

```

    use constants, only: twopi
    use constants, only: degree
    use lorentz, only: vector4_t
    use lorentz, only: vector4_moving
    use lorentz, only: lorentz_transformation_t
    use lorentz, only: inverse
    use lorentz, only: operator(+)
    use lorentz, only: operator(*)
    use lorentz, only: operator(**)
    use lorentz, only: pacify

```

```

use recoil_kinematics, only: solve_recoil
use recoil_kinematics, only: recoil_momenta
use recoil_kinematics, only: recoil_transformation
use recoil_kinematics, only: initial_transformation
use recoil_kinematics, only: generate_q2_recoil
use recoil_kinematics, only: generate_recoil

```

<Standard module head>

<Recoil kinematics: test declarations>

contains

<Recoil kinematics: tests>

end module recoil_kinematics_util

API: driver for the unit tests below.

```

<Recoil kinematics: public test>≡
  public :: recoil_kinematics_test

<Recoil kinematics: test driver>≡
  subroutine recoil_kinematics_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Recoil kinematics: execute tests>
  end subroutine recoil_kinematics_test

```

Recoil kinematics

For a set of input data, solve the kinematics constraints and generate momenta accordingly.

```

<Recoil kinematics: execute tests>≡
  call test (recoil_kinematics_1, "recoil_kinematics_1", &
    "iterative solution of non-collinear kinematics", &
    u, results)

<Recoil kinematics: test declarations>≡
  public :: recoil_kinematics_1

<Recoil kinematics: tests>≡
  subroutine recoil_kinematics_1 (u)
    integer, intent(in) :: u

    real(default) :: sqrts
    real(default), dimension(2) :: xc, xcb
    real(default), dimension(2) :: q
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: mo
    real(default), dimension(2) :: cos_th, sin_th
    real(default), dimension(2) :: x
    real(default), dimension(2) :: xb
    type(vector4_t), dimension(2) :: km

```

```

type(vector4_t), dimension(2) :: qm
type(vector4_t), dimension(2) :: qo
integer :: i
logical :: ok

character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"
character(*), parameter :: FMT4 = "(3x,ES8.1,9(1x,ES19.12))"

write (u, "(A)")  "* Test output: recoil_kinematics_1"
write (u, "(A)")  "* Purpose: compute kinematics for various input data"
write (u, "(A)")

sqrt_s = 100
write (u, FMT1) "sqrt_s =", sqrt_s

write (u, "(A)")
write (u, "(A)") "*** collinear data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = 0
mo = 0

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrt_s

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results
call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** semi-soft data set"
write (u, "(A)")

xcb= [0.1_default, 0.0001_default]
xc = 1 - xcb

```



```

phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.00001_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** hard-soft data set"
write (u, "(A)")

xcb= [0.1_default, 1.e-30_default]
xc = 1 - xcb
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 1.e-35_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** hard data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc
phi = [0.1_default, 0.8_default] * twopi
q = [0.74_default, 0.3_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** failing data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc
phi = [0.1_default, 0.8_default] * twopi
q = [0.9_default, 0.3_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
if (.not. ok) then

```

```

        write (u, "(A)")
        write (u, "(A)") "Failed as expected."
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: recoil_kinematics_1"

contains

subroutine show_data
    write (u, FMT1) "sqsh_h =", sqrt (xc(1) * xc(2)) * sqrts
    write (u, FMT1) "xc      =", xc
    write (u, FMT1) "xcb      =", xcb
    write (u, FMT1) "Q        =", Q
    write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_results
    write (u, "(A)")
    write (u, "(A)") "Result:"
    write (u, FMT1) "th/D  =", atan2 (sin_th, cos_th) / degree
    write (u, FMT1) "x      =", x
    write (u, "(A)")
end subroutine show_results

subroutine show_momenta
    type(vector4_t) :: qm0, qo0
    real(default), parameter :: tol = 1.e-7_default
    call pacify (km, tol)
    call pacify (qm, tol)
    call pacify (qo, tol)
    write (u, "(A)") "Momenta: k"
    call km(1)%write (u, testflag=.true.)
    call km(2)%write (u, testflag=.true.)
    write (u, FMT1) "k^2 =", abs (km(1)**2), abs (km(2)**2)
    write (u, "(A)")
    write (u, "(A)") "Momenta: q"
    call qm(1)%write (u, testflag=.true.)
    call qm(2)%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "Momenta: q(os)"
    call qo(1)%write (u, testflag=.true.)
    call qo(2)%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "Check: parton momentum sum: q vs q(os)"
    qm0 = qm(1) + qm(2)
    call qm0%write (u, testflag=.true.)
    qo0 = qo(1) + qo(2)
    call qo0%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "* Check: momentum transfer (off-shell/on-shell)"
    write (u, FMT2) "|q| =", abs (qm(1)**1), abs (qm(2)**1)
    write (u, FMT2) "Q  =", q
    write (u, FMT2) "|qo|=", abs (qo(1)**1), abs (qo(2)**1)

```

```

        write (u, "(A)")
        write (u, "(A)") "* Check: sqrts, sqrts_hat"
        write (u, FMT1) "|p| =", (km(1)+km(2)+qm(1)+qm(2))**1, (qm(1)+qm(2))**1
        write (u, FMT1) "sqs =", sqrts, sqrt (product (xc)) * sqrts
        write (u, FMT1) "|po| =", abs ((km(1)+km(2)+qo(1)+qo(2))**1), abs ((qo(1)+qo(2))**1)
    end subroutine show_momenta

end subroutine recoil_kinematics_1

```

Recoil Q distribution

Sample the Q distribution for equidistant bins in the input variable.

```

<Recoil kinematics: execute tests>+≡
    call test (recoil_kinematics_2, "recoil_kinematics_2", &
        "Q distribution", &
        u, results)

<Recoil kinematics: test declarations>+≡
    public :: recoil_kinematics_2

<Recoil kinematics: tests>+≡
    subroutine recoil_kinematics_2 (u)
        integer, intent(in) :: u

        real(default) :: sqrts
        real(default) :: q_max
        real(default) :: m
        real(default) :: x_bar
        real(default) :: r
        real(default) :: q2, q2_old
        integer :: i
        integer :: n_bin

        character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
        character(*), parameter :: FMT3 = "(2x,9(1x,F10.5))"

        write (u, "(A)")  "* Test output: recoil_kinematics_2"
        write (u, "(A)")  "* Purpose: compute Q distribution"
        write (u, "(A)")

        n_bin = 20

        write (u, "(A)")  "* No Q cutoff, xbar = 1"
        write (u, "(A)")

        sqrts = 100
        q_max = sqrts
        m = 0.511e-3_default
        x_bar = 1._default
        call show_table

        write (u, "(A)")
        write (u, "(A)")  "* With Q cutoff, xbar = 1"
        write (u, "(A)")
    end subroutine recoil_kinematics_2

```

```

q_max = 10
call show_table

write (u, "(A)")
write (u, "(A)") "* No Q cutoff, xbar = 0.01"
write (u, "(A)")

q_max = sqrts
x_bar = 0.01_default
call show_table

write (u, "(A)")
write (u, "(A)") "* Test output end: recoil_kinematics_2"

contains

subroutine show_table
  write (u, FMT1) "sqrts =", sqrts
  write (u, FMT1) "q_max =", q_max
  write (u, FMT1) "m      =", m
  write (u, FMT1) "x_bar =", x_bar
  write (u, "(A)")
  write (u, "(1x,A)") "Table: r          |Q|      |Q_i/Q_(i-1)|"
  q2_old = 0
  do i = 0, n_bin
    r = real (i, default) / n_bin
    call generate_q2_recoil (sqrts**2, x_bar, q_max**2, m**2, r, q2)
    if (q2_old > 0) then
      write (u, FMT3) r, sqrt (q2), sqrt (q2 / q2_old)
    else
      write (u, FMT3) r, sqrt (q2)
    end if
    q2_old = q2
  end do
end subroutine show_table

end subroutine recoil_kinematics_2

```

Generate recoil event

Combine Q^2 sampling with momentum generation.

```

<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_3, "recoil_kinematics_3", &
    "generate recoil event", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_3

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_3 (u)
    integer, intent(in) :: u

```

```

real(default) :: sqrts
real(default), dimension(2) :: q_max
real(default), dimension(2) :: m, mo
real(default), dimension(2) :: xc, xcb
real(default), dimension(4) :: r
type(vector4_t), dimension(2) :: km
type(vector4_t), dimension(2) :: qm
type(vector4_t), dimension(2) :: qo
logical :: ok

character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

write (u, "(A)")  "* Test output: recoil_kinematics_3"
write (u, "(A)")  "* Purpose: generate momenta from RNG parameters"
write (u, "(A)")

write (u, "(A)")  "*** collinear data set"
write (u, "(A)")

sqrts = 100
q_max = sqrts
m      = 0.511e-3_default
mo     = 0

xc = [0.6_default, 0.9_default]
xcb = 1 - xc

r = [0._default, 0._default, 0._default, 0._default]

call show_data
call generate_recoil (sqrts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc

r = [0.8_default, 0.2_default, 0.1_default, 0.2_default]

call show_data
call generate_recoil (sqrts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** failing data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc

```

```

r = [0.9999_default, 0.3_default, 0.1_default, 0.8_default]

call show_data
call generate_recoil (sqrts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
if (.not. ok) then
    write (u, "(A)")
    write (u, "(A)") "Failed as expected."
else
    call show_momenta
end if

contains

subroutine show_data
    write (u, FMT1) "sqrts =", sqrts
    write (u, FMT1) "q_max =", q_max
    write (u, FMT1) "m      =", m
    write (u, FMT1) "xc     =", xc
    write (u, FMT1) "xcb    =", xcb
    write (u, FMT1) "r      =", r
end subroutine show_data

subroutine show_momenta
    real(default), parameter :: tol = 1.e-7_default
    call pacify (km, tol)
    call pacify (qo, tol)
    write (u, "(A)")
    write (u, "(A)") "* Momenta: k"
    call km(1)%write (u, testflag=.true.)
    call km(2)%write (u, testflag=.true.)
    write (u, FMT1) "k^2 =", abs (km(1)**2), abs (km(2)**2)
    write (u, "(A)")
    write (u, "(A)") "* Momenta: q(os)"
    call qo(1)%write (u, testflag=.true.)
    call qo(2)%write (u, testflag=.true.)
    write (u, FMT1) "q^2 =", abs (qo(1)**2), abs (qo(2)**2)
    write (u, "(A)")
    write (u, "(A)") "* Check: momentum transfer (off-shell/on-shell)"
    write (u, FMT2) "Q    =", q_check (1), q_check (2)
    write (u, FMT2) "|q|  =", abs (qm(1)**1), abs (qm(2)**1)
    write (u, "(A)")
    write (u, "(A)") "* Check: sqrts, sqrts_hat"
    write (u, FMT1) "sqs =", sqrts, sqrt (product (xc)) * sqrts
    write (u, FMT1) "|po| =", abs ((km(1)+km(2)+qo(1)+qo(2))**1), abs ((qo(1)+qo(2))**1)
end subroutine show_momenta

function q_check (i) result (q)
    integer, intent(in) :: i
    real(default) :: q
    real(default) :: q2
    call generate_q2_recoil (sqrts**2, xcb(i), q_max(i)**2, m(i)**2, r(i), q2)
    q = sqrt (q2)
end function q_check

```

```
end subroutine recoil_kinematics_3
```

Transformation after recoil

Given a solution to recoil kinematics, compute the Lorentz transformation that transforms the old collinear parton momenta into the new parton momenta.

```
<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_4, "recoil_kinematics_4", &
    "reference frame", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_4

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_4 (u)
    integer, intent(in) :: u

    real(default) :: sqrts
    real(default), dimension(2) :: xc, xcb
    real(default), dimension(2) :: q
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: cos_th, sin_th
    real(default), dimension(2) :: mo
    real(default), dimension(2) :: x
    real(default), dimension(2) :: xb
    type(vector4_t), dimension(2) :: km
    type(vector4_t), dimension(2) :: qm
    type(vector4_t), dimension(2) :: qo
    type(lorentz_transformation_t) :: lt
    logical :: ok

    character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
    character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

    write (u, "(A)")  "* Test output: recoil_kinematics_4"
    write (u, "(A)")  "* Purpose: check Lorentz transformation for recoil"
    write (u, "(A)")

    sqrts = 100
    write (u, FMT1)  "sqrts =", sqrts

    write (u, "(A)")
    write (u, "(A)")  "*** collinear data set"
    write (u, "(A)")

    xc = [0.6_default, 0.9_default]
    xcb = 1 - xc
    phi = [0.1_default, 0.2_default] * twopi
    q = 0
    mo = 0

    call show_data
```

```

call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
call show_transformation

write (u, "(A)")
write (u, "(A)") "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
call show_transformation

write (u, "(A)")
write (u, "(A)") "* Test output end: recoil_kinematics_4"

contains

subroutine show_data
  write (u, FMT1) "sqs_h =", sqrt (xc(1) * xc(2)) * sqrts
  write (u, FMT1) "xc      =", xc
  write (u, FMT1) "xcb     =", xcb
  write (u, FMT1) "Q       =", Q
  write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_transformation
  type(vector4_t), dimension(2) :: qc
  type(vector4_t), dimension(2) :: qct
  real(default), parameter :: tol = 1.e-7_default
  qc(1) = xc(1) * vector4_moving (sqrts/2, sqrts/2, 3)
  qc(2) = xc(2) * vector4_moving (sqrts/2, -sqrts/2, 3)
  qct = lt * qc
  call pacify (qct, tol)
  write (u, "(A)")
  write (u, "(A)") "Momenta: q(os)"
  call qo(1)%write (u, testflag=.true.)
  call qo(2)%write (u, testflag=.true.)
  write (u, "(A)")
  write (u, "(A)") "Momenta: LT * qc"
  call qct(1)%write (u, testflag=.true.)
  call qct(2)%write (u, testflag=.true.)
end subroutine show_transformation

end subroutine recoil_kinematics_4

```


Transformation before recoil

Given a pair of incoming 'beam' partons (i.e., before ISR splitting), compute the transformation that transforms their common c.m. frame into the lab frame.

```
<Recoil kinematics: execute tests>+≡
    call test (recoil_kinematics_5, "recoil_kinematics_5", &
              "initial reference frame", &
              u, results)

<Recoil kinematics: test declarations>+≡
    public :: recoil_kinematics_5

<Recoil kinematics: tests>+≡
    subroutine recoil_kinematics_5 (u)
        integer, intent(in) :: u

        real(default) :: sqrts
        real(default) :: sqrtsi
        real(default), dimension(2) :: x
        type(vector4_t), dimension(2) :: p
        type(vector4_t), dimension(2) :: pi
        type(vector4_t), dimension(2) :: p0
        type(lorentz_transformation_t) :: lt
        logical :: ok

        character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
        character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

        write (u, "(A)")  "*" Test output: recoil_kinematics_5"
        write (u, "(A)")  "*" Purpose: determine initial Lorentz transformation"
        write (u, "(A)")

        sqrts = 100
        write (u, FMT1) "sqrts =", sqrts

        x = [0.6_default, 0.9_default]

        p(1) = x(1) * vector4_moving (sqrts/2, sqrts/2, 3)
        p(2) = x(2) * vector4_moving (sqrts/2, -sqrts/2, 3)

        call show_data
        call initial_transformation (p, sqrtsi, lt, ok)

        pi(1) = vector4_moving (sqrtsi/2, sqrtsi/2, 3)
        pi(2) = vector4_moving (sqrtsi/2, -sqrtsi/2, 3)

        p0 = inverse (lt) * p

        call show_momenta

        write (u, "(A)")
        write (u, "(A)")  "*" Test output end: recoil_kinematics_5"

contains
```

```

subroutine show_data
  write (u, FMT1) "sqrts =", sqrts
  write (u, FMT1) "x      =", x
end subroutine show_data

subroutine show_momenta
  real(default), parameter :: tol = 1.e-7_default
  write (u, "(A)")
  write (u, "(A)") "* Momenta: p_in(c.m.)"
  call pi(1)%write (u, testflag=.true.)
  call pi(2)%write (u, testflag=.true.)
  write (u, "(A)")
  write (u, "(A)") "* Momenta: inv(LT) * p_in(lab)"
  call p0(1)%write (u, testflag=.true.)
  call p0(2)%write (u, testflag=.true.)
end subroutine show_momenta

end subroutine recoil_kinematics_5

```

Transformation after recoil with on-shell momenta

Given a solution to recoil kinematics, compute the Lorentz transformation that transforms the old collinear parton momenta into the new parton momenta.

Compare the results for massless and massive on-shell projection.

```

<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_6, "recoil_kinematics_6", &
    "massless/massive on-shell projection", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_6

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_6 (u)
    integer, intent(in) :: u

    real(default) :: sqrts
    real(default), dimension(2) :: xc, xcb
    real(default), dimension(2) :: q
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: cos_th, sin_th
    real(default), dimension(2) :: x
    real(default), dimension(2) :: xb
    real(default), dimension(2) :: mo, z
    type(vector4_t), dimension(2) :: km
    type(vector4_t), dimension(2) :: qm
    type(vector4_t), dimension(2) :: qo
    type(lorentz_transformation_t) :: lt
    logical :: ok

    character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
    character(*), parameter :: FMT2 = "(1x,A,9(1x,F11.6))"

```

```

write (u, "(A)")  "* Test output: recoil_kinematics_6"
write (u, "(A)")  "* Purpose: check effect of mass in on-shell projection"
write (u, "(A)")

sqrts = 10
write (u, FMT1)  "sqrts =", sqrts
z = 0
mo = 0.511e-3
write (u, FMT1)  "mass =", mo

write (u, "(A)")
write (u, "(A)")  "*** collinear data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = 0

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, z, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massless projection:"
call show_momenta

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massive projection:"
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, z, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massless projection:"
call show_momenta

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
write (u, "(A)")

```

```

write (u, "(A)") "Massive projection:"
call show_momenta

write (u, "(A)")
write (u, "(A)")  "* Test output end: recoil_kinematics_6"

contains

subroutine show_data
  write (u, FMT1) "sqs_h =", sqrt (xc(1) * xc(2)) * sqrts
  write (u, FMT1) "xc    =", xc
  write (u, FMT1) "xcb   =", xcb
  write (u, FMT1) "Q     =", Q
  write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_momenta
  write (u, "(A)") "Momenta: q(os)"
  call qo(1)%write (u, testflag=.true.)
  write (u, FMT2)  "m = ", abs (qo(1)**1)
  call qo(2)%write (u, testflag=.true.)
  write (u, FMT2)  "m = ", abs (qo(2)**1)
end subroutine show_momenta

end subroutine recoil_kinematics_6

```

32.5 Transverse momentum for the ISR and EPA approximations

The ISR and EPA handler takes an event with a single radiated collinear particle (photon for ISR, beam particle for EPA) for each beam, respectively, and inserts transverse momentum for both. The four-particle kinematics allows us to generate Q^2 and azimuthal angles independently, without violating energy-momentum conservation. The Q^2 distribution is logarithmic, as required by the effective particle approximation, and reflected in the inclusive ISR/EPA structure functions. We also conserve the invariant mass of the partonic system after radiation. The total transverse-momentum kick is applied in form of a Lorentz transformation to the elementary process, both in- and out-particles. In fact, the incoming partons (beam particle for ISR, photon for EPA) which would be virtual space-like in the exact kinematics configuration, are replaced by on-shell incoming partons, such that energy, momentum, and invariant mass \sqrt{s} are conserved.

Regarding kinematics, we treat all particles as massless. The beam-particle mass only appears as the parameter `isr_mass` or `epa_mass`, respectively, and cuts off the logarithmic distribution. The upper cutoff is `isr_q_max` (`epa_q_max`), which defaults to the available energy \sqrt{s} .

The only differences between ISR and EPA, in this context, are the particle types, and an extra \bar{x} factor in the lower cutoff for EPA, see below.

(`isr_epa_handler.f90`)≡

```

<File header>

module isr_epa_handler

  <Use kinds>
  <Use strings>
    use lorentz, only: vector4_t
    use lorentz, only: energy
    use lorentz, only: lorentz_transformation_t
    use lorentz, only: identity
    use lorentz, only: inverse
    use lorentz, only: operator(*)
    use flavors, only: flavor_t
    use particles, only: particle_t
    use rng_base, only: rng_t
    use event_transforms

  <Standard module head>

  <ISR/EPA handler: public>

  <ISR/EPA handler: parameters>

  <ISR/EPA handler: types>

    interface
  <ISR/EPA handler: sub interfaces>
    end interface

  end module isr_epa_handler
<isr_epa_handler_sub.f90>≡
  <File header>

  submodule (isr_epa_handler) isr_epa_handler_s

    use diagnostics, only: msg_fatal
    use diagnostics, only: msg_bug
    use io_units
    use format_defs, only: FMT_12, FMT_19
    use format_utils, only: write_separator
    use format_utils, only: pac_fmt
    use physics_defs, only: PHOTON
    use recoil_kinematics, only: initial_transformation
    use recoil_kinematics, only: generate_recoil
    use recoil_kinematics, only: recoil_transformation

    implicit none

  contains

  <ISR/EPA handler: procedures>

  end submodule isr_epa_handler_s

```

32.5.1 Event transform type

Convention: **beam** are the incoming partons before ISR – not necessarily the actual beams, need not be in c.m. frame. **radiated** are the radiated particles (photon for ISR), and **parton** are the remainders which initiate the elementary process. These particles are copied verbatim from the event record, and must be collinear.

The kinematical parameters are **sqrts** = invariant mass of the **beam** particles, **q_max** and **m** determining the Q^2 distribution, and **xc/xcb** as the energy fraction (complement) of the partons, relative to the beams.

Transformations: **lti** is the Lorentz transformation that would boost **pi** (c.m. frame) back to the original **beam** momenta (lab frame). **lto** is the recoil transformation, transforming the partons after ISR from the collinear frame to the recoiling frame. **lt** is the combination of both, which is to be applied to all particles after the hard interaction.

Momenta: **pi** are the beams transformed to their common c.m. frame. **ki** and **qi** are the photon/parton momenta in the **pi** c.m. frame. **km** and **qm** are the photon/parton momenta with the Q distribution applied, and finally **qo** are the partons **qm** projected on-shell.

```
<ISR/EPA handler: public>≡
    public :: evt_isr_epa_t

<ISR/EPA handler: types>≡
    type, extends (evt_t) :: evt_isr_epa_t
        private
            integer :: mode = ISR_TRIVIAL_COLLINEAR
            logical :: isr_active = .false.
            logical :: epa_active = .false.
            real(default) :: isr_q_max = 0
            real(default) :: epa_q_max = 0
            real(default) :: isr_mass = 0
            real(default) :: epa_mass = 0
            logical :: isr_keep_mass = .true.
            real(default) :: sqrts = 0
            integer, dimension(2) :: rad_mode = BEAM_RAD_NONE
            real(default), dimension(2) :: q_max = 0
            real(default), dimension(2) :: m = 0
            real(default), dimension(2) :: xc = 0
            real(default), dimension(2) :: xcb = 0
            type(lorentz_transformation_t) :: lti = identity
            type(lorentz_transformation_t) :: lto = identity
            type(lorentz_transformation_t) :: lt = identity
            integer, dimension(2) :: i_beam = 0
            type(particle_t), dimension(2) :: beam
            type(vector4_t), dimension(2) :: pi
            integer, dimension(2) :: i_radiated = 0
            type(particle_t), dimension(2) :: radiated
            type(vector4_t), dimension(2) :: ki
            type(vector4_t), dimension(2) :: km
            integer, dimension(2) :: i_parton = 0
            type(particle_t), dimension(2) :: parton
            type(vector4_t), dimension(2) :: qi
            type(vector4_t), dimension(2) :: qm
```

```

        type(vector4_t), dimension(2) :: qo
contains
  <ISR/EPA handler: evt_isr: TBP>
end type evt_isr_epa_t

```

32.5.2 ISR/EPA distinction

```

<ISR/EPA handler: parameters>≡
  integer, parameter, public :: BEAM_RAD_NONE = 0
  integer, parameter, public :: BEAM_RAD_ISR = 1
  integer, parameter, public :: BEAM_RAD_EPA = 2

```

```

<ISR/EPA handler: procedures>≡
  function rad_mode_string (mode) result (string)
    type(string_t) :: string
    integer, intent(in) :: mode
    select case (mode)
      case (BEAM_RAD_NONE); string = "--"
      case (BEAM_RAD_ISR); string = "ISR"
      case (BEAM_RAD_EPA); string = "EPA"
      case default; string = "???"
    end select
  end function rad_mode_string

```

32.5.3 Photon insertion modes

```

<ISR/EPA handler: parameters>+≡
  integer, parameter, public :: ISR_TRIVIAL_COLLINEAR = 0
  integer, parameter, public :: ISR_PAIR_RECOIL = 1

```

```

<ISR/EPA handler: evt_isr: TBP>≡
  procedure :: get_mode_string => evt_isr_epa_get_mode_string

```

```

<ISR/EPA handler: sub interfaces>≡
  module function evt_isr_epa_get_mode_string (evt) result (string)
    type(string_t) :: string
    class(evt_isr_epa_t), intent(in) :: evt
  end function evt_isr_epa_get_mode_string

```

```

<ISR/EPA handler: procedures>+≡
  module function evt_isr_epa_get_mode_string (evt) result (string)
    type(string_t) :: string
    class(evt_isr_epa_t), intent(in) :: evt
    select case (evt%mode)
      case (ISR_TRIVIAL_COLLINEAR)
        string = "trivial, collinear"
      case (ISR_PAIR_RECOIL)
        string = "pair recoil"
      case default
        string = "[undefined]"
    end select
  end function

```

```
end function evt_isr_epa_get_mode_string
```

Set the numerical mode ID from a user-level string representation.

```
<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: set_mode_string => evt_isr_epa_set_mode_string

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_set_mode_string (evt, string)
    class(evt_isr_epa_t), intent(inout) :: evt
    type(string_t), intent(in) :: string
  end subroutine evt_isr_epa_set_mode_string

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_set_mode_string (evt, string)
    class(evt_isr_epa_t), intent(inout) :: evt
    type(string_t), intent(in) :: string
    select case (char (string))
    case ("trivial")
      evt%mode = ISR_TRIVIAL_COLLINEAR
    case ("recoil")
      evt%mode = ISR_PAIR_RECOIL
    case default
      call msg_fatal ("ISR handler: mode '" // char (string) &
        // "' is undefined")
    end select
  end subroutine evt_isr_epa_set_mode_string
```

32.5.4 Output

```
<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: write_name => evt_isr_epa_write_name

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_write_name (evt, unit)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
  end subroutine evt_isr_epa_write_name

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_write_name (evt, unit)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: ISR/EPA handler"
  end subroutine evt_isr_epa_write_name
```

The overall recoil-handling mode.

```
<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: write_mode => evt_isr_epa_write_mode
```



```

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_write_mode (evt, unit)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
  end subroutine evt_isr_epa_write_mode

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_write_mode (evt, unit)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,1x,I0,':',1x,A)") "Insertion mode =", evt%mode, &
      char (evt%get_mode_string ())
  end subroutine evt_isr_epa_write_mode

```

The input data for ISR and EPA, respectively.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure :: write_input => evt_isr_epa_write_input

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_write_input (evt, unit, testflag)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
  end subroutine evt_isr_epa_write_input

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_write_input (evt, unit, testflag)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    character(len=7) :: fmt
    integer :: u
    u = given_output_unit (unit)
    call pac_fmt (fmt, FMT_19, FMT_12, testflag)
    if (evt%isr_active) then
      write (u, "(3x,A,1x," // fmt // ")") "ISR: Q_max =", evt%isr_q_max
      write (u, "(3x,A,1x," // fmt // ")") "      m      =", evt%isr_mass
      write (u, "(3x,A,1x,L1)") "      keep m=", evt%isr_keep_mass
    else
      write (u, "(3x,A)") "ISR: [inactive]"
    end if
    if (evt%epa_active) then
      write (u, "(3x,A,1x," // fmt // ")") "EPA: Q_max =", evt%epa_q_max
      write (u, "(3x,A,1x," // fmt // ")") "      m      =", evt%epa_mass
    else
      write (u, "(3x,A)") "EPA: [inactive]"
    end if
  end subroutine evt_isr_epa_write_input

```

The trivial mode does not depend on any data, since it does nothing to the event.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure :: write_data => evt_isr_epa_write_data

```

<ISR/EPA handler: sub interfaces>+≡

```

module subroutine evt_isr_epa_write_data (evt, unit, testflag)
  class(evt_isr_epa_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
end subroutine evt_isr_epa_write_data

```

<ISR/EPA handler: procedures>+≡

```

module subroutine evt_isr_epa_write_data (evt, unit, testflag)
  class(evt_isr_epa_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  character(len=7), parameter :: FMTL_19 = "A3,16x"
  character(len=7), parameter :: FMTL_12 = "A3,9x"
  character(len=7) :: fmt, fmtl
  integer :: u
  u = given_output_unit (unit)
  call pac_fmt (fmt, FMT_19, FMT_12, testflag)
  call pac_fmt (fmtl, FMTL_19, FMTL_12, testflag)
  select case (evt%mode)
  case (ISR_PAIR_RECOIL)
    write (u, "(1x,A)") "Event:"
    write (u, "(3x,A,2(1x," // fmtl // "))" ) &
      "mode = ", &
      char (rad_mode_string (evt%rad_mode(1))), &
      char (rad_mode_string (evt%rad_mode(2)))
    write (u, "(3x,A,2(1x," // fmt // "))" ) "Q_max =", evt%q_max
    write (u, "(3x,A,2(1x," // fmt // "))" ) "m      =", evt%m
    write (u, "(3x,A,2(1x," // fmt // "))" ) "x      =", evt%xc
    write (u, "(3x,A,2(1x," // fmt // "))" ) "xb     =", evt%xcb
    write (u, "(3x,A,1x," // fmt // "))"    "sqrts =", evt%sqrts
    call write_separator (u)
    write (u, "(A)") "Lorentz boost (partons before radiation &
      &c.m. -> lab) ="
    call evt%lti%write (u, testflag)
    write (u, "(A)") "Lorentz transformation (collinear partons &
      &-> partons with recoil in c.m.) ="
    call evt%lto%write (u, testflag)
    write (u, "(A)") "Combined transformation (partons &
      &-> partons with recoil in lab frame) ="
    call evt%lt%write (u, testflag)
  end select
end subroutine evt_isr_epa_write_data

```

Output method.

<ISR/EPA handler: evt isr: TBP>+≡

```

procedure :: write => evt_isr_epa_write

```

<ISR/EPA handler: sub interfaces>+≡

```

module subroutine evt_isr_epa_write &
  (evt, unit, verbose, more_verbose, testflag)
  class(evt_isr_epa_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose, more_verbose, testflag
end subroutine evt_isr_epa_write

```

```

<ISR/EPA handler: procedures>+=
module subroutine evt_isr_epa_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    logical :: show_mass
    integer :: u, i
    u = given_output_unit (unit)
    if (present (testflag)) then
        show_mass = .not. testflag
    else
        show_mass = .true.
    end if
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u, 2)
    call evt%write_mode (u)
    call evt%write_input (u, testflag=testflag)
    call evt%write_data (u, testflag=testflag)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag, show_set = .false.)
    if (all (evt%i_beam > 0)) then
        call write_separator (u)
        write (u, "(A,2(1x,I0))") "Partons before radiation:", evt%i_beam
        do i = 1, 2
            call evt%beam(i)%write (u, testflag=testflag)
        end do
        call write_separator (u)
        write (u, "(A)") "... boosted to c.m.:"
        do i = 1, 2
            call evt%pi(i)%write (u, show_mass=show_mass, testflag=testflag)
        end do
    end if
    if (all (evt%i_radiated > 0)) then
        call write_separator (u)
        write (u, "(A,2(1x,I0))") "Radiated particles, collinear:", &
            evt%i_radiated
        do i = 1, 2
            call evt%radiated(i)%write (u, testflag=testflag)
        end do
        call write_separator (u)
        write (u, "(A)") "... boosted to c.m.:"
        do i = 1, 2
            call evt%ki(i)%write (u, show_mass=show_mass, testflag=testflag)
        end do
        call write_separator (u)
        write (u, "(A)") "... with kT:"
        do i = 1, 2
            call evt%km(i)%write (u, show_mass=show_mass, testflag=testflag)
        end do
    end if
    if (all (evt%i_parton > 0)) then
        call write_separator (u)

```

```

write (u, "(A,2(1x,I0))") "Partons after radiation, collinear:", &
    evt%i_parton
do i = 1, 2
    call evt%parton(i)%write (u, testflag=testflag)
end do
call write_separator (u)
write (u, "(A)") "... boosted to c.m.:"
do i = 1, 2
    call evt%qi(i)%write (u, show_mass=show_mass, testflag=testflag)
end do
call write_separator (u)
write (u, "(A)") "... with qT, off-shell:"
do i = 1, 2
    call evt%qm(i)%write (u, show_mass=show_mass, testflag=testflag)
end do
call write_separator (u)
write (u, "(A)") "... projected on-shell:"
do i = 1, 2
    call evt%qo(i)%write (u, show_mass=show_mass, testflag=testflag)
end do
call write_separator (u)
end if
if (evt%particle_set_exists) &
    call evt%particle_set%write &
    (u, summary = .true., compressed = .true., testflag = testflag)
call write_separator (u)
end subroutine evt_isr_epa_write

```

32.5.5 Initialization

Manually import a random-number generator object. This should be done only for testing purposes. The standard procedure is to **connect** a process to an event transform; this will create an appropriate **rng** from the RNG factory in the process object.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: import_rng => evt_isr_epa_import_rng

<ISR/EPA handler: sub interfaces>+≡
    module subroutine evt_isr_epa_import_rng (evt, rng)
        class(evt_isr_epa_t), intent(inout) :: evt
        class(rng_t), allocatable, intent(inout) :: rng
    end subroutine evt_isr_epa_import_rng

<ISR/EPA handler: procedures>+≡
    module subroutine evt_isr_epa_import_rng (evt, rng)
        class(evt_isr_epa_t), intent(inout) :: evt
        class(rng_t), allocatable, intent(inout) :: rng
        call move_alloc (from = rng, to = evt%rng)
    end subroutine evt_isr_epa_import_rng

```

Set constant kinematics limits and initialize for ISR. Note that **sqrts** is used only as the fallback value for **q_max**. The actual **sqrts** value for the transform

object is inferred from the incoming particles, event by event.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: set_data_isr => evt_isr_epa_set_data_isr

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_set_data_isr (evt, sqrts, q_max, m, keep_mass)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: q_max
    real(default), intent(in) :: m
    logical, intent(in) :: keep_mass
  end subroutine evt_isr_epa_set_data_isr

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_set_data_isr (evt, sqrts, q_max, m, keep_mass)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: q_max
    real(default), intent(in) :: m
    logical, intent(in) :: keep_mass
    if (sqrts <= 0) then
      call msg_fatal ("ISR handler: sqrts value must be positive")
    end if
    if (q_max <= 0 .or. q_max > sqrts) then
      evt%isr_q_max = sqrts
    else
      evt%isr_q_max = q_max
    end if
    if (m > 0) then
      evt%isr_mass = m
    else
      call msg_fatal ("ISR handler: ISR_mass value must be positive")
    end if
    evt%isr_active = .true.
    evt%isr_keep_mass = keep_mass
  end subroutine evt_isr_epa_set_data_isr

```

Set constant kinematics limits and initialize for EPA. Note that `sqrts` is used only as the fallback value for `q_max`. The actual `sqrts` value for the transform object is inferred from the incoming particles, event by event.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: set_data_epa => evt_isr_epa_set_data_epa

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_set_data_epa (evt, sqrts, q_max, m)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: q_max
    real(default), intent(in) :: m
  end subroutine evt_isr_epa_set_data_epa

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_set_data_epa (evt, sqrts, q_max, m)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(in) :: sqrts

```

```

real(default), intent(in) :: q_max
real(default), intent(in) :: m
if (sqrts <= 0) then
    call msg_fatal ("EPA handler: sqrts value must be positive")
end if
if (q_max <= 0 .or. q_max > sqrts) then
    evt%epa_q_max = sqrts
else
    evt%epa_q_max = q_max
end if
if (m > 0) then
    evt%epa_mass = m
else
    call msg_fatal ("EPA handler: EPA_mass value must be positive")
end if
evt%epa_active = .true.
end subroutine evt_isr_epa_set_data_epa

```

32.5.6 Fetch event data

Identify the radiated particles and the recoil momenta in the particle set. Without much sophistication, start from the end and find particles with the “remnant” status. Their parents should point to the recoiling parton. If successful, set the particle indices in the `evt` object, for further processing.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure, private :: identify_radiated

<ISR/EPA handler: sub interfaces>+≡
    module subroutine identify_radiated (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
    end subroutine identify_radiated

<ISR/EPA handler: procedures>+≡
    module subroutine identify_radiated (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        integer :: i, k
        k = 2
        FIND_LAST_RADIATED: do i = evt%particle_set%get_n_tot (), 1, -1
            associate (prt => evt%particle_set%prt(i))
                if (prt%is_beam_remnant ()) then
                    evt%i_radiated(k) = i
                    evt%radiated(k) = prt
                    k = k - 1
                    if (k == 0) exit FIND_LAST_RADIATED
                end if
            end associate
        end do FIND_LAST_RADIATED
        if (k /= 0) call err_count
contains
    subroutine err_count
        call evt%particle_set%write ()
        call msg_fatal ("ISR/EPA handler: &
            &event does not contain two radiated particles")
    end subroutine err_count
end module identify_radiated

```

```

    end subroutine err_count
end subroutine identify_radiated

```

When the radiated particles are known, we can fetch their parent particles and ask for the other child, the incoming parton.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure, private :: identify_partons

<ISR/EPA handler: sub interfaces>+≡
  module subroutine identify_partons (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
  end subroutine identify_partons

<ISR/EPA handler: procedures>+≡
  module subroutine identify_partons (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, dimension(:), allocatable :: parent, child
    integer :: i, j
    if (all (evt%i_radiated > 0)) then
      do i = 1, 2
        parent = evt%i_radiated(i)%get_parents ()
        if (size (parent) /= 1) call err_mismatch
        evt%i_beam(i) = parent(1)
        evt%beam(i) = evt%particle_set%prt(parent(1))
        associate (prt => evt%beam(i))
          child = prt%get_children ()
          if (size (child) /= 2) call err_mismatch
          do j = 1, 2
            if (child(j) /= evt%i_radiated(i)) then
              evt%i_parton(i) = child(j)
              evt%parton(i) = evt%particle_set%prt(child(j))
            end if
          end do
        end associate
      end do
    end if
  contains
    subroutine err_mismatch
      call evt%particle_set%write ()
      call msg_bug ("ISR/EPA handler: mismatch in parent-child relations")
    end subroutine err_mismatch
  end subroutine identify_partons

```

Check whether the radiated particle is a photon, or the incoming parton is a photon. Then set the ISR/EPA switch appropriately, for each beam.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: check_radiation => evt_isr_epa_check_radiation

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_check_radiation (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
  end subroutine evt_isr_epa_check_radiation

```

<ISR/EPA handler: procedures>+≡

```

module subroutine evt_isr_epa_check_radiation (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  type(flavor_t) :: flv
  integer :: i
  do i = 1, 2
    flv = evt%radiated(i)%get_flv ()
    if (flv%get_pdg () == PHOTON) then
      if (evt%isr_active) then
        evt%rad_mode(i) = BEAM_RAD_ISR
      else
        call err_isr_init
      end if
    else
      flv = evt%parton(i)%get_flv ()
      if (flv%get_pdg () == PHOTON) then
        if (evt%epa_active) then
          evt%rad_mode(i) = BEAM_RAD_EPA
        else
          call err_epa_init
        end if
      else
        call err_no_photon
      end if
    end if
  end do
contains
  subroutine err_isr_init
    call evt%particle_set%write ()
    call msg_fatal ("ISR/EPA handler: &
      &event contains radiated photon, but ISR is not initialized")
  end subroutine err_isr_init
  subroutine err_epa_init
    call evt%particle_set%write ()
    call msg_fatal ("ISR/EPA handler: &
      &event contains incoming photon, but EPA is not initialized")
  end subroutine err_epa_init
  subroutine err_no_photon
    call evt%particle_set%write ()
    call msg_fatal ("ISR/EPA handler: &
      &event does not appear to be ISR or EPA - missing photon")
  end subroutine err_no_photon
end subroutine evt_isr_epa_check_radiation

```

Internally set the appropriate parameters (ISR/EPA) for the two beams in the recoil mode.

<ISR/EPA handler: evt isr: TBP>+≡

```

procedure :: set_recoil_parameters => evt_isr_epa_set_recoil_parameters

```

<ISR/EPA handler: sub interfaces>+≡

```

module subroutine evt_isr_epa_set_recoil_parameters (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
end subroutine evt_isr_epa_set_recoil_parameters

```



```

<ISR/EPA handler: procedures>+≡
module subroutine evt_isr_epa_set_recoil_parameters (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  integer :: i
  do i = 1, 2
    select case (evt%rad_mode(i))
    case (BEAM_RAD_ISR)
      evt%q_max(i) = evt%isr_q_max
      evt%m(i) = evt%isr_mass
    case (BEAM_RAD_EPA)
      evt%q_max(i) = evt%epa_q_max
      evt%m(i) = evt%epa_mass
    end select
  end do
end subroutine evt_isr_epa_set_recoil_parameters

```

Boost the particles that participate in ISR to their proper c.m. frame, copying the momenta to `pi`, `ki`, `qi`. Also assign `sqrts` properly.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure, private :: boost_to_cm

<ISR/EPA handler: sub interfaces>+≡
  module subroutine boost_to_cm (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
  end subroutine boost_to_cm

<ISR/EPA handler: procedures>+≡
module subroutine boost_to_cm (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  type(vector4_t), dimension(2) :: p
  type(vector4_t), dimension(2) :: k
  type(vector4_t), dimension(2) :: q
  logical :: ok
  p = evt%beam%get_momentum ()
  k = evt%radiated%get_momentum ()
  q = evt%parton%get_momentum ()
  call initial_transformation (p, evt%sqrts, evt%lti, ok)
  if (.not. ok) call err_non_collinear
  evt%pi = inverse (evt%lti) * p
  evt%ki = inverse (evt%lti) * k
  evt%qi = inverse (evt%lti) * q
contains
  subroutine err_non_collinear
    call evt%particle_set%write ()
    call msg_fatal ("ISR/EPA handler: &
      &partons before radiation are not collinear")
  end subroutine err_non_collinear
end subroutine boost_to_cm

```

We can infer the x and \bar{x} values of the event by looking at the energy fractions of the radiated particles and incoming partons, respectively, relative to their parents. Of course, we must assume that they are all collinear, and that energy is conserved.

```

<ISR/EPA handler: evt_isr: TBP>+≡

```

```

    procedure, private :: infer_x
<ISR/EPA handler: sub interfaces>+≡
    module subroutine infer_x (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
    end subroutine infer_x
<ISR/EPA handler: procedures>+≡
    module subroutine infer_x (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        real(default) :: E_parent, E_radiated, E_parton
        integer :: i
        if (all (evt%i_radiated > 0)) then
            do i = 1, 2
                E_parent = energy (evt%pi(i))
                E_radiated = energy (evt%ki(i))
                E_parton = energy (evt%qi(i))
                if (E_parent > 0) then
                    evt%xc(i) = E_parton / E_parent
                    evt%xcb(i) = E_radiated / E_parent
                else
                    call err_energy
                end if
            end do
        end if
    contains
        subroutine err_energy
            call evt%particle_set%write ()
            call msg_bug ("ISR/EPA handler: non-positive energy in splitting")
        end subroutine err_energy
    end subroutine infer_x

```

32.5.7 Two-parton recoil

For transforming partons into recoil momenta, we make use of the routines in the `recoil_kinematics` module. In addition to the collinear momenta, we use the x energy fractions, and four numbers from the RNG.

There is one subtle difference w.r.t. ISR case: the EPA mass parameter is multiplied by the energy fraction x , separately for each beam. This is the effective lower Q cutoff.

For certain kinematics, close to the Q_{\max} endpoint, this may fail, and `ok` is set to false. In that case, we should generate new recoil momenta for the same event. This is handled by the generic unweighting procedure.

```

<ISR/EPA handler: evt isr: TBP>+≡
    procedure, private :: generate_recoil => evt_generate_recoil
<ISR/EPA handler: sub interfaces>+≡
    module subroutine evt_generate_recoil (evt, ok)
        class(evt_isr_epa_t), intent(inout) :: evt
        logical, intent(out) :: ok
    end subroutine evt_generate_recoil

```

(ISR/EPA handler: procedures)+≡

```

module subroutine evt_generate_recoil (evt, ok)
  class(evt_isr_epa_t), intent(inout) :: evt
  logical, intent(out) :: ok
  real(default), dimension(4) :: r
  real(default), dimension(2) :: m, mo
  integer :: i
  call evt%rng%generate (r)
  m = 0
  mo = 0
  do i = 1, 2
    select case (evt%rad_mode(i))
    case (BEAM_RAD_ISR)
      m(i) = evt%m(i)
      if (evt%isr_keep_mass) mo(i) = m(i)
    case (BEAM_RAD_EPA)
      m(i) = evt%xc(i) * evt%m(i)
    end select
  end do
  call generate_recoil (evt%sqrts, evt%q_max, m, mo, evt%xc, evt%xcb, r, &
    evt%km, evt%qm, evt%qo, ok)
end subroutine evt_generate_recoil

```

Replace the collinear radiated (incoming) parton momenta by the momenta that we have generated, respectively. Recall that the recoil has been applied in the c.m. system of the partons before ISR, so we apply the stored Lorentz transformation to boost them to the lab frame.

(ISR/EPA handler: evt isr: TBP)+≡

```

procedure, private :: replace_radiated
procedure, private :: replace_partons

```

(ISR/EPA handler: sub interfaces)+≡

```

module subroutine replace_radiated (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
end subroutine replace_radiated
module subroutine replace_partons (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
end subroutine replace_partons

```

(ISR/EPA handler: procedures)+≡

```

module subroutine replace_radiated (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  integer :: i
  do i = 1, 2
    associate (prt => evt%particle_set%prt(evt%i_radiated(i)))
      call prt%set_momentum (evt%lti * evt%km(i))
    end associate
  end do
end subroutine replace_radiated

module subroutine replace_partons (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  integer :: i
  do i = 1, 2

```

```

        associate (prt => evt%particle_set%prt(evt%i_parton(i)))
        call prt%set_momentum (evt%lti * evt%qo(i))
    end associate
end do
end subroutine replace_partons

```

32.5.8 Transform the event

Knowing the new incoming partons for the elementary process, we can make use of another procedure in `recoil_kinematics` to determine the Lorentz transformation that transforms the collinear frame into the frame with transverse momentum. We apply this transformation, recursively, to all particles that originate from those incoming partons in the original particle set.

We have to allow for the pre-ISR partons being not in their common c.m. frame. Taking into account non-commutativity, we actually have to first transform the outgoing particles to that c.m. frame, then apply the recoil transformation, then boost back to the lab frame.

The `mask` keep track of particles that we transform, just in case the parent-child tree is multiply connected.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: transform_outgoing => evt_transform_outgoing

<ISR/EPA handler: sub interfaces>+≡
    module subroutine evt_transform_outgoing (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
    end subroutine evt_transform_outgoing

<ISR/EPA handler: procedures>+≡
    module subroutine evt_transform_outgoing (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        logical, dimension(:), allocatable :: mask
        call recoil_transformation (evt%sqrts, evt%xc, evt%qo, evt%lto)
        evt%lt = evt%lti * evt%lto * inverse (evt%lti)
        allocate (mask (evt%particle_set%get_n_tot ()), source=.false.)
        call transform_children (evt%i_parton(1))
    contains
        recursive subroutine transform_children (i)
            integer, intent(in) :: i
            integer :: j, n_child, c
            integer, dimension(:), allocatable :: child
            child = evt%particle_set%prt(i)%get_children ()
            do j = 1, size (child)
                c = child(j)
                if (.not. mask(c)) then
                    associate (prt => evt%particle_set%prt(c))
                        call prt%set_momentum (evt%lt * prt%get_momentum ())
                        mask(c) = .true.
                        call transform_children (c)
                    end associate
                end if
            end do
        end subroutine transform_children
    end module evt_transform_outgoing

```

```
end subroutine evt_transform_outgoing
```

32.5.9 Implemented methods

Here we take the particle set from the previous event transform and copy it, then generate the transverse momentum for the radiated particles and for the incoming partons. If this fails (rarely, for large p_T), return zero for the probability, to trigger another try.

NOTE: The boost for the initial partonic system, if not in the c.m. frame, has not been implemented yet.

```
(ISR/EPA handler: evt_isr: TBP)+≡
  procedure :: generate_weighted => &
    evt_isr_epa_generate_weighted

(ISR/EPA handler: sub interfaces)+≡
  module subroutine evt_isr_epa_generate_weighted (evt, probability)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
  end subroutine evt_isr_epa_generate_weighted

(ISR/EPA handler: procedures)+≡
  module subroutine evt_isr_epa_generate_weighted (evt, probability)
    class(evt_isr_epa_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    logical :: valid
    call evt%particle_set%final ()
    evt%particle_set = evt%previous%particle_set
    evt%particle_set_exists = .true.
    select case (evt%mode)
    case (ISR_TRIVIAL_COLLINEAR)
      probability = 1
      valid = .true.
    case (ISR_PAIR_RECOIL)
      call evt%identify_radiated ()
      call evt%identify_partons ()
      call evt%check_radiation ()
      call evt%set_recoil_parameters ()
      call evt%boost_to_cm ()
      call evt%infer_x ()
      call evt%generate_recoil (valid)
      if (valid) then
        probability = 1
      else
        probability = 0
      end if
    case default
      call msg_bug ("ISR/EPA handler: generate weighted: unsupported mode")
    end select
    evt%particle_set_exists = .false.
  end subroutine evt_isr_epa_generate_weighted
```

Insert the generated radiated particles and incoming partons with p_T in their respective places.

The factorization parameters are irrelevant.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure :: make_particle_set => &
    evt_isr_epa_make_particle_set

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_isr_epa_make_particle_set

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    select case (evt%mode)
    case (ISR_TRIVIAL_COLLINEAR)
    case (ISR_PAIR_RECOIL)
      call evt%replace_radiated ()
      call evt%replace_partons ()
      call evt%transform_outgoing ()
    case default
      call msg_bug ("ISR/EPA handler: make particle set: unsupported mode")
    end select
    evt%particle_set_exists = .true.
  end subroutine evt_isr_epa_make_particle_set

<ISR/EPA handler: evt isr: TBP>+≡
  procedure :: prepare_new_event => &
    evt_isr_epa_prepare_new_event

<ISR/EPA handler: sub interfaces>+≡
  module subroutine evt_isr_epa_prepare_new_event (evt, i_mci, i_term)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_isr_epa_prepare_new_event

<ISR/EPA handler: procedures>+≡
  module subroutine evt_isr_epa_prepare_new_event (evt, i_mci, i_term)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_isr_epa_prepare_new_event

```

32.5.10 Unit tests: ISR

Test module, followed by the corresponding implementation module.

This test module differs from most of the other test modules, since it contains two test subroutines: one for ISR and one for EPA below.

```
<isr_epa_handler_ut.f90>≡
  <File header>

  module isr_epa_handler_ut
    use unit_tests
    use isr_epa_handler_uti

  <Standard module head>

  <ISR/EPA handler: public test>

  contains

  <ISR/EPA handler: test driver>

  end module isr_epa_handler_ut
<isr_epa_handler_uti.f90>≡
  <File header>

  module isr_epa_handler_uti

  <Use kinds>
  <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use lorentz, only: vector4_t, vector4_moving, operator(*)
    use rng_base, only: rng_t
    use models, only: syntax_model_file_init, syntax_model_file_final
    use models, only: model_list_t, model_t
    use particles, only: particle_set_t, pacify

    use event_transforms
    use isr_epa_handler, only: evt_isr_epa_t

    use rng_base_ut, only: rng_test_t

  <Standard module head>

  <ISR/EPA handler: test declarations>

  contains

  <ISR/EPA handler: tests>

  end module isr_epa_handler_uti
```

API: driver for the unit tests below.

```
<ISR/EPA handler: public test>≡
```

```

public :: isr_handler_test
<ISR/EPA handler: test driver>≡
  subroutine isr_handler_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <ISR/EPA handler: execute ISR tests>
  end subroutine isr_handler_test

```

Trivial case

Handle photons resulting from ISR radiation. This test is for the trivial case where the event is kept collinear.

```

<ISR/EPA handler: execute ISR tests>≡
  call test (isr_handler_1, "isr_handler_1", &
    "collinear case, no modification", &
    u, results)

<ISR/EPA handler: test declarations>≡
  public :: isr_handler_1

<ISR/EPA handler: tests>≡
  subroutine isr_handler_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x, xb
    real(default) :: probability

    write (u, "(A)")  "* Test output: isr_handler_1"
    write (u, "(A)")  "* Purpose: apply photon handler trivially (no-op)"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

    call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

```



```

sqrt s = 100._default
x = [0.6_default, 0.9_default]
xb= 1 - x

p(1) = vector4_moving (sqrt s/2, sqrt s/2, 3)
p(2) = vector4_moving (sqrt s/2,-sqrt s/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call pacify (evt_trivial%particle_set)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill ISR handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: isr_handler_1"

end subroutine isr_handler_1

```

Photon pair with recoil

Handle photons resulting from ISR radiation. This test invokes the two-photon recoil mechanism. Both photons acquire transverse momentum, the parton momenta recoil, such that total energy-momentum is conserved, and all outgoing photons and partons are on-shell (massless).

```
<ISR/EPA handler: execute ISR tests>+≡
  call test (isr_handler_2, "isr_handler_2", &
    "two-photon recoil", &
    u, results)

<ISR/EPA handler: test declarations>+≡
  public :: isr_handler_2

<ISR/EPA handler: tests>+≡
  subroutine isr_handler_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: isr_handler_2"
    write (u, "(A)")  "* Purpose: apply photon handler with two-photon recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

    call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

    sqrts = 100._default
    x = [0.6_default, 0.9_default]
    xb= 1 - x
```

```

p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call pacify (evt_trivial%particle_set)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_isr ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default, &
    keep_mass = .false. &
)

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill ISR handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: isr_handler_2"

end subroutine isr_handler_2

```

Boosted beams

Handle photons resulting from ISR radiation. This test invokes the two-photon recoil mechanism, in the case that the partons before ISR are not in their c.m. frame (but collinear).

```

<ISR/EPA handler: execute ISR tests>+≡
  call test (isr_handler_3, "isr_handler_3", &
    "two-photon recoil with boost", &
    u, results)

<ISR/EPA handler: test declarations>+≡
  public :: isr_handler_3

<ISR/EPA handler: tests>+≡
  subroutine isr_handler_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x0
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: isr_handler_3"
    write (u, "(A)")  "* Purpose: apply photon handler for boosted beams &
      &and two-photon recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"

```

```

write (u, "(A)")

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
    pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

write (u, "(A)")  "* Event data"
write (u, "(A)")

sqrts = 100._default
write (u, "(A,2(1x,F12.7))")  "sqrts  =", sqrts

x0 = [0.9_default, 0.4_default]
write (u, "(A,2(1x,F12.7))")  "x0      =", x0

write (u, "(A)")
write (u, "(A,2(1x,F12.7))")  "sqs_hat =", sqrts * sqrt (product (x0))

x = [0.6_default, 0.9_default]
xb= 1 - x
write (u, "(A,2(1x,F12.7))")  "x      =", x

write (u, "(A)")
write (u, "(A,2(1x,F12.7))")  "x0 * x =", x0 * x

p(1) = x0(1) * vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = x0(2) * vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")
write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call pacify (evt_trivial%particle_set)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_isr ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default, &

```

```

        keep_mass = .false. &
    )

    allocate (rng_test_t :: rng)
    call rng%init (3) ! default would produce pi for azimuthal angle
    call evt_isr_epa%import_rng (rng)

    call evt_isr_epa%write (u, testflag=.true.)

    write (u, "(A)")
    write (u, "(A)")  "* Fill ISR handler transform"
    write (u, "(A)")

    call evt_isr_epa%prepare_new_event (1, 1)
    call evt_isr_epa%generate_weighted (probability)
    call evt_isr_epa%make_particle_set (0, .false.)

    call evt_isr_epa%write (u, testflag=.true.)

    write (u, "(A)")
    write (u, "(A,1x,F8.5)")  "Event probability =", probability

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call evt_isr_epa%final ()
    call evt_trivial%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: isr_handler_3"

end subroutine isr_handler_3

```

32.5.11 Unit tests: EPA

API: Extra driver for the unit tests below.

```

<ISR/EPA handler: public test>+≡
    public :: epa_handler_test
<ISR/EPA handler: test driver>+≡
    subroutine epa_handler_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <ISR/EPA handler: execute EPA tests>
    end subroutine epa_handler_test

```

Trivial case

Handle events resulting from the EPA approximation. This test is for the trivial case where the event is kept collinear.

```

<ISR/EPA handler: execute EPA tests>≡

```

```

call test (epa_handler_1, "epa_handler_1", &
          "collinear case, no modification", &
          u, results)

<ISR/EPA handler: test declarations>+≡
public :: epa_handler_1

<ISR/EPA handler: tests>+≡
subroutine epa_handler_1 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(particle_set_t) :: pset
  type(model_list_t) :: model_list
  type(model_t), pointer :: model
  type(evt_trivial_t), target :: evt_trivial
  type(evt_isr_epa_t), target :: evt_isr_epa
  type(vector4_t), dimension(8) :: p
  real(default) :: sqrts
  real(default), dimension(2) :: x, xb
  real(default) :: probability

  write (u, "(A)")  "* Test output: epa_handler_1"
  write (u, "(A)")  "* Purpose: apply beam handler trivially (no-op)"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize environment"
  write (u, "(A)")

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)

  write (u, "(A)")  "* Initialize particle set"
  write (u, "(A)")

  call pset%init_direct &
    (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
    pdg = [11, -11, 22, 22, 11, -11, 13, -13], &
    model = model)

  sqrts = 100._default
  x = [0.6_default, 0.9_default]
  xb = 1 - x

  p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
  p(2) = vector4_moving (sqrts/2, -sqrts/2, 3)
  p(3:4) = x * p(1:2)
  p(5:6) = xb * p(1:2)
  p(7:8) = p(3:4)

  call pset%set_momentum (p, on_shell = .false.)

  write (u, "(A)")  "* Fill trivial event transform"

```

```

write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call pacify (evt_trivial%particle_set)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_1"

end subroutine epa_handler_1

```

Beam pair with recoil

Handle beams resulting from the EPA approximation. This test invokes the two-beam recoil mechanism. Both beam remnants acquire transverse momentum, the photon momenta recoil, such that total energy-momentum is conserved, and all outgoing beam remnants and photons are on-shell (massless).

```

<ISR/EPA handler: execute EPA tests>+≡
call test (epa_handler_2, "epa_handler_2", &
  "two-beam recoil", &
  u, results)

```



```

<ISR/EPA handler: test declarations>+=
  public :: epa_handler_2
<ISR/EPA handler: tests>+=
  subroutine epa_handler_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: epa_handler_2"
    write (u, "(A)")  "*   Purpose: apply beam handler with two-beam recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
       os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

    call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 22, 22, 11, -11, 13, -13], model = model)

    sqrts = 100._default
    x = [0.6_default, 0.9_default]
    xb = 1 - x

    p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
    p(2) = vector4_moving (sqrts/2, -sqrts/2, 3)
    p(3:4) = x * p(1:2)
    p(5:6) = xb * p(1:2)
    p(7:8) = p(3:4)

    call pset%set_momentum (p, on_shell = .false.)

    write (u, "(A)")  "* Fill trivial event transform"
    write (u, "(A)")

    call evt_trivial%reset ()
    call evt_trivial%set_particle_set (pset, 1, 1)
    call pacify (evt_trivial%particle_set)

```

```

call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_epa ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default &
    )

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_2"

end subroutine epa_handler_2

```

Boosted beams

Handle radiated beam remnants resulting from EPA radiation. This test invokes the two-beam recoil mechanism, in the case that the partons before EPA are

not in their c.m. frame (but collinear).

```

<ISR/EPA handler: execute EPA tests>+=
  call test (epa_handler_3, "epa_handler_3", &
    "two-beam recoil with boost", &
    u, results)

<ISR/EPA handler: test declarations>+=
  public :: epa_handler_3

<ISR/EPA handler: tests>+=
  subroutine epa_handler_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x0
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: epa_handler_3"
    write (u, "(A)")  "* Purpose: apply beam handler for boosted beams &
      &and two-beam recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

    call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 22, 22, 11, -11, 13, -13], model = model)

    write (u, "(A)")  "* Event data"
    write (u, "(A)")

    sqrts = 100._default
    write (u, "(A,2(1x,F12.7))")  "sqrts  =", sqrts

    x0 = [0.9_default, 0.4_default]
    write (u, "(A,2(1x,F12.7))")  "x0      =", x0

    write (u, "(A)")

```

```

write (u, "(A,2(1x,F12.7))") "sqs_hat =", sqrts * sqrt (product (x0))

x = [0.6_default, 0.9_default]
xb= 1 - x
write (u, "(A,2(1x,F12.7))") "x      =", x

write (u, "(A)")
write (u, "(A,2(1x,F12.7))") "x0 * x =", x0 * x

p(1) = x0(1) * vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = x0(2) * vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")
write (u, "(A)") "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call pacify (evt_trivial%particle_set)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)") "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_epa ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default &
)

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)") "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

```

```

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)") "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_3"

end subroutine epa_handler_3

```

32.6 Decays

```

<decays.f90>≡
<File header>

module decays

<Use kinds>
<Use strings>
  use diagnostics
  use flavors
  use interactions
  use evaluators
  use variables, only: var_list_t
  use model_data
  use rng_base
  use selectors
  use parton_states
  use process, only: process_t
  use instances, only: process_instance_t, pacify
  use process_stacks
  use event_transforms

<Standard module head>

<Decays: public>

<Decays: types>

<Decays: interfaces>

  interface
<Decays: sub interfaces>
  end interface

```

```

contains

  <Decays: main procedures>

end module decays

<decays_sub.f90>≡
  <File header>

  submodule (decays) decays_s

    use io_units
    use format_utils, only: write_indent, write_separator
    use format_defs, only: FMT_15
    use numeric_utils
    use helicities
    use quantum_numbers

    implicit none

  contains

    <Decays: procedures>

  end submodule decays_s

```

32.6.1 Final-State Particle Configuration

A final-state particle may be either stable or unstable. Here is an empty abstract type as the parent of both, with holds just the flavor information.

```

<Decays: types>≡
  type, abstract :: any_config_t
    private
    contains
    <Decays: any config: TBP>
  end type any_config_t

```

Finalizer, depends on the implementation.

```

<Decays: any config: TBP>≡
  procedure (any_config_final), deferred :: final

<Decays: interfaces>≡
  interface
    subroutine any_config_final (object)
      import
      class(any_config_t), intent(inout) :: object
    end subroutine any_config_final
  end interface

```

The output is also deferred:

```

<Decays: any config: TBP>+≡
  procedure (any_config_write), deferred :: write

<Decays: interfaces>+≡
  interface
    subroutine any_config_write (object, unit, indent, verbose)
      import
      class(any_config_t), intent(in) :: object
      integer, intent(in), optional :: unit, indent
      logical, intent(in), optional :: verbose
    end subroutine any_config_write
  end interface

```

This is a container for a stable or unstable particle configurator. We need this wrapper for preparing arrays that mix stable and unstable particles.

```

<Decays: types>+≡
  type :: particle_config_t
  private
    class(any_config_t), allocatable :: c
  end type particle_config_t

```

32.6.2 Final-State Particle

In theory, for the particle instance we only need to consider the unstable case. However, it is more straightforward to treat configuration and instance on the same footing, and to introduce a wrapper for particle objects as above.

```

<Decays: types>+≡
  type, abstract :: any_t
  private
    contains
    <Decays: any: TBP>
  end type any_t

```

Finalizer, depends on the implementation.

```

<Decays: any: TBP>≡
  procedure (any_final), deferred :: final

<Decays: interfaces>+≡
  interface
    subroutine any_final (object)
      import
      class(any_t), intent(inout) :: object
    end subroutine any_final
  end interface

```

The output is also deferred:

```

<Decays: any: TBP>+≡
  procedure (any_write), deferred :: write

```

```

<Decays: interfaces>+=
  interface
    subroutine any_write (object, unit, indent)
      import
      class(any_t), intent(in) :: object
      integer, intent(in), optional :: unit, indent
    end subroutine any_write
  end interface

```

This is a container for a stable or unstable outgoing particle. We need this wrapper for preparing arrays that mix stable and unstable particles.

```

<Decays: types>+=
  type :: particle_out_t
  private
    class(any_t), allocatable :: c
  end type particle_out_t

```

32.6.3 Decay Term Configuration

A decay term is a distinct final state, corresponding to a process term. Each decay process may give rise to several terms with, possibly, differing flavor content.

```

<Decays: types>+=
  type :: decay_term_config_t
  private
    type(particle_config_t), dimension(:), allocatable :: prt
  contains
    <Decays: decay term config: TBP>
  end type decay_term_config_t

```

Finalizer, recursive.

```

<Decays: decay term config: TBP>=
  procedure :: final => decay_term_config_final

<Decays: sub interfaces>=
  recursive module subroutine decay_term_config_final (object)
    class(decay_term_config_t), intent(inout) :: object
  end subroutine decay_term_config_final

<Decays: procedures>=
  recursive module subroutine decay_term_config_final (object)
    class(decay_term_config_t), intent(inout) :: object
    integer :: i
    if (allocated (object%prt)) then
      do i = 1, size (object%prt)
        if (allocated (object%prt(i)%c)) call object%prt(i)%c%final ()
      end do
    end if
  end subroutine decay_term_config_final

```


Output, with optional indentation

```

<Decays: decay term config: TBP>+≡
    procedure :: write => decay_term_config_write

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_config_write &
        (object, unit, indent, verbose)
        class(decay_term_config_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        logical, intent(in), optional :: verbose
    end subroutine decay_term_config_write

<Decays: procedures>+≡
    recursive module subroutine decay_term_config_write &
        (object, unit, indent, verbose)
        class(decay_term_config_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        logical, intent(in), optional :: verbose
        integer :: i, j, u, ind
        logical :: verb
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        verb = .true.; if (present (verbose)) verb = verbose
        call write_indent (u, ind)
        write (u, "(1x,A)", advance="no") "Final state:"
        do i = 1, size (object%prt)
            select type (prt_config => object%prt(i)%c)
                type is (stable_config_t)
                    write (u, "(1x,A)", advance="no") &
                        char (prt_config%flv(1)%get_name ())
                    do j = 2, size (prt_config%flv)
                        write (u, "(:',A)", advance="no") &
                            char (prt_config%flv(j)%get_name ())
                    end do
                type is (unstable_config_t)
                    write (u, "(1x,A)", advance="no") &
                        char (prt_config%flv%get_name ())
            end select
        end do
        write (u, *)
        if (verb) then
            do i = 1, size (object%prt)
                call object%prt(i)%c%write (u, ind)
            end do
        end if
    end subroutine decay_term_config_write

```

Initialize, given a set of flavors. For each flavor, we must indicate whether the particle is stable. The second index of the flavor array runs over alternatives for each decay product; alternatives are allowed only if the decay product is itself stable. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Decays: decay term config: TBP>+≡
    procedure :: init => decay_term_config_init

```

```

<Decays: main procedures>≡
recursive subroutine decay_term_config_init &
  (term, flv, stable, model, process_stack, var_list)
  class(decay_term_config_t), intent(out) :: term
  type(flavor_t), dimension(:,:), intent(in) :: flv
  logical, dimension(:), intent(in) :: stable
  class(model_data_t), intent(in), target :: model
  type(process_stack_t), intent(in), optional :: process_stack
  type(var_list_t), intent(in), optional :: var_list
  type(string_t), dimension(:), allocatable :: decay
  integer :: i
  allocate (term%prt (size (flv, 1)))
  do i = 1, size (flv, 1)
    associate (prt => term%prt(i))
      if (stable(i)) then
        allocate (stable_config_t :: prt%c)
      else
        allocate (unstable_config_t :: prt%c)
      end if
      select type (prt_config => prt%c)
      type is (stable_config_t)
        call prt_config%init (flv(i,:))
      type is (unstable_config_t)
        if (all (flv(i,:) == flv(i,1))) then
          call prt_config%init (flv(i,1))
          call flv(i,1)%get_decays (decay)
          call prt_config%init_decays &
            (decay, model, process_stack, var_list)
        else
          call prt_config%write ()
          call msg_fatal ("Decay configuration: &
            &unstable product must be unique")
        end if
      end select
    end associate
  end do
end subroutine decay_term_config_init

```

Recursively compute widths and branching ratios for all unstable particles.

```

<Decays: decay term config: TBP>+≡
procedure :: compute => decay_term_config_compute

<Decays: sub interfaces>+≡
recursive module subroutine decay_term_config_compute (term)
  class(decay_term_config_t), intent(inout) :: term
end subroutine decay_term_config_compute

<Decays: procedures>+≡
recursive module subroutine decay_term_config_compute (term)
  class(decay_term_config_t), intent(inout) :: term
  integer :: i
  do i = 1, size (term%prt)
    select type (unstable_config => term%prt(i)%c)
    type is (unstable_config_t)
      call unstable_config%compute ()
    end select
  end do
end subroutine decay_term_config_compute

```

```

        end select
    end do
end subroutine decay_term_config_compute

```

32.6.4 Decay Term

A decay term instance is selected when we generate an event for the associated process instance. When evaluated, it triggers further decays down the chain.

Only unstable products are allocated as child particles.

```

<Decays: types>+≡
    type :: decay_term_t
    private
        type(decay_term_config_t), pointer :: config => null ()
        type(particle_out_t), dimension(:), allocatable :: particle_out
    contains
        <Decays: decay term: TBP>
    end type decay_term_t

```

Finalizer.

```

<Decays: decay term: TBP>≡
    procedure :: final => decay_term_final

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_final (object)
        class(decay_term_t), intent(inout) :: object
    end subroutine decay_term_final

<Decays: procedures>+≡
    recursive module subroutine decay_term_final (object)
        class(decay_term_t), intent(inout) :: object
        integer :: i
        if (allocated (object%particle_out)) then
            do i = 1, size (object%particle_out)
                call object%particle_out(i)%c%final ()
            end do
        end if
    end subroutine decay_term_final

```

Output.

```

<Decays: decay term: TBP>+≡
    procedure :: write => decay_term_write

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_write (object, unit, indent)
        class(decay_term_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
    end subroutine decay_term_write

<Decays: procedures>+≡
    recursive module subroutine decay_term_write (object, unit, indent)
        class(decay_term_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        integer :: i, u, ind

```

```

u = given_output_unit (unit)
ind = 0; if (present (indent)) ind = indent
call object%config%write (u, ind, verbose = .false.)
do i = 1, size (object%particle_out)
    call object%particle_out(i)%c%write (u, ind)
end do
end subroutine decay_term_write

```

Recursively write the embedded process instances.

```

<Decays: decay term: TBP>+≡
    procedure :: write_process_instances => decay_term_write_process_instances

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_write_process_instances &
        (term, unit, verbose)
        class(decay_term_t), intent(in) :: term
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine decay_term_write_process_instances

<Decays: procedures>+≡
    recursive module subroutine decay_term_write_process_instances &
        (term, unit, verbose)
        class(decay_term_t), intent(in) :: term
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: i
    do i = 1, size (term%particle_out)
        select type (unstable => term%particle_out(i)%c)
            type is (unstable_t)
                call unstable%write_process_instances (unit, verbose)
            end select
        end do
    end subroutine decay_term_write_process_instances

```

Initialization, using the configuration object. We allocate particle objects in parallel to the particle configuration objects which we use to initialize them, one at a time. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Decays: decay term: TBP>+≡
    procedure :: init => decay_term_init

<Decays: main procedures>+≡
    recursive subroutine decay_term_init (term, config)
        class(decay_term_t), intent(out) :: term
        type(decay_term_config_t), intent(in), target :: config
        integer :: i
        term%config => config
        allocate (term%particle_out (size (config%prt)))
        do i = 1, size (config%prt)
            select type (prt_config => config%prt(i)%c)
                type is (stable_config_t)
                    allocate (stable_t :: term%particle_out(i)%c)
                    select type (stable => term%particle_out(i)%c)
                        type is (stable_t)

```

```

        call stable%init (prt_config)
    end select
    type is (unstable_config_t)
    allocate (unstable_t :: term%particle_out(i)%c)
    select type (unstable => term%particle_out(i)%c)
    type is (unstable_t)
        call unstable%init (prt_config)
    end select
end select
end do
end subroutine decay_term_init

```

Implement a RNG instance, spawned by the process object.

```

<Decays: decay term: TBP>+≡
    procedure :: make_rng => decay_term_make_rng

<Decays: sub interfaces>+≡
    module subroutine decay_term_make_rng (term, process)
        class(decay_term_t), intent(inout) :: term
        type(process_t), intent(inout) :: process
        class(rng_t), allocatable :: rng
    end subroutine decay_term_make_rng

<Decays: procedures>+≡
    module subroutine decay_term_make_rng (term, process)
        class(decay_term_t), intent(inout) :: term
        type(process_t), intent(inout) :: process
        class(rng_t), allocatable :: rng
        integer :: i
        do i = 1, size (term%particle_out)
            select type (unstable => term%particle_out(i)%c)
            type is (unstable_t)
                call process%make_rng (rng)
                call unstable%import_rng (rng)
            end select
        end do
    end subroutine decay_term_make_rng

Link the interactions for unstable decay products to the interaction of the parent
process.

<Decays: decay term: TBP>+≡
    procedure :: link_interactions => decay_term_link_interactions

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_link_interactions (term, trace)
        class(decay_term_t), intent(inout) :: term
        type(interaction_t), intent(in), target :: trace
    end subroutine decay_term_link_interactions

<Decays: procedures>+≡
    recursive module subroutine decay_term_link_interactions (term, trace)
        class(decay_term_t), intent(inout) :: term
        type(interaction_t), intent(in), target :: trace
        integer :: i
        do i = 1, size (term%particle_out)

```

```

        select type (unstable => term%particle_out(i)%c)
        type is (unstable_t)
            call unstable%link_interactions (i, trace)
        end select
    end do
end subroutine decay_term_link_interactions

```

Recursively generate a decay chain, for each of the unstable particles in the final state.

```

<Decays: decay term: TBP>+≡
    procedure :: select_chain => decay_term_select_chain

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_select_chain (term)
        class(decay_term_t), intent(inout) :: term
        end subroutine decay_term_select_chain

<Decays: procedures>+≡
    recursive module subroutine decay_term_select_chain (term)
        class(decay_term_t), intent(inout) :: term
        integer :: i
        do i = 1, size (term%particle_out)
            select type (unstable => term%particle_out(i)%c)
            type is (unstable_t)
                call unstable%select_chain ()
            end select
        end do
    end subroutine decay_term_select_chain

```

Recursively generate a decay event, for each of the unstable particles in the final state.

```

<Decays: decay term: TBP>+≡
    procedure :: generate => decay_term_generate

<Decays: sub interfaces>+≡
    recursive module subroutine decay_term_generate (term)
        class(decay_term_t), intent(inout) :: term
        end subroutine decay_term_generate

<Decays: procedures>+≡
    recursive module subroutine decay_term_generate (term)
        class(decay_term_t), intent(inout) :: term
        integer :: i
        do i = 1, size (term%particle_out)
            select type (unstable => term%particle_out(i)%c)
            type is (unstable_t)
                call unstable%generate ()
            end select
        end do
    end subroutine decay_term_generate

```

32.6.5 Decay Root Configuration

At the root of a decay chain, there is a parent process. The decay root stores a pointer to the parent process and the set of decay configurations.

```
<Decays: public>≡
    public :: decay_root_config_t

<Decays: types>+≡
    type :: decay_root_config_t
    private
        type(string_t) :: process_id
        type(process_t), pointer :: process => null ()
        class(model_data_t), pointer :: model => null ()
        type(decay_term_config_t), dimension(:), allocatable :: term_config
    contains
        <Decays: decay root config: TBP>
    end type decay_root_config_t
```

The finalizer is recursive since there may be cascade decays.

```
<Decays: decay root config: TBP>≡
    procedure :: final => decay_root_config_final

<Decays: sub interfaces>+≡
    recursive module subroutine decay_root_config_final (object)
        class(decay_root_config_t), intent(inout) :: object
    end subroutine decay_root_config_final

<Decays: procedures>+≡
    recursive module subroutine decay_root_config_final (object)
        class(decay_root_config_t), intent(inout) :: object
        integer :: i
        if (allocated (object%term_config)) then
            do i = 1, size (object%term_config)
                call object%term_config(i)%final ()
            end do
        end if
    end subroutine decay_root_config_final
```

The output routine is also recursive, and it contains an adjustable indentation.

```
<Decays: decay root config: TBP>+≡
    procedure :: write => decay_root_config_write
    procedure :: write_header => decay_root_config_write_header
    procedure :: write_terms => decay_root_config_write_terms

<Decays: sub interfaces>+≡
    recursive module subroutine decay_root_config_write &
        (object, unit, indent, verbose)
        class(decay_root_config_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        logical, intent(in), optional :: verbose
    end subroutine decay_root_config_write
    module subroutine decay_root_config_write_header (object, unit, indent)
        class(decay_root_config_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
    end subroutine decay_root_config_write_header
```

```

module recursive subroutine decay_root_config_write_terms &
    (object, unit, indent, verbose)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
end subroutine decay_root_config_write_terms

<Decays: procedures>+≡
recursive module subroutine decay_root_config_write &
    (object, unit, indent, verbose)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,A)") "Final-state decay tree:"
    call object%write_header (unit, indent)
    call object%write_terms (unit, indent, verbose)
end subroutine decay_root_config_write

module subroutine decay_root_config_write_header (object, unit, indent)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    if (associated (object%process)) then
        write (u, 3) "process ID      =", char (object%process_id), "*"
    else
        write (u, 3) "process ID      =", char (object%process_id)
    end if
3   format (3x,A,2(1x,A))
end subroutine decay_root_config_write_header

module recursive subroutine decay_root_config_write_terms &
    (object, unit, indent, verbose)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: i, u, ind
    logical :: verb
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    verb = .true.; if (present (verbose)) verb = verbose
    if (verb .and. allocated (object%term_config)) then
        do i = 1, size (object%term_config)
            call object%term_config(i)%write (u, ind + 1)
        end do
    end if
end subroutine decay_root_config_write_terms

```


Initialize for a named process and (optionally) a pre-determined number of terms.

```

<Decays: decay root config: TBP>+≡
    procedure :: init => decay_root_config_init

<Decays: sub interfaces>+≡
    module subroutine decay_root_config_init (decay, model, process_id, n_terms)
        class(decay_root_config_t), intent(out) :: decay
        class(model_data_t), intent(in), target :: model
        type(string_t), intent(in) :: process_id
        integer, intent(in), optional :: n_terms
    end subroutine decay_root_config_init

<Decays: procedures>+≡
    module subroutine decay_root_config_init (decay, model, process_id, n_terms)
        class(decay_root_config_t), intent(out) :: decay
        class(model_data_t), intent(in), target :: model
        type(string_t), intent(in) :: process_id
        integer, intent(in), optional :: n_terms
        decay%model => model
        decay%process_id = process_id
        if (present (n_terms)) then
            allocate (decay%term_config (n_terms))
        end if
    end subroutine decay_root_config_init

```

Declare a decay term, given an array of flavors.

```

<Decays: decay root config: TBP>+≡
    procedure :: init_term => decay_root_config_init_term

<Decays: sub interfaces>+≡
    recursive module subroutine decay_root_config_init_term &
        (decay, i, flv, stable, model, process_stack, var_list)
        class(decay_root_config_t), intent(inout) :: decay
        integer, intent(in) :: i
        type(flavor_t), dimension(:,:), intent(in) :: flv
        logical, dimension(:), intent(in) :: stable
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        type(var_list_t), intent(in), optional, target :: var_list
    end subroutine decay_root_config_init_term

<Decays: procedures>+≡
    recursive module subroutine decay_root_config_init_term &
        (decay, i, flv, stable, model, process_stack, var_list)
        class(decay_root_config_t), intent(inout) :: decay
        integer, intent(in) :: i
        type(flavor_t), dimension(:,:), intent(in) :: flv
        logical, dimension(:), intent(in) :: stable
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        type(var_list_t), intent(in), optional, target :: var_list
        call decay%term_config(i)%init (flv, stable, model, process_stack, var_list)
    end subroutine decay_root_config_init_term

```

Connect the decay root configuration with a process object (which should represent the parent process). This includes initialization, therefore `intent(out)`.

The flavor state is retrieved from the process term object. However, we have to be careful: the flavor object points to the model instance that is stored in the process object. This model instance may not contain the current setting for unstable particles and decay. Therefore, we assign the model directly.

If the `process_instance` argument is provided, we use this for the flavor state. This applies to the decay root only, where the process can be entangled with a beam setup, and the latter contains beam remnants as further outgoing particles. These must be included in the set of outgoing flavors, since the decay application is also done on the connected state.

Infer stability from the particle properties, using the first row in the set of flavor states. For unstable particles, we look for decays, recursively, available from the process stack (if present).

For the unstable particles, we have to check whether their masses match between the production and the decay. Fortunately, both versions are available for comparison.

The optional `var_list` argument may override integral/error values for decay processes.

```

<Decays: decay root config: TBP>+=
  procedure :: connect => decay_root_config_connect

<Decays: sub interfaces>+=
  recursive module subroutine decay_root_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_root_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
  end subroutine decay_root_config_connect

<Decays: procedures>+=
  recursive module subroutine decay_root_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_root_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
    type(connected_state_t), pointer :: connected_state
    type(interaction_t), pointer :: int
    type(flavor_t), dimension(:,:), allocatable :: flv
    logical, dimension(:), allocatable :: stable
    real(default), dimension(:), allocatable :: m_prod, m_dec
    integer :: i
    call decay%init (model, process%get_id (), process%get_n_terms ())
    do i = 1, size (decay%term_config)
      if (present (process_instance)) then
        connected_state => process_instance%get_connected_state_ptr (i)
        int => connected_state%get_matrix_int_ptr ()

```

```

        call int%get_flv_out (flv)
    else
        call process%get_term_flv_out (i, flv)
    end if
    allocate (m_prod (size (flv(:,1)%get_mass ())))
    m_prod = flv(:,1)%get_mass ()
    call flv%set_model (model)
    allocate (m_dec (size (flv(:,1)%get_mass ())))
    m_dec = flv(:,1)%get_mass ()
    allocate (stable (size (flv, 1)))
    stable = flv(:,1)%is_stable ()
    call check_masses ()
    call decay%init_term (i, flv, stable, model, process_stack, var_list)
    deallocate (flv, stable, m_prod, m_dec)
end do
decay%process => process
contains
subroutine check_masses ()
    integer :: i
    logical :: ok
    ok = .true.
    do i = 1, size (m_prod)
        if (.not. stable(i)) then
            if (.not. nearly_equal (m_prod(i), m_dec(i))) then
                write (msg_buffer, "(A,A,A)") "particle '", &
                    char (flv(i,1)%get_name ()), "':"
                call msg_message
                write (msg_buffer, &
                    "(2x,A,1x," // FMT_15 // ",3x,A,1x," // FMT_15 // ")") &
                    "m_prod =", m_prod(i), "m_dec =", m_dec(i)
                call msg_message
                ok = .false.
            end if
        end if
    end do
    if (.not. ok) call msg_fatal &
        ("Particle mass mismatch between production and decay")
end subroutine check_masses
end subroutine decay_root_config_connect

```

Recursively compute widths, errors, and branching ratios.

```

<Decays: decay root config: TBP>+≡
    procedure :: compute => decay_root_config_compute

<Decays: sub interfaces>+≡
    recursive module subroutine decay_root_config_compute (decay)
        class(decay_root_config_t), intent(inout) :: decay
    end subroutine decay_root_config_compute

<Decays: procedures>+≡
    recursive module subroutine decay_root_config_compute (decay)
        class(decay_root_config_t), intent(inout) :: decay
        integer :: i
        do i = 1, size (decay%term_config)
            call decay%term_config(i)%compute ()

```

```

    end do
end subroutine decay_root_config_compute

```

32.6.6 Decay Root Instance

This is the common parent type for decay and decay root. The process instance points to the parent process. The model pointer is separate because particle settings may be updated w.r.t. the parent process object.

```

<Decays: types>+≡
  type, abstract :: decay_gen_t
  private
    type(decay_term_t), dimension(:), allocatable :: term
    type(process_instance_t), pointer :: process_instance => null ()
    integer :: selected_mci = 0
    integer :: selected_term = 0
  contains
    <Decays: decay gen: TBP>
  end type decay_gen_t

```

The decay root represents the parent process. When an event is generated, the generator selects the term to which the decay chain applies (if possible).

The process instance is just a pointer.

```

<Decays: public>+≡
  public :: decay_root_t

<Decays: types>+≡
  type, extends (decay_gen_t) :: decay_root_t
  private
    type(decay_root_config_t), pointer :: config => null ()
  contains
    <Decays: decay root: TBP>
  end type decay_root_t

```

The finalizer has to recursively finalize the terms, but we can skip the process instance which is not explicitly allocated.

```

<Decays: decay gen: TBP>≡
  procedure :: base_final => decay_gen_final

<Decays: sub interfaces>+≡
  recursive module subroutine decay_gen_final (object)
    class(decay_gen_t), intent(inout) :: object
  end subroutine decay_gen_final

<Decays: procedures>+≡
  recursive module subroutine decay_gen_final (object)
    class(decay_gen_t), intent(inout) :: object
    integer :: i
    if (allocated (object%term)) then
      do i = 1, size (object%term)
        call object%term(i)%final ()
      end do
    end if
  end subroutine decay_gen_final

```

```
end subroutine decay_gen_final
```

No extra finalization for the decay root.

```
<Decays: decay root: TBP>≡
  procedure :: final => decay_root_final

<Decays: sub interfaces>+≡
  module subroutine decay_root_final (object)
    class(decay_root_t), intent(inout) :: object
  end subroutine decay_root_final

<Decays: procedures>+≡
  module subroutine decay_root_final (object)
    class(decay_root_t), intent(inout) :: object
    call object%base_final ()
  end subroutine decay_root_final
```

Output.

```
<Decays: decay root: TBP>+≡
  procedure :: write => decay_root_write

<Decays: sub interfaces>+≡
  module subroutine decay_root_write (object, unit)
    class(decay_root_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine decay_root_write

<Decays: procedures>+≡
  module subroutine decay_root_write (object, unit)
    class(decay_root_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%config)) then
      call object%config%write (unit, verbose = .false.)
    else
      write (u, "(1x,A)") "Final-state decay tree: [not configured]"
    end if
    if (object%selected_mci > 0) then
      write (u, "(3x,A,I0)") "Selected MCI      = ", object%selected_mci
    else
      write (u, "(3x,A)") "Selected MCI      = [undefined]"
    end if
    if (object%selected_term > 0) then
      write (u, "(3x,A,I0)") "Selected term    = ", object%selected_term
      call object%term(object%selected_term)%write (u, 1)
    else
      write (u, "(3x,A)") "Selected term    = [undefined]"
    end if
  end subroutine decay_root_write
```

Write the process instances, recursively.

```
<Decays: decay gen: TBP>+≡
  procedure :: write_process_instances => decay_gen_write_process_instances
```

```

<Decays: sub interfaces>+≡
    recursive module subroutine decay_gen_write_process_instances &
        (decay, unit, verbose)
        class(decay_gen_t), intent(in) :: decay
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine decay_gen_write_process_instances
<Decays: procedures>+≡
    recursive module subroutine decay_gen_write_process_instances &
        (decay, unit, verbose)
        class(decay_gen_t), intent(in) :: decay
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        logical :: verb
        verb = .true.; if (present (verbose)) verb = verbose
        if (associated (decay%process_instance)) then
            if (verb) then
                call decay%process_instance%write (unit)
            else
                call decay%process_instance%write_header (unit)
            end if
        end if
        if (decay%selected_term > 0) then
            call decay%term(decay%selected_term)%write_process_instances (unit, verb)
        end if
    end subroutine decay_gen_write_process_instances

```

Generic initializer. All can be done recursively.

```

<Decays: decay gen: TBP>+≡
    procedure :: base_init => decay_gen_init
<Decays: sub interfaces>+≡
    recursive module subroutine decay_gen_init (decay, term_config)
        class(decay_gen_t), intent(out) :: decay
        type(decay_term_config_t), dimension(:), intent(in), target :: term_config
    end subroutine decay_gen_init
<Decays: procedures>+≡
    recursive module subroutine decay_gen_init (decay, term_config)
        class(decay_gen_t), intent(out) :: decay
        type(decay_term_config_t), dimension(:), intent(in), target :: term_config
        integer :: i
        allocate (decay%term (size (term_config)))
        do i = 1, size (decay%term)
            call decay%term(i)%init (term_config(i))
        end do
    end subroutine decay_gen_init

```

Specific initializer. We assign the configuration object, which should correspond to a completely initialized decay configuration tree. We also connect to an existing process instance. Then, we recursively link the child interactions to the parent process.

```

<Decays: decay root: TBP>+≡
    procedure :: init => decay_root_init

```

```

<Decays: sub interfaces>+≡
  module subroutine decay_root_init (decay_root, config, process_instance)
    class(decay_root_t), intent(out) :: decay_root
    type(decay_root_config_t), intent(in), target :: config
    type(process_instance_t), intent(in), target :: process_instance
  end subroutine decay_root_init

```

```

<Decays: procedures>+≡
  module subroutine decay_root_init (decay_root, config, process_instance)
    class(decay_root_t), intent(out) :: decay_root
    type(decay_root_config_t), intent(in), target :: config
    type(process_instance_t), intent(in), target :: process_instance
    call decay_root%base_init (config%term_config)
    decay_root%config => config
    decay_root%process_instance => process_instance
    call decay_root%make_term_rng (config%process)
    call decay_root%link_term_interactions ()
  end subroutine decay_root_init

```

Explicitly set/get mci and term indices. (Used in unit test.)

```

<Decays: decay gen: TBP>+≡
  procedure :: set_mci => decay_gen_set_mci
  procedure :: set_term => decay_gen_set_term
  procedure :: get_mci => decay_gen_get_mci
  procedure :: get_term => decay_gen_get_term

```

```

<Decays: sub interfaces>+≡
  module subroutine decay_gen_set_mci (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
  end subroutine decay_gen_set_mci
  module subroutine decay_gen_set_term (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
  end subroutine decay_gen_set_term
  module function decay_gen_get_mci (decay) result (i)
    class(decay_gen_t), intent(inout) :: decay
    integer :: i
  end function decay_gen_get_mci
  module function decay_gen_get_term (decay) result (i)
    class(decay_gen_t), intent(inout) :: decay
    integer :: i
  end function decay_gen_get_term

```

```

<Decays: procedures>+≡
  module subroutine decay_gen_set_mci (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
    decay%selected_mci = i
  end subroutine decay_gen_set_mci

  module subroutine decay_gen_set_term (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
    decay%selected_term = i
  end subroutine decay_gen_set_term

```

```

end subroutine decay_gen_set_term

module function decay_gen_get_mci (decay) result (i)
  class(decay_gen_t), intent(inout) :: decay
  integer :: i
  i = decay%selected_mci
end function decay_gen_get_mci

module function decay_gen_get_term (decay) result (i)
  class(decay_gen_t), intent(inout) :: decay
  integer :: i
  i = decay%selected_term
end function decay_gen_get_term

```

Implement random-number generators for unstable decay selection in all terms. This is not recursive.

We also make use of the fact that `process` is a pointer; the (state of the RNG factory inside the) target process will be modified by the rng-spawning method, but not the pointer.

```

<Decays: decay gen: TBP>+≡
  procedure :: make_term_rng => decay_gen_make_term_rng

<Decays: sub interfaces>+≡
  module subroutine decay_gen_make_term_rng (decay, process)
    class(decay_gen_t), intent(inout) :: decay
    type(process_t), intent(in), pointer :: process
  end subroutine decay_gen_make_term_rng

<Decays: procedures>+≡
  module subroutine decay_gen_make_term_rng (decay, process)
    class(decay_gen_t), intent(inout) :: decay
    type(process_t), intent(in), pointer :: process
    integer :: i
    do i = 1, size (decay%term)
      call decay%term(i)%make_rng (process)
    end do
  end subroutine decay_gen_make_term_rng

```

Recursively link interactions of the enclosed decay terms to the corresponding terms in the current process instance.

```

<Decays: decay gen: TBP>+≡
  procedure :: link_term_interactions => decay_gen_link_term_interactions

<Decays: sub interfaces>+≡
  recursive module subroutine decay_gen_link_term_interactions (decay)
    class(decay_gen_t), intent(inout) :: decay
  end subroutine decay_gen_link_term_interactions

<Decays: procedures>+≡
  recursive module subroutine decay_gen_link_term_interactions (decay)
    class(decay_gen_t), intent(inout) :: decay
    integer :: i
    type(interaction_t), pointer :: trace
    associate (instance => decay%process_instance)

```



```

do i = 1, size (decay%term)
  trace => instance%get_trace_int_ptr (i)
  call decay%term(i)%link_interactions (trace)
end do
end associate
end subroutine decay_gen_link_term_interactions

```

Select a decay chain: decay modes and process components.

```

<Decays: decay root: TBP>+≡
  procedure :: select_chain => decay_root_select_chain

<Decays: sub interfaces>+≡
  module subroutine decay_root_select_chain (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    end subroutine decay_root_select_chain

<Decays: procedures>+≡
  module subroutine decay_root_select_chain (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    if (decay_root%selected_term > 0) then
      call decay_root%term(decay_root%selected_term)%select_chain ()
    else
      call msg_bug ("Decays: no term selected for parent process")
    end if
  end subroutine decay_root_select_chain

```

Generate a decay tree, i.e., for the selected term in the parent process, recursively generate a decay event for all unstable particles.

Factor out the trace of the connected state of the parent process. This trace should not be taken into account for unweighting the decay chain, since it was already used for unweighting the parent event, or it determines the overall event weight.

```

<Decays: decay root: TBP>+≡
  procedure :: generate => decay_root_generate

<Decays: sub interfaces>+≡
  module subroutine decay_root_generate (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    end subroutine decay_root_generate

<Decays: procedures>+≡
  module subroutine decay_root_generate (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    type(connected_state_t), pointer :: connected_state
    if (decay_root%selected_term > 0) then
      connected_state => decay_root%process_instance%get_connected_state_ptr &
        (decay_root%selected_term)
      call connected_state%normalize_matrix_by_trace ()
      call decay_root%term(decay_root%selected_term)%generate ()
    else
      call msg_bug ("Decays: no term selected for parent process")
    end if
  end subroutine decay_root_generate

```

32.6.7 Decay Configuration

A decay configuration describes a distinct decay mode of a particle. Each decay mode may include several terms, which correspond to the terms in the associated process. In addition to the base type, the decay configuration object contains the integral of the parent process and the selector for the MCI group inside this process.

The flavor component should be identical to the flavor component of the parent particle (`unstable` object).

```

<Decays: types>+≡
  type, extends (decay_root_config_t) :: decay_config_t
  private
    type(flavor_t) :: flv
    real(default) :: weight = 0
    real(default) :: integral = 0
    real(default) :: abs_error = 0
    real(default) :: rel_error = 0
    type(selector_t) :: mci_selector
  contains
    <Decays: decay config: TBP>
  end type decay_config_t

```

The output routine extends the decay-root writer by listing numerical component values.

```

<Decays: decay config: TBP>≡
  procedure :: write => decay_config_write

<Decays: sub interfaces>+≡
  recursive module subroutine decay_config_write &
    (object, unit, indent, verbose)
    class(decay_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
  end subroutine decay_config_write

<Decays: procedures>+≡
  recursive module subroutine decay_config_write (object, unit, indent, verbose)
    class(decay_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,A)") "Decay:"
    call object%write_header (unit, indent)
    call write_indent (u, ind)
    write (u, 2) "branching ratio =", object%weight * 100
    call write_indent (u, ind)
    write (u, 1) "partial width   =", object%integral
    call write_indent (u, ind)
    write (u, 1) "error (abs)      =", object%abs_error
    call write_indent (u, ind)
    write (u, 1) "error (rel)     =", object%rel_error
  end subroutine decay_config_write

```

```

1  format (3x,A,ES19.12)
2  format (3x,A,F11.6,1x,'%')
   call object%write_terms (unit, indent, verbose)
end subroutine decay_config_write

```

Connect a decay configuration with a process object (which should represent the decay). This includes initialization, therefore intent(out). We first connect the process itself, then do initializations that are specific for this decay.

Infer stability from the particle properties, using the first row in the set of flavor states. Once we can deal with predetermined decay chains, they should be used instead.

If there is an optional `var_list`, check if the stored values for the decay partial width and error have been overridden there.

```

<Decays: decay config: TBP>+≡
  procedure :: connect => decay_config_connect

<Decays: sub interfaces>+≡
  recursive module subroutine decay_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
  end subroutine decay_config_connect

<Decays: procedures>+≡
  recursive module subroutine decay_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
    real(default), dimension(:), allocatable :: integral_mci
    type(string_t) :: process_id
    integer :: i, n_mci
    call decay%decay_root_config_t%connect &
      (process, model, process_stack, var_list=var_list)
    process_id = process%get_id ()
    if (process%lab_is_cm ()) then
      call msg_fatal ("Decay process " // char (process_id) &
        // ": unusable because rest frame is fixed.")
    end if
    decay%integral = process%get_integral ()
    decay%abs_error = process%get_error ()
    if (present (var_list)) then
      call update (decay%integral, "integral(" // process_id // ")")
      call update (decay%abs_error, "error(" // process_id // ")")
    end if
    n_mci = process%get_n_mci ()
    allocate (integral_mci (n_mci))

```

```

do i = 1, n_mci
  integral_mci(i) = process%get_integral_mci (i)
end do
call decay%mci_selector%init (integral_mci)
contains
  subroutine update (var, var_name)
    real(default), intent(inout) :: var
    type(string_t), intent(in) :: var_name
    if (var_list%contains (var_name)) then
      var = var_list%get_rval (var_name)
    end if
  end subroutine update
end subroutine decay_config_connect

```

Set the flavor entry, which repeats the flavor of the parent unstable particle.

```

<Decays: decay config: TBP>+≡
  procedure :: set_flv => decay_config_set_flv

<Decays: sub interfaces>+≡
  module subroutine decay_config_set_flv (decay, flv)
    class(decay_config_t), intent(inout) :: decay
    type(flavor_t), intent(in) :: flv
  end subroutine decay_config_set_flv

<Decays: procedures>+≡
  module subroutine decay_config_set_flv (decay, flv)
    class(decay_config_t), intent(inout) :: decay
    type(flavor_t), intent(in) :: flv
    decay%flv = flv
  end subroutine decay_config_set_flv

```

Compute embedded branchings and the relative error. This method does not apply to the decay root.

```

<Decays: decay config: TBP>+≡
  procedure :: compute => decay_config_compute

<Decays: sub interfaces>+≡
  recursive module subroutine decay_config_compute (decay)
    class(decay_config_t), intent(inout) :: decay
  end subroutine decay_config_compute

<Decays: procedures>+≡
  recursive module subroutine decay_config_compute (decay)
    class(decay_config_t), intent(inout) :: decay
    call decay%decay_root_config_t%compute ()
    if (.not. vanishes (decay%integral)) then
      decay%rel_error = decay%abs_error / decay%integral
    else
      decay%rel_error = 0
    end if
  end subroutine decay_config_compute

```

32.6.8 Decay Instance

The decay contains a collection of terms. One of them is selected when the decay is evaluated. This is similar to the decay root, but we implement it independently.

The process instance object is allocated via a pointer, so it automatically behaves as a target.

```
<Decays: types>+≡
  type, extends (decay_gen_t) :: decay_t
  private
    type(decay_config_t), pointer :: config => null ()
    class(rng_t), allocatable :: rng
  contains
    <Decays: decay: TBP>
  end type decay_t
```

The finalizer is recursive.

```
<Decays: decay: TBP>≡
  procedure :: final => decay_final

<Decays: sub interfaces>+≡
  recursive module subroutine decay_final (object)
    class(decay_t), intent(inout) :: object
  end subroutine decay_final

<Decays: procedures>+≡
  recursive module subroutine decay_final (object)
    class(decay_t), intent(inout) :: object
    integer :: i
    call object%base_final ()
    do i = 1, object%config%process%get_n_mci ()
      call object%process_instance%final_simulation (i)
    end do
    call object%process_instance%final ()
    deallocate (object%process_instance)
  end subroutine decay_final
```

Output.

```
<Decays: decay: TBP>+≡
  procedure :: write => decay_write

<Decays: sub interfaces>+≡
  recursive module subroutine decay_write (object, unit, indent, recursive)
    class(decay_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent, recursive
  end subroutine decay_write

<Decays: procedures>+≡
  recursive module subroutine decay_write (object, unit, indent, recursive)
    class(decay_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent, recursive
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call object%config%write (unit, indent, verbose = .false.)
```

```

if (allocated (object%rng)) then
  call object%rng%write (u, ind + 1)
end if
call write_indent (u, ind)
if (object%selected_mci > 0) then
  write (u, "(3x,A,I0)") "Selected MCI    = ", object%selected_mci
else
  write (u, "(3x,A)") "Selected MCI    = [undefined]"
end if
call write_indent (u, ind)
if (object%selected_term > 0) then
  write (u, "(3x,A,I0)") "Selected term  = ", object%selected_term
  call object%term(object%selected_term)%write (u, ind + 1)
else
  write (u, "(3x,A)") "Selected term  = [undefined]"
end if
end subroutine decay_write

```

Initializer. Base initialization is done recursively. Then, we prepare the current process instance and allocate a random-number generator for term selection. For all unstable particles, we also allocate a r.n.g. as spawned by the current process.

```

<Decays: decay: TBP>+≡
  procedure :: init => decay_init

<Decays: sub interfaces>+≡
  recursive module subroutine decay_init (decay, config)
    class(decay_t), intent(out) :: decay
    type(decay_config_t), intent(in), target :: config
  end subroutine decay_init

<Decays: procedures>+≡
  recursive module subroutine decay_init (decay, config)
    class(decay_t), intent(out) :: decay
    type(decay_config_t), intent(in), target :: config
    integer :: i
    call decay%base_init (config%term_config)
    decay%config => config
    allocate (decay%process_instance)
    call decay%process_instance%init (decay%config%process)
    call decay%process_instance%setup_event_data (decay%config%model)
    do i = 1, decay%config%process%get_n_mci ()
      call decay%process_instance%init_simulation (i)
    end do
    call decay%config%process%make_rng (decay%rng)
    call decay%make_term_rng (decay%config%process)
  end subroutine decay_init

```

Link interactions to the parent process. `i_prt` is the index of the current outgoing particle in the parent interaction, for which we take the trace evaluator. We link it to the beam particle in the beam interaction of the decay process instance. Then, repeat the procedure for the outgoing particles.

```

<Decays: decay: TBP>+≡
  procedure :: link_interactions => decay_link_interactions

```

```

<Decays: sub interfaces>+≡
    recursive module subroutine decay_link_interactions (decay, i_prt, trace)
        class(decay_t), intent(inout) :: decay
        integer, intent(in) :: i_prt
        type(interaction_t), intent(in), target :: trace
    end subroutine decay_link_interactions

<Decays: procedures>+≡
    recursive module subroutine decay_link_interactions (decay, i_prt, trace)
        class(decay_t), intent(inout) :: decay
        integer, intent(in) :: i_prt
        type(interaction_t), intent(in), target :: trace
        type(interaction_t), pointer :: beam_int
        integer :: n_in, n_vir
        beam_int => decay%process_instance%get_beam_int_ptr ()
        n_in = trace%get_n_in ()
        n_vir = trace%get_n_vir ()
        call beam_int%set_source_link (1, trace, &
            n_in + n_vir + i_prt)
        call decay%link_term_interactions ()
    end subroutine decay_link_interactions

```

Determine a decay chain. For each unstable particle we select one of the possible decay modes, and for each decay process we select one of the possible decay MCI components, calling the random-number generators. We do not generate momenta, yet.

```

<Decays: decay: TBP>+≡
    procedure :: select_chain => decay_select_chain

<Decays: sub interfaces>+≡
    recursive module subroutine decay_select_chain (decay)
        class(decay_t), intent(inout) :: decay
    end subroutine decay_select_chain

<Decays: procedures>+≡
    recursive module subroutine decay_select_chain (decay)
        class(decay_t), intent(inout) :: decay
        real(default) :: x
        integer :: i
        call decay%rng%generate (x)
        decay%selected_mci = decay%config%mc_selector%select (x)
        call decay%process_instance%choose_mci (decay%selected_mci)
        decay%selected_term = decay%process_instance%select_i_term ()
        do i = 1, size (decay%term)
            call decay%term(i)%select_chain ()
        end do
    end subroutine decay_select_chain

```

Generate a decay. We first receive the beam momenta from the parent process (assuming that this is properly linked), then call the associated process object for a new event.

Factor out the trace of the helicity density matrix of the isolated state (the one that will be used for the decay chain). The trace is taken into account

for unweighting the individual decay event and should therefore be ignored for unweighting the correlated decay chain afterwards.

```

<Decays: decay: TBP>+≡
    procedure :: generate => decay_generate

<Decays: sub interfaces>+≡
    recursive module subroutine decay_generate (decay)
        class(decay_t), intent(inout) :: decay
    end subroutine decay_generate

<Decays: procedures>+≡
    recursive module subroutine decay_generate (decay)
        class(decay_t), intent(inout) :: decay
        type(isolated_state_t), pointer :: isolated_state
        integer :: i
        call decay%process_instance%receive_beam_momenta ()
        call decay%process_instance%generate_unweighted_event (decay%selected_mci)
        if (signal_is_pending ()) return
        call decay%process_instance%evaluate_event_data ()
        isolated_state => &
            decay%process_instance%get_isolated_state_ptr (decay%selected_term)
        call isolated_state%normalize_matrix_by_trace ()
        do i = 1, size (decay%term)
            call decay%term(i)%generate ()
            if (signal_is_pending ()) return
        end do
    end subroutine decay_generate

```

32.6.9 Stable Particles

This is a stable particle. The flavor can be ambiguous (e.g., partons).

```

<Decays: types>+≡
    type, extends (any_config_t) :: stable_config_t
    private
        type(flavor_t), dimension(:), allocatable :: flv
    contains
        <Decays: stable config: TBP>
    end type stable_config_t

```

The finalizer is empty:

```

<Decays: stable config: TBP>≡
    procedure :: final => stable_config_final

<Decays: sub interfaces>+≡
    module subroutine stable_config_final (object)
        class(stable_config_t), intent(inout) :: object
    end subroutine stable_config_final

<Decays: procedures>+≡
    module subroutine stable_config_final (object)
        class(stable_config_t), intent(inout) :: object
    end subroutine stable_config_final

```


Output.

```

<Decays: stable config: TBP>+=
  procedure :: write => stable_config_write

<Decays: sub interfaces>+=
  recursive module subroutine stable_config_write &
    (object, unit, indent, verbose)
    class(stable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
  end subroutine stable_config_write

<Decays: procedures>+=
  recursive module subroutine stable_config_write &
    (object, unit, indent, verbose)
    class(stable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, i, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,'+',1x,A)", advance = "no") "Stable:"
    write (u, "(1x,A)", advance = "no") char (object%flv(1)%get_name ())
    do i = 2, size (object%flv)
      write (u, "(:',A)", advance = "no") &
        char (object%flv(i)%get_name ())
    end do
    write (u, *)
  end subroutine stable_config_write

```

Initializer. We are presented with an array of flavors, but there may be double entries which we remove, so we store only the distinct flavors.

```

<Decays: stable config: TBP>+=
  procedure :: init => stable_config_init

<Decays: sub interfaces>+=
  module subroutine stable_config_init (config, flv)
    class(stable_config_t), intent(out) :: config
    type(flavor_t), dimension(:), intent(in) :: flv
  end subroutine stable_config_init

<Decays: procedures>+=
  module subroutine stable_config_init (config, flv)
    class(stable_config_t), intent(out) :: config
    type(flavor_t), dimension(:), intent(in) :: flv
    integer, dimension (size (flv)) :: pdg
    logical, dimension (size (flv)) :: mask
    integer :: i
    pdg = flv%get_pdg ()
    mask(1) = .true.
    forall (i = 2 : size (pdg))
      mask(i) = all (pdg(i) /= pdg(1:i-1))
    end forall
    allocate (config%flv (count (mask)))

```

```

    config%flv = pack (flv, mask)
end subroutine stable_config_init

```

Here is the corresponding object instance. Except for the pointer to the configuration, there is no content.

```

<Decays: types>+≡
    type, extends (any_t) :: stable_t
    private
        type(stable_config_t), pointer :: config => null ()
    contains
        <Decays: stable: TBP>
    end type stable_t

```

The finalizer does nothing.

```

<Decays: stable: TBP>≡
    procedure :: final => stable_final

<Decays: sub interfaces>+≡
    module subroutine stable_final (object)
        class(stable_t), intent(inout) :: object
    end subroutine stable_final

<Decays: procedures>+≡
    module subroutine stable_final (object)
        class(stable_t), intent(inout) :: object
    end subroutine stable_final

```

We can delegate output to the configuration object.

```

<Decays: stable: TBP>+≡
    procedure :: write => stable_write

<Decays: sub interfaces>+≡
    module subroutine stable_write (object, unit, indent)
        class(stable_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
    end subroutine stable_write

<Decays: procedures>+≡
    module subroutine stable_write (object, unit, indent)
        class(stable_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        call object%config%write (unit, indent)
    end subroutine stable_write

```

Initializer: just assign the configuration.

```

<Decays: stable: TBP>+≡
    procedure :: init => stable_init

<Decays: sub interfaces>+≡
    module subroutine stable_init (stable, config)
        class(stable_t), intent(out) :: stable
        type(stable_config_t), intent(in), target :: config
    end subroutine stable_init

```

```

<Decays: procedures>+≡
  module subroutine stable_init (stable, config)
    class(stable_t), intent(out) :: stable
    type(stable_config_t), intent(in), target :: config
    stable%config => config
  end subroutine stable_init

```

32.6.10 Unstable Particles

A branching configuration enables us to select among distinct decay modes of a particle. We store the particle flavor (with its implicit link to a model), an array of decay configurations, and a selector object.

The total width, absolute and relative error are stored as `integral`, `abs_error`, and `rel_error`, respectively.

The flavor must be unique in this case.

```

<Decays: public>+≡
  public :: unstable_config_t

<Decays: types>+≡
  type, extends (any_config_t) :: unstable_config_t
    private
    type(flavor_t) :: flv
    real(default) :: integral = 0
    real(default) :: abs_error = 0
    real(default) :: rel_error = 0
    type(selector_t) :: selector
    type(decay_config_t), dimension(:), allocatable :: decay_config
  contains
    <Decays: unstable config: TBP>
  end type unstable_config_t

```

Finalizer. The branching configuration can be a recursive structure.

```

<Decays: unstable config: TBP>≡
  procedure :: final => unstable_config_final

<Decays: sub interfaces>+≡
  recursive module subroutine unstable_config_final (object)
    class(unstable_config_t), intent(inout) :: object
  end subroutine unstable_config_final

<Decays: procedures>+≡
  recursive module subroutine unstable_config_final (object)
    class(unstable_config_t), intent(inout) :: object
    integer :: i
    if (allocated (object%decay_config)) then
      do i = 1, size (object%decay_config)
        call object%decay_config(i)%final ()
      end do
    end if
  end subroutine unstable_config_final

```

Output. Since this may be recursive, we include indentation.

```

<Decays: unstable config: TBP>+≡
  procedure :: write => unstable_config_write

<Decays: sub interfaces>+≡
  recursive module subroutine unstable_config_write &
    (object, unit, indent, verbose)
    class(unstable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
  end subroutine unstable_config_write

<Decays: procedures>+≡
  recursive module subroutine unstable_config_write &
    (object, unit, indent, verbose)
    class(unstable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, i, ind
    logical :: verb
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    verb = .true.; if (present (verbose)) verb = verbose
    call write_indent (u, ind)
    write (u, "(1x,'+',1x,A,1x,A)") "Unstable:", &
      char (object%flv%get_name ())
    call write_indent (u, ind)
    write (u, 1) "total width =", object%integral
    call write_indent (u, ind)
    write (u, 1) "error (abs) =", object%abs_error
    call write_indent (u, ind)
    write (u, 1) "error (rel) =", object%rel_error
1   format (5x,A,ES19.12)
    if (verb .and. allocated (object%decay_config)) then
      do i = 1, size (object%decay_config)
        call object%decay_config(i)%write (u, ind + 1)
      end do
    end if
  end subroutine unstable_config_write

```

Initializer. For the unstable particle, the flavor is unique.

```

<Decays: unstable config: TBP>+≡
  procedure :: init => unstable_config_init

<Decays: sub interfaces>+≡
  module subroutine unstable_config_init (unstable, flv, set_decays, model)
    class(unstable_config_t), intent(out) :: unstable
    type(flavor_t), intent(in) :: flv
    logical, intent(in), optional :: set_decays
    class(model_data_t), intent(in), optional, target :: model
  end subroutine unstable_config_init

<Decays: procedures>+≡
  module subroutine unstable_config_init (unstable, flv, set_decays, model)
    class(unstable_config_t), intent(out) :: unstable

```

```

type(flavor_t), intent(in) :: flv
logical, intent(in), optional :: set_decays
class(model_data_t), intent(in), optional, target :: model
type(string_t), dimension(:), allocatable :: decay
unstable%flv = flv
if (present (set_decays)) then
    call unstable%flv%get_decays (decay)
    call unstable%init_decays (decay, model)
end if
end subroutine unstable_config_init

```

Further initialization: determine the number of decay modes. We can assume that the flavor of the particle has been set already.

If the process stack is given, we can delve recursively into actually assigning decay processes. Otherwise, we just initialize with decay process names.

```

<Decays: unstable config: TBP>+≡
    procedure :: init_decays => unstable_config_init_decays

<Decays: sub interfaces>+≡
    recursive module subroutine unstable_config_init_decays &
        (unstable, decay_id, model, process_stack, var_list)
        class(unstable_config_t), intent(inout) :: unstable
        type(string_t), dimension(:), intent(in) :: decay_id
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        type(var_list_t), intent(in), optional :: var_list
    end subroutine unstable_config_init_decays

<Decays: procedures>+≡
    recursive module subroutine unstable_config_init_decays &
        (unstable, decay_id, model, process_stack, var_list)
        class(unstable_config_t), intent(inout) :: unstable
        type(string_t), dimension(:), intent(in) :: decay_id
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        type(var_list_t), intent(in), optional :: var_list
        integer :: i
        allocate (unstable%decay_config (size (decay_id)))
        do i = 1, size (decay_id)
            associate (decay => unstable%decay_config(i))
                if (present (process_stack)) then
                    call decay%connect (process_stack%get_process_ptr (decay_id(i)), &
                        model, process_stack, var_list=var_list)
                else
                    call decay%init (model, decay_id(i))
                end if
                call decay%set_flv (unstable%flv)
            end associate
        end do
    end subroutine unstable_config_init_decays

```

Explicitly connect a specific decay with a process. This is used only in unit tests.

```

<Decays: unstable config: TBP>+≡

```

```

    procedure :: connect_decay => unstable_config_connect_decay
  <Decays: sub interfaces>+≡
    module subroutine unstable_config_connect_decay &
      (unstable, i, process, model)
      class(unstable_config_t), intent(inout) :: unstable
      integer, intent(in) :: i
      type(process_t), intent(in), target :: process
      class(model_data_t), intent(in), target :: model
    end subroutine unstable_config_connect_decay

  <Decays: procedures>+≡
    module subroutine unstable_config_connect_decay (unstable, i, process, model)
      class(unstable_config_t), intent(inout) :: unstable
      integer, intent(in) :: i
      type(process_t), intent(in), target :: process
      class(model_data_t), intent(in), target :: model
      associate (decay => unstable%decay_config(i))
        call decay%connect (process, model)
      end associate
    end subroutine unstable_config_connect_decay

```

Compute the total width and branching ratios, initializing the decay selector.

```

  <Decays: unstable config: TBP>+≡
    procedure :: compute => unstable_config_compute

  <Decays: sub interfaces>+≡
    recursive module subroutine unstable_config_compute (unstable)
      class(unstable_config_t), intent(inout) :: unstable
    end subroutine unstable_config_compute

  <Decays: procedures>+≡
    recursive module subroutine unstable_config_compute (unstable)
      class(unstable_config_t), intent(inout) :: unstable
      integer :: i
      do i = 1, size (unstable%decay_config)
        call unstable%decay_config(i)%compute ()
      end do
      unstable%integral = sum (unstable%decay_config%integral)
      if (unstable%integral <= 0) then
        call unstable%write ()
        call msg_fatal ("Decay configuration: computed total width is zero")
      end if
      unstable%abs_error = sqrt (sum (unstable%decay_config%abs_error ** 2))
      unstable%rel_error = unstable%abs_error / unstable%integral
      call unstable%selector%init (unstable%decay_config%integral)
      do i = 1, size (unstable%decay_config)
        unstable%decay_config(i)%weight &
          = unstable%selector%get_weight (i)
      end do
    end subroutine unstable_config_compute

```

Now we define the instance of an unstable particle.

```

  <Decays: public>+≡
    public :: unstable_t

```

```

<Decays: types>+≡
  type, extends (any_t) :: unstable_t
  private
    type(unstable_config_t), pointer :: config => null ()
    class(rng_t), allocatable :: rng
    integer :: selected_decay = 0
    type(decay_t), dimension(:), allocatable :: decay
  contains
    <Decays: unstable: TBP>
  end type unstable_t

```

Recursive finalizer.

```

<Decays: unstable: TBP>≡
  procedure :: final => unstable_final

<Decays: sub interfaces>+≡
  recursive module subroutine unstable_final (object)
    class(unstable_t), intent(inout) :: object
  end subroutine unstable_final

<Decays: procedures>+≡
  recursive module subroutine unstable_final (object)
    class(unstable_t), intent(inout) :: object
    integer :: i
    if (allocated (object%decay)) then
      do i = 1, size (object%decay)
        call object%decay(i)%final ()
      end do
    end if
  end subroutine unstable_final

```

Output.

```

<Decays: unstable: TBP>+≡
  procedure :: write => unstable_write

<Decays: sub interfaces>+≡
  recursive module subroutine unstable_write (object, unit, indent)
    class(unstable_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
  end subroutine unstable_write

<Decays: procedures>+≡
  recursive module subroutine unstable_write (object, unit, indent)
    class(unstable_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call object%config%write (u, ind, verbose=.false.)
    if (allocated (object%rng)) then
      call object%rng%write (u, ind + 2)
    end if
    call write_indent (u, ind)
    if (object%selected_decay > 0) then
      write (u, "(5x,A,I0)") "Sel. decay = ", object%selected_decay
    end if
  end subroutine unstable_write

```

```

        call object%decay(object%selected_decay)%write (u, ind + 1)
    else
        write (u, "(5x,A)") "Sel. decay = [undefined]"
    end if
end subroutine unstable_write

```

Write the embedded process instances.

```

<Decays: unstable: TBP>+≡
    procedure :: write_process_instances => unstable_write_process_instances

<Decays: sub interfaces>+≡
    recursive module subroutine unstable_write_process_instances &
        (unstable, unit, verbose)
        class(unstable_t), intent(in) :: unstable
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine unstable_write_process_instances

<Decays: procedures>+≡
    recursive module subroutine unstable_write_process_instances &
        (unstable, unit, verbose)
        class(unstable_t), intent(in) :: unstable
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        if (unstable%selected_decay > 0) then
            call unstable%decay(unstable%selected_decay)% &
                write_process_instances (unit, verbose)
        end if
    end subroutine unstable_write_process_instances

```

Initialization, using the configuration object.

```

<Decays: unstable: TBP>+≡
    procedure :: init => unstable_init

<Decays: sub interfaces>+≡
    recursive module subroutine unstable_init (unstable, config)
        class(unstable_t), intent(out) :: unstable
        type(unstable_config_t), intent(in), target :: config
    end subroutine unstable_init

<Decays: procedures>+≡
    recursive module subroutine unstable_init (unstable, config)
        class(unstable_t), intent(out) :: unstable
        type(unstable_config_t), intent(in), target :: config
        integer :: i
        unstable%config => config
        allocate (unstable%decay (size (config%decay_config)))
        do i = 1, size (config%decay_config)
            call unstable%decay(i)%init (config%decay_config(i))
        end do
    end subroutine unstable_init

```

Recursively link interactions to the parent process. `i_prt` is the index of the current outgoing particle in the parent interaction.

```

<Decays: unstable: TBP>+≡

```



```

    procedure :: link_interactions => unstable_link_interactions
<Decays: sub interfaces>+≡
    recursive module subroutine unstable_link_interactions &
        (unstable, i_prt, trace)
        class(unstable_t), intent(inout) :: unstable
        integer, intent(in) :: i_prt
        type(interaction_t), intent(in), target :: trace
    end subroutine unstable_link_interactions
<Decays: procedures>+≡
    recursive module subroutine unstable_link_interactions &
        (unstable, i_prt, trace)
        class(unstable_t), intent(inout) :: unstable
        integer, intent(in) :: i_prt
        type(interaction_t), intent(in), target :: trace
        integer :: i
        do i = 1, size (unstable%decay)
            call unstable%decay(i)%link_interactions (i_prt, trace)
        end do
    end subroutine unstable_link_interactions

```

Import the random-number generator state.

```

<Decays: unstable: TBP>+≡
    procedure :: import_rng => unstable_import_rng
<Decays: sub interfaces>+≡
    module subroutine unstable_import_rng (unstable, rng)
        class(unstable_t), intent(inout) :: unstable
        class(rng_t), intent(inout), allocatable :: rng
    end subroutine unstable_import_rng
<Decays: procedures>+≡
    module subroutine unstable_import_rng (unstable, rng)
        class(unstable_t), intent(inout) :: unstable
        class(rng_t), intent(inout), allocatable :: rng
        call move_alloc (from = rng, to = unstable%rng)
    end subroutine unstable_import_rng

```

Generate a decay chain. First select a decay mode, then call the `select_chain` method of the selected mode.

```

<Decays: unstable: TBP>+≡
    procedure :: select_chain => unstable_select_chain
<Decays: sub interfaces>+≡
    recursive module subroutine unstable_select_chain (unstable)
        class(unstable_t), intent(inout) :: unstable
    end subroutine unstable_select_chain
<Decays: procedures>+≡
    recursive module subroutine unstable_select_chain (unstable)
        class(unstable_t), intent(inout) :: unstable
        real(default) :: x
        call unstable%rng%generate (x)
        unstable%selected_decay = unstable%config%selector%select (x)
        call unstable%decay(unstable%selected_decay)%select_chain ()
    end subroutine unstable_select_chain

```

```
end subroutine unstable_select_chain
```

Generate a decay event.

```
<Decays: unstable: TBP>+≡
  procedure :: generate => unstable_generate

<Decays: sub interfaces>+≡
  recursive module subroutine unstable_generate (unstable)
    class(unstable_t), intent(inout) :: unstable
  end subroutine unstable_generate

<Decays: procedures>+≡
  recursive module subroutine unstable_generate (unstable)
    class(unstable_t), intent(inout) :: unstable
    call unstable%decay(unstable%selected_decay)%generate ()
  end subroutine unstable_generate
```

32.6.11 Decay Chain

While the decay configuration tree and the decay tree are static entities (during a simulation run), the decay chain is dynamically generated for each event. The reason is that with the possibility of several decay modes for each particle, and several terms for each process, the total number of distinct decay chains is not under control.

Each entry in the decay chain is a connected parton state. The origin of the chain is a connected state in the parent process (not part of the chain itself). For each decay, mode and term chosen, we convolute this with the isolated (!) state of the current decay, to generate a new connected state. We accumulate this chain by recursively traversing the allocated decay tree. Whenever a particle decays, it becomes virtual and is replaced by its decay product, while all other particles stay in the parton state as spectators.

Technically, we implement the decay chain as a stack structure and include information from the associated decay object for easier debugging. This is a decay chain entry:

```
<Decays: types>+≡
  type, extends (connected_state_t) :: decay_chain_entry_t
  private
  integer :: index = 0
  type(decay_config_t), pointer :: config => null ()
  integer :: selected_mci = 0
  integer :: selected_term = 0
  type(decay_chain_entry_t), pointer :: previous => null ()
end type decay_chain_entry_t
```

This is the complete chain; we need just a pointer to the last entry. We also include a pointer to the master process instance, which serves as the seed for the decay chain.

The evaluator `correlated_trace` traces over all quantum numbers for the final spin-correlated (but color-summed) evaluator of the decay chain. This allows us to compute the probability for a momentum configuration, given that

all individual density matrices (of the initial process and the subsequent decays) have been normalized to one.

Note: This trace is summed over color, so color is treated exactly when computing spin correlations. However, we do not keep non-diagonal color correlations. When an event is accepted, we compute probabilities for all color states and can choose one of them.

```

<Decays: public>+≡
    public :: decay_chain_t

<Decays: types>+≡
    type :: decay_chain_t
    private
    type(process_instance_t), pointer :: process_instance => null ()
    integer :: selected_term = 0
    type(evaluator_t) :: correlated_trace
    type(decay_chain_entry_t), pointer :: last => null ()
    contains
    <Decays: decay chain: TBP>
end type decay_chain_t

```

The finalizer recursively deletes and deallocates the entries.

```

<Decays: decay chain: TBP>≡
    procedure :: final => decay_chain_final

<Decays: sub interfaces>+≡
    module subroutine decay_chain_final (object)
        class(decay_chain_t), intent(inout) :: object
    end subroutine decay_chain_final

<Decays: procedures>+≡
    module subroutine decay_chain_final (object)
        class(decay_chain_t), intent(inout) :: object
        type(decay_chain_entry_t), pointer :: entry
        do while (associated (object%last))
            entry => object%last
            object%last => entry%previous
            call entry%final ()
            deallocate (entry)
        end do
        call object%correlated_trace%final ()
    end subroutine decay_chain_final

```

Doing output recursively allows us to display the chain in chronological order.

```

<Decays: decay chain: TBP>+≡
    procedure :: write => decay_chain_write

<Decays: sub interfaces>+≡
    module subroutine decay_chain_write (object, unit)
        class(decay_chain_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine decay_chain_write

```

```

<Decays: procedures>+≡
module subroutine decay_chain_write (object, unit)
  class(decay_chain_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  call write_separator (u, 2)
  write (u, "(1x,A)") "Decay chain:"
  call write_entries (object%last)
  call write_separator (u, 2)
  write (u, "(1x,A)") "Evaluator (correlated trace of the decay chain):"
  call write_separator (u)
  call object%correlated_trace%write (u)
  call write_separator (u, 2)
contains
  recursive subroutine write_entries (entry)
    type(decay_chain_entry_t), intent(in), pointer :: entry
    if (associated (entry)) then
      call write_entries (entry%previous)
      call write_separator (u, 2)
      write (u, "(1x,A,I0)") "Decay #", entry%index
      call entry%config%write_header (u)
      write (u, "(3x,A,I0)") "Selected MCI    = ", entry%selected_mci
      write (u, "(3x,A,I0)") "Selected term  = ", entry%selected_term
      call entry%config%term_config(entry%selected_term)%write (u, indent=1)
      call entry%write (u)
    end if
  end subroutine write_entries
end subroutine decay_chain_write

```

Build a decay chain, recursively following the selected decays and terms in a decay tree. Before start, we finalize the chain, deleting any previous contents.

```

<Decays: decay chain: TBP>+≡
  procedure :: build => decay_chain_build

<Decays: sub interfaces>+≡
  module subroutine decay_chain_build (chain, decay_root)
    class(decay_chain_t), intent(inout), target :: chain
    type(decay_root_t), intent(in) :: decay_root
  end subroutine decay_chain_build

<Decays: procedures>+≡
module subroutine decay_chain_build (chain, decay_root)
  class(decay_chain_t), intent(inout), target :: chain
  type(decay_root_t), intent(in) :: decay_root
  type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
  type(interaction_t), pointer :: int_last_decay
  call chain%final ()
  if (decay_root%selected_term > 0) then
    chain%process_instance => decay_root%process_instance
    chain%selected_term = decay_root%selected_term
    call chain%build_term_entries (decay_root%term(decay_root%selected_term))
  end if
  int_last_decay => chain%last%get_matrix_int_ptr ()
  allocate (qn_mask (int_last_decay%get_n_tot ()))

```

```

    call qn_mask%init (mask_f = .true., mask_c = .true., mask_h = .true.)
    call chain%correlated_trace%init_qn_sum (int_last_decay, qn_mask)
end subroutine decay_chain_build

```

Build the entries that correspond to a decay term. We have to scan all unstable particles.

```

<Decays: decay chain: TBP>+≡
  procedure :: build_term_entries => decay_chain_build_term_entries

<Decays: sub interfaces>+≡
  recursive module subroutine decay_chain_build_term_entries (chain, term)
    class(decay_chain_t), intent(inout) :: chain
    type(decay_term_t), intent(in) :: term
  end subroutine decay_chain_build_term_entries

<Decays: procedures>+≡
  recursive module subroutine decay_chain_build_term_entries (chain, term)
    class(decay_chain_t), intent(inout) :: chain
    type(decay_term_t), intent(in) :: term
    integer :: i
    do i = 1, size (term%particle_out)
      select type (unstable => term%particle_out(i)%c)
        type is (unstable_t)
          if (unstable%selected_decay > 0) then
            call chain%build_decay_entries &
              (unstable%decay(unstable%selected_decay))
          end if
        end select
      end do
    end subroutine decay_chain_build_term_entries

```

Build the entries that correspond to a specific decay. The decay term should have been determined, so we allocate a decay chain entry and fill it, then proceed to child decays.

For the first entry, we convolute the connected state of the parent process instance with the isolated state of the current decay (which does not contain an extra beam entry for the parent). For subsequent entries, we take the previous entry as first factor.

In principle, each chain entry (as a parton state) is capable of holding a subevent object and associated expressions. We currently do not make use of that feature.

Before generating the decays, factor out the trace of the helicity density matrix of the parent parton state. This trace has been used for unweighting the original event (unweighted case) or it determines the overall weight, so it should not be taken into account in the decay chain generation.

```

<Decays: decay chain: TBP>+≡
  procedure :: build_decay_entries => decay_chain_build_decay_entries

<Decays: sub interfaces>+≡
  recursive module subroutine decay_chain_build_decay_entries (chain, decay)
    class(decay_chain_t), intent(inout) :: chain
    type(decay_t), intent(in) :: decay
  end subroutine decay_chain_build_decay_entries

```

<Decays: procedures>+≡

```

recursive module subroutine decay_chain_build_decay_entries (chain, decay)
  class(decay_chain_t), intent(inout) :: chain
  type(decay_t), intent(in) :: decay
  type(decay_chain_entry_t), pointer :: entry
  type(connected_state_t), pointer :: previous_state
  type(isolated_state_t), pointer :: current_decay
  type(helicity_t) :: hel
  type(quantum_numbers_t) :: qn_filter_conn
  allocate (entry)
  if (associated (chain%last)) then
    entry%previous => chain%last
    entry%index = entry%previous%index + 1
    previous_state => entry%previous%connected_state_t
  else
    entry%index = 1
    previous_state => &
      chain%process_instance%get_connected_state_ptr (chain%selected_term)
  end if
  entry%config => decay%config
  entry%selected_mci = decay%selected_mci
  entry%selected_term = decay%selected_term
  current_decay => decay%process_instance%get_isolated_state_ptr &
    (decay%selected_term)
  call entry%setup_connected_trace &
    (current_decay, previous_state%get_trace_int_ptr (), resonant=.true.)
  if (entry%config%flv%has_decay_helicity ()) then
    call hel%init (entry%config%flv%get_decay_helicity ())
    call qn_filter_conn%init (hel)
    call entry%setup_connected_matrix &
      (current_decay, previous_state%get_matrix_int_ptr (), &
        resonant=.true., qn_filter_conn = qn_filter_conn)
    call entry%setup_connected_flows &
      (current_decay, previous_state%get_flows_int_ptr (), &
        resonant=.true., qn_filter_conn = qn_filter_conn)
  else
    call entry%setup_connected_matrix &
      (current_decay, previous_state%get_matrix_int_ptr (), &
        resonant=.true.)
    call entry%setup_connected_flows &
      (current_decay, previous_state%get_flows_int_ptr (), &
        resonant=.true.)
  end if
  chain%last => entry
  call chain%build_term_entries (decay%term(decay%selected_term))
end subroutine decay_chain_build_decay_entries

```

Recursively fill the decay chain with momenta and evaluate the matrix elements. Since all evaluators should have correct source entries at this point, momenta are automatically retrieved from the appropriate process instance.

Like we did above for the parent process, factor out the trace for each subsequent decay (the helicity density matrix in the isolated state, which is taken for the convolution).

```

<Decays: decay chain: TBP>+≡
  procedure :: evaluate => decay_chain_evaluate

<Decays: sub interfaces>+≡
  module subroutine decay_chain_evaluate (chain)
    class(decay_chain_t), intent(inout) :: chain
    end subroutine decay_chain_evaluate

<Decays: procedures>+≡
  module subroutine decay_chain_evaluate (chain)
    class(decay_chain_t), intent(inout) :: chain
    call evaluate (chain%last)
    call chain%correlated_trace%receive_momenta ()
    call chain%correlated_trace%evaluate ()
  contains
    recursive subroutine evaluate (entry)
      type(decay_chain_entry_t), intent(inout), pointer :: entry
      if (associated (entry)) then
        call evaluate (entry%previous)
        call entry%receive_kinematics ()
        call entry%evaluate_trace ()
        call entry%evaluate_event_data ()
      end if
    end subroutine evaluate
  end subroutine decay_chain_evaluate

```

Return the probability of a decay chain. This is given as the trace of the density matrix with intermediate helicity correlations, normalized by the product of the uncorrelated density matrix traces. This works only if an event has been evaluated and the `correlated_trace` evaluator is filled. By definition, this evaluator has only one matrix element, and this must be real.

```

<Decays: decay chain: TBP>+≡
  procedure :: get_probability => decay_chain_get_probability

<Decays: sub interfaces>+≡
  module function decay_chain_get_probability (chain) result (x)
    class(decay_chain_t), intent(in) :: chain
    real(default) :: x
    end function decay_chain_get_probability

<Decays: procedures>+≡
  module function decay_chain_get_probability (chain) result (x)
    class(decay_chain_t), intent(in) :: chain
    real(default) :: x
    x = real (chain%correlated_trace%get_matrix_element (1))
  end function decay_chain_get_probability

```

32.6.12 Decay as Event Transform

The `evt_decay` object combines decay configuration, decay tree, and chain in a single object, as an implementation of the `evt` (event transform) abstract type.

The `var_list` may be a pointer to the user variable list, which could contain overridden parameters for the decay processes.

```

<Decays: public>+≡

```

```

    public :: evt_decay_t
<Decays: types>+≡
    type, extends (evt_t) :: evt_decay_t
        private
            type(decay_root_config_t) :: decay_root_config
            type(decay_root_t) :: decay_root
            type(decay_chain_t) :: decay_chain
            type(var_list_t), pointer :: var_list => null ()
        contains
            <Decays: evt decay: TBP>
        end type evt_decay_t

<Decays: evt decay: TBP>≡
    procedure :: write_name => evt_decay_write_name

<Decays: sub interfaces>+≡
    module subroutine evt_decay_write_name (evt, unit)
        class(evt_decay_t), intent(in) :: evt
        integer, intent(in), optional :: unit
    end subroutine evt_decay_write_name

<Decays: procedures>+≡
    module subroutine evt_decay_write_name (evt, unit)
        class(evt_decay_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: partonic decays"
    end subroutine evt_decay_write_name

```

Output. We display the currently selected decay tree, which includes configuration data, and the decay chain, i.e., the evaluators.

```

<Decays: evt decay: TBP>+≡
    procedure :: write => evt_decay_write

<Decays: sub interfaces>+≡
    module subroutine evt_decay_write &
        (evt, unit, verbose, more_verbose, testflag)
        class(evt_decay_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
    end subroutine evt_decay_write

<Decays: procedures>+≡
    module subroutine evt_decay_write (evt, unit, verbose, more_verbose, testflag)
        class(evt_decay_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
        logical :: verb, verb2
        integer :: u
        u = given_output_unit (unit)
        verb = .true.; if (present (verbose)) verb = verbose
        verb2 = .false.; if (present (more_verbose)) verb2 = more_verbose
        call write_separator (u, 2)
    end subroutine evt_decay_write

```



```

call evt%write_name (u)
call write_separator (u, 2)
call evt%base_write (u, testflag = testflag)
if (associated (evt%var_list)) then
    call write_separator (u)
    write (u, "(1x,A)" "Variable list for simulation: &
        &[associated, not shown]"
end if
if (verb) then
    call write_separator (u)
    call evt%decay_root%write (u)
    if (verb2) then
        call evt%decay_chain%write (u)
        call evt%decay_root%write_process_instances (u, verb)
    end if
else
    call write_separator (u, 2)
end if
end subroutine evt_decay_write

```

Set the pointer to a user variable list.

```

<Decays: evt decay: TBP>+≡
    procedure :: set_var_list => evt_decay_set_var_list

<Decays: sub interfaces>+≡
    module subroutine evt_decay_set_var_list (evt, var_list)
        class(evt_decay_t), intent(inout) :: evt
        type(var_list_t), intent(in), target :: var_list
    end subroutine evt_decay_set_var_list

<Decays: procedures>+≡
    module subroutine evt_decay_set_var_list (evt, var_list)
        class(evt_decay_t), intent(inout) :: evt
        type(var_list_t), intent(in), target :: var_list
        evt%var_list => var_list
    end subroutine evt_decay_set_var_list

```

Connect with a process instance and process. This initializes the decay configuration. The process stack is used to look for process objects that implement daughter decays.

When all processes are assigned, configure the decay tree instance, using the decay tree configuration. First obtain the branching ratios, then allocate the decay tree. This is done once for all events.

```

<Decays: evt decay: TBP>+≡
    procedure :: connect => evt_decay_connect

<Decays: sub interfaces>+≡
    module subroutine evt_decay_connect &
        (evt, process_instance, model, process_stack)
        class(evt_decay_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
    end subroutine evt_decay_connect

```

```

<Decays: procedures>+≡
  module subroutine evt_decay_connect &
    (evt, process_instance, model, process_stack)
    class(evt_decay_t), intent(inout), target :: evt
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    call evt%base_connect (process_instance, model)
    if (associated (evt%var_list)) then
      call evt%decay_root_config%connect (process_instance%process, &
        model, process_stack, process_instance, evt%var_list)
    else
      call evt%decay_root_config%connect (process_instance%process, &
        model, process_stack, process_instance)
    end if
    call evt%decay_root_config%compute ()
    call evt%decay_root%init (evt%decay_root_config, evt%process_instance)
  end subroutine evt_decay_connect

```

Prepare a new event: Select a decay chain and build the corresponding chain object.

```

<Decays: evt decay: TBP>+≡
  procedure :: prepare_new_event => evt_decay_prepare_new_event

<Decays: sub interfaces>+≡
  module subroutine evt_decay_prepare_new_event (evt, i_mci, i_term)
    class(evt_decay_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_decay_prepare_new_event

<Decays: procedures>+≡
  module subroutine evt_decay_prepare_new_event (evt, i_mci, i_term)
    class(evt_decay_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
    evt%decay_root%selected_mci = i_mci
    evt%decay_root%selected_term = i_term
    call evt%decay_root%select_chain ()
    call evt%decay_chain%build (evt%decay_root)
  end subroutine evt_decay_prepare_new_event

```

Generate a weighted event and assign the resulting weight (probability). We use a chain initialized by the preceding subroutine, fill it with momenta and evaluate.

```

<Decays: evt decay: TBP>+≡
  procedure :: generate_weighted => evt_decay_generate_weighted

<Decays: sub interfaces>+≡
  module subroutine evt_decay_generate_weighted (evt, probability)
    class(evt_decay_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
  end subroutine evt_decay_generate_weighted

```

```

<Decays: procedures>+≡
  module subroutine evt_decay_generate_weighted (evt, probability)
    class(evt_decay_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    call evt%decay_root%generate ()
    if (signal_is_pending ()) return
    call evt%decay_chain%evaluate ()
    probability = evt%decay_chain%get_probability ()
  end subroutine evt_decay_generate_weighted

```

To create a usable event, we have to transform the interaction into a particle set; this requires factorization for the correlated density matrix, according to the factorization mode.

```

<Decays: evt decay: TBP>+≡
  procedure :: make_particle_set => evt_decay_make_particle_set

<Decays: sub interfaces>+≡
  module subroutine evt_decay_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_decay_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_decay_make_particle_set

<Decays: procedures>+≡
  module subroutine evt_decay_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_decay_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    type(interaction_t), pointer :: int_matrix, int_flows
    type(decay_chain_entry_t), pointer :: last_entry
    last_entry => evt%decay_chain%last
    int_matrix => last_entry%get_matrix_int_ptr ()
    int_flows => last_entry%get_flows_int_ptr ()
    call evt%factorize_interactions (int_matrix, int_flows, &
      factorization_mode, keep_correlations, r)
    call evt%tag_incoming ()
  end subroutine evt_decay_make_particle_set

```

Auxiliary

Eliminate numerical noise for the associated process instances.

```

<Decays: public>+≡
  public :: pacify

<Decays: interfaces>+≡
  interface pacify
    module procedure pacify_decay
    module procedure pacify_decay_gen
    module procedure pacify_term
  end interface

```

```

        module procedure pacify_unstable
    end interface pacify
<Decays: sub interfaces>+≡
    module subroutine pacify_decay (evt)
        class(evt_decay_t), intent(inout) :: evt
    end subroutine pacify_decay
    recursive module subroutine pacify_decay_gen (decay)
        class(decay_gen_t), intent(inout) :: decay
    end subroutine pacify_decay_gen
    recursive module subroutine pacify_term (term)
        class(decay_term_t), intent(inout) :: term
    end subroutine pacify_term
    recursive module subroutine pacify_unstable (unstable)
        class(unstable_t), intent(inout) :: unstable
    end subroutine pacify_unstable
<Decays: procedures>+≡
    module subroutine pacify_decay (evt)
        class(evt_decay_t), intent(inout) :: evt
        call pacify_decay_gen (evt%decay_root)
    end subroutine pacify_decay

    recursive module subroutine pacify_decay_gen (decay)
        class(decay_gen_t), intent(inout) :: decay
        if (associated (decay%process_instance)) then
            call pacify (decay%process_instance)
        end if
        if (decay%selected_term > 0) then
            call pacify_term (decay%term(decay%selected_term))
        end if
    end subroutine pacify_decay_gen

    recursive module subroutine pacify_term (term)
        class(decay_term_t), intent(inout) :: term
        integer :: i
        do i = 1, size (term%particle_out)
            select type (unstable => term%particle_out(i)%c)
                type is (unstable_t); call pacify_unstable (unstable)
            end select
        end do
    end subroutine pacify_term

    recursive module subroutine pacify_unstable (unstable)
        class(unstable_t), intent(inout) :: unstable
        if (unstable%selected_decay > 0) then
            call pacify_decay_gen (unstable%decay(unstable%selected_decay))
        end if
    end subroutine pacify_unstable

```

Prepare specific configurations for use in unit tests.

```

<Decays: unstable config: TBP>+≡
    procedure :: init_test_case1
    procedure :: init_test_case2

```

```

<Decays: sub interfaces>+≡
  module subroutine init_test_case1 &
    (unstable, i, flv, integral, relerr, model)
    class(unstable_config_t), intent(inout) :: unstable
    integer, intent(in) :: i
    type(flavor_t), dimension(:, :), intent(in) :: flv
    real(default), intent(in) :: integral
    real(default), intent(in) :: relerr
    class(model_data_t), intent(in), target :: model
  end subroutine init_test_case1
  module subroutine init_test_case2 (unstable, flv1, flv21, flv22, model)
    class(unstable_config_t), intent(inout) :: unstable
    type(flavor_t), dimension(:, :), intent(in) :: flv1, flv21, flv22
    class(model_data_t), intent(in), target :: model
  end subroutine init_test_case2

<Decays: procedures>+≡
  module subroutine init_test_case1 (unstable, i, flv, integral, relerr, model)
    class(unstable_config_t), intent(inout) :: unstable
    integer, intent(in) :: i
    type(flavor_t), dimension(:, :), intent(in) :: flv
    real(default), intent(in) :: integral
    real(default), intent(in) :: relerr
    class(model_data_t), intent(in), target :: model
    associate (decay => unstable%decay_config(i))
      allocate (decay%term_config (1))
      call decay%init_term (1, flv, stable = [.true., .true.], model=model)
      decay%integral = integral
      decay%abs_error = integral * relerr
    end associate
  end subroutine init_test_case1

  module subroutine init_test_case2 (unstable, flv1, flv21, flv22, model)
    class(unstable_config_t), intent(inout) :: unstable
    type(flavor_t), dimension(:, :), intent(in) :: flv1, flv21, flv22
    class(model_data_t), intent(in), target :: model
    associate (decay => unstable%decay_config(1))
      decay%integral = 1.e-3_default
      decay%abs_error = decay%integral * .01_default

      allocate (decay%term_config (1))
      call decay%init_term (1, flv1, stable = [.false., .true.], model=model)

      select type (w => decay%term_config(1)%prt(1)%c)
      type is (unstable_config_t)

        associate (w_decay => w%decay_config(1))
          w_decay%integral = 2._default
          allocate (w_decay%term_config (1))
          call w_decay%init_term (1, flv21, stable = [.true., .true.], &
            model=model)
        end associate
        associate (w_decay => w%decay_config(2))
          w_decay%integral = 1._default
          allocate (w_decay%term_config (1))

```

```

        call w_decay%init_term (1, flv22, stable = [.true., .true.], &
            model=model)
    end associate
    call w%compute ()

    end select
end associate
end subroutine init_test_case2

```

32.6.13 Unit tests

Test module, followed by the corresponding implementation module.

<decays_ut.f90>≡
<File header>

```

module decays_ut
    use unit_tests
    use decays_util

```

<Standard module head>

<Decays: public test>

<Decays: public test auxiliary>

contains

<Decays: test driver>

```

end module decays_ut

```

<decays_util.f90>≡
<File header>

```

module decays_util

```

<Use kinds>

<Use strings>

```

    use os_interface
    use sm_qcd
    use model_data
    use models
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions, only: reset_interaction_counter
    use flavors
    use process_libraries
    use rng_base
    use mci_base
    use mci_midpoint
    use phs_base
    use phs_single
    use prc_core
    use prc_test, only: prc_test_create_library

```

```

    use process, only: process_t
    use instances, only: process_instance_t
    use process_stacks

    use decays

    use rng_base_ut, only: rng_test_t, rng_test_factory_t

    <Standard module head>

    <Decays: public test auxiliary>

    <Decays: test declarations>

    contains

    <Decays: tests>

    <Decays: test auxiliary>

    end module decays_utl

```

API: driver for the unit tests below.

```

<Decays: public test>≡
    public :: decays_test

<Decays: test driver>≡
    subroutine decays_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Decays: execute tests>
    end subroutine decays_test

```

Testbed

As a variation of the `prepare_test_process` routine used elsewhere, we define here a routine that creates two processes (scattering $ss \rightarrow ss$ and decay $s \rightarrow f\bar{f}$), compiles and integrates them and prepares for event generation.

```

<Decays: public test auxiliary>≡
    public :: prepare_testbed

<Decays: test auxiliary>≡
    subroutine prepare_testbed &
        (lib, process_stack, prefix, os_data, &
         scattering, decay, decay_rest_frame)
        type(process_library_t), intent(out), target :: lib
        type(process_stack_t), intent(out) :: process_stack
        type(string_t), intent(in) :: prefix
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: scattering, decay
        logical, intent(in), optional :: decay_rest_frame

        type(model_t), target :: model

```

```

type(model_t), target :: model_copy
type(string_t) :: libname, procname1, procname2
type(process_entry_t), pointer :: process
type(process_instance_t), allocatable, target :: process_instance
class(phs_config_t), allocatable :: phs_config_template
type(field_data_t), pointer :: field_data
real(default) :: sqrts

libname = prefix // "_lib"
procname1 = prefix // "_p"
procname2 = prefix // "_d"

call model%init_test ()
call model%set_par (var_str ("ff"), 0.4_default)
call model%set_par (var_str ("mf"), &
    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

if (scattering .and. decay) then
    field_data => model%get_field_ptr (25)
    call field_data%set (p_is_stable = .false.)
end if

call prc_test_create_library (libname, lib, &
    scattering = .true., decay = .true., &
    procname1 = procname1, procname2 = procname2)

call reset_interaction_counter ()

allocate (phs_single_config_t :: phs_config_template)

if (scattering) then

    call model_copy%init (model%get_name (), &
        model%get_n_real (), &
        model%get_n_complex (), &
        model%get_n_field (), &
        model%get_n_vtx ())
    call model_copy%copy_from (model)

    allocate (process)
    call process%init (procname1, lib, os_data, model_copy)
    call process%setup_test_cores ()
    call process%init_components (phs_config_template)
    sqrts = 1000
    call process%setup_beams_sqrts (sqrts, i_core = 1)
    call process%configure_phs ()
    call process%setup_mci (dispatch_mci_test_midpoint)
    call process%setup_terms ()

    allocate (process_instance)
    call process_instance%init (process%process_t)
    call process_instance%integrate (1, n_it = 1, n_calls = 100)
    call process_instance%final_integration (1)
    call process_instance%final ()

```



```

        deallocate (process_instance)

        call process%prepare_simulation (1)
        call process_stack%push (process)
    end if

    if (decay) then
        call model_copy%init (model%get_name (), &
            model%get_n_real (), &
            model%get_n_complex (), &
            model%get_n_field (), &
            model%get_n_vtx ())
        call model_copy%copy_from (model)

        allocate (process)
        call process%init (procname2, lib, os_data, model_copy)
        call process%setup_test_cores ()
        call process%init_components (phs_config_template)
        if (present (decay_rest_frame)) then
            call process%setup_beams_decay (rest_frame = decay_rest_frame, i_core = 1)
        else
            call process%setup_beams_decay (rest_frame = .not. scattering, i_core = 1)
        end if
        call process%configure_phs ()
        call process%setup_mci (dispatch_mci_test_midpoint)
        call process%setup_terms ()

        allocate (process_instance)
        call process_instance%init (process%process_t)
        call process_instance%integrate (1, n_it=1, n_calls=100)
        call process%final_integration (1)
        call process_instance%final ()
        deallocate (process_instance)

        call process%prepare_simulation (1)
        call process_stack%push (process)
    end if

    call model%final ()
    call model_copy%final ()

end subroutine prepare_testbed

```

MCI record prepared for midpoint integrator.

<Decays: test auxiliary>+≡

```

subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
    use variables, only: var_list_t
    class(mci_t), allocatable, intent(out) :: mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    logical, intent(in), optional :: is_nlo
    allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

Simple decay configuration

We define a branching configuration with two decay modes. We set the integral values by hand, so we do not need to evaluate processes, yet.

```
<Decays: execute tests>≡
  call test (decays_1, "decays_1", &
    "branching and decay configuration", &
    u, results)

<Decays: test declarations>≡
  public :: decays_1

<Decays: tests>≡
  subroutine decays_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t) :: flv_h
    type(flavor_t), dimension(2,1) :: flv_hbb, flv_hgg
    type(unstable_config_t), allocatable :: unstable

    write (u, "(A)")  "* Test output: decays_1"
    write (u, "(A)")  "* Purpose: Set up branching and decay configuration"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call os_data%init ()
    call model%init_sm_test ()

    call flv_h%init (25, model)
    call flv_hbb(:,1)%init ([5, -5], model)
    call flv_hgg(:,1)%init ([22, 22], model)

    write (u, "(A)")  "* Set up branching and decay"
    write (u, "(A)")

    allocate (unstable)
    call unstable%init (flv_h)
    call unstable%init_decays ([var_str ("h_bb"), var_str ("h_gg")], model)

    call unstable%init_test_case1 &
      (1, flv_hbb, 1.234e-3_default, .02_default, model)

    call unstable%init_test_case1 &
      (2, flv_hgg, 3.085e-4_default, .08_default, model)

    call unstable%compute ()
    call unstable%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
```

```

call unstable%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: decays_1"

end subroutine decays_1

```

Cascade decay configuration

We define a branching configuration with one decay, which is followed by another branching.

```

<Decays: execute tests> +=
  call test (decays_2, "decays_2", &
    "cascade decay configuration", &
    u, results)

<Decays: test declarations> +=
  public :: decays_2

<Decays: tests> +=
  subroutine decays_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t) :: flv_h, flv_wp, flv_wm
    type(flavor_t), dimension(2,1) :: flv_hww, flv_wud, flv_wen
    type(unstable_config_t), allocatable :: unstable

    write (u, "(A)")  "** Test output: decays_2"
    write (u, "(A)")  "** Purpose: Set up cascade branching"
    write (u, "(A)")

    write (u, "(A)")  "** Initialize environment"
    write (u, "(A)")

    call os_data%init ()
    call model%init_sm_test ()

    call model%set_unstable (25, [var_str ("h_ww")])
    call model%set_unstable (24, [var_str ("w_ud"), var_str ("w_en")])

    call flv_h%init (25, model)
    call flv_hww(:,1)%init ([24, -24], model)
    call flv_wp%init (24, model)
    call flv_wm%init (-24, model)
    call flv_wud(:,1)%init ([2, -1], model)
    call flv_wen(:,1)%init ([-11, 12], model)

    write (u, "(A)")  "** Set up branching and decay"
    write (u, "(A)")

```

```

allocate (unstable)
call unstable%init (flv_h, set_decays=.true., model=model)

call unstable%init_test_case2 (flv_hww, flv_wud, flv_wen, model)

call unstable%compute ()
call unstable%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call unstable%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_2"

end subroutine decays_2

```

Decay and Process Object

We define a branching configuration with one decay and connect this with an actual process object.

```

<Decays: execute tests>+=
  call test (decays_3, "decays_3", &
    "associate process", &
    u, results)

<Decays: test declarations>+=
  public :: decays_3

<Decays: tests>+=
  subroutine decays_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(process_library_t), target :: lib
    type(string_t) :: prefix
    type(string_t) :: procname2
    type(process_stack_t) :: process_stack
    type(process_t), pointer :: process
    type(unstable_config_t), allocatable :: unstable
    type(flavor_t) :: flv

    write (u, "(A)")  "* Test output: decays_3"
    write (u, "(A)")  "*   Purpose: Connect a decay configuration &
      &with a process"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment and integrate process"
    write (u, "(A)")

```

```

call os_data%init ()

prefix = "decays_3"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.false., decay=.true., decay_rest_frame=.false.)

procname2 = prefix // "_d"
process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Set up branching and decay"
write (u, "(A)")

call flv%init (25, model)

allocate (unstable)
call unstable%init (flv)
call unstable%init_decays ([procname2], model)

write (u, "(A)")  "* Connect decay with process object"
write (u, "(A)")

call unstable%connect_decay (1, process, model)

call unstable%compute ()
call unstable%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call unstable%final ()
call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_3"

end subroutine decays_3

```

Decay and Process Object

Building upon the previous test, we set up a decay instance and generate a decay event.

```

<Decays: execute tests>+≡
    call test (decays_4, "decays_4", &
        "decay instance", &
        u, results)

<Decays: test declarations>+≡
    public :: decays_4

```

<Decays: tests>+≡

```
subroutine decays_4 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  class(model_data_t), pointer :: model
  type(process_library_t), target :: lib
  type(string_t) :: prefix, procname2
  class(rng_t), allocatable :: rng
  type(process_stack_t) :: process_stack
  type(process_t), pointer :: process
  type(unstable_config_t), allocatable, target :: unstable
  type(flavor_t) :: flv
  type(unstable_t), allocatable :: instance

  write (u, "(A)")  "* Test output: decays_4"
  write (u, "(A)")  "*   Purpose: Create a decay process and evaluate &
    &an instance"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize environment, process, &
    &and decay configuration"
  write (u, "(A)")

  call os_data%init ()

  prefix = "decays_4"
  call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.false., decay=.true., decay_rest_frame = .false.)

  procname2 = prefix // "_d"
  process => process_stack%get_process_ptr (procname2)
  model => process%get_model_ptr ()

  call flv%init (25, model)

  allocate (unstable)
  call unstable%init (flv)
  call unstable%init_decays ([procname2], model)

  call model%set_unstable (25, [procname2])

  call unstable%connect_decay (1, process, model)

  call unstable%compute ()

  allocate (rng_test_t :: rng)

  allocate (instance)
  call instance%init (unstable)
  call instance%import_rng (rng)

  call instance%select_chain ()
  call instance%generate ()
```

```

call instance%write (u)

write (u, *)
call instance%write_process_instances (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call instance%final ()
call process_stack%final ()
call unstable%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_4"

end subroutine decays_4

```

Decay with Parent Process

We define a scattering process $ss \rightarrow ss$ and subsequent decays $s \rightarrow f\bar{f}$.

```

<Decays: execute tests>+≡
  call test (decays_5, "decays_5", &
    "parent process and decay", &
    u, results)

<Decays: test declarations>+≡
  public :: decays_5

<Decays: tests>+≡
  subroutine decays_5 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(process_library_t), target :: lib
    type(string_t) :: prefix, procname1, procname2
    type(process_stack_t) :: process_stack
    type(process_t), pointer :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(decay_root_config_t), target :: decay_root_config
    type(decay_root_t) :: decay_root
    type(decay_chain_t) :: decay_chain

    write (u, "(A)")  "* Test output: decays_5"
    write (u, "(A)")  "* Purpose: Handle a process with subsequent decays"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment and parent process"
    write (u, "(A)")

    call os_data%init ()

    prefix = "decays_5"
    procname1 = prefix // "_p"
    procname2 = prefix // "_d"

```

```

call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
     scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"
write (u, "(A)")

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

write (u, "(A)")  "* Initialize decay tree configuration"
write (u, "(A)")

call decay_root_config%connect (process, model, process_stack)
call decay_root_config%compute ()
call decay_root_config%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize decay tree"

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

call decay_root%init (decay_root_config, process_instance)

write (u, "(A)")
write (u, "(A)")  "* Select decay chain"
write (u, "(A)")

call decay_root%set_mci (1)
!!! Not yet implemented; there is only one term anyway:
! call process_instance%select_i_term (decay_root%selected_term)
call decay_root%set_term (1)
call decay_root%select_chain ()

call decay_chain%build (decay_root)

call decay_root%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call process_instance%generate_unweighted_event (decay_root%get_mci ())
call process_instance%evaluate_event_data ()

call decay_root%generate ()

call pacify (decay_root)

write (u, "(A)")  "* Process instances"

```



```

write (u, "(A)")

call decay_root%write_process_instances (u)

write (u, "(A)")
write (u, "(A)")  "* Generate decay chain"
write (u, "(A)")

call decay_chain%evaluate ()
call decay_chain%write (u)

write (u, *)
write (u, "(A,ES19.12)")  "chain probability =", &
    decay_chain%get_probability ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call decay_chain%final ()
call decay_root%final ()
call decay_root_config%final ()
call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_5"

end subroutine decays_5

```

Decay as Event Transform

Again, we define a scattering process $ss \rightarrow ss$ and subsequent decays $s \rightarrow f\bar{f}$.

```

<Decays: execute tests>+≡
    call test (decays_6, "decays_6", &
        "evt_decay object", &
        u, results)

<Decays: test declarations>+≡
    public :: decays_6

<Decays: tests>+≡
    subroutine decays_6 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        class(model_data_t), pointer :: model
        type(process_library_t), target :: lib
        type(string_t) :: prefix, procname1, procname2
        type(process_stack_t) :: process_stack
        type(process_t), pointer :: process
        type(process_instance_t), allocatable, target :: process_instance
        type(evt_decay_t), target :: evt_decay
        integer :: factorization_mode

```

```

logical :: keep_correlations

write (u, "(A)")  "* Test output: decays_6"
write (u, "(A)")  "* Purpose: Handle a process with subsequent decays"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment and parent process"
write (u, "(A)")

call os_data%init ()

prefix = "decays_6"
procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")
write (u, "(A)")  "* Initialize decay object"

call evt_decay%connect (process_instance, model, process_stack)

write (u, "(A)")
write (u, "(A)")  "* Generate scattering event"

call process_instance%generate_unweighted_event (1)
call process_instance%evaluate_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Select decay chain and generate event"
write (u, "(A)")

call evt_decay%prepare_new_event (1, 1)
call evt_decay%generate_unweighted ()

factorization_mode = FM_IGNORE_HELICITY
keep_correlations = .false.
call evt_decay%make_particle_set (factorization_mode, keep_correlations)

call evt_decay%write (u, verbose = .true.)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call evt_decay%final ()
call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_6"

end subroutine decays_6

```

32.7 Tau decays

```

⟨tau_decays.f90⟩≡
  ⟨File header⟩

  module tau_decays

    ⟨Use kinds⟩
    use sm_qcd
    use model_data
    use models
    use event_transforms

    ⟨Standard module head⟩

    ⟨Tau decays: public⟩

    ⟨Tau decays: types⟩

    interface
    ⟨Tau decays: sub interfaces⟩
    end interface

  end module tau_decays

⟨tau_decays_sub.f90⟩≡
  ⟨File header⟩

  submodule (tau_decays) tau_decays_s

    use io_units
    use format_utils, only: write_separator

    implicit none

  contains

    ⟨Tau decays: procedures⟩

```

```
end submodule tau_decays_s
```

32.7.1 Tau Decays Event Transform

This is the type for the tau decay event transform.

```
<Tau decays: public>≡
  public :: evt_tau_decays_t

<Tau decays: types>≡
  type, extends (evt_t) :: evt_tau_decays_t
    type(model_t), pointer :: model_hadrons => null()
    type(qcd_t) :: qcd
  contains
    <Tau decays: evt tau decays: TBP>
  end type evt_tau_decays_t

<Tau decays: evt tau decays: TBP>≡
  procedure :: write_name => evt_tau_decays_write_name

<Tau decays: sub interfaces>≡
  module subroutine evt_tau_decays_write_name (evt, unit)
    class(evt_tau_decays_t), intent(in) :: evt
    integer, intent(in), optional :: unit
  end subroutine evt_tau_decays_write_name

<Tau decays: procedures>≡
  module subroutine evt_tau_decays_write_name (evt, unit)
    class(evt_tau_decays_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: tau decays"
  end subroutine evt_tau_decays_write_name
```

Output.

```
<Tau decays: evt tau decays: TBP>+≡
  procedure :: write => evt_tau_decays_write

<Tau decays: sub interfaces>+≡
  module subroutine evt_tau_decays_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_tau_decays_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
  end subroutine evt_tau_decays_write

<Tau decays: procedures>+≡
  module subroutine evt_tau_decays_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_tau_decays_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u
    u = given_output_unit (unit)
```

```

call write_separator (u, 2)
call evt%write_name (u)
call write_separator (u)
call evt%base_write (u, testflag = testflag, show_set = .false.)
if (evt%particle_set_exists) &
    call evt%particle_set%write &
    (u, summary = .true., compressed = .true., testflag = testflag)
call write_separator (u)
end subroutine evt_tau_decays_write

```

Here we take the particle set from the previous event transform and apply the tau decays. What probability should be given back, the product of branching ratios of the corresponding tau decays?

```

<Tau decays: evt tau decays: TBP>+≡
    procedure :: generate_weighted => evt_tau_decays_generate_weighted

<Tau decays: sub interfaces>+≡
    module subroutine evt_tau_decays_generate_weighted (evt, probability)
        class(evt_tau_decays_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
    end subroutine evt_tau_decays_generate_weighted

<Tau decays: procedures>+≡
    module subroutine evt_tau_decays_generate_weighted (evt, probability)
        class(evt_tau_decays_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        logical :: valid
        evt%particle_set = evt%previous%particle_set
        !!! To be checked or expanded
        probability = 1
        valid = .true.
        evt%particle_set_exists = valid
    end subroutine evt_tau_decays_generate_weighted

```

The factorization parameters are irrelevant.

```

<Tau decays: evt tau decays: TBP>+≡
    procedure :: make_particle_set => evt_tau_decays_make_particle_set

<Tau decays: sub interfaces>+≡
    module subroutine evt_tau_decays_make_particle_set &
        (evt, factorization_mode, keep_correlations, r)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
    end subroutine evt_tau_decays_make_particle_set

<Tau decays: procedures>+≡
    module subroutine evt_tau_decays_make_particle_set &
        (evt, factorization_mode, keep_correlations, r)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
        logical :: valid

```

```

    !!! to be checked and expanded
    valid = .true.
    evt%particle_set_exists = evt%particle_set_exists .and. valid
end subroutine evt_tau_decays_make_particle_set

<Tau decays: evt tau decays: TBP>+≡
    procedure :: prepare_new_event => evt_tau_decays_prepare_new_event

<Tau decays: sub interfaces>+≡
    module subroutine evt_tau_decays_prepare_new_event (evt, i_mci, i_term)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
    end subroutine evt_tau_decays_prepare_new_event

<Tau decays: procedures>+≡
    module subroutine evt_tau_decays_prepare_new_event (evt, i_mci, i_term)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
        call evt%reset ()
    end subroutine evt_tau_decays_prepare_new_event

```

32.8 Shower

We might use matrix elements of LO and NLO to increase the accuracy of the shower in the sense of matching as well as merging.

```

<shower.f90>≡
    <File header>

    module shower

    <Use kinds>
    <Use strings>
    use os_interface
    use pdf

    use shower_base
    use matching_base

    use sm_qcd
    use model_data

    use event_transforms
    use models
    use process, only: process_t
    use instances, only: process_instance_t
    use process_stacks

    <Standard module head>

    <Shower: public>

    <Shower: parameters>

```

```

    <Shower: types>

    interface
    <Shower: sub interfaces>
    end interface

    end module shower

    <shower_sub.f90>≡
    <File header>

    submodule (shower) shower_s

    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use system_defs, only: LF
    use diagnostics
    use lorentz
    use subevents, only: PRT_BEAM_REMNANT, PRT_INCOMING, PRT_OUTGOING
    use powheg_matching, only: powheg_matching_t
    use rng_base
    use hep_common

    implicit none

    contains

    <Shower: procedures>

    end submodule shower_s

```

32.8.1 Configuration Parameters

POWHEG_TESTING allows to disable the parton shower for validation and testing of the POWHEG procedure.

```

<Shower: parameters>≡
    logical, parameter :: POWHEG_TESTING = .true.

```

32.8.2 Event Transform

The event transforms can do more than mere showering. Especially, it may reweight showered events to fixed-order matrix elements. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that can be generated in the shower.

```

<Shower: public>≡
    public :: evt_shower_t

```

```

<Shower: types>≡
  type, extends (evt_t) :: evt_shower_t
    class(shower_base_t), allocatable :: shower
    class(matching_t), allocatable :: matching
    type(model_t), pointer :: model_hadrons => null ()
    type(qcd_t) :: qcd
    type(pdf_data_t) :: pdf_data
    type(os_data_t) :: os_data
    logical :: is_first_event
  contains
    <Shower: evt shower: TBP>
  end type evt_shower_t

```

```

<Shower: evt shower: TBP>≡
  procedure :: write_name => evt_shower_write_name

```

```

<Shower: sub interfaces>≡
  module subroutine evt_shower_write_name (evt, unit)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
  end subroutine evt_shower_write_name

```

```

<Shower: procedures>≡
  module subroutine evt_shower_write_name (evt, unit)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: shower"
  end subroutine evt_shower_write_name

```

Output.

```

<Shower: evt shower: TBP>+≡
  procedure :: write => evt_shower_write

```

```

<Shower: sub interfaces>+≡
  module subroutine evt_shower_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
  end subroutine evt_shower_write

```

```

<Shower: procedures>+≡
  module subroutine evt_shower_write &
    (evt, unit, verbose, more_verbose, testflag)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag, show_set = .false.)

```



```

    if (evt%particle_set_exists) call evt%particle_set%write &
        (u, summary = .true., compressed = .true., testflag = testflag)
    call write_separator (u)
    call evt%shower%settings%write (u)
end subroutine evt_shower_write

```

```

<Shower: evt shower: TBP>+≡
    procedure :: connect => evt_shower_connect

```

```

<Shower: sub interfaces>+≡
    module subroutine evt_shower_connect &
        (evt, process_instance, model, process_stack)
        class(evt_shower_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
    end subroutine evt_shower_connect

```

```

<Shower: procedures>+≡
    module subroutine evt_shower_connect &
        (evt, process_instance, model, process_stack)
        class(evt_shower_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        call evt%base_connect (process_instance, model, process_stack)
        call evt%make_rng (evt%process)
        if (allocated (evt%matching)) then
            call evt%matching%connect (process_instance, model, evt%shower)
        end if
    end subroutine evt_shower_connect

```

Initialize the event transformation. This will be executed once during dispatching. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that may be generated in the shower.

```

<Shower: evt shower: TBP>+≡
    procedure :: init => evt_shower_init

```

```

<Shower: sub interfaces>+≡
    module subroutine evt_shower_init (evt, model_hadrons, os_data)
        class(evt_shower_t), intent(out) :: evt
        type(model_t), intent(in), target :: model_hadrons
        type(os_data_t), intent(in) :: os_data
    end subroutine evt_shower_init

```

```

<Shower: procedures>+≡
    module subroutine evt_shower_init (evt, model_hadrons, os_data)
        class(evt_shower_t), intent(out) :: evt
        type(model_t), intent(in), target :: model_hadrons
        type(os_data_t), intent(in) :: os_data
        evt%os_data = os_data
        evt%model_hadrons => model_hadrons
        evt%is_first_event = .true.
    end subroutine evt_shower_init

```

Create RNG instances, spawned by the process object.

```

<Shower: evt shower: TBP>+≡
    procedure :: make_rng => evt_shower_make_rng

<Shower: sub interfaces>+≡
    module subroutine evt_shower_make_rng (evt, process)
        class(evt_shower_t), intent(inout) :: evt
        type(process_t), intent(inout) :: process
    end subroutine evt_shower_make_rng

<Shower: procedures>+≡
    module subroutine evt_shower_make_rng (evt, process)
        class(evt_shower_t), intent(inout) :: evt
        type(process_t), intent(inout) :: process
        class(rng_t), allocatable :: rng
        call process%make_rng (rng)
        call evt%shower%import_rng (rng)
        if (allocated (evt%matching)) then
            call process%make_rng (rng)
            call evt%matching%import_rng (rng)
        end if
    end subroutine evt_shower_make_rng

```

Things we want to do for a new event before the whole event transformation chain is evaluated.

```

<Shower: evt shower: TBP>+≡
    procedure :: prepare_new_event => evt_shower_prepare_new_event

<Shower: sub interfaces>+≡
    module subroutine evt_shower_prepare_new_event (evt, i_mci, i_term)
        class(evt_shower_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
    end subroutine evt_shower_prepare_new_event

<Shower: procedures>+≡
    module subroutine evt_shower_prepare_new_event (evt, i_mci, i_term)
        class(evt_shower_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
        real(default) :: fac_scale, alpha_s
        fac_scale = evt%process_instance%get_fac_scale (i_term)
        alpha_s = evt%process_instance%get_alpha_s (i_term)
        call evt%reset ()
        call evt%shower%prepare_new_event (fac_scale, alpha_s)
    end subroutine evt_shower_prepare_new_event

<Shower: evt shower: TBP>+≡
    procedure :: first_event => evt_shower_first_event

<Shower: sub interfaces>+≡
    module subroutine evt_shower_first_event (evt)
        class(evt_shower_t), intent(inout) :: evt
    end subroutine evt_shower_first_event

```

<Shower: procedures>+≡

```

module subroutine evt_shower_first_event (evt)
  class(evt_shower_t), intent(inout) :: evt
  double precision :: pdftest
  if (debug_on) call msg_debug (D_TRANSFORMS, "evt_shower_first_event")
  associate (settings => evt%shower%settings)
    settings%hadron_collision = .false.
    !!! !!! !!! Workaround for PGF90 v16.1
    !!! if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () <= 39)) then
    if (evt%particle_set%prt(1)%flv%get_pdg_abs () <= 39 .and. &
        evt%particle_set%prt(2)%flv%get_pdg_abs () <= 39) then
      settings%hadron_collision = .false.
    !!! else if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () >= 100)) then
    else if (evt%particle_set%prt(1)%flv%get_pdg_abs () >= 100 .and. &
        evt%particle_set%prt(2)%flv%get_pdg_abs () >= 100) then
      settings%hadron_collision = .true.
    else
      call msg_fatal ("evt_shower didn't recognize beams setup")
    end if
    if (debug_on) call msg_debug (D_TRANSFORMS, "hadron_collision", settings%hadron_collision)
    if (allocated (evt%matching)) then
      evt%matching%is_hadron_collision = settings%hadron_collision
      call evt%matching%first_event ()
    end if
    if (.not. settings%hadron_collision .and. settings%isr_active) then
      call msg_fatal ("?ps_isr_active is only intended for hadron-collisions")
    end if
    if (evt%pdf_data%type == STRF_LHAPDF5) then
      if (settings%isr_active .and. settings%hadron_collision) then
        call GetQ2max (0, pdftest)
        if (pdftest < epsilon (pdftest)) then
          call msg_bug ("ISR QCD shower enabled, but LHAPDF not " // &
              "initialized," // LF // "      aborting simulation")
          return
        end if
      end if
    else if (evt%pdf_data%type == STRF_PDF_BUILTIN .and. &
        settings%method == PS_PYTHIA6) then
      call msg_fatal ("Builtin PDFs cannot be used for PYTHIA showers," &
          // LF // "      aborting simulation")
      return
    end if
  end associate
  evt%is_first_event = .false.
end subroutine evt_shower_first_event

```

Here we take the particle set from the previous event transform (assuming that there is always one) and apply the shower algorithm. The result is stored in the event transform of the current object. We always return a probability of unity as we don't have the analytic weight of the combination of shower, MLM matching and hadronization. A subdivision into multiple event transformations is under construction. Invalid or vetoed events have to be discarded by the caller which is why we mark the particle set as invalid. This procedure directly

takes the (MLM) matching into account.

```

(Shower: evt shower: TBP)+≡
    procedure :: generate_weighted => evt_shower_generate_weighted

(Shower: sub interfaces)+≡
    module subroutine evt_shower_generate_weighted (evt, probability)
        class(evt_shower_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
    end subroutine evt_shower_generate_weighted

(Shower: procedures)+≡
    module subroutine evt_shower_generate_weighted (evt, probability)
        class(evt_shower_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        logical :: valid, vetoed, is_powheg_matching
        if (debug_on) call msg_debug (D_TRANSFORMS, "evt_shower_generate_weighted")
        if (signal_is_pending ()) return
        evt%particle_set = evt%previous%particle_set
        valid = .true.; vetoed = .false.; is_powheg_matching = .false.
        if (evt%is_first_event) call evt%first_event ()
        call evt%shower%import_particle_set (evt%particle_set)
        if (allocated (evt%matching)) then
            call evt%matching%before_shower (evt%particle_set, vetoed)
            if (msg_level(D_TRANSFORMS) >= DEBUG) then
                if (debug_on) call msg_debug &
                    (D_TRANSFORMS, "Matching before generate emissions")
                call evt%matching%write ()
            end if
        end if
        if (allocated (evt%matching)) then
            select type (matching => evt%matching)
            type is (powheg_matching_t)
                is_powheg_matching = .true.
            end select
        end if
        if (.not. vetoed) then
            if (.not. POWHEG_TESTING .or. .not. is_powheg_matching) then
                if (evt%shower%settings%method == PS_PYTHIA6 .or. &
                    evt%shower%settings%hadronization_active) then
                    call assure_heprup (evt%particle_set)
                end if
                call evt%shower%generate_emissions (valid)
            end if
        end if
        probability = 1
        evt%particle_set_exists = valid .and. .not. vetoed
    end subroutine evt_shower_generate_weighted

```

Here, we fill the particle set with the partons from the shower. The factorization parameters are irrelevant. We make a sanity check that the initial energy lands either in the outgoing particles or add to the beam remnant.

```

(Shower: evt shower: TBP)+≡
    procedure :: make_particle_set => evt_shower_make_particle_set

```

```

<Shower: sub interfaces>+=
  module subroutine evt_shower_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_shower_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
  end subroutine evt_shower_make_particle_set

<Shower: procedures>+=
  module subroutine evt_shower_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_shower_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    type(vector4_t) :: sum_vec_in, sum_vec_out, sum_vec_beamrem, &
      sum_vec_beamrem_before
    logical :: vetoed, sane
    if (evt%particle_set_exists) then
      vetoed = .false.
      sum_vec_beamrem_before = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_BEAM_REMNANT)
      call evt%shower%make_particle_set (evt%particle_set, &
        evt%model, evt%model_hadrons)
      if (allocated (evt%matching)) then
        call evt%matching%after_shower (evt%particle_set, vetoed)
      end if
      if (debug_active (D_TRANSFORMS)) then
        call msg_debug (D_TRANSFORMS, &
          "Shower: obtained particle set after shower + matching")
        call evt%particle_set%write (summary = .true., compressed = .true.)
      end if
      sum_vec_in = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_INCOMING)
      sum_vec_out = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_OUTGOING)
      sum_vec_beamrem = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_BEAM_REMNANT)
      sum_vec_beamrem = sum_vec_beamrem - sum_vec_beamrem_before
      sane = abs(sum_vec_out%p(0) - sum_vec_in%p(0)) < &
        sum_vec_in%p(0) / 10 .or. &
        abs((sum_vec_out%p(0) + sum_vec_beamrem%p(0)) - sum_vec_in%p(0)) < &
        sum_vec_in%p(0) / 10
      sane = .true.
      evt%particle_set_exists = .not. vetoed .and. sane
    end if
  end subroutine evt_shower_make_particle_set

<Shower: evt shower: TBP>+=
  procedure :: contains_powheg_matching => evt_shower_contains_powheg_matching

<Shower: sub interfaces>+=
  module function evt_shower_contains_powheg_matching (evt) result (val)
    logical :: val

```

```

        class(evt_shower_t), intent(in) :: evt
        end function evt_shower_contains_powheg_matching
    <Shower: procedures>+≡
    module function evt_shower_contains_powheg_matching (evt) result (val)
        logical :: val
        class(evt_shower_t), intent(in) :: evt
        val = .false.
        if (allocated (evt%matching)) &
            val = evt%matching%get_method () == "POWHEG"
        end function evt_shower_contains_powheg_matching

    <Shower: evt shower: TBP>+≡
    procedure :: disable_powheg_matching => evt_shower_disable_powheg_matching

    <Shower: sub interfaces>+≡
    module subroutine evt_shower_disable_powheg_matching (evt)
        class(evt_shower_t), intent(inout) :: evt
        end subroutine evt_shower_disable_powheg_matching

    <Shower: procedures>+≡
    module subroutine evt_shower_disable_powheg_matching (evt)
        class(evt_shower_t), intent(inout) :: evt
        select type (matching => evt%matching)
            type is (powheg_matching_t)
                matching%active = .false.
            class default
                call msg_fatal ("Trying to disable powheg but " // &
                    "no powheg matching is allocated!")
            end select
        end subroutine evt_shower_disable_powheg_matching

    <Shower: evt shower: TBP>+≡
    procedure :: enable_powheg_matching => evt_shower_enable_powheg_matching

    <Shower: sub interfaces>+≡
    module subroutine evt_shower_enable_powheg_matching (evt)
        class(evt_shower_t), intent(inout) :: evt
        end subroutine evt_shower_enable_powheg_matching

    <Shower: procedures>+≡
    module subroutine evt_shower_enable_powheg_matching (evt)
        class(evt_shower_t), intent(inout) :: evt
        select type (matching => evt%matching)
            type is (powheg_matching_t)
                matching%active = .true.
            class default
                call msg_fatal &
                    ("Trying to enable powheg but no powheg matching is allocated!")
            end select
        end subroutine evt_shower_enable_powheg_matching

    <Shower: evt shower: TBP>+≡
    procedure :: final => evt_shower_final

```

```

<Shower: sub interfaces>+≡
    module subroutine evt_shower_final (evt)
        class(evt_shower_t), intent(inout) :: evt
    end subroutine evt_shower_final

<Shower: procedures>+≡
    module subroutine evt_shower_final (evt)
        class(evt_shower_t), intent(inout) :: evt
        call evt%base_final ()
        if (allocated (evt%matching)) call evt%matching%final ()
    end subroutine evt_shower_final

```

32.8.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<shower_ut.f90>≡
    <File header>

    module shower_ut
        use unit_tests
        use shower_util

    <Standard module head>

    <Shower: public test>

    contains

    <Shower: test driver>

    end module shower_ut

<shower_util.f90>≡
    <File header>

    module shower_util

    <Use kinds>
    <Use strings>
        use format_utils, only: write_separator
        use os_interface
        use sm_qcd
        use physics_defs, only: BORN
        use model_data
        use models
        use state_matrices, only: FM_IGNORE_HELICITY
        use process_libraries
        use rng_base
        use rng_tao
        use dispatch_rng, only: dispatch_rng_factory_fallback
        use mci_base
        use mci_midpoint
        use phs_base

```

```

use phs_single
use prc_core_def, only: prc_core_def_t
use prc_core
use prc_omega
use variables
use event_transforms
use tauola_interface !NODEP!

use process, only: process_t
use instances, only: process_instance_t

use pdf
use shower_base
use shower_core

use dispatch_rng_ut, only: dispatch_rng_factory_tao

use shower

<Standard module head>

<Shower: test declarations>

contains

<Shower: tests>

end module shower_util

```

API: driver for the unit tests below.

```

<Shower: public test>≡
  public :: shower_test

<Shower: test driver>≡
  subroutine shower_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Shower: execute tests>
  end subroutine shower_test

```

Testbed

This sequence sets up a two-jet process, ready for generating events.

```

<Shower: tests>≡
  <setup testbed>

<setup testbed>≡
  subroutine setup_testbed &
    (prefix, os_data, lib, model_list, process, process_instance)
    type(string_t), intent(in) :: prefix
    type(os_data_t), intent(out) :: os_data
    type(process_library_t), intent(out), target :: lib
    type(model_list_t), intent(out) :: model_list
  end subroutine

```



```

type(model_t), pointer :: model
type(model_t), pointer :: model_tmp
type(process_t), target, intent(out) :: process
type(process_instance_t), target, intent(out) :: process_instance
type(var_list_t), pointer :: model_vars
type(string_t) :: model_name, libname, procname
type(process_def_entry_t), pointer :: entry
type(string_t), dimension(:), allocatable :: prt_in, prt_out
class(prc_core_t), allocatable :: core_template
class(phs_config_t), allocatable :: phs_config_template
real(default) :: sqrts

model_name = "SM"
libname = prefix // "_lib"
procname = prefix // "p"

call os_data%init ()
dispatch_rng_factory_fallback => dispatch_rng_factory_tao
allocate (model_tmp)
call model_list%read_model (model_name, model_name // ".mdl", &
    os_data, model_tmp)
model_vars => model_tmp%get_var_list_ptr ()
call model_vars%set_real (var_str ("me"), 0._default, &
    is_known = .true.)
model => model_tmp

call lib%init (libname)

allocate (prt_in (2), source = [var_str ("e-"), var_str ("e+")])
allocate (prt_out (2), source = [var_str ("d"), var_str ("dbar")])

allocate (entry)
call entry%init (procname, model, n_in = 2, n_components = 1)
call omega_make_process_component (entry, 1, &
    model_name, prt_in, prt_out, &
    report_progress=.true.)
call lib%append (entry)

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

call process%init (procname, lib, os_data, model)

allocate (prc_omega_t :: core_template)
allocate (phs_single_config_t :: phs_config_template)

call process%setup_cores (dispatch_core_omega_test)

call process%init_components (phs_config_template)

sqrts = 1000

```

```

call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_test_midpoint)
call process%setup_terms ()

call process_instance%init (process)
call process_instance%integrate (1, 1, 1000)
call process%final_integration (1)

call process_instance%setup_event_data (i_core = 1)
call process_instance%init_simulation (1)
call process_instance%generate_weighted_event (1)
call process_instance%evaluate_event_data ()

end subroutine setup_testbed

```

A minimal dispatcher version that allocates the core object for testing.

```

<setup_testbed>+≡
subroutine dispatch_core_omega_test (core, core_def, model, &
    helicity_selection, qcd, use_color_factors, has_beam_pol)
class(prc_core_t), allocatable, intent(inout) :: core
class(prc_core_def_t), intent(in) :: core_def
class(model_data_t), intent(in), target, optional :: model
type(helicity_selection_t), intent(in), optional :: helicity_selection
type(qcd_t), intent(in), optional :: qcd
logical, intent(in), optional :: use_color_factors
logical, intent(in), optional :: has_beam_pol
allocate (prc_omega_t :: core)
select type (core)
type is (prc_omega_t)
    call core%set_parameters (model)
end select
end subroutine dispatch_core_omega_test

```

MCI record prepared for midpoint integrator.

```

<setup_testbed>+≡
subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
use variables, only: var_list_t
class(mci_t), allocatable, intent(out) :: mci
type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_id
logical, intent(in), optional :: is_nlo
allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

Trivial Test

We generate a two-jet event and shower it using default settings, i.e. in disabled mode.

```

<Shower: execute tests>≡
call test (shower_1, "shower_1", &

```

```

        "disabled shower", &
        u, results)
<Shower: test declarations>≡
    public :: shower_1
<Shower: tests>+≡
    subroutine shower_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t), target :: lib
        type(model_list_t) :: model_list
        class(model_data_t), pointer :: model
        type(model_t), pointer :: model_hadrons
        type(process_t), target :: process
        type(process_instance_t), target :: process_instance
        type(pdf_data_t) :: pdf_data
        integer :: factorization_mode
        logical :: keep_correlations
        class(evt_t), allocatable, target :: evt_trivial
        class(evt_t), allocatable, target :: evt_shower
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings

        write (u, "(A)")  "* Test output: shower_1"
        write (u, "(A)")  "*   Purpose: Two-jet event with disabled shower"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"), &
            os_data, model_hadrons)
        call setup_testbed (var_str ("shower_1"), &
            os_data, lib, model_list, process, process_instance)

        write (u, "(A)")  "* Set up trivial transform"
        write (u, "(A)")

        allocate (evt_trivial_t :: evt_trivial)
        model => process%get_model_ptr ()
        call evt_trivial%connect (process_instance, model)
        call evt_trivial%prepare_new_event (1, 1)
        call evt_trivial%generate_unweighted ()

        factorization_mode = FM_IGNORE_HELICITY
        keep_correlations = .false.
        call evt_trivial%make_particle_set (factorization_mode, keep_correlations)

        select type (evt_trivial)
        type is (evt_trivial_t)
            call evt_trivial%write (u)

```

```

        call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Set up shower event transform"
write (u, "(A)")

allocate (evt_shower_t :: evt_shower)
select type (evt_shower)
type is (evt_shower_t)
    call evt_shower%init (model_hadrons, os_data)
    allocate (shower_t :: evt_shower%shower)
    call evt_shower%shower%init (settings, taudec_settings, pdf_data, os_data)
    call evt_shower%connect (process_instance, model)
end select

evt_trivial%next => evt_shower
evt_shower%previous => evt_trivial

call evt_shower%prepare_new_event (1, 1)
call evt_shower%generate_unweighted ()
call evt_shower%make_particle_set (factorization_mode, keep_correlations)

select type (evt_shower)
type is (evt_shower_t)
    call evt_shower%write (u)
    call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_shower%final ()
call evt_trivial%final ()
call process_instance%final ()
call process%final ()
call lib%final ()
call model_hadrons%final ()
deallocate (model_hadrons)
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_1"

end subroutine shower_1

```

FSR Shower

We generate a two-jet event and shower it with the Whizard FSR shower.

```

<Shower: execute tests>+≡
    call test (shower_2, "shower_2", &
        "final-state shower", &
        u, results)

```

```

<Shower: test declarations>+≡
    public :: shower_2

<Shower: tests>+≡
    subroutine shower_2 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t), target :: lib
        type(model_list_t) :: model_list
        type(model_t), pointer :: model_hadrons
        class(model_data_t), pointer :: model
        type(process_t), target :: process
        type(process_instance_t), target :: process_instance
        integer :: factorization_mode
        logical :: keep_correlations
        type(pdf_data_t) :: pdf_data
        class(evt_t), allocatable, target :: evt_trivial
        class(evt_t), allocatable, target :: evt_shower
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings

        write (u, "(A)")  "* Test output: shower_2"
        write (u, "(A)")  "*   Purpose: Two-jet event with FSR shower"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"), &
             os_data, model_hadrons)
        call setup_testbed (var_str ("shower_2"), &
            os_data, lib, model_list, process, process_instance)
        model => process%get_model_ptr ()

        write (u, "(A)")  "* Set up trivial transform"
        write (u, "(A)")

        allocate (evt_trivial_t :: evt_trivial)
        call evt_trivial%connect (process_instance, model)
        call evt_trivial%prepare_new_event (1, 1)
        call evt_trivial%generate_unweighted ()

        factorization_mode = FM_IGNORE_HELICITY
        keep_correlations = .false.
        call evt_trivial%make_particle_set (factorization_mode, keep_correlations)

        select type (evt_trivial)
        type is (evt_trivial_t)
            call evt_trivial%write (u)
            call write_separator (u, 2)
        end select
    end subroutine shower_2

```

```

write (u, "(A)")
write (u, "(A)")  "* Set up shower event transform"
write (u, "(A)")

settings%fsr_active = .true.

allocate (evt_shower_t :: evt_shower)
select type (evt_shower)
type is (evt_shower_t)
  call evt_shower%init (model_hadrons, os_data)
  allocate (shower_t :: evt_shower%shower)
  call evt_shower%shower%init (settings, taudec_settings, pdf_data, os_data)
  call evt_shower%connect (process_instance, model)
end select

evt_trivial%next => evt_shower
evt_shower%previous => evt_trivial

call evt_shower%prepare_new_event (1, 1)
call evt_shower%generate_unweighted ()
call evt_shower%make_particle_set (factorization_mode, keep_correlations)

select type (evt_shower)
type is (evt_shower_t)
  call evt_shower%write (u, testflag = .true.)
  call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_shower%final ()
call evt_trivial%final ()
call process_instance%final ()
call process%final ()
call lib%final ()
call model_hadrons%final ()
deallocate (model_hadrons)
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_2"

end subroutine shower_2

```

32.9 Fixed Order NLO Events

This section deals with the generation of weighted event samples which take into account next-to-leading order corrections. An approach generating unweighted events is not possible here, because negative weights might occur due to subtraction. Note that the events produced this way are not physical in the sense

that they will not keep NLO-accuracy when interfaced to a parton shower. They are rather useful for theoretical consistency checks and a fast estimate of NLO effects.

We generate NLO events in the following way: First, the integration is carried out using the complete divergence-subtracted NLO matrix element. In the subsequent simulation, N -particle kinematics are generated using $\mathcal{B} + \mathcal{V} + \mathcal{C}$ as weight. After that, the program loops over all singular regions and for each of them generates an event with $N + 1$ -particle kinematics. The weight for those events corresponds to the real matrix element \mathcal{R}^α evaluated at the α -region's emitter's phase space point, multiplied with S_α . This procedure is implemented using the `evt_nlo` transform.

```

<evt_nlo.f90>≡
  <File header>

  module evt_nlo

    <Use kinds>
    <Use strings>
    use constants
    use phs_points, only: phs_point_t
    use phs_points, only: assignment(=), operator(*), size
    use sm_qcd
    use model_data
    use particles
    use instances, only: process_instance_t
    use process_stacks
    use event_transforms
    use quantum_numbers, only: quantum_numbers_t

    use phs_fks, only: phs_fks_t, phs_fks_generator_t
    use phs_fks, only: phs_identifier_t, phs_point_set_t
    use resonances, only: resonance_contributors_t
    use fks_regions, only: region_data_t

    <Standard module head>

    <Evt NLO: public>

    <Evt NLO: public parameters>

    <Evt NLO: types>

    interface
    <Evt NLO: sub interfaces>
    end interface

  end module evt_nlo

<evt_nlo_sub.f90>≡
  <File header>

  submodule (evt_nlo) evt_nlo_s

```

```

    <Use debug>
    use io_units, only: given_output_unit
    use diagnostics
    use format_utils, only: write_separator
    use numeric_utils, only: nearly_equal
    use physics_defs, only: BORN, NLO_REAL
    use lorentz
    use interactions, only: interaction_t
    use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t
    use prc_core, only: prc_core_t
    use prc_external, only: prc_external_t
    use phs_fks, only: SQRTS_FIXED, SQRTS_VAR

    implicit none

contains

    <Evt NLO: procedures>

end submodule evt_nlo_s

<Evt NLO: types>≡
type :: nlo_event_deps_t
    logical :: lab_is_cm = .true.
    type(phs_point_set_t) :: p_born_cms
    type(phs_point_set_t) :: p_born_lab
    type(phs_point_set_t) :: p_real_cms
    type(phs_point_set_t) :: p_real_lab
    type(resonance_contributors_t), dimension(:), allocatable :: contributors
    type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
    integer, dimension(:), allocatable :: alr_to_i_con
    integer :: n_phs = 0
end type nlo_event_deps_t

```

This event transformation is for the generation of fixed-order NLO events. It takes an event with Born kinematics and creates $N_\alpha + 1$ modified weighted events. The first one has Born kinematics and its weight is the sum of Born, virtual, subtraction and, if present, also DGLAP matrix elements. The other N_α events have a weight which is equal to the real matrix element, evaluated with the phase space corresponding to the emitter of the α -region.

As the NLO event transforms have different kinematics, they also differ in their `particle_sets`. The `NLO event_t` object carries a single pointer to a `particle_set`. To avoid interference between the different NLO `particle_sets`, we save the `particle_set` of the current α -region in the array `particle_set_nlo`. Otherwise it would be unretrievable if the usual particle set of the event object was used.

```

<Evt NLO: public parameters>≡
integer, parameter, public :: EVT_NLO_UNDEFINED = 0
integer, parameter, public :: EVT_NLO_SEPARATE_BORNLIKE = 1
integer, parameter, public :: EVT_NLO_SEPARATE_REAL = 2
integer, parameter, public :: EVT_NLO_COMBINED = 3

```



```

<Evt NLO: public>≡
    public :: evt_nlo_t

<Evt NLO: types>+≡
    type, extends (evt_t) :: evt_nlo_t
        type(phs_fks_generator_t) :: phs_fks_generator
        real(default) :: sqme_rad = zero
        integer :: i_evaluation = 0
        type(particle_set_t), dimension(:), allocatable :: particle_set_nlo
        type(qcd_t) :: qcd
        type(nlo_event_deps_t) :: event_deps
        integer :: mode = EVT_NLO_UNDEFINED
        integer, dimension(:), allocatable :: &
            i_evaluation_to_i_phs, i_evaluation_to_emitter, &
            i_evaluation_to_i_term
        logical :: keep_failed_events = .false.
        integer :: selected_i_flv = 0
    contains
        <Evt NLO: evt nlo: TBP>
    end type evt_nlo_t

<Evt NLO: evt nlo: TBP>≡
    procedure :: write_name => evt_nlo_write_name

<Evt NLO: sub interfaces>≡
    module subroutine evt_nlo_write_name (evt, unit)
        class(evt_nlo_t), intent(in) :: evt
        integer, intent(in), optional :: unit
    end subroutine evt_nlo_write_name

<Evt NLO: procedures>≡
    module subroutine evt_nlo_write_name (evt, unit)
        class(evt_nlo_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: NLO"
    end subroutine evt_nlo_write_name

<Evt NLO: evt nlo: TBP>+≡
    procedure :: write => evt_nlo_write

<Evt NLO: sub interfaces>+≡
    module subroutine evt_nlo_write (evt, unit, verbose, more_verbose, testflag)
        class(evt_nlo_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
    end subroutine evt_nlo_write

<Evt NLO: procedures>+≡
    module subroutine evt_nlo_write (evt, unit, verbose, more_verbose, testflag)
        class(evt_nlo_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
        integer :: u, i
        u = given_output_unit (unit)

```

```

call write_separator (u, 2)
call evt%write_name (u)
call write_separator (u)
call evt%base_write (u, testflag = testflag, show_set = .true.)
write (u,'(A,ES16.9)') "sqme_rad = ", evt%sqme_rad
write (u, "(3x,A,I0)") "i_evaluation = ", evt%i_evaluation
call write_separator (u)
write (u, "(1x,A)") "Radiated particle sets:"
do i = 1, size (evt%particle_set_nlo)
    call evt%particle_set_nlo(i)%write (u, testflag = testflag)
    call write_separator (u)
end do
end subroutine evt_nlo_write

```

Connects the event transform to the process. Here also the phase space is set up by making `real_kinematics` point to the corresponding object in the `pcm_instance`.

```

(Evt NLO: evt_nlo: TBP)+≡
    procedure :: connect => evt_nlo_connect

(Evt NLO: sub interfaces)+≡
    module subroutine evt_nlo_connect &
        (evt, process_instance, model, process_stack)
        class(evt_nlo_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
    end subroutine evt_nlo_connect

(Evt NLO: procedures)+≡
    module subroutine evt_nlo_connect &
        (evt, process_instance, model, process_stack)
        class(evt_nlo_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_connect")
        call evt%base_connect (process_instance, model, process_stack)
        select type (pcm_work => process_instance%pcm_work)
        class is (pcm_nlo_workspace_t)
            select type (pcm => process_instance%pcm)
            type is (pcm_nlo_t)
                call pcm%setup_phs_generator (pcm_work, evt%phs_fks_generator, &
                    process_instance%get_sqrts ())
                call evt%set_i_evaluation_mappings (pcm%region_data, &
                    pcm_work%real_kinematics%alr_to_i_phs)
            end select
        end select
        call evt%set_mode (process_instance)
        call evt%setup_general_event_kinematics (process_instance)
        if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) &
            call evt%setup_real_event_kinematics (process_instance)
        if (debug_on) call msg_debug2 (D_TRANSFORMS, "evt_nlo_connect: success")
    end subroutine evt_nlo_connect

```

```

(Evt NLO: evt_nlo: TBP)+≡
    procedure :: set_i_evaluation_mappings => evt_nlo_set_i_evaluation_mappings

(Evt NLO: sub interfaces)+≡
    module subroutine evt_nlo_set_i_evaluation_mappings &
        (evt, reg_data, alr_to_i_phs)
        class(evt_nlo_t), intent(inout) :: evt
        type(region_data_t), intent(in) :: reg_data
        integer, intent(in), dimension(:) :: alr_to_i_phs
    end subroutine evt_nlo_set_i_evaluation_mappings

(Evt NLO: types)+≡
    type :: registered_triple_t
        integer, dimension(2) :: phs_em
        type(registered_triple_t), pointer :: next => null ()
    end type registered_triple_t

(Evt NLO: procedures)+≡
    module subroutine evt_nlo_set_i_evaluation_mappings &
        (evt, reg_data, alr_to_i_phs)
        class(evt_nlo_t), intent(inout) :: evt
        type(region_data_t), intent(in) :: reg_data
        integer, intent(in), dimension(:) :: alr_to_i_phs
        integer :: n_phs, alr
        integer :: i_evaluation, i_phs, emitter
        logical :: checked
        type(registered_triple_t), allocatable, target :: check_list
        i_evaluation = 1
        n_phs = reg_data%n_phs
        allocate (evt%i_evaluation_to_i_phs (n_phs), source = 0)
        allocate (evt%i_evaluation_to_emitter (n_phs), source = -1)
        allocate (evt%i_evaluation_to_i_term (0 : n_phs), source = 0)
        do alr = 1, reg_data%n_regions
            i_phs = alr_to_i_phs (alr)
            emitter = reg_data%regions(alr)%emitter
            call search_check_list (checked)
            if (.not. checked) then
                evt%i_evaluation_to_i_phs (i_evaluation) = i_phs
                evt%i_evaluation_to_emitter (i_evaluation) = emitter
                i_evaluation = i_evaluation + 1
            end if
        end do
        call fill_i_evaluation_to_i_term ()
        if (.not. (all (evt%i_evaluation_to_i_phs > 0) &
            .and. all (evt%i_evaluation_to_emitter > -1))) then
            call msg_fatal ("evt_nlo: Inconsistent mappings!")
        else
            if (debug2_active (D_TRANSFORMS)) then
                print *, 'evt_nlo Mappings, i_evaluation -> '
                print *, 'i_phs: ', evt%i_evaluation_to_i_phs
                print *, 'emitter: ', evt%i_evaluation_to_emitter
            end if
        end if
    contains
        subroutine fill_i_evaluation_to_i_term ()
            integer :: i_term, i_evaluation, term_emitter

```

```

!!! First find subtraction component
i_evaluation = 1
do i_term = 1, evt%process%get_n_terms ()
  if (evt%process_instance%term(i_term)%nlo_type /= NLO_REAL) cycle
  term_emitter = evt%process_instance%kin(i_term)%emitter
  if (term_emitter < 0) then
    evt%i_evaluation_to_i_term (0) = i_term
  else if (evt%i_evaluation_to_emitter(i_evaluation) == term_emitter) then
    evt%i_evaluation_to_i_term (i_evaluation) = i_term
    i_evaluation = i_evaluation + 1
  end if
end do
end subroutine fill_i_evaluation_to_i_term

subroutine search_check_list (found)
  logical, intent(out) :: found
  type(registered_triple_t), pointer :: current_triple => null ()
  if (allocated (check_list)) then
    current_triple => check_list
    do
      if (all (current_triple%phs_em == [i_phs, emitter])) then
        found = .true.
        exit
      end if
      if (.not. associated (current_triple%next)) then
        allocate (current_triple%next)
        current_triple%next%phs_em = [i_phs, emitter]
        found = .false.
        exit
      else
        current_triple => current_triple%next
      end if
    end do
  else
    allocate (check_list)
    check_list%phs_em = [i_phs, emitter]
    found = .false.
  end if
end subroutine search_check_list
end subroutine evt_nlo_set_i_evaluation_mappings

```

```

<Evt NLO: evt nlo: TBP>+≡
  procedure :: get_i_phs => evt_nlo_get_i_phs

<Evt NLO: sub interfaces>+≡
  module function evt_nlo_get_i_phs (evt) result (i_phs)
    integer :: i_phs
    class(evt_nlo_t), intent(in) :: evt
  end function evt_nlo_get_i_phs

<Evt NLO: procedures>+≡
  module function evt_nlo_get_i_phs (evt) result (i_phs)
    integer :: i_phs
    class(evt_nlo_t), intent(in) :: evt
    i_phs = evt%i_evaluation_to_i_phs (evt%i_evaluation)
  end function

```

```

end function evt_nlo_get_i_phs

<Evt NLO: evt nlo: TBP>+=
  procedure :: get_emitter => evt_nlo_get_emitter

<Evt NLO: sub interfaces>+=
  module function evt_nlo_get_emitter (evt) result (emitter)
    integer :: emitter
    class(evt_nlo_t), intent(in) :: evt
  end function evt_nlo_get_emitter

<Evt NLO: procedures>+=
  module function evt_nlo_get_emitter (evt) result (emitter)
    integer :: emitter
    class(evt_nlo_t), intent(in) :: evt
    emitter = evt%i_evaluation_to_emitter (evt%i_evaluation)
  end function evt_nlo_get_emitter

<Evt NLO: evt nlo: TBP>+=
  procedure :: get_i_term => evt_nlo_get_i_term

<Evt NLO: sub interfaces>+=
  module function evt_nlo_get_i_term (evt) result (i_term)
    integer :: i_term
    class(evt_nlo_t), intent(in) :: evt
  end function evt_nlo_get_i_term

<Evt NLO: procedures>+=
  module function evt_nlo_get_i_term (evt) result (i_term)
    integer :: i_term
    class(evt_nlo_t), intent(in) :: evt
    if (evt%mode >= EVT_NLO_SEPARATE_REAL) then
      i_term = evt%i_evaluation_to_i_term (evt%i_evaluation)
    else
      i_term = evt%process_instance%get_first_active_i_term ()
    end if
  end function evt_nlo_get_i_term

```

The event transform has a variable which counts the number of times it has already been called for one generation point. If this variable, `i_evaluation`, is zero, this means that `evt_nlo_generate_weighted` is called for the first time, so that the generation of an N -particle event is required. In all other cases, emission events are generated.

During a separate integration of the real component, the first event of each event group will become the counterevent. In this case, we return the sum of all subtraction matrix elements.

During a combined integration, the first event will be a combination of all Born-like events. To get the sum of their matrix elements, we subtract the sum of all real emissions from the sum of all matrix elements as the real contribution is the only non-Born contribution.

Note that the argument named `probability`, the use of the routine `generate_weighted` and the procedure we use to generate NLO events via an event transformation is an abuse of the interface which should be refactored.

```

<Evt NLO: evt nlo: TBP>+=

```

```

    procedure :: generate_weighted => evt_nlo_generate_weighted
<Evt NLO: sub interfaces>+≡
    module subroutine evt_nlo_generate_weighted (evt, probability)
        class(evt_nlo_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
    end subroutine evt_nlo_generate_weighted
<Evt NLO: procedures>+≡
    module subroutine evt_nlo_generate_weighted (evt, probability)
        class(evt_nlo_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        real(default) :: sqme
        call print_debug_info ()
        sqme = probability
        if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) then
            if (evt%i_evaluation == 0) then
                call evt%reset_phs_identifiers ()
                call evt%evaluate_real_kinematics ()
                if (evt%mode == EVT_NLO_SEPARATE_REAL) then
                    sqme = evt%compute_subtraction_sqmes ()
                else
                    sqme = sqme - evt%compute_all_sqme_rad ()
                end if
            else
                call evt%compute_real ()
                sqme = evt%sqme_rad
            end if
        end if
        probability = sqme
        if (debug_on) call msg_debug &
            (D_TRANSFORMS, "probability (after)", probability)
contains
        function status_code_to_string (mode) result (smode)
            type(string_t) :: smode
            integer, intent(in) :: mode
            select case (mode)
            case (EVT_NLO_UNDEFINED)
                smode = var_str ("Undefined")
            case (EVT_NLO_SEPARATE_BORNLIKE)
                smode = var_str ("Born-like")
            case (EVT_NLO_SEPARATE_REAL)
                smode = var_str ("Real")
            case (EVT_NLO_COMBINED)
                smode = var_str ("Combined")
            end select
        end function status_code_to_string

        subroutine print_debug_info ()
            if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_generate_weighted")
            if (debug_on) call msg_debug &
                (D_TRANSFORMS, char ("mode: " // status_code_to_string (evt%mode)))
            if (debug_on) call msg_debug &
                (D_TRANSFORMS, "probability (before)", probability)
            if (debug_on) call msg_debug &

```

```

        (D_TRANSFORMS, "evt%i_evaluation", evt%i_evaluation)
    if (debug2_active (D_TRANSFORMS)) then
        if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) then
            if (evt%i_evaluation == 0) then
                print *, 'Evaluate subtraction component'
            else
                print *, 'Evaluate radiation component'
            end if
        end if
    end if
end subroutine print_debug_info
end subroutine evt_nlo_generate_weighted

```

```

<Evt NLO: evt nlo: TBP>+=
    procedure :: reset_phs_identifiers => evt_nlo_reset_phs_identifiers

<Evt NLO: sub interfaces>+=
    module subroutine evt_nlo_reset_phs_identifiers (evt)
        class(evt_nlo_t), intent(inout) :: evt
    end subroutine evt_nlo_reset_phs_identifiers

<Evt NLO: procedures>+=
    module subroutine evt_nlo_reset_phs_identifiers (evt)
        class(evt_nlo_t), intent(inout) :: evt
        evt%event_deps%phs_identifiers%evaluated = .false.
    end subroutine evt_nlo_reset_phs_identifiers

```

The routine `make_factorized_particle_set` will setup the subevent momenta from the `connected%matrix`. Its initial state momenta correspond to the Born process without IS splitting and thus need to be updated with the real momenta from the `int_hard` to get correct momenta in the events with real radiation.

Ideally the `int_hard` and the `connected` would be setup with correct `source_links` to real momenta so that we would not need to replace momenta of the `connected` here.

The parameter `n_in` from the `int_matrix` is still 0 as it has been shifted to `n_vir`. We thus take `n_in` from the `particle_set`.

```

<Evt NLO: evt nlo: TBP>+=
    procedure :: connected_set_real_IS_momenta => &
        evt_nlo_connected_set_real_IS_momenta

<Evt NLO: sub interfaces>+=
    module subroutine evt_nlo_connected_set_real_IS_momenta (evt)
        class(evt_nlo_t), intent(inout) :: evt
    end subroutine evt_nlo_connected_set_real_IS_momenta

<Evt NLO: procedures>+=
    module subroutine evt_nlo_connected_set_real_IS_momenta (evt)
        class(evt_nlo_t), intent(inout) :: evt
        type(vector4_t) :: p_hard, p_beam, p_remn
        type(interaction_t), pointer :: int_matrix
        integer :: i, i_term, n_in, i_in_beam, i_in_hard, i_in_remn
        i_term = evt%get_i_term ()
        int_matrix => evt%process_instance%get_matrix_int_ptr (i_term)
        n_in = evt%particle_set%get_n_in ()
    end subroutine

```

```

do i = 1, n_in
  i_in_beam = i
  i_in_hard = n_in + i
  i_in_remn = 2 * n_in + i
  p_hard = evt%process_instance%term(i_term)%int_hard%get_momentum (i)
  p_beam = int_matrix%get_momentum (i_in_beam)
  p_remn = p_beam - p_hard
  call int_matrix%set_momentum (p_hard , i_in_hard)
  call int_matrix%set_momentum (p_remn , i_in_remn)
end do
end subroutine evt_nlo_connected_set_real_IS_momenta

```

(Evt NLO: evt nlo: TBP)+≡

```

procedure :: make_particle_set => evt_nlo_make_particle_set

```

(Evt NLO: sub interfaces)+≡

```

module subroutine evt_nlo_make_particle_set &
  (evt, factorization_mode, keep_correlations, r)
  class(evt_nlo_t), intent(inout) :: evt
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
end subroutine evt_nlo_make_particle_set

```

(Evt NLO: procedures)+≡

```

module subroutine evt_nlo_make_particle_set &
  (evt, factorization_mode, keep_correlations, r)
  class(evt_nlo_t), intent(inout) :: evt
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
  if (evt%mode >= EVT_NLO_SEPARATE_BORNLIKE) then
    call make_factorized_particle_set (evt, factorization_mode, &
      keep_correlations, r, evt%get_i_term (), &
      evt%get_selected_quantum_numbers (evt%selected_i_flv))
  else
    call make_factorized_particle_set (evt, factorization_mode, &
      keep_correlations, r)
  end if
end subroutine evt_nlo_make_particle_set

```

(Evt NLO: evt nlo: TBP)+≡

```

procedure :: evaluate_real_kinematics => evt_nlo_evaluate_real_kinematics

```

(Evt NLO: sub interfaces)+≡

```

module subroutine evt_nlo_evaluate_real_kinematics (evt)
  class(evt_nlo_t), intent(inout) :: evt
end subroutine evt_nlo_evaluate_real_kinematics

```

(Evt NLO: procedures)+≡

```

module subroutine evt_nlo_evaluate_real_kinematics (evt)
  class(evt_nlo_t), intent(inout) :: evt
  integer :: alr, i_phs, i_con, emitter
  real(default), dimension(3) :: x_rad
  logical :: use_contributors

```



```

integer :: n_regions
integer :: i_term
type(vector4_t), dimension(:), allocatable :: p_real

select type (pcm_work => evt%process_instance%pcm_work)
class is (pcm_nlo_workspace_t)
  x_rad = pcm_work%real_kinematics%x_rad
  associate (event_deps => evt%event_deps)
    i_term = evt%get_i_term ()
    event_deps%p_born_lab%phs_point(1) = &
      evt%process_instance%term(i_term)%p_seed
    event_deps%p_born_cms%phs_point(1) &
      = evt%boost_to_cms (event_deps%p_born_lab%phs_point(1))
    call evt%phs_fks_generator%set_sqrts_hat &
      (event_deps%p_born_cms%get_energy (1, 1))
    use_contributors = allocated (event_deps%contributors)
    select type (pcm => evt%process_instance%pcm)
    type is (pcm_nlo_t)
      n_regions = pcm%region_data%n_regions
    end select
    do alr = 1, n_regions
      i_phs = pcm_work%real_kinematics%alr_to_i_phs(alr)
      if (event_deps%phs_identifiers(i_phs)%evaluated) cycle
      emitter = event_deps%phs_identifiers(i_phs)%emitter
      associate (generator => evt%phs_fks_generator)
        if (emitter <= evt%process%get_n_in ()) then
          call generator%prepare_generation (x_rad, i_phs, emitter, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            event_deps%phs_identifiers)
          ! TODO wk 19-02-28: intent of p_real (also below)?
          p_real = event_deps%p_real_lab%phs_point(i_phs)
          select case (generator%isr_kinematics%isr_mode)
          case (SQRTS_FIXED)
            call generator%generate_isr_fixed_beam_energy (i_phs, &
              event_deps%p_born_cms%phs_point(1)%get (), &
              p_real)
          case (SQRTS_VAR)
            call generator%generate_isr (i_phs, &
              event_deps%p_born_lab%phs_point(1)%get (), &
              p_real)
          end select
          event_deps%p_real_lab%phs_point(i_phs) = p_real
          event_deps%p_real_cms%phs_point(i_phs) &
            = evt%boost_to_cms (event_deps%p_real_lab%phs_point(i_phs))
        else
          if (use_contributors) then
            i_con = event_deps%alr_to_i_con(alr)
            call generator%prepare_generation (x_rad, i_phs, emitter, &
              event_deps%p_born_cms%phs_point(1)%get (), &
              event_deps%phs_identifiers, event_deps%contributors, i_con)
            p_real = event_deps%p_real_cms%phs_point(i_phs)
            call generator%generate_fsr (emitter, i_phs, i_con, &
              event_deps%p_born_cms%phs_point(1)%get (), &
              p_real)
          end if
        end associate
      end do
    end associate
  end class
end select

```

```

        event_deps%p_real_cms%phs_point(i_phs) = p_real
    else
        call generator%prepare_generation (x_rad, i_phs, emitter, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            event_deps%phs_identifiers)
        p_real = event_deps%p_real_cms%phs_point(i_phs)
        call generator%generate_fsr (emitter, i_phs, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            p_real)
        event_deps%p_real_cms%phs_point(i_phs) = p_real
    end if
    event_deps%p_real_lab%phs_point(i_phs) &
        = evt%boost_to_lab (event_deps%p_real_cms%phs_point(i_phs))
    end if
end associate
call pcm_work%set_momenta &
    (event_deps%p_born_lab%phs_point(1)%get (), &
    event_deps%p_real_lab%phs_point(i_phs)%get (), &
    i_phs)
call pcm_work%set_momenta &
    (event_deps%p_born_cms%phs_point(1)%get (), &
    event_deps%p_real_cms%phs_point(i_phs)%get (), &
    i_phs, cms = .true.)
event_deps%phs_identifiers(i_phs)%evaluated = .true.
end do
end associate
end select
end subroutine evt_nlo_evaluate_real_kinematics

```

This routine calls the evaluation of the singular regions only for the subtraction terms.

```

<Evt NLO: evt nlo: TBP>+=
    procedure :: compute_subtraction_sqmes => evt_nlo_compute_subtraction_sqmes

<Evt NLO: sub interfaces>+=
    module function evt_nlo_compute_subtraction_sqmes (evt) result (sqme)
        class(evt_nlo_t), intent(inout) :: evt
        real(default) :: sqme
    end function evt_nlo_compute_subtraction_sqmes

<Evt NLO: procedures>+=
    module function evt_nlo_compute_subtraction_sqmes (evt) result (sqme)
        class(evt_nlo_t), intent(inout) :: evt
        real(default) :: sqme
        integer :: i_phs, i_term
        if (debug_on) call msg_debug &
            (D_TRANSFORMS, "evt_nlo_compute_subtraction_sqmes")
        sqme = zero
        associate (event_deps => evt%event_deps)
            i_phs = 1; i_term = evt%i_evaluation_to_i_term(0)
            call evt%process_instance%compute_sqme_rad &
                (i_term, i_phs, is_subtraction = .true.)
            sqme = sqme + evt%process_instance%get_sqme (i_term)
        end associate
    end function evt_nlo_compute_subtraction_sqmes

```

This routine calls the evaluation of the singular regions only for emission matrix elements.

```

(Evt NLO: evt nlo: TBP)+≡
  procedure :: compute_real => evt_nlo_compute_real

(Evt NLO: sub interfaces)+≡
  module subroutine evt_nlo_compute_real (evt)
    class(evt_nlo_t), intent(inout) :: evt
  end subroutine evt_nlo_compute_real

(Evt NLO: procedures)+≡
  module subroutine evt_nlo_compute_real (evt)
    class(evt_nlo_t), intent(inout) :: evt
    integer :: i_phs, i_term
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_compute_real")
    i_phs = evt%get_i_phs ()
    i_term = evt%i_evaluation_to_i_term (evt%i_evaluation)
    associate (event_deps => evt%event_deps)
      call evt%process_instance%compute_sqme_rad (i_term, i_phs, &
        is_subtraction = .false.)
      evt%sqme_rad = evt%process_instance%get_sqme (i_term)
    end associate
  end subroutine evt_nlo_compute_real

```

This routine calls the evaluation of the singular regions only for all emission matrix elements. This is needed for the combined mode. It returns the sum of all valid real matrix elements.

```

(Evt NLO: evt nlo: TBP)+≡
  procedure :: compute_all_sqme_rad => evt_nlo_compute_all_sqme_rad

(Evt NLO: sub interfaces)+≡
  module function evt_nlo_compute_all_sqme_rad (evt) result (sqme)
    class(evt_nlo_t), intent(inout) :: evt
    real(default) :: sqme
  end function evt_nlo_compute_all_sqme_rad

(Evt NLO: procedures)+≡
  module function evt_nlo_compute_all_sqme_rad (evt) result (sqme)
    class(evt_nlo_t), intent(inout) :: evt
    real(default) :: sqme
    integer :: i_phs, i_term
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_compute_all_sqme_rad")
    sqme = zero
    do i_term = 1, size (evt%process_instance%term)
      if (evt%is_valid_event (i_term)) then
        associate (term => evt%process_instance%term(i_term))
          if (term%nlo_type == NLO_REAL .and. &
            .not. term%is_subtraction ()) then
            i_phs = evt%process_instance%kin(i_term)%i_phs
            call evt%process_instance%compute_sqme_rad ( &
              i_term, i_phs, is_subtraction = .false.)
            sqme = sqme + evt%process_instance%get_sqme (i_term)
          end if
        end associate
      end if
    end do
  end function

```

```

        end if
    end do
end function evt_nlo_compute_all_sqme_rad

```

Boosts the given four vector `p_lab` to the Born or real CMS depending on the number of given momenta. Unfortunately, all boosts available via `get_boost_to_cms` are Born-like, so we need to compute the boost to the real CMS here manually. We cannot rely on `i_term` in order to determine whether to apply a Born-like or a real boost as we also need a real boost to compute the weights of the Born-like subevents as implemented in `evt_nlo_generate_weighted`.

```

(Evt NLO: evt_nlo: TBP)+≡
    procedure :: boost_to_cms => evt_nlo_boost_to_cms

(Evt NLO: sub interfaces)+≡
    module function evt_nlo_boost_to_cms (evt, p_lab) result (p_cms)
        type(phs_point_t), intent(in) :: p_lab
        class(evt_nlo_t), intent(in) :: evt
        type(phs_point_t) :: p_cms
    end function evt_nlo_boost_to_cms

(Evt NLO: procedures)+≡
    module function evt_nlo_boost_to_cms (evt, p_lab) result (p_cms)
        type(phs_point_t), intent(in) :: p_lab
        class(evt_nlo_t), intent(in) :: evt
        type(phs_point_t) :: p_cms
        type(vector4_t) :: p0, p1
        type(lorentz_transformation_t) :: lt_lab_to_cms, lt
        real(default) :: sqrts_hat
        integer :: i_boost, n_legs_born
        if (evt%event_deps%lab_is_cm) then
            lt_lab_to_cms = identity
        else
            n_legs_born = size (evt%event_deps%p_born_lab%phs_point(1))
            if (size (p_lab) == n_legs_born) then
                i_boost = evt%get_i_term ()
                lt_lab_to_cms = evt%process_instance%get_boost_to_cms (i_boost)
            else
                sqrts_hat = (p_lab%select (1) + p_lab%select (2))*1
                p0 = p_lab%select (1) + p_lab%select (2)
                lt = boost (p0, sqrts_hat)
                p1 = inverse(lt) * p_lab%select (1)
                lt_lab_to_cms = inverse (lt * rotation_to_2nd (3, space_part (p1)))
            end if
        end if
        p_cms = lt_lab_to_cms * p_lab
    end function evt_nlo_boost_to_cms

```

Boosts the given four vector `p_cms` from the Born CMS to the lab system. It should not be called for ISR as in this case, the Born CMS and the real CMS differ.

```

(Evt NLO: evt_nlo: TBP)+≡
    procedure :: boost_to_lab => evt_nlo_boost_to_lab

```

```

(Evt NLO: sub interfaces)+≡
    module function evt_nlo_boost_to_lab (evt, p_cms) result (p_lab)
        type(phs_point_t) :: p_lab
        class(evt_nlo_t), intent(in) :: evt
        type(phs_point_t), intent(in) :: p_cms
    end function evt_nlo_boost_to_lab

(Evt NLO: procedures)+≡
    module function evt_nlo_boost_to_lab (evt, p_cms) result (p_lab)
        type(phs_point_t) :: p_lab
        class(evt_nlo_t), intent(in) :: evt
        type(phs_point_t), intent(in) :: p_cms
        type(lorentz_transformation_t) :: lt_cms_to_lab
        integer :: i_boost
        if (evt%event_deps%lab_is_cm) then
            lt_cms_to_lab = identity
        else
            i_boost = evt%get_i_term ()
            lt_cms_to_lab = evt%process_instance%get_boost_to_lab (i_boost)
        end if
        p_lab = lt_cms_to_lab * p_cms
    end function evt_nlo_boost_to_lab

(Evt NLO: evt nlo: TBP)+≡
    procedure :: setup_general_event_kinematics => &
        evt_nlo_setup_general_event_kinematics

(Evt NLO: sub interfaces)+≡
    module subroutine evt_nlo_setup_general_event_kinematics &
        (evt, process_instance)
        class(evt_nlo_t), intent(inout) :: evt
        type(process_instance_t), intent(in) :: process_instance
    end subroutine evt_nlo_setup_general_event_kinematics

(Evt NLO: procedures)+≡
    module subroutine evt_nlo_setup_general_event_kinematics &
        (evt, process_instance)
        class(evt_nlo_t), intent(inout) :: evt
        type(process_instance_t), intent(in) :: process_instance
        integer :: n_born
        associate (event_deps => evt%event_deps)
            event_deps%lab_is_cm = process_instance%lab_is_cm (1)
            select type (pcm => process_instance%pcm)
                type is (pcm_nlo_t)
                    n_born = pcm%region_data%n_legs_born
                end select
            call event_deps%p_born_cms%init (n_born, 1)
            call event_deps%p_born_lab%init (n_born, 1)
        end associate
    end subroutine evt_nlo_setup_general_event_kinematics

(Evt NLO: evt nlo: TBP)+≡
    procedure :: setup_real_event_kinematics => &
        evt_nlo_setup_real_event_kinematics

```

<Evt NLO: sub interfaces>+≡

```

module subroutine evt_nlo_setup_real_event_kinematics &
  (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance
end subroutine evt_nlo_setup_real_event_kinematics

```

<Evt NLO: procedures>+≡

```

module subroutine evt_nlo_setup_real_event_kinematics (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance
  integer :: n_real, n_phs
  integer :: i_real
  associate (event_deps => evt%event_deps)
    select type (pcm => process_instance%pcm)
    class is (pcm_nlo_t)
      n_real = pcm%region_data%n_legs_real
    end select
    i_real = evt%process%get_first_real_term ()
    select type (phs => process_instance%kin(i_real)%phs)
    type is (phs_fks_t)
      event_deps%phs_identifiers = phs%phs_identifiers
    end select
    n_phs = size (event_deps%phs_identifiers)
    call event_deps%p_real_cms%init (n_real, n_phs)
    call event_deps%p_real_lab%init (n_real, n_phs)
    select type (pcm => process_instance%pcm)
    type is (pcm_nlo_t)
      if (allocated (pcm%region_data%alr_contributors)) then
        allocate (event_deps%contributors &
          (size (pcm%region_data%alr_contributors)))
        event_deps%contributors = pcm%region_data%alr_contributors
      end if
      if (allocated (pcm%region_data%alr_to_i_contributor)) then
        allocate (event_deps%alr_to_i_con &
          (size (pcm%region_data%alr_to_i_contributor)))
        event_deps%alr_to_i_con = pcm%region_data%alr_to_i_contributor
      end if
    end select
  end associate
end subroutine evt_nlo_setup_real_event_kinematics

```

<Evt NLO: evt nlo: TBP>+≡

```

procedure :: set_mode => evt_nlo_set_mode

```

<Evt NLO: sub interfaces>+≡

```

module subroutine evt_nlo_set_mode (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance
end subroutine evt_nlo_set_mode

```

<Evt NLO: procedures>+≡

```

module subroutine evt_nlo_set_mode (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance

```

```

integer :: i_real
select type (pcm => process_instance%pcm)
type is (pcm_nlo_t)
  if (pcm%settings%combined_integration) then
    evt%mode = EVT_NLO_COMBINED
  else
    i_real = evt%process%get_first_real_component ()
    if (i_real == evt%process%extract_active_component_mci ()) then
      evt%mode = EVT_NLO_SEPARATE_REAL
    else
      evt%mode = EVT_NLO_SEPARATE_BORNLIKE
    end if
  end if
end select
end subroutine evt_nlo_set_mode

```

<Evt NLO: evt nlo: TBP>+≡
 procedure :: is_valid_event => evt_nlo_is_valid_event

<Evt NLO: sub interfaces>+≡
 module function evt_nlo_is_valid_event (evt, i_term) result (valid)
 logical :: valid
 class(evt_nlo_t), intent(in) :: evt
 integer, intent(in) :: i_term
 end function evt_nlo_is_valid_event

<Evt NLO: procedures>+≡
 module function evt_nlo_is_valid_event (evt, i_term) result (valid)
 logical :: valid
 class(evt_nlo_t), intent(in) :: evt
 integer, intent(in) :: i_term
 valid = evt%process_instance%term(i_term)%passed
 end function evt_nlo_is_valid_event

Retrieves the actual quantum numbers chosen in evt_nlo_prepare_new_event.

<Evt NLO: evt nlo: TBP>+≡
 procedure :: get_selected_quantum_numbers => &
 evt_nlo_get_selected_quantum_numbers

<Evt NLO: sub interfaces>+≡
 module function evt_nlo_get_selected_quantum_numbers &
 (evt, i_flv) result (qn_select)
 class(evt_nlo_t), intent(in) :: evt
 integer, intent(in) :: i_flv
 type(quantum_numbers_t), dimension(:), allocatable :: qn_select
 end function evt_nlo_get_selected_quantum_numbers

<Evt NLO: procedures>+≡
 module function evt_nlo_get_selected_quantum_numbers &
 (evt, i_flv) result (qn_select)
 class(evt_nlo_t), intent(in) :: evt
 integer, intent(in) :: i_flv
 type(quantum_numbers_t), dimension(:), allocatable :: qn_select
 integer :: i_term, index
 i_term = evt%get_i_term ()

```

associate (term => evt%process_instance%term(i_term))
  index = term%connected%matrix%get_qn_index (i_flv, i_sub = 0)
  qn_select = term%connected%matrix%get_quantum_numbers (index)
end associate
end function evt_nlo_get_selected_quantum_numbers

```

Selects a flavor structure for Born subevents, such that each possible flavor structure is as probable as its portion of the sum of Born matrix elements over all flavors. For non-Born Born-like subevents, no Born matrix elements are available. We always choose `i_flv = 1` in this case. If all terms are active, i.e. in a full NLO calculation, the flavors of Born-like subevents will be distributed according to the Born matrix elements only, to avoid issues with matrix elements of different sign and assure a LO flavor distribution.

Likewise, the real-like event flavors are distributed according to the real matrix elements. Here, we need to make sure to not mix matrix elements from different real terms and instead determine the flavor for each subevent based on just the matrix elements for one of the terms. The implementation below assumes that in the sequence of NLO terms, the Born term is immediately followed by all the real terms which are again followed by the subtraction, the virtual and the DGLAP term.

Both flavor structures can be determined without correlation as the flavors will only become important for events to be matched to a parton shower and in this case we will only generate either a single Born-like or a single real-like event which are not part of an event group.

In case all subevents failed the cuts, all `sqmes` were set to 0 so we cannot determine the flavor in this way. In this case, we always choose the first flavor structure given by the matrix-element generator with `i_flv = 1`.

Ideally, having to choose a particle set here would not be necessary as it is also chosen in `particle_set_init_interaction` which in the current approach is disabled by supplying `qn_select` explicitly based on the flavors chosen here.

```

(Evt NLO: evt_nlo: TBP)+≡
  procedure :: prepare_new_event => evt_nlo_prepare_new_event

(Evt NLO: sub interfaces)+≡
  module subroutine evt_nlo_prepare_new_event (evt, i_mci, i_term)
    class(evt_nlo_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
  end subroutine evt_nlo_prepare_new_event

(Evt NLO: procedures)+≡
  module subroutine evt_nlo_prepare_new_event (evt, i_mci, i_term)
    class(evt_nlo_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    real(default) :: s, x
    real(default) :: sqme_total
    real(default), dimension(:), allocatable :: sqme_flv
    integer :: i, i_flv, i_core, emitter, n_in
    logical, save :: warn_once = .true.
    class(prc_core_t), pointer :: core => null ()
    call evt%reset ()
    call evt%rng%generate (x)
    do i = 1, size (evt%process_instance%term)

```



```

associate (term => evt%process_instance%term(i))
  if (evt%i_evaluation == 0) then
    if (term%nlo_type == BORN) then
      allocate (sqme_flv (term%config%data%n_flv))
      exit
    end if
  else
    if (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction()) then
      allocate (sqme_flv (term%config%data%n_flv))
      exit
    end if
  end if
end associate
end do
sqme_total = zero
sqme_flv = zero
i_core = evt%process%get_i_core (i_term)
core => evt%process%get_core_ptr (i_core)
do i = 1, size (evt%process_instance%term)
  associate (term => evt%process_instance%term(i))
    if (i == evt%i_evaluation + 1 .and. (term%nlo_type == BORN .or. &
      (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction())) ) then
      sqme_total = sqme_total + real (sum ( term%connected%matrix%get_matrix_element ()))
      !!! TODO (VR 2020-02-19) figure out why this select type is needed for prc_omega_t
      !!! For NLO and prc_omega_t the connected trace seems to be set up incorrectly!
      !!! (PS 2020-11-05) This leads to real events of processes with structure functions
      !!! having a wrong flavor distribution if computed with 0'Mega.
      !!! The flavor distributions are identical with and also without the special case
      !!! for 0'Mega and wrong in both cases.
      !!! However, this case it is not critical as long as 0'Mega does not provide matrix e
      !!! exclusive in coupling orders and is thus only rarely used for NLO applications an
      select type (core)
      class is (prc_external_t)
        do i_flv = 1, size (sqme_flv)
          if (allocated (term%passed_array)) then
            if (term%passed .and. .not. term%passed_array(i_flv)) cycle
          end if
          sqme_flv(i_flv) = sqme_flv(i_flv) &
            + real (term%connected%matrix%get_matrix_element ( &
              term%connected%matrix%get_qn_index (i_flv, i_sub = 0)))
        end do
      class default
        sqme_flv = sqme_flv &
          + real (term%connected%matrix%get_matrix_element ())
        emitter = evt%process_instance%kin(i)%emitter
        n_in = evt%process_instance%kin(i)%n_in
        if (warn_once .and. term%nlo_type == NLO_REAL .and. emitter <= n_in) then
          warn_once = .false.
          call msg_warning("evt_nlo_prepare_new_event: fNLO flavor&
            & distributions with 0'Mega are wrong.")
        end if
      end select
    end if
  end associate
end do
end associate

```

```

end do
if (debug2_active (D_TRANSFORMS)) then
  if (.not. nearly_equal(sqme_total, sum (sqme_flv))) then
    call msg_warning ("evt_nlo_prepare_new_event: &
      &sum over flavored sqmes does not match total sqme.")
  end if
end if
!!! Need absolute values to take into account negative weights
x = x * abs (sqme_total)
s = abs (sqme_flv (1))
evt%selected_i_flv = 1
if (s < x) then
  do i_flv = 2, size (sqme_flv)
    s = s + abs (sqme_flv (i_flv))
    if (s > x) then
      evt%selected_i_flv = i_flv
      exit
    end if
  end do
end if
if (debug2_active (D_TRANSFORMS)) then
  call msg_print_color ("Selected i_flv: ", COL_GREEN)
  print *, evt%selected_i_flv
end if
end subroutine evt_nlo_prepare_new_event

```

32.10 Complete Events

This module combines hard processes with decay chains, shower, and hadronization (not implemented yet) to complete events. It also manages the input and output of event records in various formats.

`<events.f90>`≡
<File header>

`module events`

<Use kinds>

<Use strings>

`use diagnostics`

`use variables`

`use expr_base`

`use model_data`

`use state_matrices, only: FM_IGNORE_HELICITY, &`

`FM_SELECT_HELICITY, FM_FACTOR_HELICITY, FM_CORRELATED_HELICITY`

`use particles`

`use subevt_expr`

`use rng_base`

`use process, only: process_t`

`use instances, only: process_instance_t`

`use process_stacks`

`use event_base`

```

        use event_transforms

        <Standard module head>

        <Events: public>

        <Events: types>

        <Events: interfaces>

        interface
        <Events: sub interfaces>
        end interface

contains

        <Events: main procedures>

    end module events

<events_sub.f90>≡
    <File header>

    submodule (events) events_s

        <Use debug>
        use constants, only: one
        use io_units
        use format_utils, only: pac_fmt, write_separator
        use format_defs, only: FMT_12, FMT_19
        use numeric_utils
        use pcm, only: pcm_nlo_workspace_t
        use decays
        use evt_nlo
        use phs_fks, only: SQRTS_FIXED, SQRTS_VAR

        implicit none

contains

        <Events: procedures>

    end submodule events_s

```

32.10.1 Event configuration

The parameters govern the transformation of an event to a particle set.

The **safety_factor** reduces the acceptance probability for unweighting. If greater than one, excess events become less likely, but the reweighting efficiency also drops.

The **sigma** and **n** values, if nontrivial, allow for reweighting the events according to the requested **norm_mode**.

Various `parse_node_t` objects are taken from the SINDARIN input. They encode expressions that apply to the current event. The workspaces for evaluating those expressions are set up in the `event_expr_t` objects. Note that these are really pointers, so the actual nodes are not stored inside the event object.

```

<Events: types>≡
type :: event_config_t
  logical :: unweighted = .false.
  integer :: norm_mode = NORM_UNDEFINED
  integer :: factorization_mode = FM_IGNORE_HELICITY
  logical :: keep_correlations = .false.
  logical :: colorize_subevt = .false.
  real(default) :: sigma = 1
  integer :: n = 1
  real(default) :: safety_factor = 1
  class(expr_factory_t), allocatable :: ef_selection
  class(expr_factory_t), allocatable :: ef_reweight
  class(expr_factory_t), allocatable :: ef_analysis
contains
  <Events: event config: TBP>
end type event_config_t

```

Output.

```

<Events: event config: TBP>≡
  procedure :: write => event_config_write

<Events: sub interfaces>≡
  module subroutine event_config_write (object, unit, show_expressions)
    class(event_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_expressions
  end subroutine event_config_write

<Events: procedures>≡
  module subroutine event_config_write (object, unit, show_expressions)
    class(event_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_expressions
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,L1)") "Unweighted          = ", object%unweighted
    write (u, "(3x,A,A)") "Normalization      = ", &
      char (event_normalization_string (object%norm_mode))
    write (u, "(3x,A)", advance="no") "Helicity handling = "
    select case (object%factorization_mode)
    case (FM_IGNORE_HELICITY)
      write (u, "(A)") "drop"
    case (FM_SELECT_HELICITY)
      write (u, "(A)") "select"
    case (FM_FACTOR_HELICITY)
      write (u, "(A)") "factorize"
    end select
    write (u, "(3x,A,L1)") "Keep correlations = ", object%keep_correlations
    if (object%colorize_subevt) then
      write (u, "(3x,A,L1)") "Colorize subevent = ", object%colorize_subevt
    end if
  end subroutine event_config_write

```

```

end if
if (.not. nearly_equal (object%safety_factor, one)) then
  write (u, "(3x,A," // FMT_12 // ")") &
    "Safety factor      = ", object%safety_factor
end if
if (present (show_expressions)) then
  if (show_expressions) then
    if (allocated (object%ef_selection)) then
      call write_separator (u)
      write (u, "(3x,A)") "Event selection expression:"
      call object%ef_selection%write (u)
    end if
    if (allocated (object%ef_reweight)) then
      call write_separator (u)
      write (u, "(3x,A)") "Event reweighting expression:"
      call object%ef_reweight%write (u)
    end if
    if (allocated (object%ef_analysis)) then
      call write_separator (u)
      write (u, "(3x,A)") "Analysis expression:"
      call object%ef_analysis%write (u)
    end if
  end if
end if
end subroutine event_config_write

```

32.10.2 The event type

This is the concrete implementation of the `generic_event_t` core that is defined above in the `event_base` module. The core manages the main (dressed) particle set pointer and the current values for weights and `sqme`. The implementation adds configuration data, expressions, process references, and event transforms.

Each event refers to a single elementary process. This process may be dressed by a shower, a decay chain etc. We maintain pointers to a process instance.

A list of event transforms (class `evt_t`) transform the connected interactions of the process instance into the final particle set. In this list, the first transform is always the trivial one, which just factorizes the process instance. Subsequent transforms may apply decays, etc. The `particle_set` pointer identifies the particle set that we want to be analyzed and returned by the event, usually the last one.

Squared matrix element and weight values: when reading events from file, the `ref` value is the number in the file, while the `prc` value is the number that we calculate from the momenta in the file, possibly with different parameters. When generating events the first time, or if we do not recalculate, the numbers should coincide. Furthermore, the array of `alt` values is copied from an array of alternative event records. These values should represent calculated values.

The `sqme` and `weight` values mirror corresponding values in the `expr` sub-object. The idea is that when generating or reading events, the event record is filled first, then the `expr` object acquires copies. These copies are used for writing events and as targets for pointer variables in the analysis expression.

All data that involve user-provided expressions (selection, reweighting, analysis) are handled by the `expr` subobject. In particular, evaluating the event-selection expression sets the `passed` flag. Furthermore, the `expr` subobject collects data that can be used in the analysis and should be written to file, including copies of `sqme` and `weight`.

```

<Events: public>≡
    public :: event_t

<Events: types>+≡
    type, extends (generic_event_t) :: event_t
        type(event_config_t) :: config
        type(process_t), pointer :: process => null ()
        type(process_instance_t), pointer :: instance => null ()
        class(rng_t), allocatable :: rng
        integer :: selected_i_mci = 0
        integer :: selected_i_term = 0
        integer :: selected_channel = 0
        logical :: is_complete = .false.
        class(evt_t), pointer :: transform_first => null ()
        class(evt_t), pointer :: transform_last => null ()
        type(event_expr_t) :: expr
        logical :: selection_evaluated = .false.
        logical :: passed = .false.
        real(default), allocatable :: alpha_qcd_forced
        real(default), allocatable :: scale_forced
        real(default) :: reweight = 1
        logical :: analysis_flag = .false.
        integer :: i_event = 0
    contains
        <Events: event: TBP>
    end type event_t

<Events: event: TBP>≡
    procedure :: clone => event_clone

<Events: sub interfaces>+≡
    module subroutine event_clone (event, event_new)
        class(event_t), intent(in), target :: event
        class(event_t), intent(out), target :: event_new
    end subroutine event_clone

<Events: procedures>+≡
    module subroutine event_clone (event, event_new)
        class(event_t), intent(in), target :: event
        class(event_t), intent(out), target :: event_new
        type(string_t) :: id
        integer :: num_id
        event_new%config = event%config
        event_new%process => event%process
        event_new%instance => event%instance
        if (allocated (event%rng)) &
            allocate(event_new%rng, source=event%rng)
        event_new%selected_i_mci = event%selected_i_mci
        event_new%selected_i_term = event%selected_i_term
        event_new%selected_channel = event%selected_channel

```

```

event_new%is_complete = event%is_complete
event_new%transform_first => event%transform_first
event_new%transform_last => event%transform_last
event_new%selection_evaluated = event%selection_evaluated
event_new%passed = event%passed
if (allocated (event%alpha_qcd_forced)) &
    allocate(event_new%alpha_qcd_forced, source=event%alpha_qcd_forced)
if (allocated (event%scale_forced)) &
    allocate(event_new%scale_forced, source=event%scale_forced)
event_new%reweight = event%reweight
event_new%analysis_flag = event%analysis_flag
event_new%i_event = event%i_event
id = event_new%process%get_id ()
if (id /= "") call event_new%expr%set_process_id (id)
num_id = event_new%process%get_num_id ()
if (num_id /= 0) call event_new%expr%set_process_num_id (num_id)
call event_new%expr%setup_vars (event_new%process%get_sqrts ())
call event_new%expr%link_var_list (event_new%process%get_var_list_ptr ())
end subroutine event_clone

```

Finalizer: the list of event transforms is deleted iteratively.

```

<Events: event: TBP>+≡
    procedure :: final => event_final

<Events: sub interfaces>+≡
    module subroutine event_final (object)
        class(event_t), intent(inout) :: object
    end subroutine event_final

<Events: procedures>+≡
    module subroutine event_final (object)
        class(event_t), intent(inout) :: object
        class(evt_t), pointer :: evt
        if (allocated (object%rng)) call object%rng%final ()
        call object%expr%final ()
        do while (associated (object%transform_first))
            evt => object%transform_first
            object%transform_first => evt%next
            call evt%final ()
            deallocate (evt)
        end do
    end subroutine event_final

```

Output.

The event index is written in the header, it should coincide with the `event_index` variable that can be used in selection and analysis.

Particle set: this is a pointer to one of the event transforms, so it should suffice to print the latter.

```

<Events: event: TBP>+≡
    procedure :: write => event_write

<Events: sub interfaces>+≡
    module subroutine event_write (object, unit, show_process, &
        show_transforms, show_decay, verbose, testflag)

```

```

        class(event_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_process, show_transforms, show_decay
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: testflag
    end subroutine event_write

<Events: procedures>+≡
    module subroutine event_write (object, unit, show_process, &
        show_transforms, show_decay, verbose, testflag)
        class(event_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_process, show_transforms, show_decay
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: testflag
        logical :: prc, trans, dec, verb
        class(evt_t), pointer :: evt
        character(len=7) :: fmt
        integer :: u, i
        call pac_fmt (fmt, FMT_19, FMT_12, testflag)
        u = given_output_unit (unit)
        prc = .true.; if (present (show_process)) prc = show_process
        trans = .true.; if (present (show_transforms)) trans = show_transforms
        dec = .true.; if (present (show_decay)) dec = show_decay
        verb = .false.; if (present (verbose)) verb = verbose
        call write_separator (u, 2)
        write (u, "(1x,A)", advance="no") "Event"
        if (object%has_index ()) then
            write (u, "(1x,'#',I0)", advance="no") object%get_index ()
        end if
        if (object%is_complete) then
            write (u, *)
        else
            write (u, "(1x,A)") "[incomplete]"
        end if
        call write_separator (u)
        call object%config%write (u)
        if (object%sqme_ref_is_known () .or. object%weight_ref_is_known ()) then
            call write_separator (u)
        end if
        if (object%sqme_ref_is_known ()) then
            write (u, "(3x,A," // fmt // ")") &
                "Squared matrix el. (ref) = ", object%get_sqme_ref ()
            if (object%sqme_alt_is_known ()) then
                do i = 1, object%get_n_alt ()
                    write (u, "(5x,A," // fmt // ",1x,I0)") &
                        "alternate sqme   = ", object%get_sqme_alt(i), i
                end do
            end if
        end if
        if (object%sqme_prc_is_known ()) &
            write (u, "(3x,A," // fmt // ")") &
                "Squared matrix el. (prc) = ", object%get_sqme_prc ()

        if (object%weight_ref_is_known ()) then

```



```

write (u, "(3x,A," // fmt // ")") &
    "Event weight (ref)          = ", object%get_weight_ref ()
if (object%weight_alt_is_known ()) then
    do i = 1, object%get_n_alt ()
        write (u, "(5x,A," // fmt // ",1x,I0)") &
            "alternate weight      = ", object%get_weight_alt(i), i
    end do
end if
end if
if (object%weight_prc_is_known ()) &
    write (u, "(3x,A," // fmt // ")") &
        "Event weight (prc)          = ", object%get_weight_prc ()

if (object%selected_i_mci /= 0) then
    call write_separator (u)
    write (u, "(3x,A,I0)") "Selected MCI group = ", object%selected_i_mci
    write (u, "(3x,A,I0)") "Selected term      = ", object%selected_i_term
    write (u, "(3x,A,I0)") "Selected channel   = ", object%selected_channel
end if
if (object%selection_evaluated) then
    call write_separator (u)
    write (u, "(3x,A,L1)") "Passed selection   = ", object%passed
    if (object%passed) then
        write (u, "(3x,A," // fmt // ")") &
            "Reweighting factor = ", object%reweight
        write (u, "(3x,A,L1)") &
            "Analysis flag      = ", object%analysis_flag
    end if
end if
if (associated (object%instance)) then
    if (prc) then
        if (verb) then
            call object%instance%write (u, testflag)
        else
            call object%instance%write_header (u)
        end if
    end if
    if (trans) then
        evt => object%transform_first
        do while (associated (evt))
            select type (evt)
            type is (evt_decay_t)
                call evt%write (u, verbose = dec, more_verbose = verb, &
                    testflag = testflag)
            class default
                call evt%write (u, verbose = verb, testflag = testflag)
            end select
            call write_separator (u, 2)
            evt => evt%next
        end do
    else
        call write_separator (u, 2)
    end if
    if (object%expr%subevt_filled) then

```

```

        call object%expr%write (u, pacified = testflag)
        call write_separator (u, 2)
    end if
else
    call write_separator (u, 2)
    write (u, "(1x,A)") "Process instance: [undefined]"
    call write_separator (u, 2)
end if
end subroutine event_write

```

32.10.3 Initialization

Initialize: set configuration parameters, using a variable list. We do not call this `init`, because this method name will be used by a type extension.

The default normalization is `NORM_SIGMA`, since the default generation mode is weighted.

For unweighted events, we may want to apply a safety factor to event rejection. (By default, this factor is unity and can be ignored.)

We also allocate the trivial event transform, which is always the first one. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Events: event: TBP>+≡
    procedure :: basic_init => event_init

<Events: main procedures>≡
    subroutine event_init (event, var_list, n_alt)
        class(event_t), intent(out) :: event
        type(var_list_t), intent(in), optional :: var_list
        integer, intent(in), optional :: n_alt
        type(string_t) :: norm_string, mode_string
        logical :: polarized_events
        if (present (n_alt)) then
            call event%base_init (n_alt)
            call event%expr%init (n_alt)
        else
            call event%base_init (0)
        end if
        if (present (var_list)) then
            event%config%unweighted = var_list%get_lval (&
                var_str ("?unweighted"))
            norm_string = var_list%get_sval (&
                var_str ("sample_normalization"))
            event%config%norm_mode = &
                event_normalization_mode (norm_string, event%config%unweighted)
            polarized_events = &
                var_list%get_lval (var_str ("?polarized_events"))
            if (polarized_events) then
                mode_string = &
                    var_list%get_sval (var_str ("polarization_mode"))
                select case (char (mode_string))
                case ("ignore")
                    event%config%factorization_mode = FM_IGNORE_HELICITY
                case ("helicity")

```

```

        event%config%factorization_mode = FM_SELECT_HELICITY
    case ("factorized")
        event%config%factorization_mode = FM_FACTOR_HELICITY
    case ("correlated")
        event%config%factorization_mode = FM_CORRELATED_HELICITY
    case default
        call msg_fatal ("Polarization mode " &
            // char (mode_string) // " is undefined")
    end select
else
    event%config%factorization_mode = FM_IGNORE_HELICITY
end if
event%config%colorize_subevt = &
    var_list%get_lval (var_str ("?colorize_subevt"))
if (event%config%unweighted) then
    event%config%safety_factor = var_list%get_rval (&
        var_str ("safety_factor"))
end if
else
    event%config%norm_mode = NORM_SIGMA
end if
allocate (evt_trivial_t :: event%transform_first)
event%transform_last => event%transform_first
end subroutine event_init

```

Set the `sigma` and `n` values in the configuration record that determine non-standard event normalizations. If these numbers are not set explicitly, the default value for both is unity, and event renormalization has no effect.

(Events: event: TBP)+≡

```

    procedure :: set_sigma => event_set_sigma
    procedure :: set_n => event_set_n

```

(Events: sub interfaces)+≡

```

    elemental module subroutine event_set_sigma (event, sigma)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: sigma
    end subroutine event_set_sigma
    elemental module subroutine event_set_n (event, n)
        class(event_t), intent(inout) :: event
        integer, intent(in) :: n
    end subroutine event_set_n

```

(Events: procedures)+≡

```

    elemental module subroutine event_set_sigma (event, sigma)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: sigma
        event%config%sigma = sigma
    end subroutine event_set_sigma

    elemental module subroutine event_set_n (event, n)
        class(event_t), intent(inout) :: event
        integer, intent(in) :: n
        event%config%n = n
    end subroutine event_set_n

```

Append an event transform (decays, etc.). The transform is not yet connected to a process. The transform is then considered to belong to the event object, and will be finalized together with it. The original pointer is removed.

We can assume that the trivial transform is already present in the event object, at least.

```

<Events: event: TBP>+≡
  procedure :: import_transform => event_import_transform

<Events: sub interfaces>+≡
  module subroutine event_import_transform (event, evt)
    class(event_t), intent(inout) :: event
    class(evt_t), intent(inout), pointer :: evt
  end subroutine event_import_transform

<Events: procedures>+≡
  module subroutine event_import_transform (event, evt)
    class(event_t), intent(inout) :: event
    class(evt_t), intent(inout), pointer :: evt
    event%transform_last%next => evt
    evt%previous => event%transform_last
    event%transform_last => evt
    evt => null ()
  end subroutine event_import_transform

```

We link the event to an existing process instance. This includes the variable list, which is linked to the process variable list. Note that this is not necessarily identical to the variable list used for event initialization.

The variable list will contain pointers to **event** subobjects, therefore the **target** attribute.

Once we have a process connected, we can use it to obtain an event generator instance.

The model and process stack may be needed by event transforms. The current model setting may be different from the model in the process (regarding unstable particles, etc.). The process stack can be used for assigning extra processes that we need for the event transforms.

```

<Events: event: TBP>+≡
  procedure :: connect => event_connect

<Events: sub interfaces>+≡
  module subroutine event_connect &
    (event, process_instance, model, process_stack)
    class(event_t), intent(inout), target :: event
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
  end subroutine event_connect

<Events: procedures>+≡
  module subroutine event_connect &
    (event, process_instance, model, process_stack)
    class(event_t), intent(inout), target :: event
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack

```

```

type(string_t) :: id
integer :: num_id
class(evt_t), pointer :: evt
event%process => process_instance%process
event%instance => process_instance
id = event%process%get_id ()
if (id /= "") call event%expr%set_process_id (id)
num_id = event%process%get_num_id ()
if (num_id /= 0) call event%expr%set_process_num_id (num_id)
call event%expr%setup_vars (event%process%get_sqrts ())
call event%expr%link_var_list (event%process%get_var_list_ptr ())
call event%process%make_rng (event%rng)
evt => event%transform_first
do while (associated (evt))
    call evt%connect (process_instance, model, process_stack)
    evt => evt%next
end do
end subroutine event_connect

```

Set the parse nodes for the associated expressions, individually. The parse-node pointers may be null.

(Events: event: TBP)+≡

```

procedure :: set_selection => event_set_selection
procedure :: set_reweight => event_set_reweight
procedure :: set_analysis => event_set_analysis

```

(Events: sub interfaces)+≡

```

module subroutine event_set_selection (event, ef_selection)
    class(event_t), intent(inout) :: event
    class(expr_factory_t), intent(in) :: ef_selection
end subroutine event_set_selection
module subroutine event_set_reweight (event, ef_reweight)
    class(event_t), intent(inout) :: event
    class(expr_factory_t), intent(in) :: ef_reweight
end subroutine event_set_reweight
module subroutine event_set_analysis (event, ef_analysis)
    class(event_t), intent(inout) :: event
    class(expr_factory_t), intent(in) :: ef_analysis
end subroutine event_set_analysis

```

(Events: procedures)+≡

```

module subroutine event_set_selection (event, ef_selection)
    class(event_t), intent(inout) :: event
    class(expr_factory_t), intent(in) :: ef_selection
    allocate (event%config%ef_selection, source = ef_selection)
end subroutine event_set_selection

module subroutine event_set_reweight (event, ef_reweight)
    class(event_t), intent(inout) :: event
    class(expr_factory_t), intent(in) :: ef_reweight
    allocate (event%config%ef_reweight, source = ef_reweight)
end subroutine event_set_reweight

module subroutine event_set_analysis (event, ef_analysis)
    class(event_t), intent(inout) :: event

```

```

class(expr_factory_t), intent(in) :: ef_analysis
allocate (event%config%ef_analysis, source = ef_analysis)
end subroutine event_set_analysis

```

Create evaluation trees from the parse trees. The `target` attribute is required because the expressions contain pointers to event subobjects.

```

<Events: event: TBP>+≡
  procedure :: setup_expressions => event_setup_expressions

<Events: sub interfaces>+≡
  module subroutine event_setup_expressions (event)
    class(event_t), intent(inout), target :: event
  end subroutine event_setup_expressions

<Events: procedures>+≡
  module subroutine event_setup_expressions (event)
    class(event_t), intent(inout), target :: event
    call event%expr%setup_selection (event%config%ef_selection)
    call event%expr%setup_analysis (event%config%ef_analysis)
    call event%expr%setup_reweight (event%config%ef_reweight)
    call event%expr%colorize (event%config%colorize_subevt)
  end subroutine event_setup_expressions

```

32.10.4 Evaluation

To fill the `particle_set`, i.e., the event record proper, we have to apply all event transforms in order. The last transform should fill its associated particle set, factorizing the state matrix according to the current settings. There are several parameters in the event configuration that control this.

We always fill the particle set for the first transform (the hard process) and the last transform, if different from the first (the fully dressed process).

Each event transform is an event generator of its own. We choose to generate an *unweighted* event for each of them, even if the master event is assumed to be weighted. Thus, the overall event weight is the one of the hard process only. (There may be more options in future extensions.)

We can generate the two random numbers that the factorization needs. For testing purpose, we allow for providing them explicitly, as an option.

```

<Events: event: TBP>+≡
  procedure :: evaluate_transforms => event_evaluate_transforms

<Events: sub interfaces>+≡
  module subroutine event_evaluate_transforms (event, r)
    class(event_t), intent(inout) :: event
    real(default), dimension(:), intent(in), optional :: r
  end subroutine event_evaluate_transforms

<Events: procedures>+≡
  module subroutine event_evaluate_transforms (event, r)
    class(event_t), intent(inout) :: event
    real(default), dimension(:), intent(in), optional :: r
    class(evt_t), pointer :: evt
    real(default) :: weight_over_sqme
    integer :: i_term, emitter, n_in

```

```

logical :: failed_but_keep
failed_but_keep = .false.
if (debug_on) call msg_debug (D_TRANSFORMS, "event_evaluate_transforms")
call event%discard_particle_set ()
call event%check ()
if (event%instance%is_complete_event ()) then
  i_term = event%instance%select_i_term ()
  event%selected_i_term = i_term
  evt => event%transform_first
  do while (associated (evt))
    call evt%prepare_new_event &
      (event%selected_i_mci, event%selected_i_term)
    evt => evt%next
  end do
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "Before event transformations")
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%weight_prc", event%weight_prc)
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%sqme_prc", event%sqme_prc)
  evt => event%transform_first
  do while (associated (evt))
    call print_transform_name_if_debug ()
    if (evt%only_weighted_events) then
      select type (evt)
      type is (evt_nlo_t)
        i_term = evt%get_i_term ()
        failed_but_keep = .not. evt%is_valid_event (i_term) &
          .and. evt%keep_failed_events
        if (.not. any(evt%process_instance%term%passed .and. evt%process_instance%term%act
          .and. .not. evt%keep_failed_events) return
      end select
      if (abs (event%weight_prc) > 0._default) then
        weight_over_sqme = event%weight_prc / event%sqme_prc
        call evt%generate_weighted (event%sqme_prc)
        event%weight_prc = weight_over_sqme * event%sqme_prc
        select type (evt)
        type is (evt_nlo_t)
          if (.not. evt%is_valid_event (i_term)) event%weight_prc = 0
        end select
      else
        if (.not. failed_but_keep) exit
      end if
    else
      call evt%generate_unweighted ()
    end if
    if (signal_is_pending ()) return
    select type (evt)
    type is (evt_nlo_t)
      if (evt%i_evaluation > 0) then
        emitter = evt%process_instance%kin(i_term)%emitter
        n_in = evt%process_instance%kin(i_term)%n_in
        select type (pcm_work => evt%process_instance%term(i_term)%pcm_work)
        type is (pcm_nlo_workspace_t)

```

```

        if (emitter <= n_in .and. pcm_work%isr_kinematics%isr_mode == SQRTS_VAR) then
            call evt%connected_set_real_IS_momenta ()
        end if
    end select
end if
end select
call evt%make_particle_set (event%config%factorization_mode, &
    event%config%keep_correlations)
if (signal_is_pending ()) return
if (.not. evt%particle_set_exists) exit
evt => evt%next
end do
evt => event%transform_last
if ((associated (evt) .and. evt%particle_set_exists) .or. failed_but_keep) then
    if (event%is_nlo ()) then
        select type (evt)
        type is (evt_nlo_t)
            evt%particle_set_nlo (event%i_event + 1) = evt%particle_set
            evt%i_evaluation = evt%i_evaluation + 1
            call event%link_particle_set &
                (evt%particle_set_nlo(event%i_event + 1))
        end select
    else
        call event%link_particle_set (evt%particle_set)
    end if
end if
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "After event transformations")
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%weight_prc", event%weight_prc)
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%sqme_prc", event%sqme_prc)
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "evt%particle_set_exists", evt%particle_set_exists)
end if
contains
subroutine print_transform_name_if_debug ()
    if (debug_active (D_TRANSFORMS)) then
        print *, 'Current event transform: '
        call evt%write_name ()
    end if
end subroutine print_transform_name_if_debug
end subroutine event_evaluate_transforms

```

Set / increment the event index for the current event. There is no condition for this to happen. The event index is actually stored in the subevent expression, because this allows us to access it in subevent expressions as a variable.

(Events: event: TBP)+≡

```

    procedure :: set_index => event_set_index
    procedure :: increment_index => event_increment_index

```

(Events: sub interfaces)+≡

```

    module subroutine event_set_index (event, index)
        class(event_t), intent(inout) :: event

```



```

        integer, intent(in) :: index
    end subroutine event_set_index
    module subroutine event_increment_index (event, offset)
        class(event_t), intent(inout) :: event
        integer, intent(in), optional :: offset
    end subroutine event_increment_index
<Events: procedures>+≡
    module subroutine event_set_index (event, index)
        class(event_t), intent(inout) :: event
        integer, intent(in) :: index
        call event%expr%set_event_index (index)
    end subroutine event_set_index

    module subroutine event_increment_index (event, offset)
        class(event_t), intent(inout) :: event
        integer, intent(in), optional :: offset
        call event%expr%increment_event_index (offset)
    end subroutine event_increment_index

```

Evaluate the event-related expressions, given a valid `particle_set`. If `update_sqme` is set, we use the process instance for the `sqme_prc` value. The `sqme_ref` value is always taken from the event record.

```

<Events: event: TBP>+≡
    procedure :: evaluate_expressions => event_evaluate_expressions
<Events: sub interfaces>+≡
    module subroutine event_evaluate_expressions (event)
        class(event_t), intent(inout) :: event
    end subroutine event_evaluate_expressions
<Events: procedures>+≡
    module subroutine event_evaluate_expressions (event)
        class(event_t), intent(inout) :: event
        if (event%has_valid_particle_set ()) then
            call event%expr%fill_subevt (event%get_particle_set_ptr ())
        end if
        if (event%weight_ref_is_known ()) then
            call event%expr%set (weight_ref = event%get_weight_ref ())
        end if
        if (event%weight_prc_is_known ()) then
            call event%expr%set (weight_prc = event%get_weight_prc ())
        end if
        if (event%excess_prc_is_known ()) then
            call event%expr%set (excess_prc = event%get_excess_prc ())
        end if
        if (event%sqme_ref_is_known ()) then
            call event%expr%set (sqme_ref = event%get_sqme_ref ())
        end if
        if (event%sqme_prc_is_known ()) then
            call event%expr%set (sqme_prc = event%get_sqme_prc ())
        end if
        if (event%has_valid_particle_set ()) then
            call event%expr%evaluate &
                (event%passed, event%reweight, event%analysis_flag)

```

```

        event%selection_evaluated = .true.
    end if
end subroutine event_evaluate_expressions

```

Report the result of the selection evaluation.

```

<Events: event: TBP>+≡
    procedure :: passed_selection => event_passed_selection

<Events: sub interfaces>+≡
    module function event_passed_selection (event) result (flag)
        class(event_t), intent(in) :: event
        logical :: flag
    end function event_passed_selection

<Events: procedures>+≡
    module function event_passed_selection (event) result (flag)
        class(event_t), intent(in) :: event
        logical :: flag
        flag = event%passed
    end function event_passed_selection

```

Set alternate sqme and weight arrays. This should be merged with the previous routine, if the expressions are allowed to refer to these values.

```

<Events: event: TBP>+≡
    procedure :: store_alt_values => event_store_alt_values

<Events: sub interfaces>+≡
    module subroutine event_store_alt_values (event)
        class(event_t), intent(inout) :: event
    end subroutine event_store_alt_values

<Events: procedures>+≡
    module subroutine event_store_alt_values (event)
        class(event_t), intent(inout) :: event
        if (event%weight_alt_is_known ()) then
            call event%expr%set (weight_alt = event%get_weight_alt ())
        end if
        if (event%sqme_alt_is_known ()) then
            call event%expr%set (sqme_alt = event%get_sqme_alt ())
        end if
    end subroutine event_store_alt_values

```

```

<Events: event: TBP>+≡
    procedure :: is_nlo => event_is_nlo

<Events: sub interfaces>+≡
    module function event_is_nlo (event) result (is_nlo)
        logical :: is_nlo
        class(event_t), intent(in) :: event
    end function event_is_nlo

<Events: procedures>+≡
    module function event_is_nlo (event) result (is_nlo)
        logical :: is_nlo
        class(event_t), intent(in) :: event

```

```

if (associated (event%instance)) then
  select type (pcm_work => event%instance%pcm_work)
  type is (pcm_nlo_workspace_t)
    is_nlo = pcm_work%is_fixed_order_nlo_events ()
  class default
    is_nlo = .false.
  end select
else
  is_nlo = .false.
end if
end function event_is_nlo

```

32.10.5 Reset to empty state

Applying this, current event contents are marked as incomplete but are not deleted. In particular, the initialization is kept. The event index is also kept, this can be reset separately.

(Events: event: TBP)+≡

```

procedure :: reset_contents => event_reset_contents
procedure :: reset_index => event_reset_index

```

(Events: sub interfaces)+≡

```

module subroutine event_reset_contents (event)
  class(event_t), intent(inout) :: event
end subroutine event_reset_contents
module subroutine event_reset_index (event)
  class(event_t), intent(inout) :: event
end subroutine event_reset_index

```

(Events: procedures)+≡

```

module subroutine event_reset_contents (event)
  class(event_t), intent(inout) :: event
  class(evt_t), pointer :: evt
  call event%base_reset_contents ()
  event%selected_i_mci = 0
  event%selected_i_term = 0
  event%selected_channel = 0
  event%is_complete = .false.
  call event%expr%reset_contents ()
  event%selection_evaluated = .false.
  event%passed = .false.
  event%analysis_flag = .false.
  if (associated (event%instance)) then
    call event%instance%reset (reset_mci = .true.)
  end if
  if (allocated (event%alpha_qcd_forced)) deallocate (event%alpha_qcd_forced)
  if (allocated (event%scale_forced)) deallocate (event%scale_forced)
  evt => event%transform_first
  do while (associated (evt))
    call evt%reset ()
    evt => evt%next
  end do
end subroutine event_reset_contents

```

```

module subroutine event_reset_index (event)
  class(event_t), intent(inout) :: event
  call event%expr%reset_event_index ()
end subroutine event_reset_index

```

32.10.6 Squared Matrix Element and Weight

Transfer the result of the process instance calculation to the event record header.

```

<Events: event: TBP>+≡
  procedure :: import_instance_results => event_import_instance_results

<Events: sub interfaces>+≡
  module subroutine event_import_instance_results (event)
    class(event_t), intent(inout) :: event
    end subroutine event_import_instance_results

<Events: procedures>+≡
  module subroutine event_import_instance_results (event)
    class(event_t), intent(inout) :: event
    if (associated (event%instance)) then
      if (event%instance%has_evaluated_trace ()) then
        call event%set ( &
          sqme_prc = event%instance%get_sqme (), &
          weight_prc = event%instance%get_weight (), &
          excess_prc = event%instance%get_excess (), &
          n_dropped = event%instance%get_n_dropped () &
          )
      end if
    end if
  end subroutine event_import_instance_results

```

Duplicate the instance result / the reference result in the event record.

```

<Events: event: TBP>+≡
  procedure :: accept_sqme_ref => event_accept_sqme_ref
  procedure :: accept_sqme_prc => event_accept_sqme_prc
  procedure :: accept_weight_ref => event_accept_weight_ref
  procedure :: accept_weight_prc => event_accept_weight_prc

<Events: sub interfaces>+≡
  module subroutine event_accept_sqme_ref (event)
    class(event_t), intent(inout) :: event
  end subroutine event_accept_sqme_ref
  module subroutine event_accept_sqme_prc (event)
    class(event_t), intent(inout) :: event
  end subroutine event_accept_sqme_prc
  module subroutine event_accept_weight_ref (event)
    class(event_t), intent(inout) :: event
  end subroutine event_accept_weight_ref
  module subroutine event_accept_weight_prc (event)
    class(event_t), intent(inout) :: event
  end subroutine event_accept_weight_prc

```

<Events: procedures>+≡

```

module subroutine event_accept_sqme_ref (event)
  class(event_t), intent(inout) :: event
  if (event%sqme_ref_is_known ()) then
    call event%set (sqme_prc = event%get_sqme_ref ())
  end if
end subroutine event_accept_sqme_ref

module subroutine event_accept_sqme_prc (event)
  class(event_t), intent(inout) :: event
  if (event%sqme_prc_is_known ()) then
    call event%set (sqme_ref = event%get_sqme_prc ())
  end if
end subroutine event_accept_sqme_prc

module subroutine event_accept_weight_ref (event)
  class(event_t), intent(inout) :: event
  if (event%weight_ref_is_known ()) then
    call event%set (weight_prc = event%get_weight_ref ())
  end if
end subroutine event_accept_weight_ref

module subroutine event_accept_weight_prc (event)
  class(event_t), intent(inout) :: event
  if (event%weight_prc_is_known ()) then
    call event%set (weight_ref = event%get_weight_prc ())
  end if
end subroutine event_accept_weight_prc

```

Update the weight normalization, just after generation. Unweighted and weighted events are generated with a different default normalization. The intended normalization is stored in the configuration record.

<Events: event: TBP>+≡

```

procedure :: update_normalization => event_update_normalization

```

<Events: sub interfaces>+≡

```

module subroutine event_update_normalization (event, mode_ref)
  class(event_t), intent(inout) :: event
  integer, intent(in), optional :: mode_ref
end subroutine event_update_normalization

```

<Events: procedures>+≡

```

module subroutine event_update_normalization (event, mode_ref)
  class(event_t), intent(inout) :: event
  integer, intent(in), optional :: mode_ref
  integer :: mode_old
  real(default) :: weight, excess
  if (present (mode_ref)) then
    mode_old = mode_ref
  else if (event%config%unweighted) then
    mode_old = NORM_UNIT
  else
    mode_old = NORM_SIGMA
  end if

```

```

weight = event%get_weight_prc ()
call event_normalization_update (weight, &
event%config%sigma, event%config%n, &
mode_new = event%config%norm_mode, &
mode_old = mode_old)
call event%set_weight_prc (weight)
excess = event%get_excess_prc ()
call event_normalization_update (excess, &
event%config%sigma, event%config%n, &
mode_new = event%config%norm_mode, &
mode_old = mode_old)
call event%set_excess_prc (excess)
end subroutine event_update_normalization

```

The event is complete if it has a particle set plus valid entries for the sqme and weight values.

```

<Events: event: TBP>+≡
  procedure :: check => event_check

<Events: sub interfaces>+≡
  module subroutine event_check (event)
    class(event_t), intent(inout) :: event
  end subroutine event_check

<Events: procedures>+≡
  module subroutine event_check (event)
    class(event_t), intent(inout) :: event
    event%is_complete = event%has_valid_particle_set () &
      .and. event%sqme_ref_is_known () &
      .and. event%sqme_prc_is_known () &
      .and. event%weight_ref_is_known () &
      .and. event%weight_prc_is_known ()
    if (event%get_n_alt () /= 0) then
      event%is_complete = event%is_complete &
        .and. event%sqme_alt_is_known () &
        .and. event%weight_alt_is_known ()
    end if
  end subroutine event_check

```

32.10.7 Generation

Assuming that we have a valid process associated to the event, we generate an event. We complete the event data, then factorize the spin density matrix and transfer it to the particle set.

When done, we retrieve squared matrix element and weight. In case of explicit generation, the reference values coincide with the process values, so we accept the latter.

The explicit random number argument `r` should be generated by a random-number generator. It is taken for the factorization algorithm, bypassing the event-specific random-number generator. This is useful for deterministic testing.

```

<Events: event: TBP>+≡
  procedure :: generate => event_generate

```

```

<Events: sub interfaces>+≡
  module subroutine event_generate (event, i_mci, r, i_nlo)
    class(event_t), intent(inout) :: event
    integer, intent(in) :: i_mci
    real(default), dimension(:), intent(in), optional :: r
    integer, intent(in), optional :: i_nlo
  end subroutine event_generate

```

```

<Events: procedures>+≡
  module subroutine event_generate (event, i_mci, r, i_nlo)
    class(event_t), intent(inout) :: event
    integer, intent(in) :: i_mci
    real(default), dimension(:), intent(in), optional :: r
    integer, intent(in), optional :: i_nlo
    logical :: generate_new
    generate_new = .true.
    if (present (i_nlo)) generate_new = (i_nlo == 1)
    if (generate_new) call event%reset_contents ()
    event%selected_i_mci = i_mci
    if (event%config%unweighted) then
      call event%instance%generate_unweighted_event (i_mci)
      if (signal_is_pending ()) return
      call event%instance%evaluate_event_data ()
      call event%instance%normalize_weight ()
    else
      if (generate_new) &
        call event%instance%generate_weighted_event (i_mci)
      if (signal_is_pending ()) return
      call event%instance%evaluate_event_data ()
    end if
    event%selected_channel = event%instance%get_channel ()
    call event%import_instance_results ()
    call event%accept_sqme_prc ()
    call event%update_normalization ()
    call event%accept_weight_prc ()
    call event%evaluate_transforms (r)
    if (signal_is_pending ()) return
    call event%check ()
  end subroutine event_generate

```

Get a copy of the particle set belonging to the hard process.

```

<Events: event: TBP>+≡
  procedure :: get_hard_particle_set => event_get_hard_particle_set

```

```

<Events: sub interfaces>+≡
  module subroutine event_get_hard_particle_set (event, pset)
    class(event_t), intent(in) :: event
    type(particle_set_t), intent(out) :: pset
  end subroutine event_get_hard_particle_set

```

```

<Events: procedures>+≡
  module subroutine event_get_hard_particle_set (event, pset)
    class(event_t), intent(in) :: event
    type(particle_set_t), intent(out) :: pset
    class(evt_t), pointer :: evt

```

```

    evt => event%transform_first
    pset = evt%particle_set
end subroutine event_get_hard_particle_set

```

32.10.8 Recovering an event

Select MC group, term, and integration channel.

```

<Events: event: TBP>+≡
  procedure :: select => event_select

<Events: sub interfaces>+≡
  module subroutine event_select (event, i_mci, i_term, channel)
    class(event_t), intent(inout) :: event
    integer, intent(in) :: i_mci, i_term, channel
  end subroutine event_select

<Events: procedures>+≡
  module subroutine event_select (event, i_mci, i_term, channel)
    class(event_t), intent(inout) :: event
    integer, intent(in) :: i_mci, i_term, channel
    if (associated (event%instance)) then
      event%selected_i_mci = i_mci
      event%selected_i_term = i_term
      event%selected_channel = channel
    else
      event%selected_i_mci = 0
      event%selected_i_term = 0
      event%selected_channel = 0
    end if
  end subroutine event_select

```

Copy a particle set into the event record.

We deliberately use the first (the trivial) transform for this, i.e., the hard process. The event reader may either read in the transformed event separately, or apply all event transforms to the hard particle set to (re)generate a fully dressed event.

Since this makes all subsequent event transforms invalid, we call `reset` on them.

```

<Events: event: TBP>+≡
  procedure :: set_hard_particle_set => event_set_hard_particle_set

<Events: sub interfaces>+≡
  module subroutine event_set_hard_particle_set (event, particle_set)
    class(event_t), intent(inout) :: event
    type(particle_set_t), intent(in) :: particle_set
  end subroutine event_set_hard_particle_set

<Events: procedures>+≡
  module subroutine event_set_hard_particle_set (event, particle_set)
    class(event_t), intent(inout) :: event
    type(particle_set_t), intent(in) :: particle_set
    class(evt_t), pointer :: evt
    evt => event%transform_first

```



```

call evt%set_particle_set (particle_set, &
    event%selected_i_mci, event%selected_i_term)
call event%link_particle_set (evt%particle_set)
evt => evt%next
do while (associated (evt))
    call evt%reset ()
    evt => evt%next
end do
end subroutine event_set_hard_particle_set

```

Set the α_s value that should be used in a recalculation. This should be called only if we explicitly want to override the QCD setting of the process core.

```

<Events: event: TBP>+≡
    procedure :: set_alpha_qcd_forced => event_set_alpha_qcd_forced

<Events: sub interfaces>+≡
    module subroutine event_set_alpha_qcd_forced (event, alpha_qcd)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: alpha_qcd
    end subroutine event_set_alpha_qcd_forced

<Events: procedures>+≡
    module subroutine event_set_alpha_qcd_forced (event, alpha_qcd)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: alpha_qcd
        if (allocated (event%alpha_qcd_forced)) then
            event%alpha_qcd_forced = alpha_qcd
        else
            allocate (event%alpha_qcd_forced, source = alpha_qcd)
        end if
    end subroutine event_set_alpha_qcd_forced

```

Analogously, for the common scale. This forces also renormalization and factorization scale.

```

<Events: event: TBP>+≡
    procedure :: set_scale_forced => event_set_scale_forced

<Events: sub interfaces>+≡
    module subroutine event_set_scale_forced (event, scale)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: scale
    end subroutine event_set_scale_forced

<Events: procedures>+≡
    module subroutine event_set_scale_forced (event, scale)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: scale
        if (allocated (event%scale_forced)) then
            event%scale_forced = scale
        else
            allocate (event%scale_forced, source = scale)
        end if
    end subroutine event_set_scale_forced

```

Here we try to recover an event from the `particle_set` subobject and recalculate the structure functions and matrix elements. We have the appropriate `process` object and an initialized `process_instance` at hand, so beam and configuration data are known. From the `particle_set`, we get the momenta.

The quantum-number information may be incomplete, e.g., helicity information may be partial or absent. We recover the event just from the momentum configuration.

We do not transfer the matrix element from the process instance to the event record, as we do when generating an event. The event record may contain the matrix element as read from file, and the current calculation may use different parameters. We thus can compare old and new values.

The event `weight` may also be known already. If yes, we pass it to the `evaluate_event_data` procedure. It should already be normalized. If we have a `weight_factor` value, we obtain the event weight by multiplying the computed `sqme` by this factor. Otherwise, we make use of the MCI setup (which should be valid then) to compute the event weight, and we should normalize the result just as when generating events.

Evaluating event expressions must also be done separately.

If `recover_phs` is set (and false), do not attempt any phase-space calculation, including MCI evaluation. Useful if we need only matrix elements.

(Events: event: TBP)+≡

```
procedure :: recalculate => event_recalculate
```

(Events: sub interfaces)+≡

```
module subroutine event_recalculate (event, update_sqme, weight_factor, &
    recover_beams, recover_phs, check_match, success)
    class(event_t), intent(inout) :: event
    logical, intent(in) :: update_sqme
    real(default), intent(in), optional :: weight_factor
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: recover_phs
    logical, intent(in), optional :: check_match
    logical, intent(out), optional :: success
end subroutine event_recalculate
```

(Events: procedures)+≡

```
module subroutine event_recalculate (event, update_sqme, weight_factor, &
    recover_beams, recover_phs, check_match, success)
    class(event_t), intent(inout) :: event
    logical, intent(in) :: update_sqme
    real(default), intent(in), optional :: weight_factor
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: recover_phs
    logical, intent(in), optional :: check_match
    logical, intent(out), optional :: success
    type(particle_set_t), pointer :: particle_set
    integer :: i_mci, i_term, channel
    logical :: rec_phs_mci
    rec_phs_mci = .true.; if (present (recover_phs)) rec_phs_mci = recover_phs
    if (present (success)) success = .false.
    if (event%has_valid_particle_set ()) then
        particle_set => event%get_particle_set_ptr ()
        i_mci = event%selected_i_mci
```

```

i_term = event%selected_i_term
channel = event%selected_channel
if (i_mci == 0 .or. i_term == 0 .or. channel == 0) then
    call msg_bug ("Event: recalculate: undefined selection parameters")
end if
call event%instance%choose_mci (i_mci)
call event%instance%set_trace &
    (particle_set, i_term, recover_beams, check_match, success)
if (present (success)) then
    if (.not. success) return
end if
if (allocated (event%alpha_qcd_forced)) then
    call event%instance%set_alpha_qcd_forced &
        (i_term, event%alpha_qcd_forced)
end if
call event%instance%recover (channel, i_term, &
    update_sqme, rec_phs_mci, event%scale_forced)
if (signal_is_pending ()) return
if (update_sqme .and. present (weight_factor)) then
    call event%instance%evaluate_event_data &
        (weight = event%instance%get_sqme () * weight_factor)
else if (event%weight_ref_is_known ()) then
    call event%instance%evaluate_event_data &
        (weight = event%get_weight_ref ())
else if (rec_phs_mci) then
    call event%instance%recover_event ()
    if (signal_is_pending ()) return
    call event%instance%evaluate_event_data ()
    if (event%config%unweighted) then
        call event%instance%normalize_weight ()
    end if
end if
end if
if (signal_is_pending ()) return
if (update_sqme) then
    call event%import_instance_results ()
else
    call event%accept_sqme_ref ()
    call event%accept_weight_ref ()
end if
else
    call msg_bug ("Event: can't recalculate, particle set is undefined")
end if
end subroutine event_recalculate

```

32.10.9 Access content

Pointer to the associated process object (the associated model).

(Events: event: TBP)+≡

```

procedure :: get_process_ptr => event_get_process_ptr
procedure :: get_process_instance_ptr => event_get_process_instance_ptr
procedure :: get_model_ptr => event_get_model_ptr

```

```

<Events: sub interfaces>+≡
  module function event_get_process_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_t), pointer :: ptr
  end function event_get_process_ptr
  module function event_get_process_instance_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_instance_t), pointer :: ptr
  end function event_get_process_instance_ptr
  module function event_get_model_ptr (event) result (model)
    class(event_t), intent(in) :: event
    class(model_data_t), pointer :: model
  end function event_get_model_ptr

<Events: procedures>+≡
  module function event_get_process_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_t), pointer :: ptr
    ptr => event%process
  end function event_get_process_ptr

  module function event_get_process_instance_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_instance_t), pointer :: ptr
    ptr => event%instance
  end function event_get_process_instance_ptr

  module function event_get_model_ptr (event) result (model)
    class(event_t), intent(in) :: event
    class(model_data_t), pointer :: model
    if (associated (event%process)) then
      model => event%process%get_model_ptr ()
    else
      model => null ()
    end if
  end function event_get_model_ptr

```

Return the current values of indices: the MCI group of components, the term index (different terms corresponding, potentially, to different effective kinematics), and the MC integration channel. The `i_mci` call is delegated to the current process instance.

```

<Events: event: TBP>+≡
  procedure :: get_i_mci => event_get_i_mci
  procedure :: get_i_term => event_get_i_term
  procedure :: get_channel => event_get_channel

<Events: sub interfaces>+≡
  module function event_get_i_mci (event) result (i_mci)
    class(event_t), intent(in) :: event
    integer :: i_mci
  end function event_get_i_mci
  module function event_get_i_term (event) result (i_term)
    class(event_t), intent(in) :: event
    integer :: i_term

```

```

end function event_get_i_term
module function event_get_channel (event) result (channel)
  class(event_t), intent(in) :: event
  integer :: channel
end function event_get_channel

<Events: procedures>+≡
module function event_get_i_mci (event) result (i_mci)
  class(event_t), intent(in) :: event
  integer :: i_mci
  i_mci = event%selected_i_mci
end function event_get_i_mci

module function event_get_i_term (event) result (i_term)
  class(event_t), intent(in) :: event
  integer :: i_term
  i_term = event%selected_i_term
end function event_get_i_term

module function event_get_channel (event) result (channel)
  class(event_t), intent(in) :: event
  integer :: channel
  channel = event%selected_channel
end function event_get_channel

```

This flag tells us whether the event consists just of a hard process (i.e., holds at most the first, trivial transform), or is a dressed events with additional transforms.

```

<Events: event: TBP>+≡
  procedure :: has_transform => event_has_transform

<Events: sub interfaces>+≡
  module function event_has_transform (event) result (flag)
    class(event_t), intent(in) :: event
    logical :: flag
  end function event_has_transform

<Events: procedures>+≡
  module function event_has_transform (event) result (flag)
    class(event_t), intent(in) :: event
    logical :: flag
    if (associated (event%transform_first)) then
      flag = associated (event%transform_first%next)
    else
      flag = .false.
    end if
  end function event_has_transform

```

Return the currently selected normalization mode, or alternate normalization mode.

```

<Events: event: TBP>+≡
  procedure :: get_norm_mode => event_get_norm_mode

```

```

<Events: sub interfaces>+≡
    elemental module function event_get_norm_mode (event) result (norm_mode)
        class(event_t), intent(in) :: event
        integer :: norm_mode
    end function event_get_norm_mode

```

```

<Events: procedures>+≡
    elemental module function event_get_norm_mode (event) result (norm_mode)
        class(event_t), intent(in) :: event
        integer :: norm_mode
        norm_mode = event%config%norm_mode
    end function event_get_norm_mode

```

Return the kinematical weight, defined as the ratio of event weight and squared matrix element.

```

<Events: event: TBP>+≡
    procedure :: get_kinematical_weight => event_get_kinematical_weight

<Events: sub interfaces>+≡
    module function event_get_kinematical_weight (event) result (f)
        class(event_t), intent(in) :: event
        real(default) :: f
    end function event_get_kinematical_weight

<Events: procedures>+≡
    module function event_get_kinematical_weight (event) result (f)
        class(event_t), intent(in) :: event
        real(default) :: f
        if (event%sqme_ref_is_known () .and. event%weight_ref_is_known () &
            .and. abs (event%get_sqme_ref ()) > 0) then
            f = event%get_weight_ref () / event%get_sqme_ref ()
        else
            f = 0
        end if
    end function event_get_kinematical_weight

```

Return data used by external event formats.

```

<Events: event: TBP>+≡
    procedure :: has_index => event_has_index
    procedure :: get_index => event_get_index
    procedure :: get_fac_scale => event_get_fac_scale
    procedure :: get_alpha_s => event_get_alpha_s
    procedure :: get_sqrts => event_get_sqrts
    procedure :: get_polarization => event_get_polarization
    procedure :: get_beam_file => event_get_beam_file
    procedure :: get_process_name => event_get_process_name

<Events: sub interfaces>+≡
    module function event_has_index (event) result (flag)
        class(event_t), intent(in) :: event
        logical :: flag
    end function event_has_index
    module function event_get_index (event) result (index)
        class(event_t), intent(in) :: event
        integer :: index

```

```

end function event_get_index
module function event_get_fac_scale (event) result (fac_scale)
  class(event_t), intent(in) :: event
  real(default) :: fac_scale
end function event_get_fac_scale
module function event_get_alpha_s (event) result (alpha_s)
  class(event_t), intent(in) :: event
  real(default) :: alpha_s
end function event_get_alpha_s
module function event_get_sqrts (event) result (sqrts)
  class(event_t), intent(in) :: event
  real(default) :: sqrts
end function event_get_sqrts
module function event_get_polarization (event) result (pol)
  class(event_t), intent(in) :: event
  real(default), dimension(:), allocatable :: pol
end function event_get_polarization
module function event_get_beam_file (event) result (file)
  class(event_t), intent(in) :: event
  type(string_t) :: file
end function event_get_beam_file
module function event_get_process_name (event) result (name)
  class(event_t), intent(in) :: event
  type(string_t) :: name
end function event_get_process_name

```

(Events: procedures)+≡

```

module function event_has_index (event) result (flag)
  class(event_t), intent(in) :: event
  logical :: flag
  flag = event%expr%has_event_index ()
end function event_has_index

module function event_get_index (event) result (index)
  class(event_t), intent(in) :: event
  integer :: index
  index = event%expr%get_event_index ()
end function event_get_index

module function event_get_fac_scale (event) result (fac_scale)
  class(event_t), intent(in) :: event
  real(default) :: fac_scale
  fac_scale = event%instance%get_fac_scale (event%selected_i_term)
end function event_get_fac_scale

module function event_get_alpha_s (event) result (alpha_s)
  class(event_t), intent(in) :: event
  real(default) :: alpha_s
  alpha_s = event%instance%get_alpha_s (event%selected_i_term)
end function event_get_alpha_s

module function event_get_sqrts (event) result (sqrts)
  class(event_t), intent(in) :: event
  real(default) :: sqrts
  sqrts = event%instance%get_sqrts ()

```

```

end function event_get_sqrts

module function event_get_polarization (event) result (pol)
  class(event_t), intent(in) :: event
  real(default), dimension(:), allocatable :: pol
  pol = event%instance%get_polarization ()
end function event_get_polarization

module function event_get_beam_file (event) result (file)
  class(event_t), intent(in) :: event
  type(string_t) :: file
  file = event%instance%get_beam_file ()
end function event_get_beam_file

module function event_get_process_name (event) result (name)
  class(event_t), intent(in) :: event
  type(string_t) :: name
  name = event%instance%get_process_name ()
end function event_get_process_name

```

Return the actual number of calls, as stored in the process instance.

```

<Events: event: TBP>+≡
  procedure :: get_actual_calls_total => event_get_actual_calls_total

<Events: sub interfaces>+≡
  elemental module function event_get_actual_calls_total (event) result (n)
    class(event_t), intent(in) :: event
    integer :: n
  end function event_get_actual_calls_total

<Events: procedures>+≡
  elemental module function event_get_actual_calls_total (event) result (n)
    class(event_t), intent(in) :: event
    integer :: n
    if (associated (event%instance)) then
      n = event%instance%get_actual_calls_total ()
    else
      n = 0
    end if
  end function event_get_actual_calls_total

```

Eliminate numerical noise in the subevt expression and in the event transforms (which includes associated process instances).

```

<Events: public>+≡
  public :: pacify

<Events: interfaces>≡
  interface pacify
    module procedure pacify_event
  end interface pacify

<Events: sub interfaces>+≡
  module subroutine pacify_event (event)
    class(event_t), intent(inout) :: event
    class(evt_t), pointer :: evt
  end subroutine pacify_event

```



```

<Events: procedures>+≡
  module subroutine pacify_event (event)
    class(event_t), intent(inout) :: event
    class(evt_t), pointer :: evt
    call event%pacify_particle_set ()
    if (event%expr%subevt_filled) call pacify (event%expr)
    evt => event%transform_first
    do while (associated (evt))
      select type (evt)
        type is (evt_decay_t); call pacify (evt)
      end select
      evt => evt%next
    end do
  end subroutine pacify_event

```

32.10.10 Unit tests

Test module, followed by the corresponding implementation module.

```

<events_ut.f90>≡
  <File header>

  module events_ut
    use unit_tests
    use events_uti

    <Standard module head>

    <Events: public test>

    contains

    <Events: test driver>

  end module events_ut

<events_uti.f90>≡
  <File header>

  module events_uti

    <Use kinds>
    <Use strings>
    use os_interface
    use model_data
    use particles
    use process_libraries
    use process_stacks
    use event_transforms
    use decays
    use decays_ut, only: prepare_testbed

    use process, only: process_t
    use instances, only: process_instance_t

```

```

    use events

    <Standard module head>

    <Events: test declarations>

    contains

    <Events: tests>

end module events_util

```

API: driver for the unit tests below.

```

<Events: public test>≡
    public :: events_test

<Events: test driver>≡
    subroutine events_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Events: execute tests>
    end subroutine events_test

```

Empty event record

```

<Events: execute tests>≡
    call test (events_1, "events_1", &
        "empty event record", &
        u, results)

<Events: test declarations>≡
    public :: events_1

<Events: tests>≡
    subroutine events_1 (u)
        integer, intent(in) :: u
        type(event_t), target :: event

        write (u, "(A)")  "* Test output: events_1"
        write (u, "(A)")  "* Purpose: display an empty event object"
        write (u, "(A)")

        call event%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: events_1"

    end subroutine events_1

```

Simple event

```

<Events: execute tests>+≡

```

```

call test (events_2, "events_2", &
          "generate event", &
          u, results)
<Events: test declarations>+≡
public :: events_2
<Events: tests>+≡
subroutine events_2 (u)
  use processes_ut, only: prepare_test_process, cleanup_test_process
  integer, intent(in) :: u
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(model_data_t), target :: model

  write (u, "(A)")  "* Test output: events_2"
  write (u, "(A)")  "* Purpose: generate and display an event"
  write (u, "(A)")

  call model%init_test ()

  write (u, "(A)")  "* Generate test process event"

  allocate (process)
  allocate (process_instance)
  call prepare_test_process (process, process_instance, model)
  call process_instance%setup_event_data ()

  write (u, "(A)")
  write (u, "(A)")  "* Initialize event object"

  allocate (event)
  call event%basic_init ()
  call event%connect (process_instance, process%get_model_ptr ())

  write (u, "(A)")
  write (u, "(A)")  "* Generate test process event"

  call process_instance%generate_weighted_event (1)

  write (u, "(A)")
  write (u, "(A)")  "* Fill event object"
  write (u, "(A)")

  call event%generate (1, [0.4_default, 0.4_default])
  call event%increment_index ()
  call event%evaluate_expressions ()
  call event%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call event%final ()
  deallocate (event)

```

```

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_2"

end subroutine events_2

```

Recovering an event

Generate an event and store the particle set. Then reset the event record, recall the particle set, and recover the event from that.

```

<Events: execute tests>+≡
  call test (events_4, "events_4", &
    "recover event", &
    u, results)

<Events: test declarations>+≡
  public :: events_4

<Events: tests>+≡
  subroutine events_4 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(process_t), allocatable, target :: process2
    type(process_instance_t), allocatable, target :: process2_instance
    type(particle_set_t) :: particle_set
    type(model_data_t), target :: model

    write (u, "(A)")  "* Test output: events_4"
    write (u, "(A)")  "* Purpose: generate and recover an event"
    write (u, "(A)")

    call model%init_test ()

    write (u, "(A)")  "* Generate test process event and save particle set"
    write (u, "(A)")

    allocate (process)
    allocate (process_instance)
    call prepare_test_process (process, process_instance, model)
    call process_instance%setup_event_data ()

    allocate (event)
    call event%basic_init ()
    call event%connect (process_instance, process%get_model_ptr ())

```

```

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

particle_set = event%get_particle_set_ptr ()
! NB: 'particle_set' contains pointers to the model within 'process'

call event%final ()
deallocate (event)

write (u, "(A)")
write (u, "(A)")  "* Recover event from particle set"
write (u, "(A)")

allocate (process2)
allocate (process2_instance)
call prepare_test_process (process2, process2_instance, model)
call process2_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process2_instance, process2%get_model_ptr ())

call event%select (1, 1, 1)
call event%set_hard_particle_set (particle_set)
call event%recalculate (update_sqme = .true.)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer sqme and evaluate expressions"
write (u, "(A)")

call event%accept_sqme_prc ()
call event%accept_weight_prc ()
call event%check ()
call event%set_index (1)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Reset contents"
write (u, "(A)")

call event%reset_contents ()
call event%reset_index ()
event%transform_first%particle_set_exists = .false.
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set%final ()

```

```

call event%final ()
deallocate (event)

call cleanup_test_process (process2, process2_instance)
deallocate (process2_instance)
deallocate (process2)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_4"

end subroutine events_4

```

Partially Recovering an event

Generate an event and store the particle set. Then reset the event record, recall the particle set, and recover the event as far as possible without recomputing the squared matrix element.

```

<Events: execute tests>+≡
  call test (events_5, "events_5", &
    "partially recover event", &
    u, results)

<Events: test declarations>+≡
  public :: events_5

<Events: tests>+≡
  subroutine events_5 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(process_t), allocatable, target :: process2
    type(process_instance_t), allocatable, target :: process2_instance
    type(particle_set_t) :: particle_set
    real(default) :: sqme, weight
    type(model_data_t), target :: model

    write (u, "(A)")  "* Test output: events_5"
    write (u, "(A)")  "* Purpose: generate and recover an event"
    write (u, "(A)")

    call model%init_test ()

    write (u, "(A)")  "* Generate test process event and save particle set"
    write (u, "(A)")

```

```

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model)
call process_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

particle_set = event%get_particle_set_ptr ()
sqme = event%get_sqme_ref ()
weight = event%get_weight_ref ()

call event%final ()
deallocate (event)

write (u, "(A)")
write (u, "(A)")  "* Recover event from particle set"
write (u, "(A)")

allocate (process2)
allocate (process2_instance)
call prepare_test_process (process2, process2_instance, model)
call process2_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process2_instance, process2%get_model_ptr ())

call event%select (1, 1, 1)
call event%set_hard_particle_set (particle_set)
call event%recalculate (update_sqme = .false.)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set sqme and evaluate expressions"
write (u, "(A)")

call event%set (sqme_ref = sqme, weight_ref = weight)
call event%accept_sqme_ref ()
call event%accept_weight_ref ()
call event%set_index (1)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call particle_set%final ()

call event%final ()
deallocate (event)

call cleanup_test_process (process2, process2_instance)
deallocate (process2_instance)
deallocate (process2)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_5"

end subroutine events_5

```

Decays

Generate an event with subsequent decays.

```

<Events: execute tests>+≡
  call test (events_6, "events_6", &
    "decays", &
    u, results)

<Events: test declarations>+≡
  public :: events_6

<Events: tests>+≡
  subroutine events_6 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(string_t) :: prefix, procname1, procname2
    type(process_library_t), target :: lib
    type(process_stack_t) :: process_stack
    class(evt_t), pointer :: evt_decay
    type(event_t), allocatable, target :: event
    type(process_t), pointer :: process
    type(process_instance_t), allocatable, target :: process_instance

    write (u, "(A)")  "* Test output: events_6"
    write (u, "(A)")  "* Purpose: generate an event with subsequent decays"
    write (u, "(A)")

    write (u, "(A)")  "* Generate test process and decay"
    write (u, "(A)")

    call os_data%init ()

    prefix = "events_6"

```



```

procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
     scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")
write (u, "(A)")  "* Initialize event transform: decay"

allocate (evt_decay_t :: evt_decay)
call evt_decay%connect (process_instance, model, process_stack)

write (u, "(A)")
write (u, "(A)")  "* Initialize event object"
write (u, "(A)")

allocate (event)
call event%basic_init ()
call event%connect (process_instance, model)
call event%import_transform (evt_decay)

call event%write (u, show_decay = .true.)

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call event%final ()
deallocate (event)

call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_6"

end subroutine events_6

```

Decays

Generate a decay event with varying options.

```

<Events: execute tests>+≡
  call test (events_7, "events_7", &
    "decay options", &
    u, results)

<Events: test declarations>+≡
  public :: events_7

<Events: tests>+≡
  subroutine events_7 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(string_t) :: prefix, procname2
    type(process_library_t), target :: lib
    type(process_stack_t) :: process_stack
    type(process_t), pointer :: process
    type(process_instance_t), allocatable, target :: process_instance

    write (u, "(A)")  "* Test output: events_7"
    write (u, "(A)")  "* Purpose: check decay options"
    write (u, "(A)")

    write (u, "(A)")  "* Prepare test process"
    write (u, "(A)")

    call os_data%init ()

    prefix = "events_7"
    procname2 = prefix // "_d"
    call prepare_testbed &
      (lib, process_stack, prefix, os_data, &
        scattering=.false., decay=.true.)

    write (u, "(A)")  "* Generate decay event, default options"
    write (u, "(A)")

    process => process_stack%get_process_ptr (procname2)
    model => process%get_model_ptr ()
    call model%set_unstable (25, [procname2])

    allocate (process_instance)
    call process_instance%init (process)
    call process_instance%setup_event_data (model)
    call process_instance%init_simulation (1)

```

```

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Generate decay event, helicity-diagonal decay"
write (u, "(A)")

process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2], diagonal = .true.)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data (model)
call process_instance%init_simulation (1)

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Generate decay event, isotropic decay, &
                  &polarized final state"
write (u, "(A)")

process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2], isotropic = .true.)
call model%set_polarized (6)
call model%set_polarized (-6)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data (model)
call process_instance%init_simulation (1)

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_7"

```

```
end subroutine events_7
```

32.11 Raw Event I/O

The raw format is for internal use only. All data are stored unformatted, so they can be efficiently be re-read on the same machine, but not necessarily on another machine.

This module explicitly depends on the `events` module which provides the concrete implementation of `event_base`. The other I/O formats access only the methods that are defined in `event_base`.

```
(eio_raw.f90)≡
  <File header>

  module eio_raw

    <Use kinds>
    <Use strings>
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base
    use events

    <Standard module head>

    <EIO raw: public>

    <EIO raw: parameters>

    <EIO raw: types>

    interface
    <EIO raw: sub interfaces>
    end interface

  end module eio_raw

(eio_raw_sub.f90)≡
  <File header>

  submodule (eio_raw) eio_raw_s

    use io_units
    use diagnostics
    use model_data
    use particles

    implicit none

  contains
```

```
⟨EIO raw: procedures⟩
```

```
end submodule eio_raw_s
```

32.11.1 File Format Version

This is the current default file version.

```
⟨EIO raw: parameters⟩≡
```

```
integer, parameter :: CURRENT_FILE_VERSION = 2
```

The user may change this number; this should force some compatibility mode for reading and writing. In any case, the file version stored in a event file that we read has to match the expected file version.

History of version numbers:

1. Format for WHIZARD 2.2.0 to 2.2.3. No version number stored in the raw file.
2. Format from 2.2.4 on. File contains version number. The file contains the transformed particle set (if applicable) after the hard-process particle set.

32.11.2 Type

Note the file version number. The default may be reset during initialization, which should enforce some compatibility mode.

```
⟨EIO raw: public⟩≡
```

```
public :: eio_raw_t
```

```
⟨EIO raw: types⟩≡
```

```
type, extends (eio_t) :: eio_raw_t
  logical :: reading = .false.
  logical :: writing = .false.
  integer :: unit = 0
  integer :: norm_mode = NORM_UNDEFINED
  real(default) :: sigma = 1
  integer :: n = 1
  integer :: n_alt = 0
  logical :: check = .false.
  logical :: use_alphas_from_file = .false.
  logical :: use_scale_from_file = .false.
  logical :: fixed_order_nlo = .false.
  integer :: file_version = CURRENT_FILE_VERSION
contains
  ⟨EIO raw: eio raw: TBP⟩
end type eio_raw_t
```

Output. This is not the actual event format, but a readable account of the current object status.

```
⟨EIO raw: eio raw: TBP⟩≡
```

```
procedure :: write => eio_raw_write
```

```

<EIO raw: sub interfaces>≡
    module subroutine eio_raw_write (object, unit)
        class(eio_raw_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine eio_raw_write

<EIO raw: procedures>≡
    module subroutine eio_raw_write (object, unit)
        class(eio_raw_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Raw event stream:"
        write (u, "(3x,A,L1)") "Check MD5 sum      = ", object%check
        if (object%n_alt > 0) then
            write (u, "(3x,A,I0)") "Alternate weights = ", object%n_alt
        end if
        write (u, "(3x,A,L1)") "Alpha_s from file = ", &
            object%use_alphas_from_file
        write (u, "(3x,A,L1)") "Scale from file   = ", &
            object%use_scale_from_file
        write (u, "(3x,A,L1)") "Events for fNLO   = ", &
            object%fixed_order_nlo
        if (object%reading) then
            write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
        else if (object%writing) then
            write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
        else
            write (u, "(3x,A)") "[closed]"
        end if
    end subroutine eio_raw_write

```

Finalizer: close any open file.

```

<EIO raw: eio raw: TBP>+≡
    procedure :: final => eio_raw_final

<EIO raw: sub interfaces>+≡
    module subroutine eio_raw_final (object)
        class(eio_raw_t), intent(inout) :: object
    end subroutine eio_raw_final

<EIO raw: procedures>+≡
    module subroutine eio_raw_final (object)
        class(eio_raw_t), intent(inout) :: object
        if (object%reading .or. object%writing) then
            write (msg_buffer, "(A,A,A)") "Events: closing raw file '", &
                char (object%filename), "'"
            call msg_message ()
            close (object%unit)
            object%reading = .false.
            object%writing = .false.
        end if
    end subroutine eio_raw_final

```

Set the check flag which determines whether we compare checksums on input.

```

(EIO raw: eio raw: TBP)+≡
    procedure :: set_parameters => eio_raw_set_parameters

(EIO raw: sub interfaces)+≡
    module subroutine eio_raw_set_parameters (eio, check, &
        use_alphas_from_file, use_scale_from_file, fixed_order_nlo, &
        version_string, extension)
        class(eio_raw_t), intent(inout) :: eio
        logical, intent(in), optional :: check, use_alphas_from_file, &
            use_scale_from_file, fixed_order_nlo
        type(string_t), intent(in), optional :: version_string
        type(string_t), intent(in), optional :: extension
    end subroutine eio_raw_set_parameters

(EIO raw: procedures)+≡
    module subroutine eio_raw_set_parameters (eio, check, use_alphas_from_file, &
        use_scale_from_file, fixed_order_nlo, version_string, extension)
        class(eio_raw_t), intent(inout) :: eio
        logical, intent(in), optional :: check, use_alphas_from_file, &
            use_scale_from_file, fixed_order_nlo
        type(string_t), intent(in), optional :: version_string
        type(string_t), intent(in), optional :: extension
        if (present (check)) eio%check = check
        if (present (use_alphas_from_file)) eio%use_alphas_from_file = &
            use_alphas_from_file
        if (present (use_scale_from_file)) eio%use_scale_from_file = &
            use_scale_from_file
        if (present (fixed_order_nlo)) eio%fixed_order_nlo = &
            fixed_order_nlo
        if (present (version_string)) then
            select case (char (version_string))
            case ("", "2.2.4")
                eio%file_version = CURRENT_FILE_VERSION
            case ("2.2")
                eio%file_version = 1
            case default
                call msg_fatal ("Raw event I/O: unsupported version '" &
                    // char (version_string) // "'")
                eio%file_version = 0
            end select
        end if
        if (present (extension)) then
            eio%extension = extension
        else
            eio%extension = "evx"
        end if
    end subroutine eio_raw_set_parameters

```

Initialize event writing.

```

(EIO raw: eio raw: TBP)+≡
    procedure :: init_out => eio_raw_init_out

(EIO raw: sub interfaces)+≡
    module subroutine eio_raw_init_out (eio, sample, data, success, extension)

```

```

class(eio_raw_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(event_sample_data_t), intent(in), optional :: data
logical, intent(out), optional :: success
type(string_t), intent(in), optional :: extension
end subroutine eio_raw_init_out

```

(EIO raw: procedures)+≡

```

module subroutine eio_raw_init_out (eio, sample, data, success, extension)
class(eio_raw_t), intent(inout) :: eio
type(string_t), intent(in) :: sample
type(event_sample_data_t), intent(in), optional :: data
logical, intent(out), optional :: success
type(string_t), intent(in), optional :: extension
character(32) :: md5sum_prc, md5sum_cfg
character(32), dimension(:), allocatable :: md5sum_alt
integer :: i
if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "evx"
end if
eio%filename = sample // "." // eio%extension
eio%unit = free_unit ()
write (msg_buffer, "(A,A,A)") "Events: writing to raw file '", &
    char (eio%filename), "'"
call msg_message ()
eio%writing = .true.
if (present (data)) then
    md5sum_prc = data%md5sum_prc
    md5sum_cfg = data%md5sum_cfg
    eio%norm_mode = data%norm_mode
    eio%sigma = data%total_cross_section
    eio%n = data%n_evt
    eio%n_alt = data%n_alt
    if (eio%n_alt > 0) then
        !!! !!! !!! Workaround for gfortran 5.0 ICE
        allocate (md5sum_alt (data%n_alt))
        md5sum_alt = data%md5sum_alt
        !!! allocate (md5sum_alt (data%n_alt), source = data%md5sum_alt)
    end if
else
    md5sum_prc = ""
    md5sum_cfg = ""
end if
open (eio%unit, file = char (eio%filename), form = "unformatted", &
    action = "write", status = "replace")
select case (eio%file_version)
case (2:); write (eio%unit) eio%file_version
end select
write (eio%unit) md5sum_prc
write (eio%unit) md5sum_cfg
write (eio%unit) eio%norm_mode
write (eio%unit) eio%n_alt
if (allocated (md5sum_alt)) then

```



```

        do i = 1, eio%n_alt
            write (eio%unit) md5sum_alt(i)
        end do
    end if
    if (present (success)) success = .true.
end subroutine eio_raw_init_out

```

Initialize event reading.

```

(EIO raw: eio raw: TBP)+≡
    procedure :: init_in => eio_raw_init_in

(EIO raw: sub interfaces)+≡
    module subroutine eio_raw_init_in (eio, sample, data, success, extension)
        class(eio_raw_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        type(string_t), intent(in), optional :: extension
    end subroutine eio_raw_init_in

(EIO raw: procedures)+≡
    module subroutine eio_raw_init_in (eio, sample, data, success, extension)
        class(eio_raw_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        type(string_t), intent(in), optional :: extension
        character(32) :: md5sum_prc, md5sum_cfg
        character(32), dimension(:), allocatable :: md5sum_alt
        integer :: i, file_version
        if (present (success)) success = .true.
        if (present (extension)) then
            eio%extension = extension
        else
            eio%extension = "evx"
        end if
        eio%filename = sample // "." // eio%extension
        eio%unit = free_unit ()
        if (present (data)) then
            eio%sigma = data%total_cross_section
            eio%n = data%n_evt
        end if
        write (msg_buffer, "(A,A,A)") "Events: reading from raw file '", &
            char (eio%filename), "'"
        call msg_message ()
        eio%reading = .true.
        open (eio%unit, file = char (eio%filename), form = "unformatted", &
            action = "read", status = "old")
        select case (eio%file_version)
        case (2:); read (eio%unit) file_version
        case default; file_version = 1
        end select
        if (file_version /= eio%file_version) then
            call msg_error ("Reading event file: raw-file version mismatch.")
            if (present (success)) success = .false.

```

```

        return
    else if (file_version /= CURRENT_FILE_VERSION) then
        call msg_warning ("Reading event file: compatibility mode.")
    end if
    read (eio%unit) md5sum_prc
    read (eio%unit) md5sum_cfg
    read (eio%unit) eio%norm_mode
    read (eio%unit) eio%n_alt
    if (present (data)) then
        if (eio%n_alt /= data%n_alt) then
            if (present (success)) success = .false.
            return
        end if
    end if
    allocate (md5sum_alt (eio%n_alt))
    do i = 1, eio%n_alt
        read (eio%unit) md5sum_alt(i)
    end do
    if (present (success)) then
        if (present (data)) then
            if (eio%check) then
                if (data%md5sum_prc /= "") then
                    success = success .and. md5sum_prc == data%md5sum_prc
                end if
                if (data%md5sum_cfg /= "") then
                    success = success .and. md5sum_cfg == data%md5sum_cfg
                end if
                do i = 1, eio%n_alt
                    if (data%md5sum_alt(i) /= "") then
                        success = success .and. md5sum_alt(i) == data%md5sum_alt(i)
                    end if
                end do
            else
                call msg_warning ("Reading event file: MD5 sum check disabled")
            end if
        end if
    end if
end subroutine eio_raw_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO raw: eio raw: TBP>+≡
    procedure :: switch_inout => eio_raw_switch_inout

<EIO raw: sub interfaces>+≡
    module subroutine eio_raw_switch_inout (eio, success)
        class(eio_raw_t), intent(inout) :: eio
        logical, intent(out), optional :: success
    end subroutine eio_raw_switch_inout

<EIO raw: procedures>+≡
    module subroutine eio_raw_switch_inout (eio, success)
        class(eio_raw_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        write (msg_buffer, "(A,A,A)") "Events: appending to raw file '", &
            char (eio%filename), ""
    end subroutine eio_raw_switch_inout

```

```

call msg_message ()
close (eio%unit, status = "keep")
eio%reading = .false.
open (eio%unit, file = char (eio%filename), form = "unformatted", &
      action = "write", position = "append", status = "old")
eio%writing = .true.
if (present (success)) success = .true.
end subroutine eio_raw_switch_inout

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

We always write the particle set of the hard process. (Note: this should be reconsidered.) We do make a physical copy.

On output, we write the `prc` values for weight and `sqme`, since these are the values just computed. On input, we store the values as `ref` values. The caller can then decide whether to recompute values and thus obtain distinct `prc` values, or just accept them.

The `passed` flag is not written. This allow us to apply different selection criteria upon rereading.

```

<EIO raw: eio raw: TBP>+≡
  procedure :: output => eio_raw_output

<EIO raw: sub interfaces>+≡
  module subroutine eio_raw_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_raw_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    integer, intent(in) :: i_prc
  end subroutine eio_raw_output

<EIO raw: procedures>+≡
  module subroutine eio_raw_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_raw_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    integer, intent(in) :: i_prc
    type(particle_set_t), pointer :: pset
    integer :: i
    if (eio%writing) then
      if (event%has_valid_particle_set ()) then
        select type (event)
          type is (event_t)
            write (eio%unit) i_prc
            write (eio%unit) event%get_index ()
            write (eio%unit) event%get_i_mci ()
            write (eio%unit) event%get_i_term ()
            write (eio%unit) event%get_channel ()
            write (eio%unit) event%expr%weight_prc
            write (eio%unit) event%expr%excess_prc
            write (eio%unit) event%get_n_dropped ()

```

```

write (eio%unit) event%expr%sqme_prc
do i = 1, eio%n_alt
  write (eio%unit) event%expr%weight_alt(i)
  write (eio%unit) event%expr%sqme_alt(i)
end do
allocate (pset)
call event%get_hard_particle_set (pset)
call pset%write_raw (eio%unit)
call pset%final ()
deallocate (pset)
select case (eio%file_version)
case (2:)
  if (event%has_transform ()) then
    write (eio%unit) .true.
    pset => event%get_particle_set_ptr ()
    call pset%write_raw (eio%unit)
  else
    write (eio%unit) .false.
  end if
end select
class default
  call msg_bug ("Event: write raw: defined only for full event_t")
end select
else
  call msg_bug ("Event: write raw: particle set is undefined")
end if
else
  call eio%write ()
  call msg_fatal ("Raw event file is not open for writing")
end if
end subroutine eio_raw_output

```

Input an event.

Note: the particle set is physically copied. If there is a performance issue, we might choose to pointer-assign it instead, with a different version of `event%set_hard_particle_set`.

(EIO raw: TBP)+≡

```

procedure :: input_i_prc => eio_raw_input_i_prc
procedure :: input_event => eio_raw_input_event

```

(EIO raw: sub interfaces)+≡

```

module subroutine eio_raw_input_i_prc (eio, i_prc, iostat)
  class(eio_raw_t), intent(inout) :: eio
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
end subroutine eio_raw_input_i_prc
module subroutine eio_raw_input_event (eio, event, iostat, event_handle)
  class(eio_raw_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
end subroutine eio_raw_input_event

```

(EIO raw: procedures)+≡

```

module subroutine eio_raw_input_i_prc (eio, i_prc, iostat)
  class(eio_raw_t), intent(inout) :: eio
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
  if (eio%reading) then
    read (eio%unit, iostat = iostat) i_prc
  else
    call eio%write ()
    call msg_fatal ("Raw event file is not open for reading")
  end if
end subroutine eio_raw_input_i_prc

module subroutine eio_raw_input_event (eio, event, iostat, event_handle)
  class(eio_raw_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  integer :: event_index, i_mci, i_term, channel, i
  real(default) :: weight, excess, sqme
  integer :: n_dropped
  real(default), dimension(:), allocatable :: weight_alt, sqme_alt
  logical :: has_transform
  type(particle_set_t), pointer :: pset
  class(model_data_t), pointer :: model
  if (eio%reading) then
    select type (event)
    type is (event_t)
      read (eio%unit, iostat = iostat) event_index
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) i_mci
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) i_term
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) channel
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) weight
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) excess
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) n_dropped
      if (iostat /= 0) return
      read (eio%unit, iostat = iostat) sqme
      if (iostat /= 0) return
      call event%reset_contents ()
      call event%set_index (event_index)
      call event%select (i_mci, i_term, channel)
      if (eio%norm_mode /= NORM_UNDEFINED) then
        call event_normalization_update (weight, &
          eio%sigma, eio%n, event%get_norm_mode (), eio%norm_mode)
        call event_normalization_update (excess, &
          eio%sigma, eio%n, event%get_norm_mode (), eio%norm_mode)
      end if
      call event%set (sqme_ref = sqme, weight_ref = weight, &
        excess_prc = excess, &

```

```

        n_dropped = n_dropped)
if (eio%n_alt /= 0) then
    allocate (sqme_alt (eio%n_alt), weight_alt (eio%n_alt))
    do i = 1, eio%n_alt
        read (eio%unit, iostat = iostat) weight_alt(i)
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) sqme_alt(i)
        if (iostat /= 0) return
    end do
    call event%set (sqme_alt = sqme_alt, weight_alt = weight_alt)
end if
model => null ()
if (associated (event%process)) then
    model => event%process%get_model_ptr ()
end if
allocate (pset)
call pset%read_raw (eio%unit, iostat)
if (iostat /= 0) return
if (associated (model)) call pset%set_model (model)
call event%set_hard_particle_set (pset)
if (eio%use_alphas_from_file .or. eio%use_scale_from_file) then
    call event%recalculate (update_sqme = .true.)
    if (eio%fixed_order_nlo) then
        if (event%weight_prc /= event%weight_ref .and. &
            event%weight_prc == 0) then
            event%weight_prc = event%weight_ref
        end if
    end if
end if
call pset%final ()
deallocate (pset)
select case (eio%file_version)
case (2:)
    read (eio%unit, iostat = iostat) has_transform
    if (iostat /= 0) return
    if (has_transform) then
        allocate (pset)
        call pset%read_raw (eio%unit, iostat)
        if (iostat /= 0) return
        if (associated (model)) &
            call pset%set_model (model)
        call event%link_particle_set (pset)
    end if
end select
class default
    call msg_bug ("Event: read raw: defined only for full event_t")
end select
else
    call eio%write ()
    call msg_fatal ("Raw event file is not open for reading")
end if
end subroutine eio_raw_input_event

```

(EIO raw: eio raw: TBP)+≡

```

        procedure :: skip => eio_raw_skip
    <EIO raw: sub interfaces>+≡
        module subroutine eio_raw_skip (eio, iostat)
            class(eio_raw_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            end subroutine eio_raw_skip
    <EIO raw: procedures>+≡
        module subroutine eio_raw_skip (eio, iostat)
            class(eio_raw_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            if (eio%reading) then
                read (eio%unit, iostat = iostat)
            else
                call eio%write ()
                call msg_fatal ("Raw event file is not open for reading")
            end if
            end subroutine eio_raw_skip

```

32.11.3 Unit tests

Test module, followed by the corresponding implementation module.

```

    <eio_raw_ut.f90>≡
    <File header>

    module eio_raw_ut
        use unit_tests
        use eio_raw_uti

    <Standard module head>

    <EIO raw: public test>

    contains

    <EIO raw: test driver>

    end module eio_raw_ut
    <eio_raw_uti.f90>≡
    <File header>

    module eio_raw_uti

    <Use kinds>
    <Use strings>
        use model_data
        use variables
        use events
        use eio_data
        use eio_base

        use eio_raw

```

```

    use process, only: process_t
    use instances, only: process_instance_t

```

<Standard module head>

<EIO raw: test declarations>

contains

<EIO raw: tests>

```

end module eio_raw_util

```

API: driver for the unit tests below.

<EIO raw: public test>≡

```

    public :: eio_raw_test

```

<EIO raw: test driver>≡

```

    subroutine eio_raw_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <EIO raw: execute tests>
    end subroutine eio_raw_test

```

Test I/O methods

We test the implementation of all I/O methods.

<EIO raw: execute tests>≡

```

    call test (eio_raw_1, "eio_raw_1", &
        "read and write event contents", &
        u, results)

```

<EIO raw: test declarations>≡

```

    public :: eio_raw_1

```

<EIO raw: tests>≡

```

    subroutine eio_raw_1 (u)
        use processes_util, only: prepare_test_process, cleanup_test_process
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(event_t), allocatable, target :: event
        type(process_t), allocatable, target :: process
        type(process_instance_t), allocatable, target :: process_instance
        class(eio_t), allocatable :: eio
        integer :: i_prc, iostat
        type(string_t) :: sample

        write (u, "(A)")  "*" Test output: eio_raw_1"
        write (u, "(A)")  "*" Purpose: generate and read/write an event"
        write (u, "(A)")

        write (u, "(A)")  "*" Initialize test process"

```



```

call model%init_test ()

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model, &
    run_id = var_str ("run_test"))
call process_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_raw_1"

allocate (eio_raw_t :: eio)

call eio%init_out (sample)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event"
write (u, "(A)")

call eio%init_in (sample)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (i_prc):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (event):", iostat
call eio%write (u)

```

```

write (u, "(A)")
write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)
write (u, "(A)")
write (u, "(A)")  "* Generate and append another event"
write (u, "(A)")

call eio%switch_inout ()
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 5)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read both events"
write (u, "(A)")

call eio%init_in (sample)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (i_prc/1):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (event/1):", iostat
call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (i_prc/2):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (event/2):", iostat
call eio%write (u)

write (u, "(A)")
write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_raw_1"

end subroutine eio_raw_1

```

Test I/O methods

We test the implementation of all I/O methods.

```

<EIO raw: execute tests>+≡
call test (eio_raw_2, "eio_raw_2", &
           "handle multiple weights", &
           u, results)

<EIO raw: test declarations>+≡
public :: eio_raw_2

<EIO raw: tests>+≡
subroutine eio_raw_2 (u)
  use processes_ut, only: prepare_test_process, cleanup_test_process
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(var_list_t) :: var_list
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  integer :: i_prc, iostat
  type(string_t) :: sample

  write (u, "(A)")  "* Test output: eio_raw_2"
  write (u, "(A)")  "* Purpose: generate and read/write an event"
  write (u, "(A)")  "*           with multiple weights"
  write (u, "(A)")

  call model%init_test ()

  write (u, "(A)")  "* Initialize test process"

  allocate (process)

```

```

allocate (process_instance)
call prepare_test_process (process, process_instance, model, &
    run_id = var_str ("run_test"))
call process_instance%setup_event_data ()

call data%init (n_proc = 1, n_alt = 2)

call var_list%append_log (var_str ("?unweighted"), .false., &
    intrinsic = .true.)
call var_list%append_string (var_str ("sample_normalization"), &
    var_str ("auto"), intrinsic = .true.)
call var_list%append_real (var_str ("safety_factor"), &
    1._default, intrinsic = .true.)

allocate (event)
call event%basic_init (var_list, n_alt = 2)
call event%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_raw_2"

allocate (eio_raw_t :: eio)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%set (sqme_alt = [2._default, 3._default])
call event%set (weight_alt = &
    [2 * event%get_weight_ref (), 3 * event%get_weight_ref ()])
call event%store_alt_values ()
call event%check ()

call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event"
write (u, "(A)")

call eio%init_in (sample, data)

```

```

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init (var_list, n_alt = 2)
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (i_prc):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (event):", iostat
call eio%write (u)

write (u, "(A)")
write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call eio%final ()
deallocate (eio)

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: eio_raw_2"

end subroutine eio_raw_2

```

32.12 Dispatch

An event transform is responsible for dressing a partonic event. Since event transforms are not mutually exclusive but are concatenated, we provide individual dispatchers for each of them.

Due to the gfortran 7/8/9 bug that leads to segmentation violation if polymorphic user-defined derived types are allocated in routines within submodules, this module remains without submodule until we can switch to gfortran v10 or newer.

```

(dispatch_transforms.f90)≡
  {File header}

```

```

module dispatch_transforms

```

```

<Use kinds>
<Use strings>
  use process
  use variables
  use system_defs, only: LF
  use system_dependencies, only: LHAPDF6_AVAILABLE
  use sf_lhapdf, only: lhpdf_initialize
  use pdf, only: pdf_data_t
  use diagnostics
  use models
  use os_interface
  use beam_structures
  use resonances, only: resonance_history_set_t
  use instances, only: process_instance_t, process_instance_hook_t

  use event_base, only: event_callback_t, event_callback_nop_t
  use hePMC_interface, only: HEPMC3_MODE_HEPMC2, HEPMC3_MODE_HEPMC3
  use hePMC_interface, only: HEPMC3_MODE_ROOT, HEPMC3_MODE_ROOTTREE
  use hePMC_interface, only: HEPMC3_MODE_HEPEVT
  use eio_base
  use eio_raw
  use eio_checkpoints
  use eio_callback
  use eio_lhef
  use eio_hePMC
  use eio_lcio
  use eio_stdhep
  use eio_ascii
  use eio_weights
  use eio_dump

  use event_transforms
  use resonance_insertion
  use isr_epa_handler
  use decays
  use shower_base
  use shower_core
  use shower
  use shower_pythia6
  use shower_pythia8
  use hadrons
  use mlm_matching
  use powheg_matching
  use ckkw_matching
  use tauola_interface !NODEP!
  use evt_nlo

<Standard module head>

<Dispatch transforms: public>

contains

```

```

    <Dispatch transforms: procedures>

    end module dispatch_transforms

    <Dispatch transforms: public>≡
        public :: dispatch_evt_nlo

    <Dispatch transforms: procedures>≡
        subroutine dispatch_evt_nlo (evt, keep_failed_events)
            class(evt_t), intent(out), pointer :: evt
            logical, intent(in) :: keep_failed_events
            call msg_message ("Simulate: activating fixed-order NLO events")
            allocate (evt_nlo_t :: evt)
            evt%only_weighted_events = .true.
            select type (evt)
            type is (evt_nlo_t)
                evt%i_evaluation = 0
                evt%keep_failed_events = keep_failed_events
            end select
        end subroutine dispatch_evt_nlo

    <Dispatch transforms: public>+≡
        public :: dispatch_evt_resonance

    <Dispatch transforms: procedures>+≡
        subroutine dispatch_evt_resonance (evt, var_list, res_history_set, libname)
            class(evt_t), intent(out), pointer :: evt
            type(var_list_t), intent(in) :: var_list
            type(resonance_history_set_t), dimension(:), intent(in) :: res_history_set
            type(string_t), intent(in) :: libname
            logical :: resonance_history
            resonance_history = var_list%get_lval (var_str ("?resonance_history"))
            if (resonance_history) then
                allocate (evt_resonance_t :: evt)
                call msg_message ("Simulate: activating resonance insertion")
                select type (evt)
                type is (evt_resonance_t)
                    call evt%set_resonance_data (res_history_set)
                    call evt%set_library (libname)
                end select
            else
                evt => null ()
            end if
        end subroutine dispatch_evt_resonance

```

Initialize the ISR/EPA handler, depending on active settings.

The activation is independent for both handlers, since only one may be needed at a time. However, if both handlers are active, the current implementation requires the handler modes of ISR and EPA to coincide.

```

    <Dispatch transforms: public>+≡
        public :: dispatch_evt_isr_epa_handler

    <Dispatch transforms: procedures>+≡
        subroutine dispatch_evt_isr_epa_handler (evt, var_list)
            class(evt_t), intent(out), pointer :: evt

```

```

type(var_list_t), intent(in) :: var_list
logical :: isr_recoil
logical :: epa_recoil
logical :: isr_handler_active
logical :: epa_handler_active
type(string_t) :: isr_handler_mode
type(string_t) :: epa_handler_mode
logical :: isr_keep_mass
real(default) :: sqrts
real(default) :: isr_q_max
real(default) :: epa_q_max
real(default) :: isr_mass
real(default) :: epa_mass
isr_handler_active = var_list%get_lval (var_str ("?isr_handler"))
if (isr_handler_active) then
    call msg_message ("Simulate: activating ISR handler")
    isr_recoil = &
        var_list%get_lval (var_str ("?isr_recoil"))
    isr_handler_mode = &
        var_list%get_sval (var_str ("?isr_handler_mode"))
    isr_keep_mass = &
        var_list%get_lval (var_str ("?isr_handler_keep_mass"))
    if (isr_recoil) then
        call msg_fatal ("Simulate: ISR handler is incompatible &
            &with ?isr_recoil=true")
    end if
end if
epa_handler_active = var_list%get_lval (var_str ("?epa_handler"))
if (epa_handler_active) then
    call msg_message ("Simulate: activating EPA handler")
    epa_recoil = var_list%get_lval (var_str ("?epa_recoil"))
    epa_handler_mode = var_list%get_sval (var_str ("?epa_handler_mode"))
    if (epa_recoil) then
        call msg_fatal ("Simulate: EPA handler is incompatible &
            &with ?epa_recoil=true")
    end if
end if
if (isr_handler_active .and. epa_handler_active) then
    if (isr_handler_mode /= epa_handler_mode) then
        call msg_fatal ("Simulate: ISR/EPA handler: modes must coincide")
    end if
end if
if (isr_handler_active .or. epa_handler_active) then
    allocate (evt_isr_epa_t :: evt)
    select type (evt)
    type is (evt_isr_epa_t)
        if (isr_handler_active) then
            call evt%set_mode_string (isr_handler_mode)
        else
            call evt%set_mode_string (epa_handler_mode)
        end if
        sqrts = var_list%get_rval (var_str ("sqrts"))
        if (isr_handler_active) then
            isr_q_max = var_list%get_rval (var_str ("isr_q_max"))

```



```

        isr_mass = var_list%get_rval (var_str ("isr_mass"))
        call evt%set_data_isr (sqrts, isr_q_max, isr_mass, isr_keep_mass)
    end if
    if (epa_handler_active) then
        epa_q_max = var_list%get_rval (var_str ("epa_q_max"))
        epa_mass = var_list%get_rval (var_str ("epa_mass"))
        call evt%set_data_epa (sqrts, epa_q_max, epa_mass)
    end if
    call msg_message ("Simulate: ISR/EPA handler mode: " &
        // char (evt%get_mode_string ()))
end select
else
    evt => null ()
end if
end subroutine dispatch_evt_isr_epa_handler

```

<Dispatch transforms: public>+≡
 public :: dispatch_evt_decay

<Dispatch transforms: procedures>+≡
 subroutine dispatch_evt_decay (evt, var_list)
 class(evt_t), intent(out), pointer :: evt
 type(var_list_t), intent(in), target :: var_list
 logical :: allow_decays
 allow_decays = var_list%get_lval (var_str ("?allow_decays"))
 if (allow_decays) then
 allocate (evt_decay_t :: evt)
 call msg_message ("Simulate: activating decays")
 select type (evt)
 type is (evt_decay_t)
 call evt%set_var_list (var_list)
 end select
 else
 evt => null ()
 end if
 end subroutine dispatch_evt_decay

<Dispatch transforms: public>+≡
 public :: dispatch_evt_shower

<Dispatch transforms: procedures>+≡
 subroutine dispatch_evt_shower (evt, var_list, model, fallback_model, &
 os_data, beam_structure, process)
 class(evt_t), intent(out), pointer :: evt
 type(var_list_t), intent(in) :: var_list
 type(model_t), pointer, intent(in) :: model, fallback_model
 type(os_data_t), intent(in) :: os_data
 type(beam_structure_t), intent(in) :: beam_structure
 type(process_t), intent(in), optional :: process
 type(string_t) :: lhpdf_file, lhpdf_dir, process_name
 integer :: lhpdf_member
 type(shower_settings_t) :: settings
 type(taudec_settings_t) :: taudec_settings
 call msg_message ("Simulate: activating parton shower")

```

allocate (evt_shower_t :: evt)
call settings%init (var_list)
if (associated (model)) then
    call taudec_settings%init (var_list, model)
else
    call taudec_settings%init (var_list, fallback_model)
end if
if (present (process)) then
    process_name = process%get_id ()
else
    process_name = 'dispatch_testing'
end if
select type (evt)
type is (evt_shower_t)
    call evt%init (fallback_model, os_data)
    lhpdf_member = &
        var_list%get_ival (var_str ("lhpdf_member"))
    if (LHAPDF6_AVAILABLE) then
        lhpdf_dir = &
            var_list%get_sval (var_str ("lhpdf_dir"))
        lhpdf_file = &
            var_list%get_sval (var_str ("lhpdf_file"))
        call lhpdf_initialize &
            (1, lhpdf_dir, lhpdf_file, lhpdf_member, evt%pdf_data%pdf)
    end if
    if (present (process)) call evt%pdf_data%setup ("Shower", &
        beam_structure, lhpdf_member, process%get_pdf_set ())
    select case (settings%method)
    case (PS_WHIZARD)
        allocate (shower_t :: evt%shower)
    case (PS_PYTHIA6)
        allocate (shower_pythia6_t :: evt%shower)
    case (PS_PYTHIA8)
        allocate (shower_pythia8_t :: evt%shower)
    case default
        call msg_fatal ('Shower: Method ' // &
            char (var_list%get_sval (var_str ("shower_method")))) // &
            'not implemented!')
    end select
    call evt%shower%init (settings, taudec_settings, evt%pdf_data, os_data)
    call dispatch_matching (evt, settings, var_list, process_name, evt%pdf_data)
class default
    call dispatch_matching (evt, settings, var_list, process_name)
end select
end subroutine dispatch_evt_shower

```

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_shower_hook
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_shower_hook (hook, var_list, process_instance, beam_structure, pdf_set)
class(process_instance_hook_t), pointer, intent(out) :: hook
type(var_list_t), intent(in) :: var_list
class(process_instance_t), intent(in), target :: process_instance

```

```

type(beam_structure_t), intent(in) :: beam_structure
integer, intent(in) :: pdf_set
type(pdf_data_t) :: pdf_data
type(string_t) :: lhpdf_file, lhpdf_dir
integer :: lhpdf_member
if (var_list%get_lval (var_str ('?powheg_matching')) then
  call msg_message ("Integration hook: add POWHEG hook")
  allocate (powheg_matching_hook_t :: hook)
  select type (hook)
  type is (powheg_matching_hook_t)
    lhpdf_member = var_list%get_ival (var_str ("lhpdf_member"))
    if (LHAPDF6_AVAILABLE) then
      lhpdf_dir = var_list%get_sval (var_str ("lhpdf_dir"))
      lhpdf_file = var_list%get_sval (var_str ("lhpdf_file"))
      call lhpdf_initialize (1, lhpdf_dir, lhpdf_file, lhpdf_member, pdf_data%pdf)
    end if
    call pdf_data%setup ("Shower", beam_structure, lhpdf_member, pdf_set)
    call hook%init (var_list, process_instance, pdf_data)
  end select
else
  hook => null ()
end if
end subroutine dispatch_evt_shower_hook

```

<Dispatch transforms: public>+≡
 public :: dispatch_matching

<Dispatch transforms: procedures>+≡
 subroutine dispatch_matching (evt, settings, var_list, process_name, pdf_data)
 class(evt_t), intent(inout) :: evt
 type(shower_settings_t), intent(in) :: settings
 type(var_list_t), intent(in) :: var_list
 type(string_t), intent(in) :: process_name
 type(pdf_data_t), intent(in), optional :: pdf_data
 select type (evt)
 type is (evt_shower_t)
 if (settings%mlm_matching .and. settings%ckkw_matching) then
 call msg_fatal ("Both MLM and CKKW matching activated," // &
 LF // " aborting simulation")
 end if
 if (settings%powheg_matching) then
 call msg_message ("Simulate: applying POWHEG matching")
 allocate (powheg_matching_t :: evt%matching)
 end if
 if (settings%mlm_matching) then
 call msg_message ("Simulate: applying MLM matching")
 allocate (mlm_matching_t :: evt%matching)
 end if
 if (settings%ckkw_matching) then
 call msg_warning ("Simulate: CKKW(-L) matching not yet supported")
 allocate (ckkw_matching_t :: evt%matching)
 end if
 if (allocated (evt%matching)) then
 call evt%matching%init (var_list, process_name)
 end if
 end select
end subroutine dispatch_matching

```

        if (present(pdf_data)) then
            select type (matching => evt%matching)
            type is (powheg_matching_t)
                matching%process_deps%pdf_data = pdf_data
            end select
        end if
    end if
end select
end subroutine dispatch_matching

```

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_hadrons
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_hadrons (evt, var_list, fallback_model)
    class(evt_t), intent(out), pointer :: evt
    type(var_list_t), intent(in) :: var_list
    type(model_t), pointer, intent(in) :: fallback_model
    type(shower_settings_t) :: shower_settings
    type(hadron_settings_t) :: hadron_settings
    allocate (evt_hadrons_t :: evt)
    call msg_message ("Simulate: activating hadronization")
    call shower_settings%init (var_list)
    call hadron_settings%init (var_list)
    select type (evt)
    type is (evt_hadrons_t)
        call evt%init (fallback_model)
        select case (hadron_settings%method)
        case (HADRONS_WHIZARD)
            allocate (hadrons_hadrons_t :: evt%hadrons)
        case (HADRONS_PYTHIA6)
            allocate (hadrons_pythia6_t :: evt%hadrons)
        case (HADRONS_PYTHIA8)
            allocate (hadrons_pythia8_t :: evt%hadrons)
        case default
            call msg_fatal ('Hadronization: Method ' // &
                char (var_list%get_sval (var_str ("hadronization_method")) // &
                'not implemented!')
        end select
        call evt%hadrons%init &
            (shower_settings, hadron_settings, fallback_model)
    end select
end subroutine dispatch_evt_hadrons

```

We cannot put this in the `events` subdir due to `eio_raw_t`, which is defined here.

<Dispatch transforms: public>+≡

```
public :: dispatch_eio
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_eio (eio, method, var_list, fallback_model, &
    event_callback)
    class(eio_t), allocatable, intent(inout) :: eio
    type(string_t), intent(in) :: method

```

```

type(var_list_t), intent(in) :: var_list
type(model_t), target, intent(in) :: fallback_model
class(event_callback_t), allocatable, intent(in) :: event_callback
logical :: check, keep_beams, keep_remnants, recover_beams
logical :: use_alphas_from_file, use_scale_from_file
logical :: fixed_order_nlo_events
logical :: write_sqme_prc, write_sqme_ref, write_sqme_alt
logical :: output_cross_section, ensure_order
type(string_t) :: lhef_version, lhef_extension, raw_version
type(string_t) :: extension_default, debug_extension, dump_extension, &
    extension_hepmc, &
    extension_lha, extension_hepevt, extension_ascii_short, &
    extension_ascii_long, extension_athena, extension_mokka, &
    extension_stdhep, extension_stdhep_up, extension_stdhep_ev4, &
    extension_raw, extension_hepevt_verb, extension_lha_verb, &
    extension_lcio
integer :: checkpoint
integer :: lcio_run_id, hepmc3_mode
logical :: show_process, show_transforms, show_decay, verbose, pacified
logical :: dump_weights, dump_compressed, dump_summary, dump_screen
logical :: proc_as_run_id, hepmc3_write_flows
keep_beams = &
    var_list%get_lval (var_str ("?keep_beams"))
keep_remnants = &
    var_list%get_lval (var_str ("?keep_remnants"))
ensure_order = &
    var_list%get_lval (var_str ("?hepevt_ensure_order"))
recover_beams = &
    var_list%get_lval (var_str ("?recover_beams"))
use_alphas_from_file = &
    var_list%get_lval (var_str ("?use_alphas_from_file"))
use_scale_from_file = &
    var_list%get_lval (var_str ("?use_scale_from_file"))
fixed_order_nlo_events = &
    var_list%get_lval (var_str ("?fixed_order_nlo_events"))
select case (char (method))
case ("raw")
    allocate (eio_raw_t :: eio)
    select type (eio)
    type is (eio_raw_t)
        check = &
            var_list%get_lval (var_str ("?check_event_file"))
        raw_version = &
            var_list%get_sval (var_str ("$event_file_version"))
        extension_raw = &
            var_list%get_sval (var_str ("$extension_raw"))
        call eio%set_parameters (check, use_alphas_from_file, &
            use_scale_from_file, fixed_order_nlo_events, &
            raw_version, extension_raw)
    end select
case ("checkpoint")
    allocate (eio_checkpoints_t :: eio)
    select type (eio)
    type is (eio_checkpoints_t)

```

```

        checkpoint = &
            var_list%get_ival (var_str ("checkpoint"))
        pacified = &
            var_list%get_lval (var_str ("?pacify"))
        call eio%set_parameters (checkpoint, blank = pacified)
    end select
case ("callback")
    allocate (eio_callback_t :: eio)
    select type (eio)
    type is (eio_callback_t)
        checkpoint = &
            var_list%get_ival (var_str ("event_callback_interval"))
        if (allocated (event_callback)) then
            call eio%set_parameters (event_callback, checkpoint)
        else
            call eio%set_parameters (event_callback_nop_t (), 0)
        end if
    end select
case ("lhef")
    allocate (eio_lhef_t :: eio)
    select type (eio)
    type is (eio_lhef_t)
        lhef_version = &
            var_list%get_sval (var_str ("$lhef_version"))
        lhef_extension = &
            var_list%get_sval (var_str ("$lhef_extension"))
        write_sqme_prc = &
            var_list%get_lval (var_str ("?lhef_write_sqme_prc"))
        write_sqme_ref = &
            var_list%get_lval (var_str ("?lhef_write_sqme_ref"))
        write_sqme_alt = &
            var_list%get_lval (var_str ("?lhef_write_sqme_alt"))
        call eio%set_parameters ( &
            keep_beams, keep_remnants, recover_beams, &
            use_alphas_from_file, use_scale_from_file, &
            char (lhef_version), lhef_extension, &
            write_sqme_ref, write_sqme_prc, write_sqme_alt)
    end select
case ("hepmc")
    allocate (eio_hepmc_t :: eio)
    select type (eio)
    type is (eio_hepmc_t)
        output_cross_section = &
            var_list%get_lval (var_str ("?hepmc_output_cross_section"))
        extension_hepmc = &
            var_list%get_sval (var_str ("$extension_hepmc"))
        hepmc3_write_flows = &
            var_list%get_lval (var_str ("?hepmc3_write_flows"))
        select case (char (var_list%get_sval (var_str ("$hepmc3_mode"))))
        case ("HepMC2")
            hepmc3_mode = HEPMC3_MODE_HEPMC2
        case ("HepMC3")
            hepmc3_mode = HEPMC3_MODE_HEPMC3
        case ("Root")

```

```

    hepmc3_mode = HEPMC3_MODE_ROOT
    if (extension_hepmc /= "root") then
        call msg_message ("Events: HepMC3 Root mode, using " // &
            "event sample extension 'root'")
        extension_hepmc = "root"
    end if
case ("RootTree")
    hepmc3_mode = HEPMC3_MODE_ROOTTREE
    if (extension_hepmc /= "root") then
        call msg_message ("Events: HepMC3 RootTree mode, using " // &
            "event sample extension 'root'")
        extension_hepmc = "root"
    end if
case ("HepEVT")
    hepmc3_mode = HEPMC3_MODE_HEPEVT
case default
    call msg_fatal ("Only supported HepMC3 modes are: 'HepMC2', " // &
        "'HepMC3', 'HepEVT', 'Root', and 'RootTree'.")
end select
call eio%set_parameters (recover_beams, &
    use_alphas_from_file, use_scale_from_file, &
    extension = extension_hepmc, &
    output_cross_section = output_cross_section, &
    hepmc3_mode = hepmc3_mode, &
    hepmc3_write_flows = hepmc3_write_flows)
end select
case ("lcio")
    allocate (eio_lcio_t :: eio)
    select type (eio)
    type is (eio_lcio_t)
        extension_lcio = &
            var_list%get_sval (var_str ("$extension_lcio"))
        proc_as_run_id = &
            var_list%get_lval (var_str ("?proc_as_run_id"))
        lcio_run_id = &
            var_list%get_ival (var_str ("lcio_run_id"))
        call eio%set_parameters (recover_beams, &
            use_alphas_from_file, use_scale_from_file, &
            extension_lcio, proc_as_run_id = proc_as_run_id, &
            lcio_run_id = lcio_run_id)
    end select
case ("stdhep")
    allocate (eio_stdhep_hepevt_t :: eio)
    select type (eio)
    type is (eio_stdhep_hepevt_t)
        extension_stdhep = &
            var_list%get_sval (var_str ("$extension_stdhep"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, recover_beams, &
            use_alphas_from_file, use_scale_from_file, extension_stdhep)
    end select
case ("stdhep_up")
    allocate (eio_stdhep_hepeup_t :: eio)
    select type (eio)

```

```

type is (eio_stdhep_hepeup_t)
  extension_stdhep_up = &
    var_list%get_sval (var_str ("$extension_stdhep_up"))
  call eio%set_parameters (keep_beams, keep_remnants, ensure_order, &
    recover_beams, use_alphas_from_file, &
    use_scale_from_file, extension_stdhep_up)
end select
case ("stdhep_ev4")
  allocate (eio_stdhep_hepev4_t :: eio)
  select type (eio)
  type is (eio_stdhep_hepev4_t)
    extension_stdhep_ev4 = &
      var_list%get_sval (var_str ("$extension_stdhep_ev4"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, recover_beams, &
        use_alphas_from_file, use_scale_from_file, extension_stdhep_ev4)
  end select
case ("ascii")
  allocate (eio_ascii_ascii_t :: eio)
  select type (eio)
  type is (eio_ascii_ascii_t)
    extension_default = &
      var_list%get_sval (var_str ("$extension_default"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, extension_default)
  end select
case ("athena")
  allocate (eio_ascii_athena_t :: eio)
  select type (eio)
  type is (eio_ascii_athena_t)
    extension_athena = &
      var_list%get_sval (var_str ("$extension_athena"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, extension_athena)
  end select
case ("debug")
  allocate (eio_ascii_debug_t :: eio)
  select type (eio)
  type is (eio_ascii_debug_t)
    debug_extension = &
      var_list%get_sval (var_str ("$debug_extension"))
    show_process = &
      var_list%get_lval (var_str ("?debug_process"))
    show_transforms = &
      var_list%get_lval (var_str ("?debug_transforms"))
    show_decay = &
      var_list%get_lval (var_str ("?debug_decay"))
    verbose = &
      var_list%get_lval (var_str ("?debug_verbose"))
    call eio%set_parameters ( &
      extension = debug_extension, &
      show_process = show_process, &
      show_transforms = show_transforms, &
      show_decay = show_decay, &

```



```

        verbose = verbose)
    end select
case ("dump")
    allocate (eio_dump_t :: eio)
    select type (eio)
    type is (eio_dump_t)
        dump_extension = &
            var_list%get_sval (var_str ("$_dump_extension"))
        pacified = &
            var_list%get_lval (var_str ("?pacify"))
        dump_weights = &
            var_list%get_lval (var_str ("?dump_weights"))
        dump_compressed = &
            var_list%get_lval (var_str ("?dump_compressed"))
        dump_summary = &
            var_list%get_lval (var_str ("?dump_summary"))
        dump_screen = &
            var_list%get_lval (var_str ("?dump_screen"))
        call eio%set_parameters ( &
            extension = dump_extension, &
            pacify = pacified, &
            weights = dump_weights, &
            compressed = dump_compressed, &
            summary = dump_summary, &
            screen = dump_screen)
    end select
case ("hepevt")
    allocate (eio_ascii_hepevt_t :: eio)
    select type (eio)
    type is (eio_ascii_hepevt_t)
        extension_hepevt = &
            var_list%get_sval (var_str ("$_extension_hepevt"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_hepevt)
    end select
case ("hepevt_verb")
    allocate (eio_ascii_hepevt_verb_t :: eio)
    select type (eio)
    type is (eio_ascii_hepevt_verb_t)
        extension_hepevt_verb = &
            var_list%get_sval (var_str ("$_extension_hepevt_verb"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_hepevt_verb)
    end select
case ("lha")
    allocate (eio_ascii_lha_t :: eio)
    select type (eio)
    type is (eio_ascii_lha_t)
        extension_lha = &
            var_list%get_sval (var_str ("$_extension_lha"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_lha)
    end select
case ("lha_verb")

```

```

allocate (eio_ascii_lha_verb_t :: eio)
select type (eio)
type is (eio_ascii_lha_verb_t)
    extension_lha_verb = var_list%get_sval ( &
        var_str ("$extension_lha_verb"))
    call eio%set_parameters &
        (keep_beams, keep_remnants, ensure_order, extension_lha_verb)
end select
case ("long")
allocate (eio_ascii_long_t :: eio)
select type (eio)
type is (eio_ascii_long_t)
    extension_ascii_long = &
        var_list%get_sval (var_str ("$extension_ascii_long"))
    call eio%set_parameters &
        (keep_beams, keep_remnants, ensure_order, extension_ascii_long)
end select
case ("mokka")
allocate (eio_ascii_mokka_t :: eio)
select type (eio)
type is (eio_ascii_mokka_t)
    extension_mokka = &
        var_list%get_sval (var_str ("$extension_mokka"))
    call eio%set_parameters &
        (keep_beams, keep_remnants, ensure_order, extension_mokka)
end select
case ("short")
allocate (eio_ascii_short_t :: eio)
select type (eio)
type is (eio_ascii_short_t)
    extension_ascii_short = &
        var_list%get_sval (var_str ("$extension_ascii_short"))
    call eio%set_parameters &
        (keep_beams, keep_remnants, ensure_order, extension_ascii_short)
end select
case ("weight_stream")
allocate (eio_weights_t :: eio)
select type (eio)
type is (eio_weights_t)
    pacified = &
        var_list%get_lval (var_str ("?pacify"))
    call eio%set_parameters (pacify = pacified)
end select
case default
    call msg_fatal ("Event I/O method '" // char (method) &
        // "' not implemented")
end select
call eio%set_fallback_model (fallback_model)
end subroutine dispatch_eio

```

32.12.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_transforms_ut.f90>≡
  <File header>

  module dispatch_transforms_ut
    use unit_tests
    use dispatch_transforms_uti

    <Standard module head>

    <Dispatch transforms: public test>

    contains

    <Dispatch transforms: test driver>

  end module dispatch_transforms_ut
<dispatch_transforms_uti.f90>≡
  <File header>

  module dispatch_transforms_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use variables
    use event_base, only: event_callback_t
    use models, only: model_t, model_list_t
    use models, only: syntax_model_file_init, syntax_model_file_final
    use resonances, only: resonance_history_set_t
    use beam_structures, only: beam_structure_t
    use eio_base, only: eio_t
    use os_interface, only: os_data_t
    use event_transforms, only: evt_t
    use dispatch_transforms

    <Standard module head>

    <Dispatch transforms: test declarations>

    contains

    <Dispatch transforms: tests>

  end module dispatch_transforms_uti
API: driver for the unit tests below.
<Dispatch transforms: public test>≡
  public ::dispatch_transforms_test
<Dispatch transforms: test driver>≡
  subroutine dispatch_transforms_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Dispatch transforms: execute tests>
  end subroutine dispatch_transforms_test

```

Event I/O

```
<Dispatch transforms: execute tests>≡
  call test (dispatch_transforms_1, "dispatch_transforms_1", &
    "event I/O", &
    u, results)

<Dispatch transforms: test declarations>≡
  public :: dispatch_transforms_1

<Dispatch transforms: tests>≡
  subroutine dispatch_transforms_1 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(os_data_t) :: os_data
    class(event_callback_t), allocatable :: event_callback
    class(eio_t), allocatable :: eio

    write (u, "(A)")  "* Test output: dispatch_transforms_1"
    write (u, "(A)")  "* Purpose: allocate an event I/O (eio) stream"
    write (u, "(A)")

    call var_list%init_defaults (0)
    call os_data%init ()
    call syntax_model_file_init ()
    call model_list%read_model (var_str ("SM_hadrons"), &
      var_str ("SM_hadrons.mdl"), os_data, model)

    write (u, "(A)")  "* Allocate as raw"
    write (u, "(A)")

    call dispatch_eio (eio, var_str ("raw"), var_list, &
      model, event_callback)

    call eio%write (u)

    call eio%final ()
    deallocate (eio)

    write (u, "(A)")
    write (u, "(A)")  "* Allocate as checkpoints:"
    write (u, "(A)")

    call dispatch_eio (eio, var_str ("checkpoint"), var_list, &
      model, event_callback)

    call eio%write (u)

    call eio%final ()
    deallocate (eio)
```

```

write (u, "(A)")
write (u, "(A)")  "* Allocate as LHEF:"
write (u, "(A)")

call var_list%set_string (var_str ("lhef_extension"), &
    var_str ("lhe_custom"), is_known = .true.)
call dispatch_eio (eio, var_str ("lhef"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as HepMC:"
write (u, "(A)")

call dispatch_eio (eio, var_str ("hepmc"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as weight_stream"
write (u, "(A)")

call dispatch_eio (eio, var_str ("weight_stream"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as debug format"
write (u, "(A)")

call var_list%set_log (var_str ("?debug_verbose"), &
    .false., is_known = .true.)
call dispatch_eio (eio, var_str ("debug"), var_list, &
    model, event_callback)

call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
call var_list%final ()

```

```

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_transforms_1"

end subroutine dispatch_transforms_1

```

Event transforms

This test dispatches `evt` (event transform) objects.

```

<Dispatch transforms: execute tests>+≡
  call test (dispatch_transforms_2, "dispatch_transforms_2", &
    "event transforms", &
    u, results)

<Dispatch transforms: test declarations>+≡
  public :: dispatch_transforms_2

<Dispatch transforms: tests>+≡
  subroutine dispatch_transforms_2 (u)
    integer, intent(in) :: u
    type(var_list_t), target :: var_list
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(os_data_t) :: os_data
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(beam_structure_t) :: beam_structure
    class(evt_t), pointer :: evt

    write (u, "(A)")  "* Test output: dispatch_transforms_2"
    write (u, "(A)")  "* Purpose: configure event transform"
    write (u, "(A)")

    call syntax_model_file_init ()
    call var_list%init_defaults (0)
    call os_data%init ()
    call model_list%read_model (var_str ("SM_hadrons"), &
      var_str ("SM_hadrons.mdl"), os_data, model)

    write (u, "(A)")  "* Resonance insertion"
    write (u, "(A)")

    call var_list%set_log (var_str ("?resonance_history"), .true., &
      is_known = .true.)
    call dispatch_evt_resonance (evt, var_list, &
      res_history_set, &
      var_str ("foo_R"))
    call evt%write (u, verbose = .true., more_verbose = .true.)

    call evt%final ()
    deallocate (evt)

    write (u, "(A)")
    write (u, "(A)")  "* ISR handler"

```

```

write (u, "(A)")

call var_list%set_log (var_str ("?isr_handler"), .true., &
  is_known = .true.)
call var_list%set_log (var_str ("?epa_handler"), .false., &
  is_known = .true.)
call var_list%set_string (var_str ("$isr_handler_mode"), &
  var_str ("recoil"), &
  is_known = .true.)
call var_list%set_real (var_str ("sqrts"), 100._default, &
  is_known = .true.)
call var_list%set_real (var_str ("isr_mass"), 511.e-6_default, &
  is_known = .true.)
call dispatch_evt_isr_epa_handler (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* EPA handler"
write (u, "(A)")

call var_list%set_log (var_str ("?isr_handler"), .false., &
  is_known = .true.)
call var_list%set_log (var_str ("?epa_handler"), .true., &
  is_known = .true.)
call var_list%set_string (var_str ("$epa_handler_mode"), &
  var_str ("recoil"), &
  is_known = .true.)
call var_list%set_real (var_str ("sqrts"), 100._default, &
  is_known = .true.)
call var_list%set_real (var_str ("epa_mass"), 511.e-6_default, &
  is_known = .true.)
call dispatch_evt_isr_epa_handler (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* Partonic decays"
write (u, "(A)")

call dispatch_evt_decay (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* Shower"
write (u, "(A)")

```

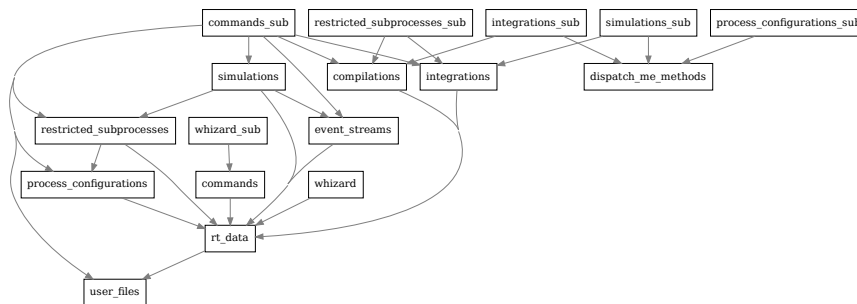


Figure 32.2: Module dependencies in `src/whizard-core`.

```

call var_list%set_log (var_str ("?allow_shower"), .true., &
    is_known = .true.)
call var_list%set_string (var_str ("$shower_method"), &
    var_str ("WHIZARD"), is_known = .true.)
call dispatch_evt_shower (evt, var_list, model, &
    model, os_data, beam_structure)
call evt%write (u)
call write_separator (u, 2)

call evt%final ()
deallocate (evt)

call var_list%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_transforms_2"

end subroutine dispatch_transforms_2

```


Chapter 33

Integration and Simulation

33.1 User-controlled File I/O

The SINDARIN language includes commands that write output to file (input may be added later). We identify files by their name, and manage the unit internally. We need procedures for opening, closing, and printing files.

```
(user_files.f90)≡  
  File header  
  
  module user_files  
  
    Use strings  
    use ifiles  
  
    Standard module head  
  
    User files: public  
  
    User files: types  
  
    User files: interfaces  
  
    interface  
    User files: sub interfaces  
    end interface  
  
  end module user_files  
  
(user_files_sub.f90)≡  
  File header  
  
  submodule (user_files) user_files_s  
  
    use io_units  
    use diagnostics  
    use analysis
```

```

        implicit none

contains

    <User files: procedures>

end submodule user_files_s

```

33.1.1 The file type

This is a type that describes an open user file and its properties. The entry is part of a doubly-linked list.

```

<User files: types>≡
    type :: file_t
    private
    type(string_t) :: name
    integer :: unit = -1
    logical :: reading = .false.
    logical :: writing = .false.
    type(file_t), pointer :: prev => null ()
    type(file_t), pointer :: next => null ()
end type file_t

```

The initializer opens the file.

```

<User files: procedures>≡
    subroutine file_init (file, name, action, status, position)
    type(file_t), intent(out) :: file
    type(string_t), intent(in) :: name
    character(len=*), intent(in) :: action, status, position
    file%unit = free_unit ()
    file%name = name
    open (unit = file%unit, file = char (file%name), &
        action = action, status = status, position = position)
    select case (action)
    case ("read")
        file%reading = .true.
    case ("write")
        file%writing = .true.
    case ("readwrite")
        file%reading = .true.
        file%writing = .true.
    end select
end subroutine file_init

```

The finalizer closes it.

```

<User files: procedures>+≡
    subroutine file_final (file)
    type(file_t), intent(inout) :: file
    close (unit = file%unit)
    file%unit = -1
end subroutine file_final

```

Check if a file is open with correct status.

<User files: procedures>+≡

```
function file_is_open (file, action) result (flag)
  logical :: flag
  type(file_t), intent(in) :: file
  character(*), intent(in) :: action
  select case (action)
  case ("read")
    flag = file%reading
  case ("write")
    flag = file%writing
  case ("readwrite")
    flag = file%reading .and. file%writing
  case default
    call msg_bug ("Checking file '" // char (file%name) &
      // "': illegal action specifier")
  end select
end function file_is_open
```

Return the unit number of a file for direct access. It should be checked first whether the file is open.

<User files: procedures>+≡

```
function file_get_unit (file) result (unit)
  integer :: unit
  type(file_t), intent(in) :: file
  unit = file%unit
end function file_get_unit
```

Write to the file. Error if in wrong mode. If there is no string, just write an empty record. If there is a string, respect the **advancing** option.

<User files: procedures>+≡

```
subroutine file_write_string (file, string, advancing)
  type(file_t), intent(in) :: file
  type(string_t), intent(in), optional :: string
  logical, intent(in), optional :: advancing
  if (file%writing) then
    if (present (string)) then
      if (present (advancing)) then
        if (advancing) then
          write (file%unit, "(A)") char (string)
        else
          write (file%unit, "(A)", advance="no") char (string)
        end if
      else
        write (file%unit, "(A)") char (string)
      end if
    else
      write (file%unit, *)
    end if
  else
    call msg_error ("Writing to file: File '" // char (file%name) &
```

```

        // " is not open for writing.")
    end if
end subroutine file_write_string

```

Write a whole ifile, line by line.

```

<User files: procedures>+≡
subroutine file_write_ifile (file, ifile)
  type(file_t), intent(in) :: file
  type(ifile_t), intent(in) :: ifile
  type(line_p) :: line
  call line_init (line, ifile)
  do while (line_is_associated (line))
    call file_write_string (file, line_get_string_advance (line))
  end do
end subroutine file_write_ifile

```

Write an analysis object (or all objects) to an open file.

```

<User files: procedures>+≡
subroutine file_write_analysis (file, tag)
  type(file_t), intent(in) :: file
  type(string_t), intent(in), optional :: tag
  if (file%writing) then
    if (present (tag)) then
      call analysis_write (tag, unit = file%unit)
    else
      call analysis_write (unit = file%unit)
    end if
  else
    call msg_error ("Writing analysis to file: File " // char (file%name) &
      // " is not open for writing.")
  end if
end subroutine file_write_analysis

```

33.1.2 The file list

We maintain a list of all open files and their attributes. The list must be doubly-linked because we may delete entries.

```

<User files: public>≡
  public :: file_list_t

<User files: types>+≡
  type :: file_list_t
    type(file_t), pointer :: first => null ()
    type(file_t), pointer :: last => null ()
  end type file_list_t

```

There is no initialization routine, but a finalizer which deletes all:

```

<User files: public>+≡
  public :: file_list_final

```

```

<User files: sub interfaces>≡
    module subroutine file_list_final (file_list)
        type(file_list_t), intent(inout) :: file_list
    end subroutine file_list_final

```

```

<User files: procedures>+≡
    module subroutine file_list_final (file_list)
        type(file_list_t), intent(inout) :: file_list
        type(file_t), pointer :: current
        do while (associated (file_list%first))
            current => file_list%first
            file_list%first => current%next
            call file_final (current)
            deallocate (current)
        end do
        file_list%last => null ()
    end subroutine file_list_final

```

Find an entry in the list. Return null pointer on failure.

```

<User files: procedures>+≡
    function file_list_get_file_ptr (file_list, name) result (current)
        type(file_t), pointer :: current
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        current => file_list%first
        do while (associated (current))
            if (current%name == name) return
            current => current%next
        end do
    end function file_list_get_file_ptr

```

Check if a file is open, public version:

```

<User files: public>+≡
    public :: file_list_is_open

<User files: sub interfaces>+≡
    module function file_list_is_open (file_list, name, action) result (flag)
        logical :: flag
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        character(len=*), intent(in) :: action
    end function file_list_is_open

<User files: procedures>+≡
    module function file_list_is_open (file_list, name, action) result (flag)
        logical :: flag
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        character(len=*), intent(in) :: action
        type(file_t), pointer :: current
        current => file_list_get_file_ptr (file_list, name)
        if (associated (current)) then
            flag = file_is_open (current, action)
        else
            flag = .false.
        end if
    end function file_list_is_open

```

```

        end if
    end function file_list_is_open

```

Return the unit number for a file. It should be checked first whether the file is open.

```

<User files: public>+=
    public :: file_list_get_unit

<User files: sub interfaces>+=
    module function file_list_get_unit (file_list, name) result (unit)
        integer :: unit
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
    end function file_list_get_unit

<User files: procedures>+=
    module function file_list_get_unit (file_list, name) result (unit)
        integer :: unit
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        type(file_t), pointer :: current
        current => file_list_get_file_ptr (file_list, name)
        if (associated (current)) then
            unit = file_get_unit (current)
        else
            unit = -1
        end if
    end function file_list_get_unit

```

Append a new file entry, i.e., open this file. Error if it is already open.

```

<User files: public>+=
    public :: file_list_open

<User files: sub interfaces>+=
    module subroutine file_list_open (file_list, name, action, status, position)
        type(file_list_t), intent(inout) :: file_list
        type(string_t), intent(in) :: name
        character(len=*), intent(in) :: action, status, position
    end subroutine file_list_open

<User files: procedures>+=
    module subroutine file_list_open (file_list, name, action, status, position)
        type(file_list_t), intent(inout) :: file_list
        type(string_t), intent(in) :: name
        character(len=*), intent(in) :: action, status, position
        type(file_t), pointer :: current
        if (.not. associated (file_list_get_file_ptr (file_list, name))) then
            allocate (current)
            call msg_message ("Opening file '" // char (name) // "' for output")
            call file_init (current, name, action, status, position)
            if (associated (file_list%last)) then
                file_list%last%next => current
                current%prev => file_list%last
            else
                file_list%first => current
            end if
        end if
    end subroutine file_list_open

```

```

        end if
        file_list%last => current
    else
        call msg_error ("Opening file: File '" // char (name) &
            // "' is already open.")
    end if
end subroutine file_list_open

```

Delete a file entry, i.e., close this file. Error if it is not open.

```

<User files: public>+≡
    public :: file_list_close

<User files: sub interfaces>+≡
    module subroutine file_list_close (file_list, name)
        type(file_list_t), intent(inout) :: file_list
        type(string_t), intent(in) :: name
    end subroutine file_list_close

<User files: procedures>+≡
    module subroutine file_list_close (file_list, name)
        type(file_list_t), intent(inout) :: file_list
        type(string_t), intent(in) :: name
        type(file_t), pointer :: current
        current => file_list_get_file_ptr (file_list, name)
        if (associated (current)) then
            if (associated (current%prev)) then
                current%prev%next => current%next
            else
                file_list%first => current%next
            end if
            if (associated (current%next)) then
                current%next%prev => current%prev
            else
                file_list%last => current%prev
            end if
            call msg_message ("Closing file '" // char (name) // "' for output")
            call file_final (current)
            deallocate (current)
        else
            call msg_error ("Closing file: File '" // char (name) &
                // "' is not open.")
        end if
    end subroutine file_list_close

```

Write a string to file. Error if it is not open.

```

<User files: public>+≡
    public :: file_list_write

<User files: interfaces>≡
    interface file_list_write
        module procedure file_list_write_string
        module procedure file_list_write_ifile
    end interface

```

```

<User files: sub interfaces>+≡
  module subroutine file_list_write_ifile (file_list, name, ifile)
    type(file_list_t), intent(in) :: file_list
    type(string_t), intent(in) :: name
    type(ifile_t), intent(in) :: ifile
  end subroutine file_list_write_ifile
  module subroutine file_list_write_string &
    (file_list, name, string, advancing)
    type(file_list_t), intent(in) :: file_list
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: string
    logical, intent(in), optional :: advancing
  end subroutine file_list_write_string

<User files: procedures>+≡
  module subroutine file_list_write_string (file_list, name, string, advancing)
    type(file_list_t), intent(in) :: file_list
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: string
    logical, intent(in), optional :: advancing
    type(file_t), pointer :: current
    current => file_list_get_file_ptr (file_list, name)
    if (associated (current)) then
      call file_write_string (current, string, advancing)
    else
      call msg_error ("Writing to file: File '" // char (name) &
        // "'is not open.")
    end if
  end subroutine file_list_write_string

  module subroutine file_list_write_ifile (file_list, name, ifile)
    type(file_list_t), intent(in) :: file_list
    type(string_t), intent(in) :: name
    type(ifile_t), intent(in) :: ifile
    type(file_t), pointer :: current
    current => file_list_get_file_ptr (file_list, name)
    if (associated (current)) then
      call file_write_ifile (current, ifile)
    else
      call msg_error ("Writing to file: File '" // char (name) &
        // "'is not open.")
    end if
  end subroutine file_list_write_ifile

```

Write an analysis object or all objects to data file. Error if it is not open. If the file name is empty, write to standard output.

```

<User files: public>+≡
  public :: file_list_write_analysis

<User files: sub interfaces>+≡
  module subroutine file_list_write_analysis (file_list, name, tag)
    type(file_list_t), intent(in) :: file_list
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: tag
  end subroutine file_list_write_analysis

```



```

<User files: procedures>+≡
module subroutine file_list_write_analysis (file_list, name, tag)
  type(file_list_t), intent(in) :: file_list
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: tag
  type(file_t), pointer :: current
  if (name == "") then
    if (present (tag)) then
      call analysis_write (tag)
    else
      call analysis_write
    end if
  else
    current => file_list_get_file_ptr (file_list, name)
    if (associated (current)) then
      call file_write_analysis (current, tag)
    else
      call msg_error ("Writing analysis to file: File '" // char (name) &
        // "' is not open.")
    end if
  end if
end subroutine file_list_write_analysis

```

33.2 Runtime data

```
<rt_data.f90>≡
  <File header>

  module rt_data

    <Use kinds>
    <Use strings>
    use os_interface
    use lexers
    use parser
    use models
    use subevents
    use pdg_arrays
    use variables, only: var_list_t
    use process_libraries
    use prclib_stacks
    use prc_core, only: helicity_selection_t
    use beam_structures
    use event_base, only: event_callback_t
    use user_files
    use process_stacks
    use iterations

    <Standard module head>

    <RT data: public>

    <RT data: types>

    interface
    <RT data: sub interfaces>
    end interface

    contains

    <RT data: main procedures>

  end module rt_data

<rt_data_sub.f90>≡
  <File header>

  submodule (rt_data) rt_data_s

    use io_units
    use format_utils, only: write_separator
    use format_defs, only: FMT_19, FMT_12
    use system_dependencies
    use diagnostics

    implicit none

    contains
```

```

    <RT data: procedures>

end submodule rt_data_s

```

33.2.1 Strategy for models and variables

The program manages its data via a main `rt_data_t` object. During program flow, various commands create and use local `rt_data_t` objects. Those transient blocks contain either pointers to global object or local copies which are deleted after use.

Each `rt_data_t` object contains a variable list component. This lists holds (local copies of) all kinds of intrinsic or user-defined variables. The variable list is linked to the variable list contained in the local process library. This, in turn, is linked to the variable list of the `rt_data_t` context, and so on.

A variable lookup will thus be recursively delegated to the linked variable lists, until a match is found. When modifying a variable which is not yet local, the program creates a local copy and uses this afterwards. Thus, when the local `rt_data_t` object is deleted, the context value is recovered.

Models are kept in a model list which is separate from the variable list. Otherwise, they are treated in a similar manner: the local list is linked to the context model list. Model lookup is thus recursively delegated. When a model or any part of it is modified, the model is copied to the local `rt_data_t` object, so the context model is not modified. Commands such as `integrate` will create their own copy of the current model (and of the current variable list) at the point where they are executed.

When a model is encountered for the first time, it is read from file. The reading is automatically delegated to the global context. Thus, this master copy survives until the main `rt_data_t` object is deleted, at program completion.

If there is a currently active model, its variable list is linked to the main variable list. Variable lookups will then start from the model variable list. When the current model is switched, the new active model will get this link instead. Consequently, a change to the current model is kept as long as this model has a local copy; it survives local model switches. On the other hand, a parameter change in the current model doesn't affect any other model, even if the parameter name is identical.

33.2.2 Container for parse nodes

The runtime data set contains a bunch of parse nodes (chunks of code that have not been compiled into evaluation trees but saved for later use). We collect them here.

This implementation has the useful effect that an assignment between two objects of this type will establish a pointer-target relationship for all components.

```

<RT data: types>≡
  type :: rt_parse_nodes_t
    type(parse_node_t), pointer :: cuts_lexpr => null ()
    type(parse_node_t), pointer :: scale_expr => null ()

```

```

        type(parse_node_t), pointer :: fac_scale_expr => null ()
        type(parse_node_t), pointer :: ren_scale_expr => null ()
        type(parse_node_t), pointer :: weight_expr => null ()
        type(parse_node_t), pointer :: selection_lexpr => null ()
        type(parse_node_t), pointer :: reweight_expr => null ()
        type(parse_node_t), pointer :: analysis_lexpr => null ()
        type(parse_node_p), dimension(:), allocatable :: alt_setup
contains
  <RT data: rt parse nodes: TBP>
end type rt_parse_nodes_t

```

Clear individual components. The parse nodes are nullified. No finalization needed since the pointer targets are part of the global parse tree.

```

  <RT data: rt parse nodes: TBP>≡
    procedure :: clear => rt_parse_nodes_clear

  <RT data: sub interfaces>≡
    module subroutine rt_parse_nodes_clear (rt_pn, name)
      class(rt_parse_nodes_t), intent(inout) :: rt_pn
      type(string_t), intent(in) :: name
    end subroutine rt_parse_nodes_clear

  <RT data: procedures>≡
    module subroutine rt_parse_nodes_clear (rt_pn, name)
      class(rt_parse_nodes_t), intent(inout) :: rt_pn
      type(string_t), intent(in) :: name
      select case (char (name))
      case ("cuts")
        rt_pn%cuts_lexpr => null ()
      case ("scale")
        rt_pn%scale_expr => null ()
      case ("factorization_scale")
        rt_pn%fac_scale_expr => null ()
      case ("renormalization_scale")
        rt_pn%ren_scale_expr => null ()
      case ("weight")
        rt_pn%weight_expr => null ()
      case ("selection")
        rt_pn%selection_lexpr => null ()
      case ("reweight")
        rt_pn%reweight_expr => null ()
      case ("analysis")
        rt_pn%analysis_lexpr => null ()
      end select
    end subroutine rt_parse_nodes_clear

```

Output for the parse nodes.

```

  <RT data: rt parse nodes: TBP>+≡
    procedure :: write => rt_parse_nodes_write

  <RT data: sub interfaces>+≡
    module subroutine rt_parse_nodes_write (object, unit)
      class(rt_parse_nodes_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine rt_parse_nodes_write

```

```

<RT data: procedures>+≡
module subroutine rt_parse_nodes_write (object, unit)
  class(rt_parse_nodes_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  call wrt ("Cuts", object%cuts_lexpr)
  call write_separator (u)
  call wrt ("Scale", object%scale_expr)
  call write_separator (u)
  call wrt ("Factorization scale", object%fac_scale_expr)
  call write_separator (u)
  call wrt ("Renormalization scale", object%ren_scale_expr)
  call write_separator (u)
  call wrt ("Weight", object%weight_expr)
  call write_separator (u, 2)
  call wrt ("Event selection", object%selection_lexpr)
  call write_separator (u)
  call wrt ("Event reweighting factor", object%reweight_expr)
  call write_separator (u)
  call wrt ("Event analysis", object%analysis_lexpr)
  if (allocated (object%alt_setup)) then
    call write_separator (u, 2)
    write (u, "(1x,A,':')") "Alternative setups"
    do i = 1, size (object%alt_setup)
      call write_separator (u)
      call wrt ("Commands", object%alt_setup(i)%ptr)
    end do
  end if
contains
  subroutine wrt (title, pn)
    character(*), intent(in) :: title
    type(parse_node_t), intent(in), pointer :: pn
    if (associated (pn)) then
      write (u, "(1x,A,':')") title
      call write_separator (u)
      call parse_node_write_rec (pn, u)
    else
      write (u, "(1x,A,':',1x,A)") title, "[undefined]"
    end if
  end subroutine wrt
end subroutine rt_parse_nodes_write

```

Screen output for individual components. (This should eventually be more condensed, currently we print the internal representation tree.)

```

<RT data: rt parse nodes: TBP>+≡
  procedure :: show => rt_parse_nodes_show

<RT data: sub interfaces>+≡
  module subroutine rt_parse_nodes_show (rt_pn, name, unit)
    class(rt_parse_nodes_t), intent(in) :: rt_pn
    type(string_t), intent(in) :: name
    integer, intent(in), optional :: unit
  end subroutine rt_parse_nodes_show

```

```

<RT data: procedures>+≡
module subroutine rt_parse_nodes_show (rt_pn, name, unit)
  class(rt_parse_nodes_t), intent(in) :: rt_pn
  type(string_t), intent(in) :: name
  integer, intent(in), optional :: unit
  type(parse_node_t), pointer :: pn
  integer :: u
  u = given_output_unit (unit)
  select case (char (name))
  case ("cuts")
    pn => rt_pn%cuts_lexpr
  case ("scale")
    pn => rt_pn%scale_expr
  case ("factorization_scale")
    pn => rt_pn%fac_scale_expr
  case ("renormalization_scale")
    pn => rt_pn%ren_scale_expr
  case ("weight")
    pn => rt_pn%weight_expr
  case ("selection")
    pn => rt_pn%selection_lexpr
  case ("reweight")
    pn => rt_pn%reweight_expr
  case ("analysis")
    pn => rt_pn%analysis_lexpr
  end select
  if (associated (pn)) then
    write (u, "(A,1x,A,1x,A)") "Expression:", char (name), "(parse tree):"
    call parse_node_write_rec (pn, u)
  else
    write (u, "(A,1x,A,A)") "Expression:", char (name), ": [undefined]"
  end if
end subroutine rt_parse_nodes_show

```

33.2.3 The data type

This is a big data container which contains everything that is used and modified during the command flow. A local copy of this can be used to temporarily override defaults. The data set is transparent.

```

<RT data: public>≡
  public :: rt_data_t

<RT data: types>+≡
  type :: rt_data_t
    type(lexer_t), pointer :: lexer => null ()
    type(rt_data_t), pointer :: context => null ()
    type(string_t), dimension(:), allocatable :: export
    type(var_list_t) :: var_list
    type(iterations_list_t) :: it_list
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model => null ()
    logical :: model_is_copy = .false.

```

```

type(model_t), pointer :: preload_model => null ()
type(model_t), pointer :: fallback_model => null ()
type(prclib_stack_t) :: prclib_stack
type(process_library_t), pointer :: prclib => null ()
type(beam_structure_t) :: beam_structure
type(rt_parse_nodes_t) :: pn
type(process_stack_t) :: process_stack
type(string_t), dimension(:), allocatable :: sample_fmt
class(event_callback_t), allocatable :: event_callback
type(file_list_t), pointer :: out_files => null ()
logical :: quit = .false.
integer :: quit_code = 0
type(string_t) :: logfile
logical :: nlo_fixed_order = .false.
logical, dimension(0:5) :: selected_nlo_parts = .false.
integer, dimension(:), allocatable :: nlo_component
contains
  <RT data: rt data: TBP>
end type rt_data_t

```

33.2.4 Output

```

<RT data: rt data: TBP>≡
  procedure :: write => rt_data_write

<RT data: sub interfaces>+≡
  module subroutine rt_data_write (object, unit, vars, pacify)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(string_t), dimension(:), intent(in), optional :: vars
    logical, intent(in), optional :: pacify
  end subroutine rt_data_write

<RT data: procedures>+≡
  module subroutine rt_data_write (object, unit, vars, pacify)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(string_t), dimension(:), intent(in), optional :: vars
    logical, intent(in), optional :: pacify
    integer :: u, i
    u = given_output_unit (unit)
    call write_separator (u, 2)
    write (u, "(1x,A)") "Runtime data:"
    if (object%get_n_export () > 0) then
      call write_separator (u, 2)
      write (u, "(1x,A)") "Exported objects and variables:"
      call write_separator (u)
      call object%write_exports (u)
    end if
    if (present (vars)) then
      if (size (vars) /= 0) then
        call write_separator (u, 2)
        write (u, "(1x,A)") "Selected variables:"
        call write_separator (u)
      end if
    end if
  end subroutine rt_data_write

```

```

        call object%write_vars (u, vars)
    end if
else
    call write_separator (u, 2)
    if (associated (object%model)) then
        call object%model%write_var_list (u, follow_link=.true.)
    else
        call object%var_list%write (u, follow_link=.true.)
    end if
end if
if (object%it_list%get_n_pass () > 0) then
    call write_separator (u, 2)
    write (u, "(1x)", advance="no")
    call object%it_list%write (u)
end if
if (associated (object%model)) then
    call write_separator (u, 2)
    call object%model%write (u)
end if
call object%prclib_stack%write (u)
call object%beam_structure%write (u)
call write_separator (u, 2)
call object%pn%write (u)
if (allocated (object%sample_fmt)) then
    call write_separator (u)
    write (u, "(1x,A)", advance="no") "Event sample formats = "
    do i = 1, size (object%sample_fmt)
        if (i > 1) write (u, "(A,1x)", advance="no") ", "
        write (u, "(A)", advance="no") char (object%sample_fmt(i))
    end do
    write (u, "(A)")
end if
call write_separator (u)
write (u, "(1x,A)", advance="no") "Event callback:"
if (allocated (object%event_callback)) then
    call object%event_callback%write (u)
else
    write (u, "(1x,A)") "[undefined]"
end if
call object%process_stack%write (u, pacify)
write (u, "(1x,A,1x,L1)") "quit      :", object%quit
write (u, "(1x,A,1x,I0)") "quit_code:", object%quit_code
call write_separator (u, 2)
write (u, "(1x,A,1x,A)") "Logfile  :", "" // trim (char (object%logfile)) // ""
call write_separator (u, 2)
end subroutine rt_data_write

```

Write only selected variables.

<RT data: rt data: TBP>+≡

```
procedure :: write_vars => rt_data_write_vars
```

<RT data: sub interfaces>+≡

```
module subroutine rt_data_write_vars (object, unit, vars)
    class(rt_data_t), intent(in), target :: object

```



```

        integer, intent(in), optional :: unit
        type(string_t), dimension(:), intent(in) :: vars
    end subroutine rt_data_write_vars

<RT data: procedures>+≡
module subroutine rt_data_write_vars (object, unit, vars)
    class(rt_data_t), intent(in), target :: object
    integer, intent(in), optional :: unit
    type(string_t), dimension(:), intent(in) :: vars
    type(var_list_t), pointer :: var_list
    integer :: u, i
    u = given_output_unit (unit)
    var_list => object%get_var_list_ptr ()
    do i = 1, size (vars)
        associate (var => vars(i))
            if (var_list%contains (var, follow_link=.true.)) then
                call var_list%write_var (var, unit = u, &
                    follow_link = .true., defined=.true.)
            end if
        end associate
    end do
end subroutine rt_data_write_vars

```

Write only the model list.

```

<RT data: rt data: TBP>+≡
    procedure :: write_model_list => rt_data_write_model_list

<RT data: sub interfaces>+≡
    module subroutine rt_data_write_model_list (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine rt_data_write_model_list

<RT data: procedures>+≡
module subroutine rt_data_write_model_list (object, unit)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    call object%model_list%write (u)
end subroutine rt_data_write_model_list

```

Write only the library stack.

```

<RT data: rt data: TBP>+≡
    procedure :: write_libraries => rt_data_write_libraries

<RT data: sub interfaces>+≡
    module subroutine rt_data_write_libraries (object, unit, libpath)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
    end subroutine rt_data_write_libraries

<RT data: procedures>+≡
module subroutine rt_data_write_libraries (object, unit, libpath)

```

```

class(rt_data_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: libpath
integer :: u
u = given_output_unit (unit)
call object%prclib_stack%write (u, libpath)
end subroutine rt_data_write_libraries

```

Write only the beam data.

```

<RT data: rt data: TBP>+≡
  procedure :: write_beams => rt_data_write_beams

<RT data: sub interfaces>+≡
  module subroutine rt_data_write_beams (object, unit)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine rt_data_write_beams

<RT data: procedures>+≡
  module subroutine rt_data_write_beams (object, unit)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call object%beam_structure%write (u)
    call write_separator (u, 2)
  end subroutine rt_data_write_beams

```

Write only the process and event expressions.

```

<RT data: rt data: TBP>+≡
  procedure :: write_expr => rt_data_write_expr

<RT data: sub interfaces>+≡
  module subroutine rt_data_write_expr (object, unit)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine rt_data_write_expr

<RT data: procedures>+≡
  module subroutine rt_data_write_expr (object, unit)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call object%pn%write (u)
    call write_separator (u, 2)
  end subroutine rt_data_write_expr

```

Write only the process stack.

```

<RT data: rt data: TBP>+≡
  procedure :: write_process_stack => rt_data_write_process_stack

```

```

<RT data: sub interfaces>+≡
    module subroutine rt_data_write_process_stack (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine rt_data_write_process_stack

<RT data: procedures>+≡
    module subroutine rt_data_write_process_stack (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call object%process_stack%write (unit)
    end subroutine rt_data_write_process_stack

<RT data: rt data: TBP>+≡
    procedure :: write_var_descriptions => rt_data_write_var_descriptions

<RT data: sub interfaces>+≡
    module subroutine rt_data_write_var_descriptions &
        (rt_data, unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output
    end subroutine rt_data_write_var_descriptions

<RT data: procedures>+≡
    module subroutine rt_data_write_var_descriptions (rt_data, unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output
        integer :: u
        logical :: ao
        u = given_output_unit (unit)
        ao = .false.; if (present (ascii_output)) ao = ascii_output
        call rt_data%var_list%write (u, follow_link=.true., &
            descriptions=.true., ascii_output=ao)
    end subroutine rt_data_write_var_descriptions

<RT data: rt data: TBP>+≡
    procedure :: show_description_of_string => rt_data_show_description_of_string

<RT data: sub interfaces>+≡
    module subroutine rt_data_show_description_of_string (rt_data, string, &
        unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        type(string_t), intent(in) :: string
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output
    end subroutine rt_data_show_description_of_string

<RT data: procedures>+≡
    module subroutine rt_data_show_description_of_string (rt_data, string, &
        unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        type(string_t), intent(in) :: string
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output

```

```

integer :: u
logical :: ao
u = given_output_unit (unit)
ao = .false.; if (present (ascii_output)) ao = ascii_output
call rt_data%var_list%write_var (string, unit=u, follow_link=.true., &
    defined=.false., descriptions=.true., ascii_output=ao)
end subroutine rt_data_show_description_of_string

```

33.2.5 Clear

The `clear` command can remove the contents of various subobjects. The objects themselves should stay.

```

<RT data: rt data: TBP>+≡
    procedure :: clear_beams => rt_data_clear_beams

<RT data: sub interfaces>+≡
    module subroutine rt_data_clear_beams (global)
        class(rt_data_t), intent(inout) :: global
    end subroutine rt_data_clear_beams

<RT data: procedures>+≡
    module subroutine rt_data_clear_beams (global)
        class(rt_data_t), intent(inout) :: global
        call global%beam_structure%final_sf ()
        call global%beam_structure%final_pol ()
        call global%beam_structure%final_mom ()
    end subroutine rt_data_clear_beams

```

33.2.6 Initialization

Initialize runtime data. This defines special variables such as `sqrts`, and should be done only for the instance that is actually global. Local copies will inherit the special variables.

We link the global variable list to the process stack variable list, so the latter is always available (and kept global).

```

<RT data: rt data: TBP>+≡
    procedure :: global_init => rt_data_global_init

<RT data: sub interfaces>+≡
    module subroutine rt_data_global_init (global, paths, logfile)
        class(rt_data_t), intent(out), target :: global
        type(paths_t), intent(in), optional :: paths
        type(string_t), intent(in), optional :: logfile
    end subroutine rt_data_global_init

<RT data: procedures>+≡
    module subroutine rt_data_global_init (global, paths, logfile)
        class(rt_data_t), intent(out), target :: global
        type(paths_t), intent(in), optional :: paths
        type(string_t), intent(in), optional :: logfile
        integer :: seed
        call global%os_data%init (paths)
    end subroutine rt_data_global_init

```

```

if (present (logfile)) then
  global%logfile = logfile
else
  global%logfile = ""
end if
allocate (global%out_files)
call system_clock (seed)
call global%var_list%init_defaults (seed, paths)
call global%init_pointer_variables ()
call global%process_stack%init_var_list (global%var_list)
end subroutine rt_data_global_init

```

33.2.7 Local copies

This is done at compile time when a local copy of runtime data is needed: Link the variable list and initialize all derived parameters. This allows for synchronizing them with local variable changes without affecting global data.

Also re-initialize pointer variables, so they point to local copies of their targets.

```

<RT data: rt data: TBP>+≡
  procedure :: local_init => rt_data_local_init

<RT data: sub interfaces>+≡
  module subroutine rt_data_local_init (local, global, env)
    class(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(in), target :: global
    integer, intent(in), optional :: env
  end subroutine rt_data_local_init

<RT data: procedures>+≡
  module subroutine rt_data_local_init (local, global, env)
    class(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(in), target :: global
    integer, intent(in), optional :: env
    local%context => global
    call local%process_stack%link (global%process_stack)
    call local%process_stack%init_var_list (local%var_list)
    call local%process_stack%link_var_list (global%var_list)
    call local%var_list%append_string (var_str ("model_name"), &
      var_str (""), intrinsic=.true.)
    call local%init_pointer_variables ()
    local%fallback_model => global%fallback_model
    local%os_data = global%os_data
    local%logfile = global%logfile
    call local%model_list%link (global%model_list)
    local%model => global%model
    if (associated (local%model)) then
      call local%model%link_var_list (local%var_list)
    end if
    if (allocated (global%event_callback)) then
      allocate (local%event_callback, source = global%event_callback)
    end if
  end subroutine rt_data_local_init

```

These variables point to objects which get local copies:

```

<RT data: rt data: TBP>+≡
    procedure :: init_pointer_variables => rt_data_init_pointer_variables

<RT data: sub interfaces>+≡
    module subroutine rt_data_init_pointer_variables (local)
        class(rt_data_t), intent(inout), target :: local
    end subroutine rt_data_init_pointer_variables

<RT data: procedures>+≡
    module subroutine rt_data_init_pointer_variables (local)
        class(rt_data_t), intent(inout), target :: local
        logical, target, save :: known = .true.
        call local%var_list%append_string_ptr (var_str ("%fc"), &
            local%os_data%fc, known, intrinsic=.true., &
            description=var_str('This string variable gives the ' // &
                '\ttt{Fortran} compiler used within \whizard. It can ' // &
                'only be accessed, not set by the user. (cf. also ' // &
                '\ttt{\$fcflags}, \ttt{\$fclibs}'))))
        call local%var_list%append_string_ptr (var_str ("%fcflags"), &
            local%os_data%fcflags, known, intrinsic=.true., &
            description=var_str('This string variable gives the ' // &
                'compiler flags for the \ttt{Fortran} compiler used ' // &
                'within \whizard. It can only be accessed, not set by ' // &
                'the user. (cf. also \ttt{\$fc}, \ttt{\$fclibs}'))))
        call local%var_list%append_string_ptr (var_str ("%fclibs"), &
            local%os_data%fclibs, known, intrinsic=.true., &
            description=var_str('This string variable gives the ' // &
                'linked libraries for the \ttt{Fortran} compiler used ' // &
                'within \whizard. It can only be accessed, not set by ' // &
                'the user. (cf. also \ttt{\$fc}, \ttt{\$fcflags}'))))
    end subroutine rt_data_init_pointer_variables

```

This is done at execution time: Copy data, transfer pointers. `local` has `intent(inout)` because its local variable list has already been prepared by the previous routine.

To be pedantic, the local pointers to model and library should point to the entries in the local copies. (However, as long as these are just shallow copies with identical content, this is actually irrelevant.)

The process library and process stacks behave as global objects. The copies of the process library and process stacks should be shallow copies, so the contents stay identical. Since objects may be pushed on the stack in the local environment, upon restoring the global environment, we should reverse the assignment. Then the added stack elements will end up on the global stack. (This should be reconsidered in a parallel environment.)

Gfortran 7/8/9 bug, has to remain in the main module:

```

<RT data: rt data: TBP>+≡
    procedure :: activate => rt_data_activate

<RT data: main procedures>≡
    subroutine rt_data_activate (local)
        class(rt_data_t), intent(inout), target :: local

```

```

class(rt_data_t), pointer :: global
global => local%context
if (associated (global)) then
    local%lexer => global%lexer
    call global%copy_globals (local)
    local%os_data = global%os_data
    local%logfile = global%logfile
    if (associated (global%prclib)) then
        local%prclib => &
            local%prclib_stack%get_library_ptr (global%prclib%get_name ())
    end if
    call local%import_values ()
    call local%process_stack%link (global%process_stack)
    local%it_list = global%it_list
    local%beam_structure = global%beam_structure
    local%pn = global%pn
    if (allocated (local%sample_fmt)) deallocate (local%sample_fmt)
    if (allocated (global%sample_fmt)) then
        allocate (local%sample_fmt (size (global%sample_fmt)), &
            source = global%sample_fmt)
    end if
    local%out_files => global%out_files
    local%model => global%model
    local%model_is_copy = .false.
else if (.not. associated (local%model)) then
    local%model => local%preload_model
    local%model_is_copy = .false.
end if
if (associated (local%model)) then
    call local%model%link_var_list (local%var_list)
    call local%var_list%set_string (var_str ("model_name"), &
        local%model%get_name (), is_known = .true.)
else
    call local%var_list%set_string (var_str ("model_name"), &
        var_str (""), is_known = .false.)
end if
end subroutine rt_data_activate

```

Restore the previous state of data, without actually finalizing the local environment. We also clear the local process stack. Some local modifications (model list and process library stack) are communicated to the global context, if there is any.

If the `keep_local` flag is set, we want to retain current settings in the local environment. In particular, we create an instance of the currently selected model (which thus becomes separated from the model library!). The local variables are also kept.

```

<RT data: rt data: TBP>+≡
    procedure :: deactivate => rt_data_deactivate

<RT data: sub interfaces>+≡
    module subroutine rt_data_deactivate (local, global, keep_local)
        class(rt_data_t), intent(inout), target :: local
        class(rt_data_t), intent(inout), optional, target :: global
    end subroutine

```

```

        logical, intent(in), optional :: keep_local
    end subroutine rt_data_deactivate

<RT data: procedures>+≡
module subroutine rt_data_deactivate (local, global, keep_local)
    class(rt_data_t), intent(inout), target :: local
    class(rt_data_t), intent(inout), optional, target :: global
    logical, intent(in), optional :: keep_local
    type(string_t) :: local_model, local_scheme
    logical :: same_model, delete
    delete = .true.; if (present (keep_local)) delete = .not. keep_local
    if (present (global)) then
        if (associated (global%model) .and. associated (local%model)) then
            local_model = local%model%get_name ()
            if (global%model%has_schemes ()) then
                local_scheme = local%model%get_scheme ()
                same_model = &
                    global%model%matches (local_model, local_scheme)
            else
                same_model = global%model%matches (local_model)
            end if
        else
            same_model = .false.
        end if
        if (delete) then
            call local%process_stack%clear ()
            call local%unselect_model ()
            call local%unset_values ()
        else if (associated (local%model)) then
            call local%ensure_model_copy ()
        end if
        if (.not. same_model .and. associated (global%model)) then
            if (global%model%has_schemes ()) then
                call msg_message ("Restoring model '" // &
                    char (global%model%get_name ()) // "', scheme '" // &
                    char (global%model%get_scheme ()) // "'")
            else
                call msg_message ("Restoring model '" // &
                    char (global%model%get_name ()) // "'")
            end if
        end if
        if (associated (global%model)) then
            call global%model%link_var_list (global%var_list)
        end if
        call global%restore_globals (local)
    else
        call local%unselect_model ()
    end if
end subroutine rt_data_deactivate

```

This imports the global objects for which local modifications should be kept. Currently, this is only the process library stack.

```

<RT data: rt data: TBP>+≡
procedure :: copy_globals => rt_data_copy_globals

```



```

<RT data: sub interfaces>+≡
  module subroutine rt_data_copy_globals (global, local)
    class(rt_data_t), intent(in) :: global
    class(rt_data_t), intent(inout) :: local
  end subroutine rt_data_copy_globals

```

```

<RT data: procedures>+≡
  module subroutine rt_data_copy_globals (global, local)
    class(rt_data_t), intent(in) :: global
    class(rt_data_t), intent(inout) :: local
    local%prclib_stack = global%prclib_stack
  end subroutine rt_data_copy_globals

```

This restores global objects for which local modifications should be kept. May also modify (remove) the local objects.

```

<RT data: rt data: TBP>+≡
  procedure :: restore_globals => rt_data_restore_globals

<RT data: sub interfaces>+≡
  module subroutine rt_data_restore_globals (global, local)
    class(rt_data_t), intent(inout) :: global
    class(rt_data_t), intent(inout) :: local
  end subroutine rt_data_restore_globals

<RT data: procedures>+≡
  module subroutine rt_data_restore_globals (global, local)
    class(rt_data_t), intent(inout) :: global
    class(rt_data_t), intent(inout) :: local
    global%prclib_stack = local%prclib_stack
    call local%handle_exports (global)
  end subroutine rt_data_restore_globals

```

33.2.8 Exported objects

Exported objects are transferred to the global state when a local environment is closed. (For the top-level global data set, there is no effect.)

The current implementation handles only the **results** object, which resolves to the local process stack. The stack elements are appended to the global stack without modification, the local stack becomes empty.

Write names of objects to be exported:

```

<RT data: rt data: TBP>+≡
  procedure :: write_exports => rt_data_write_exports

<RT data: sub interfaces>+≡
  module subroutine rt_data_write_exports (rt_data, unit)
    class(rt_data_t), intent(in) :: rt_data
    integer, intent(in), optional :: unit
  end subroutine rt_data_write_exports

<RT data: procedures>+≡
  module subroutine rt_data_write_exports (rt_data, unit)
    class(rt_data_t), intent(in) :: rt_data
    integer, intent(in), optional :: unit
    integer :: u, i

```

```

    u = given_output_unit (unit)
    do i = 1, rt_data%get_n_export ()
        write (u, "(A)") char (rt_data%export(i))
    end do
end subroutine rt_data_write_exports

```

The number of entries in the export list.

```

<RT data: rt data: TBP>+≡
    procedure :: get_n_export => rt_data_get_n_export

<RT data: sub interfaces>+≡
    module function rt_data_get_n_export (rt_data) result (n)
        class(rt_data_t), intent(in) :: rt_data
        integer :: n
    end function rt_data_get_n_export

<RT data: procedures>+≡
    module function rt_data_get_n_export (rt_data) result (n)
        class(rt_data_t), intent(in) :: rt_data
        integer :: n
        if (allocated (rt_data%export)) then
            n = size (rt_data%export)
        else
            n = 0
        end if
    end function rt_data_get_n_export

```

Return a specific export Append new names to the export list. If a duplicate occurs, do not transfer it.

```

<RT data: rt data: TBP>+≡
    procedure :: append_exports => rt_data_append_exports

<RT data: sub interfaces>+≡
    module subroutine rt_data_append_exports (rt_data, export)
        class(rt_data_t), intent(inout) :: rt_data
        type(string_t), dimension(:), intent(in) :: export
    end subroutine rt_data_append_exports

<RT data: procedures>+≡
    module subroutine rt_data_append_exports (rt_data, export)
        class(rt_data_t), intent(inout) :: rt_data
        type(string_t), dimension(:), intent(in) :: export
        logical, dimension(:), allocatable :: mask
        type(string_t), dimension(:), allocatable :: tmp
        integer :: i, j, n
        if (.not. allocated (rt_data%export)) allocate (rt_data%export (0))
        n = size (rt_data%export)
        allocate (mask (size (export)), source=.false.)
        do i = 1, size (export)
            mask(i) = all (export(i) /= rt_data%export) &
                .and. all (export(i) /= export(:i-1))
        end do
        if (count (mask) > 0) then
            allocate (tmp (n + count (mask)))
            tmp(1:n) = rt_data%export(:)

```

```

        j = n
        do i = 1, size (export)
            if (mask(i)) then
                j = j + 1
                tmp(j) = export(i)
            end if
        end do
        call move_alloc (from=tmp, to=rt_data%export)
    end if
end subroutine rt_data_append_exports

```

Transfer export-objects from the local rt data to the global rt data, as far as supported.

```

<RT data: rt data: TBP>+≡
    procedure :: handle_exports => rt_data_handle_exports

<RT data: sub interfaces>+≡
    module subroutine rt_data_handle_exports (local, global)
        class(rt_data_t), intent(inout), target :: local
        class(rt_data_t), intent(inout), target :: global
    end subroutine rt_data_handle_exports

<RT data: procedures>+≡
    module subroutine rt_data_handle_exports (local, global)
        class(rt_data_t), intent(inout), target :: local
        class(rt_data_t), intent(inout), target :: global
        type(string_t) :: export
        integer :: i
        if (local%get_n_export () > 0) then
            do i = 1, local%get_n_export ()
                export = local%export(i)
                select case (char (export))
                    case ("results")
                        call msg_message ("Exporting integration results &
                            &to outer environment")
                        call local%transfer_process_stack (global)
                    case default
                        call msg_bug ("handle exports: '" &
                            // char (export) // "' unsupported")
                end select
            end do
        end if
    end subroutine rt_data_handle_exports

```

Export the process stack. One-by-one, take the last process from the local stack and push it on the global stack. Also handle the corresponding result variables: append if the process did not exist yet in the global stack, otherwise update.

TODO: result variables do not work that way yet, require initialization in the global variable list.

```

<RT data: rt data: TBP>+≡
    procedure :: transfer_process_stack => rt_data_transfer_process_stack

<RT data: sub interfaces>+≡
    module subroutine rt_data_transfer_process_stack (local, global)

```

```

        class(rt_data_t), intent(inout), target :: local
        class(rt_data_t), intent(inout), target :: global
    end subroutine rt_data_transfer_process_stack

<RT data: procedures>+≡
module subroutine rt_data_transfer_process_stack (local, global)
    class(rt_data_t), intent(inout), target :: local
    class(rt_data_t), intent(inout), target :: global
    type(process_entry_t), pointer :: process
    type(string_t) :: process_id
    do
        call local%process_stack%pop_last (process)
        if (.not. associated (process)) exit
        process_id = process%get_id ()
        call global%process_stack%push (process)
        call global%process_stack%fill_result_vars (process_id)
        call global%process_stack%update_result_vars &
            (process_id, global%var_list)
    end do
end subroutine rt_data_transfer_process_stack

```

33.2.9 Finalization

Finalizer for the variable list and the structure-function list. This is done only for the global RT dataset; local copies contain pointers to this and do not need a finalizer.

```

<RT data: rt data: TBP>+≡
    procedure :: final => rt_data_global_final

<RT data: sub interfaces>+≡
    module subroutine rt_data_global_final (global)
        class(rt_data_t), intent(inout) :: global
    end subroutine rt_data_global_final

<RT data: procedures>+≡
module subroutine rt_data_global_final (global)
    class(rt_data_t), intent(inout) :: global
    call global%process_stack%final ()
    call global%prclib_stack%final ()
    call global%model_list%final ()
    call global%var_list%final (follow_link=.false.)
    if (associated (global%out_files)) then
        call file_list_final (global%out_files)
        deallocate (global%out_files)
    end if
end subroutine rt_data_global_final

```

The local copy needs a finalizer for the variable list, which consists of local copies. This finalizer is called only when the local environment is finally discarded. (Note that the process stack should already have been cleared after execution, which can occur many times for the same local environment.)

```

<RT data: rt data: TBP>+≡
    procedure :: local_final => rt_data_local_final

```

```

<RT data: sub interfaces>+≡
    module subroutine rt_data_local_final (local)
        class(rt_data_t), intent(inout) :: local
    end subroutine rt_data_local_final

<RT data: procedures>+≡
    module subroutine rt_data_local_final (local)
        class(rt_data_t), intent(inout) :: local
        call local%process_stack%clear ()
        call local%model_list%final ()
        call local%var_list%final (follow_link=.false.)
    end subroutine rt_data_local_final

```

33.2.10 Model Management

Read a model, so it becomes available for activation. No variables or model copies, this is just initialization.

If this is a local environment, the model will be automatically read into the global context.

```

<RT data: rt data: TBP>+≡
    procedure :: read_model => rt_data_read_model

<RT data: sub interfaces>+≡
    module subroutine rt_data_read_model (global, name, model, scheme)
        class(rt_data_t), intent(inout) :: global
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: scheme
        type(model_t), pointer, intent(out) :: model
    end subroutine rt_data_read_model

<RT data: procedures>+≡
    module subroutine rt_data_read_model (global, name, model, scheme)
        class(rt_data_t), intent(inout) :: global
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: scheme
        type(model_t), pointer, intent(out) :: model
        type(string_t) :: filename
        filename = name // ".mdl"
        call global%model_list%read_model &
            (name, filename, global%os_data, model, scheme)
    end subroutine rt_data_read_model

```

Read a UFO model. Create it on the fly if necessary.

```

<RT data: rt data: TBP>+≡
    procedure :: read_ufo_model => rt_data_read_ufo_model

<RT data: sub interfaces>+≡
    module subroutine rt_data_read_ufo_model (global, name, model, ufo_path)
        class(rt_data_t), intent(inout) :: global
        type(string_t), intent(in) :: name
        type(model_t), pointer, intent(out) :: model
        type(string_t), intent(in), optional :: ufo_path
    end subroutine rt_data_read_ufo_model

```

```

<RT data: procedures>+≡
module subroutine rt_data_read_ufo_model (global, name, model, ufo_path)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(model_t), pointer, intent(out) :: model
  type(string_t), intent(in), optional :: ufo_path
  type(string_t) :: filename
  filename = name // ".ufo.mdl"
  call global%model_list%read_model &
    (name, filename, global%os_data, model, ufo=.true., ufo_path=ufo_path)
end subroutine rt_data_read_ufo_model

```

Initialize the fallback model. This model is used whenever the current model does not describe all physical particles (hadrons, mainly). It is not supposed to be modified, and the pointer should remain linked to this model.

```

<RT data: rt data: TBP>+≡
  procedure :: init_fallback_model => rt_data_init_fallback_model

<RT data: sub interfaces>+≡
  module subroutine rt_data_init_fallback_model (global, name, filename)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name, filename
  end subroutine rt_data_init_fallback_model

```

```

<RT data: procedures>+≡
module subroutine rt_data_init_fallback_model (global, name, filename)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name, filename
  call global%model_list%read_model &
    (name, filename, global%os_data, global%fallback_model)
end subroutine rt_data_init_fallback_model

```

Activate a model: assign the current-model pointer and set the model name in the variable list. If necessary, read the model from file. Link the global variable list to the model variable list.

```

<RT data: rt data: TBP>+≡
  procedure :: select_model => rt_data_select_model

<RT data: sub interfaces>+≡
  module subroutine rt_data_select_model (global, name, scheme, ufo, ufo_path)
    class(rt_data_t), intent(inout), target :: global
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
  end subroutine rt_data_select_model

<RT data: procedures>+≡
module subroutine rt_data_select_model (global, name, scheme, ufo, ufo_path)
  class(rt_data_t), intent(inout), target :: global
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: scheme
  logical, intent(in), optional :: ufo
  type(string_t), intent(in), optional :: ufo_path
  logical :: same_model, ufo_model

```

```

ufo_model = .false.; if (present (ufo)) ufo_model = ufo
if (associated (global%model)) then
    same_model = global%model%matches (name, scheme, ufo)
else
    same_model = .false.
end if
if (.not. same_model) then
    global%model => global%model_list%get_model_ptr (name, scheme, ufo)
    if (.not. associated (global%model)) then
        if (ufo_model) then
            call global%read_ufo_model (name, global%model, ufo_path)
        else
            call global%read_model (name, global%model)
        end if
        global%model_is_copy = .false.
    else if (associated (global%context)) then
        global%model_is_copy = &
            global%model_list%model_exists (name, scheme, ufo, &
                follow_link=.false.)
    else
        global%model_is_copy = .false.
    end if
end if
if (associated (global%model)) then
    call global%model%link_var_list (global%var_list)
    call global%var_list%set_string (var_str (" $model_name"), &
        name, is_known = .true.)
    if (global%model%is_ufo_model ()) then
        call msg_message ("Switching to model '" // char (name) // "' " &
            // "(generated from UFO source)")
    else if (global%model%has_schemes ()) then
        call msg_message ("Switching to model '" // char (name) // "', " &
            // "scheme '" // char (global%model%get_scheme ()) // "'")
    else
        call msg_message ("Switching to model '" // char (name) // "'")
    end if
else
    call global%var_list%set_string (var_str (" $model_name"), &
        var_str (""), is_known = .false.)
end if
end subroutine rt_data_select_model

```

Remove the model link. Do not unset the model name variable, because this may unset the variable in a parent `rt_data` object (via linked var lists).

```

<RT data: rt data: TBP>+≡
    procedure :: unselect_model => rt_data_unselect_model

<RT data: sub interfaces>+≡
    module subroutine rt_data_unselect_model (global)
        class(rt_data_t), intent(inout), target :: global
    end subroutine rt_data_unselect_model

<RT data: procedures>+≡
    module subroutine rt_data_unselect_model (global)
        class(rt_data_t), intent(inout), target :: global

```

```

    if (associated (global%model)) then
        global%model => null ()
        global%model_is_copy = .false.
    end if
end subroutine rt_data_unselect_model

```

Create a copy of the currently selected model and append it to the local model list. The model pointer is redirected to the copy. (Not applicable for the global model list, those models will be modified in-place.)

```

<RT data: rt data: TBP>+≡
    procedure :: ensure_model_copy => rt_data_ensure_model_copy

<RT data: sub interfaces>+≡
    module subroutine rt_data_ensure_model_copy (global)
        class(rt_data_t), intent(inout), target :: global
    end subroutine rt_data_ensure_model_copy

<RT data: procedures>+≡
    module subroutine rt_data_ensure_model_copy (global)
        class(rt_data_t), intent(inout), target :: global
        if (associated (global%context)) then
            if (.not. global%model_is_copy) then
                call global%model_list%append_copy (global%model, global%model)
                global%model_is_copy = .true.
                call global%model%link_var_list (global%var_list)
            end if
        end if
    end subroutine rt_data_ensure_model_copy

```

Modify a model variable. The update mechanism will ensure that the model parameter set remains consistent. This has to take place in a local copy of the current model. If there is none yet, create one.

```

<RT data: rt data: TBP>+≡
    procedure :: model_set_real => rt_data_model_set_real

<RT data: sub interfaces>+≡
    module subroutine rt_data_model_set_real &
        (global, name, rval, verbose, pacified)
        class(rt_data_t), intent(inout), target :: global
        type(string_t), intent(in) :: name
        real(default), intent(in) :: rval
        logical, intent(in), optional :: verbose, pacified
    end subroutine rt_data_model_set_real

<RT data: procedures>+≡
    module subroutine rt_data_model_set_real &
        (global, name, rval, verbose, pacified)
        class(rt_data_t), intent(inout), target :: global
        type(string_t), intent(in) :: name
        real(default), intent(in) :: rval
        logical, intent(in), optional :: verbose, pacified
        call global%ensure_model_copy ()
        call global%model%set_real (name, rval, verbose, pacified)
    end subroutine rt_data_model_set_real

```


Modify particle properties. This has to take place in a local copy of the current model. If there is none yet, create one.

```

<RT data: rt data: TBP>+≡
    procedure :: modify_particle => rt_data_modify_particle

<RT data: sub interfaces>+≡
    module subroutine rt_data_modify_particle &
        (global, pdg, polarized, stable, decay, &
         isotropic_decay, diagonal_decay, decay_helicity)
        class(rt_data_t), intent(inout), target :: global
        integer, intent(in) :: pdg
        logical, intent(in), optional :: polarized, stable
        logical, intent(in), optional :: isotropic_decay, diagonal_decay
        integer, intent(in), optional :: decay_helicity
        type(string_t), dimension(:), intent(in), optional :: decay
    end subroutine rt_data_modify_particle

<RT data: procedures>+≡
    module subroutine rt_data_modify_particle &
        (global, pdg, polarized, stable, decay, &
         isotropic_decay, diagonal_decay, decay_helicity)
        class(rt_data_t), intent(inout), target :: global
        integer, intent(in) :: pdg
        logical, intent(in), optional :: polarized, stable
        logical, intent(in), optional :: isotropic_decay, diagonal_decay
        integer, intent(in), optional :: decay_helicity
        type(string_t), dimension(:), intent(in), optional :: decay
        call global%ensure_model_copy ()
        if (present (polarized)) then
            if (polarized) then
                call global%model%set_polarized (pdg)
            else
                call global%model%set_unpolarized (pdg)
            end if
        end if
        if (present (stable)) then
            if (stable) then
                call global%model%set_stable (pdg)
            else if (present (decay)) then
                call global%model%set_unstable &
                    (pdg, decay, isotropic_decay, diagonal_decay, decay_helicity)
            else
                call msg_bug ("Setting particle unstable: missing decay processes")
            end if
        end if
    end subroutine rt_data_modify_particle

```

33.2.11 Managing Variables

Return a pointer to the currently active variable list. If there is no model, this is the global variable list. If there is one, it is the model variable list, which should be linked to the former.

```

<RT data: rt data: TBP>+≡

```

```

        procedure :: get_var_list_ptr => rt_data_get_var_list_ptr
<RT data: sub interfaces>+≡
        module function rt_data_get_var_list_ptr (global) result (var_list)
            class(rt_data_t), intent(in), target :: global
            type(var_list_t), pointer :: var_list
        end function rt_data_get_var_list_ptr
<RT data: procedures>+≡
        module function rt_data_get_var_list_ptr (global) result (var_list)
            class(rt_data_t), intent(in), target :: global
            type(var_list_t), pointer :: var_list
            if (associated (global%model)) then
                var_list => global%model%get_var_list_ptr ()
            else
                var_list => global%var_list
            end if
        end function rt_data_get_var_list_ptr

```

Initialize a local variable: append it to the current variable list. No initial value, yet.

```

<RT data: rt data: TBP>+≡
        procedure :: append_log => rt_data_append_log
        procedure :: append_int => rt_data_append_int
        procedure :: append_real => rt_data_append_real
        procedure :: append_cmplx => rt_data_append_cmplx
        procedure :: append_subevt => rt_data_append_subevt
        procedure :: append_pdg_array => rt_data_append_pdg_array
        procedure :: append_string => rt_data_append_string
<RT data: sub interfaces>+≡
        module subroutine rt_data_append_log (local, name, lval, intrinsic, user)
            class(rt_data_t), intent(inout) :: local
            type(string_t), intent(in) :: name
            logical, intent(in), optional :: lval
            logical, intent(in), optional :: intrinsic, user
        end subroutine rt_data_append_log
        module subroutine rt_data_append_int (local, name, ival, intrinsic, user)
            class(rt_data_t), intent(inout) :: local
            type(string_t), intent(in) :: name
            integer, intent(in), optional :: ival
            logical, intent(in), optional :: intrinsic, user
        end subroutine rt_data_append_int
        module subroutine rt_data_append_real (local, name, rval, intrinsic, user)
            class(rt_data_t), intent(inout) :: local
            type(string_t), intent(in) :: name
            real(default), intent(in), optional :: rval
            logical, intent(in), optional :: intrinsic, user
        end subroutine rt_data_append_real
        module subroutine rt_data_append_cmplx (local, name, cval, intrinsic, user)
            class(rt_data_t), intent(inout) :: local
            type(string_t), intent(in) :: name
            complex(default), intent(in), optional :: cval
            logical, intent(in), optional :: intrinsic, user
        end subroutine rt_data_append_cmplx

```

```

module subroutine rt_data_append_subevt (local, name, pval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(subevt_t), intent(in), optional :: pval
  logical, intent(in) :: intrinsic, user
end subroutine rt_data_append_subevt
module subroutine rt_data_append_pdg_array &
  (local, name, aval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(pdg_array_t), intent(in), optional :: aval
  logical, intent(in), optional :: intrinsic, user
end subroutine rt_data_append_pdg_array
module subroutine rt_data_append_string (local, name, sval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: sval
  logical, intent(in), optional :: intrinsic, user
end subroutine rt_data_append_string
<RT data: procedures>+≡
module subroutine rt_data_append_log (local, name, lval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  logical, intent(in), optional :: lval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_log (name, lval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_log

module subroutine rt_data_append_int (local, name, ival, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  integer, intent(in), optional :: ival
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_int (name, ival, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_int

module subroutine rt_data_append_real (local, name, rval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  real(default), intent(in), optional :: rval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_real (name, rval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_real

module subroutine rt_data_append_cmplx (local, name, cval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  complex(default), intent(in), optional :: cval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_cmplx (name, cval, &
    intrinsic = intrinsic, user = user)

```

```

end subroutine rt_data_append_cmplx

module subroutine rt_data_append_subevt (local, name, pval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(subevt_t), intent(in), optional :: pval
  logical, intent(in) :: intrinsic, user
  call local%var_list%append_subevt (name, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_subevt

module subroutine rt_data_append_pdg_array &
  (local, name, aval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(pdg_array_t), intent(in), optional :: aval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_pdg_array (name, aval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_pdg_array

module subroutine rt_data_append_string (local, name, sval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: sval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_string (name, sval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_string

```

Import values for all local variables, given a global context environment where these variables are defined.

```

<RT data: rt data: TBP>+≡
  procedure :: import_values => rt_data_import_values

<RT data: sub interfaces>+≡
  module subroutine rt_data_import_values (local)
    class(rt_data_t), intent(inout) :: local
    end subroutine rt_data_import_values

<RT data: procedures>+≡
  module subroutine rt_data_import_values (local)
    class(rt_data_t), intent(inout) :: local
    type(rt_data_t), pointer :: global
    global => local%context
    if (associated (global)) then
      call local%var_list%import (global%var_list)
    end if
  end subroutine rt_data_import_values

```

Unset all variable values.

```

<RT data: rt data: TBP>+≡
  procedure :: unset_values => rt_data_unset_values

```

```

<RT data: sub interfaces>+≡
  module subroutine rt_data_unset_values (global)
    class(rt_data_t), intent(inout) :: global
  end subroutine rt_data_unset_values

<RT data: procedures>+≡
  module subroutine rt_data_unset_values (global)
    class(rt_data_t), intent(inout) :: global
    call global%var_list%undefine (follow_link=.false.)
  end subroutine rt_data_unset_values

```

Set a variable. (Not a model variable, these are handled separately.) We can assume that the variable has been initialized.

```

<RT data: rt data: TBP>+≡
  procedure :: set_log => rt_data_set_log
  procedure :: set_int => rt_data_set_int
  procedure :: set_real => rt_data_set_real
  procedure :: set_cmplx => rt_data_set_cmplx
  procedure :: set_subevt => rt_data_set_subevt
  procedure :: set_pdg_array => rt_data_set_pdg_array
  procedure :: set_string => rt_data_set_string

<RT data: sub interfaces>+≡
  module subroutine rt_data_set_log &
    (global, name, lval, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    logical, intent(in) :: lval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
  end subroutine rt_data_set_log
  module subroutine rt_data_set_int &
    (global, name, ival, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    integer, intent(in) :: ival
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
  end subroutine rt_data_set_int
  module subroutine rt_data_set_real &
    (global, name, rval, is_known, force, verbose, pacified)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    real(default), intent(in) :: rval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose, pacified
  end subroutine rt_data_set_real
  module subroutine rt_data_set_cmplx &
    (global, name, cval, is_known, force, verbose, pacified)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: cval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose, pacified
  end subroutine rt_data_set_cmplx

```

```

module subroutine rt_data_set_subevt &
  (global, name, pval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(subevt_t), intent(in) :: pval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
end subroutine rt_data_set_subevt
module subroutine rt_data_set_pdg_array &
  (global, name, aval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(pdg_array_t), intent(in) :: aval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
end subroutine rt_data_set_pdg_array
module subroutine rt_data_set_string &
  (global, name, sval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(string_t), intent(in) :: sval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
end subroutine rt_data_set_string

<RT data: procedures>+≡
module subroutine rt_data_set_log &
  (global, name, lval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  logical, intent(in) :: lval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
  call global%var_list%set_log (name, lval, is_known, &
    force=force, verbose=verbose)
end subroutine rt_data_set_log

module subroutine rt_data_set_int &
  (global, name, ival, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  integer, intent(in) :: ival
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
  call global%var_list%set_int (name, ival, is_known, &
    force=force, verbose=verbose)
end subroutine rt_data_set_int

module subroutine rt_data_set_real &
  (global, name, rval, is_known, force, verbose, pacified)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  real(default), intent(in) :: rval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose, pacified

```

```

        call global%var_list%set_real (name, rval, is_known, &
            force=force, verbose=verbose, pacified=pacified)
    end subroutine rt_data_set_real

module subroutine rt_data_set_cmplx &
    (global, name, cval, is_known, force, verbose, pacified)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: cval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose, pacified
    call global%var_list%set_cmplx (name, cval, is_known, &
        force=force, verbose=verbose, pacified=pacified)
end subroutine rt_data_set_cmplx

module subroutine rt_data_set_subevt &
    (global, name, pval, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    type(subevt_t), intent(in) :: pval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
    call global%var_list%set_subevt (name, pval, is_known, &
        force=force, verbose=verbose)
end subroutine rt_data_set_subevt

module subroutine rt_data_set_pdg_array &
    (global, name, aval, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    type(pdg_array_t), intent(in) :: aval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
    call global%var_list%set_pdg_array (name, aval, is_known, &
        force=force, verbose=verbose)
end subroutine rt_data_set_pdg_array

module subroutine rt_data_set_string &
    (global, name, sval, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: sval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
    call global%var_list%set_string (name, sval, is_known, &
        force=force, verbose=verbose)
end subroutine rt_data_set_string

```

Return the value of a variable, assuming that the type is correct.

```

<RT data: rt data: TBP>+≡
    procedure :: get_lval => rt_data_get_lval
    procedure :: get_ival => rt_data_get_ival
    procedure :: get_rval => rt_data_get_rval

```

```

procedure :: get_cval => rt_data_get_cval
procedure :: get_pval => rt_data_get_pval
procedure :: get_aval => rt_data_get_aval
procedure :: get_sval => rt_data_get_sval

<RT data: sub interfaces>+≡
  module function rt_data_get_lval (global, name) result (lval)
    logical :: lval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_lval
  module function rt_data_get_ival (global, name) result (ival)
    integer :: ival
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_ival
  module function rt_data_get_rval (global, name) result (rval)
    real(default) :: rval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_rval
  module function rt_data_get_cval (global, name) result (cval)
    complex(default) :: cval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_cval
  module function rt_data_get_aval (global, name) result (aval)
    type(pdg_array_t) :: aval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_aval
  module function rt_data_get_pval (global, name) result (pval)
    type(subevt_t) :: pval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_pval
  module function rt_data_get_sval (global, name) result (sval)
    type(string_t) :: sval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
  end function rt_data_get_sval

<RT data: procedures>+≡
  module function rt_data_get_lval (global, name) result (lval)
    logical :: lval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    lval = var_list%get_lval (name)
  end function rt_data_get_lval

  module function rt_data_get_ival (global, name) result (ival)
    integer :: ival
    class(rt_data_t), intent(in), target :: global

```



```

    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    ival = var_list%get_ival (name)
end function rt_data_get_ival

module function rt_data_get_rval (global, name) result (rval)
    real(default) :: rval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    rval = var_list%get_rval (name)
end function rt_data_get_rval

module function rt_data_get_cval (global, name) result (cval)
    complex(default) :: cval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    cval = var_list%get_cval (name)
end function rt_data_get_cval

module function rt_data_get_aval (global, name) result (aval)
    type(pdg_array_t) :: aval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    aval = var_list%get_aval (name)
end function rt_data_get_aval

module function rt_data_get_pval (global, name) result (pval)
    type(subvt_t) :: pval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    pval = var_list%get_pval (name)
end function rt_data_get_pval

module function rt_data_get_sval (global, name) result (sval)
    type(string_t) :: sval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    sval = var_list%get_sval (name)
end function rt_data_get_sval

```

Return true if the variable exists in the global list.

$\langle RT\ data: rt\ data: TBP \rangle + \equiv$

```

    procedure :: contains => rt_data_contains

<RT data: sub interfaces>+≡
    module function rt_data_contains (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
    end function rt_data_contains

<RT data: procedures>+≡
    module function rt_data_contains (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        lval = var_list%contains (name)
    end function rt_data_contains

```

Return true if the value of the variable is known.

```

<RT data: rt data: TBP>+≡
    procedure :: is_known => rt_data_is_known

<RT data: sub interfaces>+≡
    module function rt_data_is_known (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
    end function rt_data_is_known

<RT data: procedures>+≡
    module function rt_data_is_known (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        lval = var_list%is_known (name)
    end function rt_data_is_known

```

33.2.12 Further Content

Add a library (available via a pointer of type `prclib_entry_t`) to the stack and update the pointer and variable list to the current library. The pointer association of `prclib_entry` will be discarded.

```

<RT data: rt data: TBP>+≡
    procedure :: add_prclib => rt_data_add_prclib

<RT data: sub interfaces>+≡
    module subroutine rt_data_add_prclib (global, prclib_entry)
        class(rt_data_t), intent(inout) :: global
        type(prclib_entry_t), intent(inout), pointer :: prclib_entry
    end subroutine rt_data_add_prclib

```

```

<RT data: procedures>+≡
module subroutine rt_data_add_prclib (global, prclib_entry)
  class(rt_data_t), intent(inout) :: global
  type(prclib_entry_t), intent(inout), pointer :: prclib_entry
  call global%prclib_stack%push (prclib_entry)
  call global%update_prclib (global%prclib_stack%get_first_ptr ())
end subroutine rt_data_add_prclib

```

Given a pointer to a process library, make this the currently active library.

```

<RT data: rt data: TBP>+≡
  procedure :: update_prclib => rt_data_update_prclib

<RT data: sub interfaces>+≡
  module subroutine rt_data_update_prclib (global, lib)
    class(rt_data_t), intent(inout) :: global
    type(process_library_t), intent(in), target :: lib
  end subroutine rt_data_update_prclib

<RT data: procedures>+≡
module subroutine rt_data_update_prclib (global, lib)
  class(rt_data_t), intent(inout) :: global
  type(process_library_t), intent(in), target :: lib
  global%prclib => lib
  if (global%var_list%contains (&
    var_str ("$library_name"), follow_link = .false.)) then
    call global%var_list%set_string (var_str ("$library_name"), &
      global%prclib%get_name (), is_known=.true.)
  else
    call global%var_list%append_string ( &
      var_str ("$library_name"), global%prclib%get_name (), &
      intrinsic = .true.)
  end if
end subroutine rt_data_update_prclib

```

33.2.13 Miscellaneous

The helicity selection data are distributed among several parameters. Here, we collect them in a single record.

```

<RT data: rt data: TBP>+≡
  procedure :: get_helicity_selection => rt_data_get_helicity_selection

<RT data: sub interfaces>+≡
  module function rt_data_get_helicity_selection &
    (rt_data) result (helicity_selection)
    class(rt_data_t), intent(in) :: rt_data
    type(helicity_selection_t) :: helicity_selection
  end function rt_data_get_helicity_selection

<RT data: procedures>+≡
module function rt_data_get_helicity_selection &
  (rt_data) result (helicity_selection)
  class(rt_data_t), intent(in) :: rt_data
  type(helicity_selection_t) :: helicity_selection
  associate (var_list => rt_data%var_list)

```

```

        helicity_selection%active = var_list%get_lval (&
            var_str ("?helicity_selection_active"))
    if (helicity_selection%active) then
        helicity_selection%threshold = var_list%get_rval (&
            var_str ("helicity_selection_threshold"))
        helicity_selection%cutoff = var_list%get_ival (&
            var_str ("helicity_selection_cutoff"))
    end if
end associate
end function rt_data_get_helicity_selection

```

Show the beam setup: beam structure and relevant global variables.

<RT data: rt data: TBP>+≡

```

    procedure :: show_beams => rt_data_show_beams

```

<RT data: sub interfaces>+≡

```

    module subroutine rt_data_show_beams (rt_data, unit)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
    end subroutine rt_data_show_beams

```

<RT data: procedures>+≡

```

    module subroutine rt_data_show_beams (rt_data, unit)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
        type(string_t) :: s
        integer :: u
        u = given_output_unit (unit)
        associate (beams => rt_data%beam_structure, var_list => rt_data%var_list)
            call beams%write (u)
            if (.not. beams%asymmetric () .and. beams%get_n_beam () == 2) then
                write (u, "(2x,A," // FMT_19 // ",1x,'GeV')") "sqrts =", &
                    var_list%get_rval (var_str ("sqrts"))
            end if
            if (beams%contains ("pdf_builtin")) then
                s = var_list%get_sval (var_str ("pdf_builtin_set"))
                if (s /= "") then
                    write (u, "(2x,A,1x,3A)") "PDF set =", "'", char (s), "'"
                else
                    write (u, "(2x,A,1x,A)") "PDF set =", "[undefined]"
                end if
            end if
            if (beams%contains ("lhpdf")) then
                s = var_list%get_sval (var_str ("lhpdf_dir"))
                if (s /= "") then
                    write (u, "(2x,A,1x,3A)") "LHAPDF dir    =", "'", char (s), "'"
                end if
                s = var_list%get_sval (var_str ("lhpdf_file"))
                if (s /= "") then
                    write (u, "(2x,A,1x,3A)") "LHAPDF file    =", "'", char (s), "'"
                    write (u, "(2x,A,1x,10)") "LHAPDF member =", &
                        var_list%get_ival (var_str ("lhpdf_member"))
                else
                    write (u, "(2x,A,1x,A)") "LHAPDF file    =", "[undefined]"
                end if
            end if
        end associate
    end subroutine rt_data_show_beams

```

```

end if
if (beams%contains ("lhpdf_photon")) then
  s = var_list%get_sval (var_str ("lhpdf_dir"))
  if (s /= "") then
    write (u, "(2x,A,1x,3A)") "LHAPDF dir      =", "'", char (s), "'"
  end if
  s = var_list%get_sval (var_str ("lhpdf_photon_file"))
  if (s /= "") then
    write (u, "(2x,A,1x,3A)") "LHAPDF file      =", "'", char (s), "'"
    write (u, "(2x,A,1x,I0)") "LHAPDF member =", &
      var_list%get_ival (var_str ("lhpdf_member"))
    write (u, "(2x,A,1x,I0)") "LHAPDF scheme =", &
      var_list%get_ival (&
        var_str ("lhpdf_photon_scheme"))
  else
    write (u, "(2x,A,1x,A)") "LHAPDF file      =", "[undefined]"
  end if
end if
if (beams%contains ("isr")) then
  write (u, "(2x,A," // FMT_19 // ")") "ISR alpha      =", &
    var_list%get_rval (var_str ("isr_alpha"))
  write (u, "(2x,A," // FMT_19 // ")") "ISR Q max      =", &
    var_list%get_rval (var_str ("isr_q_max"))
  write (u, "(2x,A," // FMT_19 // ")") "ISR mass       =", &
    var_list%get_rval (var_str ("isr_mass"))
  write (u, "(2x,A,1x,I0)") "ISR order      =", &
    var_list%get_ival (var_str ("isr_order"))
  write (u, "(2x,A,1x,L1)") "ISR recoil     =", &
    var_list%get_lval (var_str ("?isr_recoil"))
  write (u, "(2x,A,1x,L1)") "ISR energy cons. =", &
    var_list%get_lval (var_str ("?isr_keep_energy"))
end if
if (beams%contains ("epa")) then
  write (u, "(2x,A," // FMT_19 // ")") "EPA alpha      =", &
    var_list%get_rval (var_str ("epa_alpha"))
  write (u, "(2x,A," // FMT_19 // ")") "EPA x min      =", &
    var_list%get_rval (var_str ("epa_x_min"))
  write (u, "(2x,A," // FMT_19 // ")") "EPA Q min      =", &
    var_list%get_rval (var_str ("epa_q_min"))
  write (u, "(2x,A," // FMT_19 // ")") "EPA Q max      =", &
    var_list%get_rval (var_str ("epa_q_max"))
  write (u, "(2x,A," // FMT_19 // ")") "EPA mass       =", &
    var_list%get_rval (var_str ("epa_mass"))
  write (u, "(2x,A,1x,L1)") "EPA recoil     =", &
    var_list%get_lval (var_str ("?epa_recoil"))
  write (u, "(2x,A,1x,L1)") "EPA energy cons. =", &
    var_list%get_lval (var_str ("?epa_keep_energy"))
end if
if (beams%contains ("ewa")) then
  write (u, "(2x,A," // FMT_19 // ")") "EWA x min      =", &
    var_list%get_rval (var_str ("ewa_x_min"))
  write (u, "(2x,A," // FMT_19 // ")") "EWA Pt max     =", &
    var_list%get_rval (var_str ("ewa_pt_max"))
  write (u, "(2x,A," // FMT_19 // ")") "EWA mass       =", &

```

```

        var_list%get_rval (var_str ("ewa_mass"))
write (u, "(2x,A,1x,L1)") "EWA recoil      =", &
        var_list%get_lval (var_str ("?ewa_recoil"))
write (u, "(2x,A,1x,L1)") "EWA energy cons. =", &
        var_list%get_lval (var_str ("ewa_keep_energy"))
end if
if (beams%contains ("circe1")) then
write (u, "(2x,A,1x,I0)") "CIRCE1 version  =", &
        var_list%get_ival (var_str ("circe1_ver"))
write (u, "(2x,A,1x,I0)") "CIRCE1 revision  =", &
        var_list%get_ival (var_str ("circe1_rev"))
s = var_list%get_sval (var_str ("$circe1_acc"))
write (u, "(2x,A,1x,A)") "CIRCE1 acceler.  =", char (s)
write (u, "(2x,A,1x,I0)") "CIRCE1 chattin.  =", &
        var_list%get_ival (var_str ("circe1_chat"))
write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 sqrts      =", &
        var_list%get_rval (var_str ("circe1_sqrts"))
write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 epsil.    =", &
        var_list%get_rval (var_str ("circe1_eps"))
write (u, "(2x,A,1x,L1)") "CIRCE1 phot. 1  =", &
        var_list%get_lval (var_str ("?circe1_photon1"))
write (u, "(2x,A,1x,L1)") "CIRCE1 phot. 2  =", &
        var_list%get_lval (var_str ("?circe1_photon2"))
write (u, "(2x,A,1x,L1)") "CIRCE1 generat. =", &
        var_list%get_lval (var_str ("?circe1_generate"))
write (u, "(2x,A,1x,L1)") "CIRCE1 mapping  =", &
        var_list%get_lval (var_str ("?circe1_map"))
write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 map. slope =", &
        var_list%get_rval (var_str ("circe1_mapping_slope"))
write (u, "(2x,A,1x,L1)") "CIRCE recoil photon =", &
        var_list%get_lval (var_str ("?circe1_with_radiation"))
end if
if (beams%contains ("circe2")) then
s = var_list%get_sval (var_str ("$circe2_design"))
write (u, "(2x,A,1x,A)") "CIRCE2 design  =", char (s)
s = var_list%get_sval (var_str ("$circe2_file"))
write (u, "(2x,A,1x,A)") "CIRCE2 file    =", char (s)
write (u, "(2x,A,1x,L1)") "CIRCE2 polarized =", &
        var_list%get_lval (var_str ("?circe2_polarized"))
end if
if (beams%contains ("gaussian")) then
write (u, "(2x,A,1x," // FMT_12 // ")") "Gaussian spread 1  =", &
        var_list%get_rval (var_str ("gaussian_spread1"))
write (u, "(2x,A,1x," // FMT_12 // ")") "Gaussian spread 2  =", &
        var_list%get_rval (var_str ("gaussian_spread2"))
end if
if (beams%contains ("beam_events")) then
s = var_list%get_sval (var_str ("$beam_events_file"))
write (u, "(2x,A,1x,A)") "Beam events file  =", char (s)
write (u, "(2x,A,1x,L1)") "Beam events EOF warn =", &
        var_list%get_lval (var_str ("?beam_events_warn_eof"))
end if
end associate
end subroutine rt_data_show_beams

```

Return the collision energy as determined by the current beam settings. Without beam setup, this is the `sqrts` variable.

If the value is meaningless for a setup, the function returns zero.

```

<RT data: rt data: TBP>+≡
  procedure :: get_sqrts => rt_data_get_sqrts

<RT data: sub interfaces>+≡
  module function rt_data_get_sqrts (rt_data) result (sqrts)
    class(rt_data_t), intent(in) :: rt_data
    real(default) :: sqrts
  end function rt_data_get_sqrts

<RT data: procedures>+≡
  module function rt_data_get_sqrts (rt_data) result (sqrts)
    class(rt_data_t), intent(in) :: rt_data
    real(default) :: sqrts
    sqrts = rt_data%var_list%get_rval (var_str ("sqrts"))
  end function rt_data_get_sqrts

```

For testing purposes, the `rt_data_t` contents can be pacified to suppress numerical fluctuations in (constant) test matrix elements.

```

<RT data: rt data: TBP>+≡
  procedure :: pacify => rt_data_pacify

<RT data: sub interfaces>+≡
  module subroutine rt_data_pacify (rt_data, efficiency_reset, error_reset)
    class(rt_data_t), intent(inout) :: rt_data
    logical, intent(in), optional :: efficiency_reset, error_reset
  end subroutine rt_data_pacify

<RT data: procedures>+≡
  module subroutine rt_data_pacify (rt_data, efficiency_reset, error_reset)
    class(rt_data_t), intent(inout) :: rt_data
    logical, intent(in), optional :: efficiency_reset, error_reset
    type(process_entry_t), pointer :: process
    process => rt_data%process_stack%first
    do while (associated (process))
      call process%pacify (efficiency_reset, error_reset)
      process => process%next
    end do
  end subroutine rt_data_pacify

<RT data: rt data: TBP>+≡
  procedure :: set_event_callback => rt_data_set_event_callback

<RT data: sub interfaces>+≡
  module subroutine rt_data_set_event_callback (global, callback)
    class(rt_data_t), intent(inout) :: global
    class(event_callback_t), intent(in) :: callback
  end subroutine rt_data_set_event_callback

```

```

<RT data: procedures>+≡
module subroutine rt_data_set_event_callback (global, callback)
  class(rt_data_t), intent(inout) :: global
  class(event_callback_t), intent(in) :: callback
  if (allocated (global%event_callback)) deallocate (global%event_callback)
  allocate (global%event_callback, source = callback)
end subroutine rt_data_set_event_callback

<RT data: rt data: TBP>+≡
procedure :: has_event_callback => rt_data_has_event_callback
procedure :: get_event_callback => rt_data_get_event_callback

<RT data: sub interfaces>+≡
module function rt_data_has_event_callback (global) result (flag)
  class(rt_data_t), intent(in) :: global
  logical :: flag
end function rt_data_has_event_callback
module function rt_data_get_event_callback (global) result (callback)
  class(rt_data_t), intent(in) :: global
  class(event_callback_t), allocatable :: callback
end function rt_data_get_event_callback

<RT data: procedures>+≡
module function rt_data_has_event_callback (global) result (flag)
  class(rt_data_t), intent(in) :: global
  logical :: flag
  flag = allocated (global%event_callback)
end function rt_data_has_event_callback

module function rt_data_get_event_callback (global) result (callback)
  class(rt_data_t), intent(in) :: global
  class(event_callback_t), allocatable :: callback
  if (allocated (global%event_callback)) then
    allocate (callback, source = global%event_callback)
  end if
end function rt_data_get_event_callback

```

Force system-dependent objects to well-defined values. Some of the variables are locked and therefore must be addressed directly.

This is, of course, only required for testing purposes. In principle, the `real_specimen` variables could be set to their values in `rt_data_t`, but this depends on the precision again, so we set them to some dummy values.

```

<RT data: public>+≡
public :: fix_system_dependencies

<RT data: sub interfaces>+≡
module subroutine fix_system_dependencies (global)
  class(rt_data_t), intent(inout), target :: global
end subroutine fix_system_dependencies

<RT data: procedures>+≡
module subroutine fix_system_dependencies (global)
  class(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list

```



```

var_list => global%get_var_list_ptr ()
call var_list%set_log (var_str ("?omega_omp"), &
    .false., is_known = .true., force=.true.)
call var_list%set_log (var_str ("?omp_is_active"), &
    .false., is_known = .true., force=.true.)
call var_list%set_int (var_str ("omp_num_threads_default"), &
    1, is_known = .true., force=.true.)
call var_list%set_int (var_str ("omp_num_threads"), &
    1, is_known = .true., force=.true.)
call var_list%set_int (var_str ("real_range"), &
    307, is_known = .true., force=.true.)
call var_list%set_int (var_str ("real_precision"), &
    15, is_known = .true., force=.true.)
call var_list%set_real (var_str ("real_epsilon"), &
    1.e-16_default, is_known = .true., force=.true.)
call var_list%set_real (var_str ("real_tiny"), &
    1.e-300_default, is_known = .true., force=.true.)

global%os_data%fc = "Fortran-compiler"
global%os_data%fcflags = "Fortran-flags"
global%os_data%fclibs = "Fortran-libs"

end subroutine fix_system_dependencies

<RT data: public>+≡
public :: show_description_of_string

<RT data: sub interfaces>+≡
module subroutine show_description_of_string (string)
    type(string_t), intent(in) :: string
end subroutine show_description_of_string

<RT data: procedures>+≡
module subroutine show_description_of_string (string)
    type(string_t), intent(in) :: string
    type(rt_data_t), target :: global
    call global%global_init ()
    call global%show_description_of_string (string, ascii_output=.true.)
end subroutine show_description_of_string

<RT data: public>+≡
public :: show_tex_descriptions

<RT data: sub interfaces>+≡
module subroutine show_tex_descriptions ()
end subroutine show_tex_descriptions

<RT data: procedures>+≡
module subroutine show_tex_descriptions ()
    type(rt_data_t), target :: global
    call global%global_init ()
    call fix_system_dependencies (global)
    call global%set_int (var_str ("seed"), 0, is_known=.true.)
    call global%var_list%sort ()
    call global%write_var_descriptions ()

```

```
end subroutine show_tex_descriptions
```

33.2.14 Unit Tests

Test module, followed by the corresponding implementation module.

```
<rt_data_ut.f90>≡  
  <File header>
```

```
module rt_data_ut  
  use unit_tests  
  use rt_data_uti
```

```
  <Standard module head>
```

```
  <RT data: public test>
```

```
contains
```

```
  <RT data: test driver>
```

```
end module rt_data_ut
```

```
<rt_data_uti.f90>≡  
  <File header>
```

```
module rt_data_uti
```

```
  <Use kinds>
```

```
  <Use strings>
```

```
    use format_defs, only: FMT_19
```

```
    use ifiles
```

```
    use lexers
```

```
    use parser
```

```
    use flavors
```

```
    use variables, only: var_list_t
```

```
    use eval_trees
```

```
    use models
```

```
    use prclib_stacks
```

```
    use rt_data
```

```
  <Standard module head>
```

```
  <RT data: test declarations>
```

```
contains
```

```
  <RT data: test auxiliary>
```

```
  <RT data: tests>
```

```
end module rt_data_uti
```

API: driver for the unit tests below.

```
<RT data: public test>≡
  public :: rt_data_test

<RT data: test driver>≡
  subroutine rt_data_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <RT data: execute tests>
  end subroutine rt_data_test
```

Initial content

Display the RT data in the state just after (global) initialization.

```
<RT data: execute tests>≡
  call test (rt_data_1, "rt_data_1", &
    "initialize", &
    u, results)

<RT data: test declarations>≡
  public :: rt_data_1

<RT data: tests>≡
  subroutine rt_data_1 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: rt_data_1"
    write (u, "(A)")  "*   Purpose: initialize global runtime data"
    write (u, "(A)")

    call global%global_init (logfile = var_str ("rt_data.log"))
    call fix_system_dependencies (global)

    call global%set_int (var_str ("seed"), 0, is_known=.true.)

    call global%it_list%init ([2, 3], [5000, 20000])

    call global%write (u)

    call global%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: rt_data_1"

  end subroutine rt_data_1
```

Fill values

Fill in empty slots in the runtime data block.

```
<RT data: execute tests>+≡
  call test (rt_data_2, "rt_data_2", &
```

```

        "fill", &
        u, results)

<RT data: test declarations>+≡
    public :: rt_data_2

<RT data: tests>+≡
    subroutine rt_data_2 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        type(flavor_t), dimension(2) :: flv
        type(string_t) :: cut_expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: parse_tree

        write (u, "(A)")  "* Test output: rt_data_2"
        write (u, "(A)")  "* Purpose: initialize global runtime data &
            &and fill contents"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call fix_system_dependencies (global)

        call global%select_model (var_str ("Test"))

        call global%set_real (var_str ("sqrts"), &
            1000._default, is_known = .true.)
        call global%set_int (var_str ("seed"), &
            0, is_known=.true.)
        call flv%init ([25,25], global%model)

        call global%set_string (var_str ("$run_id"), &
            var_str ("run1"), is_known = .true.)
        call global%set_real (var_str ("luminosity"), &
            33._default, is_known = .true.)

        call syntax_pexpr_init ()
        cut_expr_text = "all Pt > 100 [s]"
        call ifile_append (ifile, cut_expr_text)
        call stream_init (stream, ifile)
        call parse_tree_init_lexpr (parse_tree, stream, .true.)
        global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

        allocate (global%sample_fmt (2))
        global%sample_fmt(1) = "foo_fmt"
        global%sample_fmt(2) = "bar_fmt"

        call global%write (u)

        call parse_tree_final (parse_tree)
        call stream_final (stream)
        call ifile_final (ifile)

```

```

call syntax_pexpr_final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_2"

end subroutine rt_data_2

```

Save and restore

Set up a local runtime data block, change some contents, restore the global block.

```

<RT data: execute tests>+≡
  call test (rt_data_3, "rt_data_3", &
    "save/restore", &
    u, results)

<RT data: test declarations>+≡
  public :: rt_data_3

<RT data: tests>+≡
  subroutine rt_data_3 (u)
    use event_base, only: event_callback_nop_t
    integer, intent(in) :: u
    type(rt_data_t), target :: global, local
    type(flavor_t), dimension(2) :: flv
    type(string_t) :: cut_expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: parse_tree
    type(prclib_entry_t), pointer :: lib
    type(event_callback_nop_t) :: event_callback_nop

    write (u, "(A)")  "* Test output: rt_data_3"
    write (u, "(A)")  "* Purpose: initialize global runtime data &
      &and fill contents;"
    write (u, "(A)")  "*           copy to local block and back"
    write (u, "(A)")

    write (u, "(A)")  "* Init global data"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call fix_system_dependencies (global)

    call global%set_int (var_str ("seed"), &
      0, is_known=.true.)

    call global%select_model (var_str ("Test"))

```

```

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call flv%init ([25,25], global%model)

call global%beam_structure%init_sf (flv%get_name (), [1])
call global%beam_structure%set_sf (1, 1, var_str ("pdf_builtin"))

call global%set_string (var_str ("$_run_id"), &
    var_str ("run1"), is_known = .true.)
call global%set_real (var_str ("luminosity"), &
    33._default, is_known = .true.)

call syntax_pexpr_init ()
cut_expr_text = "all Pt > 100 [s]"
call ifile_append (ifile, cut_expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (parse_tree, stream, .true.)
global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

allocate (global%sample_fmt (2))
global%sample_fmt(1) = "foo_fmt"
global%sample_fmt(2) = "bar_fmt"

allocate (lib)
call lib%init (var_str ("library_1"))
call global%add_prclib (lib)

write (u, "(A)")  "* Init and modify local data"
write (u, "(A)")

call local%local_init (global)
call local%append_string (var_str ("$_integration_method"), intrinsic=.true.)
call local%append_string (var_str ("$_phs_method"), intrinsic=.true.)

call local%activate ()

write (u, "(1x,A,L1)")  "model associated   = ", associated (local%model)
write (u, "(1x,A,L1)")  "library associated = ", associated (local%prclib)
write (u, *)

call local%model_set_real (var_str ("ms"), 150._default)
call local%set_string (var_str ("$_integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call local%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)

local%os_data%fc = "Local compiler"

allocate (lib)
call lib%init (var_str ("library_2"))
call local%add_prclib (lib)

call local%set_event_callback (event_callback_nop)

```

```

call local%write (u)

write (u, "(A)")
write (u, "(A)")  "* Restore global data"
write (u, "(A)")

call local%deactivate (global)

write (u, "(1x,A,L1)") "model associated  = ", associated (global%model)
write (u, "(1x,A,L1)") "library associated = ", associated (global%prclib)
write (u, *)

call global%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call parse_tree_final (parse_tree)
call stream_final (stream)
call ifile_final (ifile)
call syntax_pexpr_final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_3"

end subroutine rt_data_3

```

Show variables

Display selected variables in the global record.

```

<RT data: execute tests>+≡
  call test (rt_data_4, "rt_data_4", &
    "show variables", &
    u, results)

<RT data: test declarations>+≡
  public :: rt_data_4

<RT data: tests>+≡
  subroutine rt_data_4 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global

    type(string_t), dimension(0) :: empty_string_array

    write (u, "(A)")  "* Test output: rt_data_4"
    write (u, "(A)")  "* Purpose: display selected variables"
    write (u, "(A)")

    call global%global_init ()

```

```

write (u, "(A)")  "* No variables:"
write (u, "(A)")

call global%write_vars (u, empty_string_array)

write (u, "(A)")  "* Two variables:"
write (u, "(A)")

call global%write_vars (u, &
    [var_str ("?unweighted"), var_str ("phs_method")])

write (u, "(A)")
write (u, "(A)")  "* Display whole record with selected variables"
write (u, "(A)")

call global%write (u, &
    vars = [var_str ("?unweighted"), var_str ("phs_method")])

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_4"

end subroutine rt_data_4

```

Show parts

Display only selected parts in the state just after (global) initialization.

```

<RT data: execute tests>+≡
    call test (rt_data_5, "rt_data_5", &
        "show parts", &
        u, results)

<RT data: test declarations>+≡
    public :: rt_data_5

<RT data: tests>+≡
    subroutine rt_data_5 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: rt_data_5"
        write (u, "(A)")  "* Purpose: display parts of rt data"
        write (u, "(A)")

        call global%global_init ()
        call global%write_libraries (u)

        write (u, "(A)")

        call global%write_beams (u)

        write (u, "(A)")

```



```

call global%write_process_stack (u)

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_5"

end subroutine rt_data_5

```

Local Model

Locally modify a model and restore the global one. We need an auxiliary function to determine the status of a model particle:

```

<RT data: test auxiliary>≡
function is_stable (pdg, global) result (flag)
  integer, intent(in) :: pdg
  type(rt_data_t), intent(in) :: global
  logical :: flag
  type(flavor_t) :: flv
  call flv%init (pdg, global%model)
  flag = flv%is_stable ()
end function is_stable

function is_polarized (pdg, global) result (flag)
  integer, intent(in) :: pdg
  type(rt_data_t), intent(in) :: global
  logical :: flag
  type(flavor_t) :: flv
  call flv%init (pdg, global%model)
  flag = flv%is_polarized ()
end function is_polarized

<RT data: execute tests>+≡
call test (rt_data_6, "rt_data_6", &
  "local model", &
  u, results)

<RT data: test declarations>+≡
public :: rt_data_6

<RT data: tests>+≡
subroutine rt_data_6 (u)
  integer, intent(in) :: u
  type(rt_data_t), target :: global, local
  type(var_list_t), pointer :: model_vars
  type(string_t) :: var_name

  write (u, "(A)")  "* Test output: rt_data_6"
  write (u, "(A)")  "* Purpose: apply and keep local modifications to model"
  write (u, "(A)")

  call syntax_model_file_init ()

```

```

call global%global_init ()
call global%select_model (var_str ("Test"))

write (u, "(A)")  "* Original model"
write (u, "(A)")

call global%write_model_list (u)
write (u, *)
write (u, "(A,L1)")  "s is stable      = ", is_stable (25, global)
write (u, "(A,L1)")  "f is polarized = ", is_polarized (6, global)

write (u, *)

var_name = "ff"

write (u, "(A)", advance="no")  "Global model variable: "
model_vars => global%model%get_var_list_ptr ()
call model_vars%write_var (var_name, u)

write (u, "(A)")
write (u, "(A)")  "* Apply local modifications: unstable"
write (u, "(A)")

call local%local_init (global)
call local%activate ()

call local%model_set_real (var_name, 0.4_default)
call local%modify_particle (25, stable = .false., decay = [var_str ("d1")])
call local%modify_particle (6, stable = .false., &
    decay = [var_str ("f1")], isotropic_decay = .true.)
call local%modify_particle (-6, stable = .false., &
    decay = [var_str ("f2"), var_str ("f3")], diagonal_decay = .true.)

call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Further modifications"
write (u, "(A)")

call local%modify_particle (6, stable = .false., &
    decay = [var_str ("f1")], &
    diagonal_decay = .true., isotropic_decay = .false.)
call local%modify_particle (-6, stable = .false., &
    decay = [var_str ("f2"), var_str ("f3")], &
    diagonal_decay = .false., isotropic_decay = .true.)
call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Further modifications: f stable but polarized"
write (u, "(A)")

call local%modify_particle (6, stable = .true., polarized = .true.)
call local%modify_particle (-6, stable = .true.)

```

```

call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Global model"
write (u, "(A)")

call global%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable    = ", is_stable (25, global)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, global)

write (u, "(A)")
write (u, "(A)")  "* Local model"
write (u, "(A)")

call local%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable    = ", is_stable (25, local)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, local)

write (u, *)

write (u, "(A)", advance="no") "Global model variable: "
model_vars => global%model%get_var_list_ptr ()
call model_vars%write_var (var_name, u)

write (u, "(A)", advance="no") "Local model variable: "
associate (model_var_list_ptr => local%model%get_var_list_ptr())
  call model_var_list_ptr%write_var (var_name, u)
end associate

write (u, "(A)")
write (u, "(A)")  "* Restore global"

call local%deactivate (global, keep_local = .true.)

write (u, "(A)")
write (u, "(A)")  "* Global model"
write (u, "(A)")

call global%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable    = ", is_stable (25, global)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, global)

write (u, "(A)")
write (u, "(A)")  "* Local model"
write (u, "(A)")

call local%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable    = ", is_stable (25, local)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, local)

```

```

write (u, *)

write (u, "(A)", advance="no") "Global model variable: "
model_vars => global%model%get_var_list_ptr ()
call model_vars%write_var (var_name, u)

write (u, "(A)", advance="no") "Local model variable: "
associate (model_var_list_ptr => local%model%get_var_list_ptr())
  call model_var_list_ptr%write_var (var_name, u)
end associate

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call local%model%final ()
deallocate (local%model)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_6"

end subroutine rt_data_6

```

Result variables

Initialize result variables and check that they are accessible via the global variable list.

```

<RT data: execute tests>+≡
  call test (rt_data_7, "rt_data_7", &
    "result variables", &
    u, results)

<RT data: test declarations>+≡
  public :: rt_data_7

<RT data: tests>+≡
  subroutine rt_data_7 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: rt_data_7"
    write (u, "(A)")  "* Purpose: set and access result variables"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process variables"
    write (u, "(A)")

    call global%global_init ()
    call global%process_stack%init_result_vars (var_str ("testproc"))

    call global%var_list%write_var (&

```

```

        var_str ("integral(testproc)", u, defined=.true.)
call global%var_list%write_var (&
        var_str ("error(testproc)", u, defined=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_7"

end subroutine rt_data_7

```

Beam energy

If beam parameters are set, the variable `sqrts` is not necessarily the collision energy. The method `get_sqrts` fetches the correct value.

```

<RT data: execute tests>+≡
call test (rt_data_8, "rt_data_8", &
        "beam energy", &
        u, results)

<RT data: test declarations>+≡
public :: rt_data_8

<RT data: tests>+≡
subroutine rt_data_8 (u)
integer, intent(in) :: u
type(rt_data_t), target :: global

write (u, "(A)")  "* Test output: rt_data_8"
write (u, "(A)")  "* Purpose: get correct collision energy"
write (u, "(A)")

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call global%global_init ()

write (u, "(A)")  "* Set sqrt s"
write (u, "(A)")

call global%set_real (var_str ("sqrts"), &
        1000._default, is_known = .true.)
write (u, "(1x,A," // FMT_19 // ")")  "sqrts =", global%get_sqrts ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: rt_data_8"

    end subroutine rt_data_8

```

Local variable modifications

```

<RT data: execute tests>+≡
    call test (rt_data_9, "rt_data_9", &
        "local variables", &
        u, results)

<RT data: test declarations>+≡
    public :: rt_data_9

<RT data: tests>+≡
    subroutine rt_data_9 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global, local
        type(var_list_t), pointer :: var_list

        write (u, "(A)")  "* Test output: rt_data_9"
        write (u, "(A)")  "* Purpose: handle local variables"
        write (u, "(A)")

        call syntax_model_file_init ()

        write (u, "(A)")  "* Initialize global record and set some variables"
        write (u, "(A)")

        call global%global_init ()
        call global%select_model (var_str ("Test"))

        call global%set_real (var_str ("sqrts"), 17._default, is_known = .true.)
        call global%set_real (var_str ("luminosity"), 2._default, is_known = .true.)
        call global%model_set_real (var_str ("ff"), 0.5_default)
        call global%model_set_real (var_str ("gy"), 1.2_default)

        var_list => global%get_var_list_ptr ()

        call var_list%write_var (var_str ("sqrts"), u, defined=.true.)
        call var_list%write_var (var_str ("luminosity"), u, defined=.true.)
        call var_list%write_var (var_str ("ff"), u, defined=.true.)
        call var_list%write_var (var_str ("gy"), u, defined=.true.)
        call var_list%write_var (var_str ("mf"), u, defined=.true.)
        call var_list%write_var (var_str ("x"), u, defined=.true.)

        write (u, "(A)")

        write (u, "(1x,A,1x,F5.2)")  "sqrts      = ", &
            global%get_rval (var_str ("sqrts"))
        write (u, "(1x,A,1x,F5.2)")  "luminosity = ", &
            global%get_rval (var_str ("luminosity"))
        write (u, "(1x,A,1x,F5.2)")  "ff          = ", &
            global%get_rval (var_str ("ff"))

```

```

write (u, "(1x,A,1x,F5.2)") "gy          = ", &
      global%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)") "mf          = ", &
      global%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)") "x           = ", &
      global%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Create local record with local variables"
write (u, "(A)")

call local%local_init (global)

call local%append_real (var_str ("luminosity"), intrinsic = .true.)
call local%append_real (var_str ("x"), user = .true.)

call local%activate ()

var_list => local%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)
call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)") "sqrts      = ", &
      local%get_rval (var_str ("sqrts"))
write (u, "(1x,A,1x,F5.2)") "luminosity = ", &
      local%get_rval (var_str ("luminosity"))
write (u, "(1x,A,1x,F5.2)") "ff         = ", &
      local%get_rval (var_str ("ff"))
write (u, "(1x,A,1x,F5.2)") "gy         = ", &
      local%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)") "mf         = ", &
      local%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)") "x          = ", &
      local%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Modify some local variables"
write (u, "(A)")

call local%set_real (var_str ("luminosity"), 42._default, is_known=.true.)
call local%set_real (var_str ("x"), 6.66_default, is_known=.true.)
call local%model_set_real (var_str ("ff"), 0.7_default)

var_list => local%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)

```

```

call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)" "sqrts      = ", &
      local%get_rval (var_str ("sqrts"))
write (u, "(1x,A,1x,F5.2)" "luminosity = ", &
      local%get_rval (var_str ("luminosity"))
write (u, "(1x,A,1x,F5.2)" "ff          = ", &
      local%get_rval (var_str ("ff"))
write (u, "(1x,A,1x,F5.2)" "gy          = ", &
      local%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)" "mf          = ", &
      local%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)" "x            = ", &
      local%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Restore globals"
write (u, "(A)")

call local%deactivate (global)

var_list => global%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)
call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)" "sqrts      = ", &
      global%get_rval (var_str ("sqrts"))
write (u, "(1x,A,1x,F5.2)" "luminosity = ", &
      global%get_rval (var_str ("luminosity"))
write (u, "(1x,A,1x,F5.2)" "ff          = ", &
      global%get_rval (var_str ("ff"))
write (u, "(1x,A,1x,F5.2)" "gy          = ", &
      global%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)" "mf          = ", &
      global%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)" "x            = ", &
      global%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call local%local_final ()

```



```

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_9"

end subroutine rt_data_9

```

Descriptions

```

<RT data: execute tests>+≡
  call test(rt_data_10, "rt_data_10", &
    "descriptions", u, results)

<RT data: test declarations>+≡
  public :: rt_data_10

<RT data: tests>+≡
  subroutine rt_data_10 (u)
    integer, intent(in) :: u
    type(rt_data_t) :: global
    ! type(var_list_t) :: var_list
    write (u, "(A)")  "* Test output: rt_data_10"
    write (u, "(A)")  "* Purpose: display descriptions"
    write (u, "(A)")

    call global%var_list%append_real (var_str ("sqrts"), &
      intrinsic=.true., &
      description=var_str ('Real variable in order to set the center-of-mass ' // &
        'energy for the collisions.'))
    call global%var_list%append_real (var_str ("luminosity"), 0._default, &
      intrinsic=.true., &
      description=var_str ('This specifier \ttt{luminosity = {\em <num>}} ' // &
        '<num>}} sets the integrated luminosity (in inverse femtobarns, ' // &
        '\fb${}^{-1}$) for the event generation of the processes in the ' // &
        '\sindarin\ input files.'))
    call global%var_list%append_int (var_str ("seed"), 1234, &
      intrinsic=.true., &
      description=var_str ('Integer variable \ttt{seed = {\em <num>}} ' // &
        'that allows to set a specific random seed \ttt{num}.'))
    call global%var_list%append_string (var_str ("method"), var_str ("omega"), &
      intrinsic=.true., &
      description=var_str ('This string variable specifies the method ' // &
        'for the matrix elements to be used in the evaluation.))
    call global%var_list%append_log (var_str ("read_color_factors"), .true., &
      intrinsic=.true., &
      description=var_str ('This flag decides whether to read QCD ' // &
        'color factors from the matrix element provided by each method, ' // &
        'or to try and calculate the color factors in \whizard\ internally.))

    call global%var_list%sort ()

    call global%write_var_descriptions (u)

```

```

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_10"
end subroutine rt_data_10

```

Export objects

Export objects are variables or other data that should be copied or otherwise applied to corresponding objects in the outer scope.

We test appending and retrieval for the export list.

```

<RT data: execute tests>+≡
call test(rt_data_11, "rt_data_11", &
         "export objects", u, results)

<RT data: test declarations>+≡
public :: rt_data_11

<RT data: tests>+≡
subroutine rt_data_11 (u)
integer, intent(in) :: u
type(rt_data_t) :: global
type(string_t), dimension(:), allocatable :: exports
integer :: i

write (u, "(A)")  "* Test output: rt_data_11"
write (u, "(A)")  "* Purpose: handle export object list"
write (u, "(A)")

write (u, "(A)")  "* Empty export list"
write (u, "(A)")

call global%write_exports (u)

write (u, "(A)")  "* Add an entry"
write (u, "(A)")

allocate (exports (1))
exports(1) = var_str ("results")
do i = 1, size (exports)
  write (u, "('+ ',A)") char (exports(i))
end do
write (u, *)

call global%append_exports (exports)
call global%write_exports (u)

write (u, "(A)")
write (u, "(A)")  "* Add more entries, including doubler"
write (u, "(A)")

deallocate (exports)
allocate (exports (3))

```

```

exports(1) = var_str ("foo")
exports(2) = var_str ("results")
exports(3) = var_str ("bar")
do i = 1, size (exports)
    write (u, "('+ ',A)") char (exports(i))
end do
write (u, *)

call global%append_exports (exports)
call global%write_exports (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_11"
end subroutine rt_data_11

```

33.3 Select implementations

For abstract types (process core, integrator, phase space, etc.), we need a way to dynamically select a concrete type, using either data given by the user or a previous selection of a concrete type. This is done by subroutines in the current module.

We would like to put this in the `me_methods` folder but it also depends on `gosam` and `openloops`, so it is unclear where to put it.

```
<dispatch_me_methods.f90>≡  
  <File header>  
  
  module dispatch_me_methods  
  
    <Use strings>  
    <Use debug>  
    use physics_defs, only: BORN  
    use diagnostics  
    use sm_qcd  
    use variables, only: var_list_t  
    use models  
    use model_data  
  
    use prc_core_def  
    use prc_core  
    use prc_test_core  
    use prc_template_me  
    use prc_test  
    use prc_omega  
    use prc_external  
    use prc_gosam  
    use prc_openloops  
    use prc_recola  
    use prc_threshold  
  
    <Standard module head>  
  
    <Dispatch ME methods: public>  
  
    interface  
    <Dispatch ME methods: sub interfaces>  
    end interface  
  
    contains  
  
    <Dispatch ME methods: main procedures>  
  
  end module dispatch_me_methods  
  
<dispatch_me_methods_sub.f90>≡  
  <File header>  
  
  submodule (dispatch_me_methods) dispatch_me_methods_s  
  
    implicit none
```

contains

<Dispatch ME methods: procedures>

end submodule dispatch_me_methods_s

33.3.1 Process Core Definition

The `prc_core_def_t` abstract type can be instantiated by providing a `$method` string variable. Gfortran 7/8/9 bug, has to remain in the main module:

<Dispatch ME methods: public>≡

public :: dispatch_core_def

<Dispatch ME methods: main procedures>≡

```
subroutine dispatch_core_def (core_def, prt_in, prt_out, &
    model, var_list, id, nlo_type, method)
    class(prc_core_def_t), allocatable, intent(out) :: core_def
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    type(model_t), pointer, intent(in) :: model
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in), optional :: id
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: method
    type(string_t) :: model_name, meth
    type(string_t) :: ufo_path
    type(string_t) :: restrictions
    logical :: ufo
    logical :: cms_scheme
    logical :: openmp_support
    logical :: report_progress
    logical :: diags, diags_color
    logical :: write_phs_output
    type(string_t) :: extra_options, correction_type
    integer :: nlo
    integer :: alpha_power
    integer :: alphas_power
    if (present (method)) then
        meth = method
    else
        meth = var_list%get_sval (var_str (" $method"))
    end if
    if (debug_on) call msg_debug2 (D_CORE, "dispatch_core_def")
    if (associated (model)) then
        model_name = model%get_name ()
        cms_scheme = model%get_scheme () == "Complex_Mass_Scheme"
        ufo = model%is_ufo_model ()
        ufo_path = model%get_ufo_path ()
    else
        model_name = ""
        cms_scheme = .false.
        ufo = .false.
```

```

end if
restrictions = var_list%get_sval (&
    var_str ("$restrictions"))
diags = var_list%get_lval (&
    var_str ("?vis_diags"))
diags_color = var_list%get_lval (&
    var_str ("?vis_diags_color"))
openmp_support = var_list%get_lval (&
    var_str ("?omega_openmp"))
report_progress = var_list%get_lval (&
    var_str ("?report_progress"))
write_phs_output = var_list%get_lval (&
    var_str ("?omega_write_phs_output"))
extra_options = var_list%get_sval (&
    var_str ("$omega_flags"))
nlo = BORN; if (present (nlo_type)) nlo = nlo_type
alpha_power = var_list%get_ival (var_str ("alpha_power"))
alphas_power = var_list%get_ival (var_str ("alphas_power"))
correction_type = var_list%get_sval (var_str ("$nlo_correction_type"))
if (debug_on) call msg_debug2 (D_CORE, "dispatching core method: ", meth)
select case (char (meth))
case ("unit_test")
    allocate (prc_test_def_t :: core_def)
    select type (core_def)
    type is (prc_test_def_t)
        call core_def%init (model_name, prt_in, prt_out)
    end select
case ("template")
    allocate (template_me_def_t :: core_def)
    select type (core_def)
    type is (template_me_def_t)
        call core_def%init (model, prt_in, prt_out, unity = .false.)
    end select
case ("template_unity")
    allocate (template_me_def_t :: core_def)
    select type (core_def)
    type is (template_me_def_t)
        call core_def%init (model, prt_in, prt_out, unity = .true.)
    end select
case ("omega")
    allocate (omega_def_t :: core_def)
    select type (core_def)
    type is (omega_def_t)
        call core_def%init (model_name, prt_in, prt_out, &
            .false., ufo, ufo_path, &
            restrictions, cms_scheme, &
            openmp_support, report_progress, write_phs_output, &
            extra_options, diags, diags_color)
    end select
case ("ovm")
    allocate (omega_def_t :: core_def)
    select type (core_def)
    type is (omega_def_t)
        call core_def%init (model_name, prt_in, prt_out, &

```

```

        .true., .false., var_str (""), &
        restrictions, cms_scheme, &
        openmp_support, report_progress, write_phs_output, &
        extra_options, diags, diags_color)
    end select
case ("gosam")
    allocate (gosam_def_t :: core_def)
    select type (core_def)
    type is (gosam_def_t)
        if (present (id)) then
            call core_def%init (id, model_name, prt_in, &
                prt_out, nlo, restrictions, var_list)
        else
            call msg_fatal ("Dispatch GoSam def: No id!")
        end if
    end select
case ("openloops")
    allocate (openloops_def_t :: core_def)
    select type (core_def)
    type is (openloops_def_t)
        if (present (id)) then
            call core_def%init (id, model_name, prt_in, &
                prt_out, nlo, restrictions, var_list)
        else
            call msg_fatal ("Dispatch OpenLoops def: No id!")
        end if
    end select
case ("recola")
    call abort_if_recola_not_active ()
    allocate (recola_def_t :: core_def)
    select type (core_def)
    type is (recola_def_t)
        if (present (id)) then
            call core_def%init (id, model_name, prt_in, prt_out, &
                nlo, alpha_power, alphas_power, correction_type, &
                restrictions)
        else
            call msg_fatal ("Dispatch RECOLA def: No id!")
        end if
    end select
case ("dummy")
    allocate (prc_external_test_def_t :: core_def)
    select type (core_def)
    type is (prc_external_test_def_t)
        if (present (id)) then
            call core_def%init (id, model_name, prt_in, prt_out)
        else
            call msg_fatal ("Dispatch User-Defined Test def: No id!")
        end if
    end select
case ("threshold")
    allocate (threshold_def_t :: core_def)
    select type (core_def)
    type is (threshold_def_t)

```

```

        if (present (id)) then
            call core_def%init (id, model_name, prt_in, prt_out, &
                               nlo, restrictions)
        else
            call msg_fatal ("Dispatch Threshold def: No id!")
        end if
    end select
case default
    call msg_fatal ("Process configuration: method '" &
                   // char (meth) // "' not implemented")
end select
end subroutine dispatch_core_def

```

33.3.2 Process core allocation

Here we allocate an object of abstract type `prc_core_t` with a concrete type that matches a process definition. The `prc_omega_t` extension will require the current parameter set, so we take the opportunity to grab it from the model. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Dispatch ME methods: public>+≡
    public :: dispatch_core

<Dispatch ME methods: main procedures>+≡
    subroutine dispatch_core (core, core_def, model, &
                             helicity_selection, qcd, use_color_factors, has_beam_pol)
        class(prc_core_t), allocatable, intent(inout) :: core
        class(prc_core_def_t), intent(in) :: core_def
        class(model_data_t), intent(in), target, optional :: model
        type(helicity_selection_t), intent(in), optional :: helicity_selection
        type(qcd_t), intent(in), optional :: qcd
        logical, intent(in), optional :: use_color_factors
        logical, intent(in), optional :: has_beam_pol
        select type (core_def)
        type is (prc_test_def_t)
            allocate (test_t :: core)
        type is (template_me_def_t)
            allocate (prc_template_me_t :: core)
            select type (core)
            type is (prc_template_me_t)
                call core%set_parameters (model)
            end select
        class is (omega_def_t)
            if (.not. allocated (core)) allocate (prc_omega_t :: core)
            select type (core)
            type is (prc_omega_t)
                call core%set_parameters (model, &
                                         helicity_selection, qcd, use_color_factors)
            end select
        type is (gosam_def_t)
            if (.not. allocated (core)) allocate (prc_gosam_t :: core)
            select type (core)
            type is (prc_gosam_t)
                call core%set_parameters (qcd)
            end select
        end select
    end subroutine dispatch_core

```



```

        end select
type is (openloops_def_t)
    if (.not. allocated (core)) allocate (prc_openloops_t :: core)
    select type (core)
    type is (prc_openloops_t)
        call core%set_parameters (qcd)
    end select
type is (recola_def_t)
    if (.not. allocated (core)) allocate (prc_recola_t :: core)
    select type (core)
    type is (prc_recola_t)
        call core%set_parameters (qcd, model)
    end select
type is (prc_external_test_def_t)
    if (.not. allocated (core)) allocate (prc_external_test_t :: core)
    select type (core)
    type is (prc_external_test_t)
        call core%set_parameters (qcd, model)
    end select
type is (threshold_def_t)
    if (.not. allocated (core)) allocate (prc_threshold_t :: core)
    select type (core)
    type is (prc_threshold_t)
        call core%set_parameters (qcd, model)
        call core%set_beam_pol (has_beam_pol)
    end select
class default
    call msg_bug ("Process core: unexpected process definition type")
end select
end subroutine dispatch_core

```

33.3.3 Process core update and restoration

Here we take an existing object of abstract type `prc_core_t` and update the parameters as given by the current state of `model`. Optionally, we can save the previous state as `saved_core`. The second routine restores the original from the save.

(In the test case, there is no possible update.)

(Dispatch ME methods: public) +≡

```

public :: dispatch_core_update
public :: dispatch_core_restore

```

(Dispatch ME methods: sub interfaces) ≡

```

module subroutine dispatch_core_update &
    (core, model, helicity_selection, qcd, saved_core)
    class(prc_core_t), allocatable, intent(inout) :: core
    class(model_data_t), intent(in), optional, target :: model
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    type(qcd_t), intent(in), optional :: qcd
    class(prc_core_t), allocatable, intent(inout), optional :: saved_core
end subroutine dispatch_core_update
module subroutine dispatch_core_restore (core, saved_core)

```

```

        class(prc_core_t), allocatable, intent(inout) :: core
        class(prc_core_t), allocatable, intent(inout) :: saved_core
    end subroutine dispatch_core_restore

    <Dispatch ME methods: procedures>≡
    module subroutine dispatch_core_update &
        (core, model, helicity_selection, qcd, saved_core)

        class(prc_core_t), allocatable, intent(inout) :: core
        class(model_data_t), intent(in), optional, target :: model
        type(helicity_selection_t), intent(in), optional :: helicity_selection
        type(qcd_t), intent(in), optional :: qcd
        class(prc_core_t), allocatable, intent(inout), optional :: saved_core

        if (present (saved_core)) then
            allocate (saved_core, source = core)
        end if
        select type (core)
        type is (test_t)
        type is (prc_omega_t)
            call core%set_parameters (model, helicity_selection, qcd)
            call core%activate_parameters ()
        class is (prc_external_t)
            call msg_message ("Updating user defined cores is not implemented yet.")
        class default
            call msg_bug ("Process core update: unexpected process definition type")
        end select
    end subroutine dispatch_core_update

    module subroutine dispatch_core_restore (core, saved_core)

        class(prc_core_t), allocatable, intent(inout) :: core
        class(prc_core_t), allocatable, intent(inout) :: saved_core

        call move_alloc (from = saved_core, to = core)
        select type (core)
        type is (test_t)
        type is (prc_omega_t)
            call core%activate_parameters ()
        class default
            call msg_bug ("Process core restore: unexpected process definition type")
        end select
    end subroutine dispatch_core_restore

```

33.3.4 Unit Tests

Test module, followed by the corresponding implementation module.

```

    <dispatch_ut.f90>≡
    <File header>

    module dispatch_ut
        use unit_tests
        use dispatch_uti

```

```

    <Standard module head>

    <Dispatch: public test>

    <Dispatch: public test auxiliary>

contains

    <Dispatch: test driver>

end module dispatch_ut

(dispatch_uti.f90)≡
    <File header>

module dispatch_uti
    <Use kinds>
    <Use strings>
    use os_interface, only: os_data_t
    use physics_defs, only: ELECTRON, PROTON
    use sm_qcd, only: qcd_t
    use flavors, only: flavor_t
    use interactions, only: reset_interaction_counter
    use pdg_arrays, only: pdg_array_t, assignment(=)
    use prc_core_def, only: prc_core_def_t
    use prc_test_core, only: test_t
    use prc_core, only: prc_core_t
    use prc_test, only: prc_test_def_t
    use prc_omega, only: omega_def_t, prc_omega_t
    use sf_mappings, only: sf_channel_t
    use sf_base, only: sf_data_t, sf_config_t
    use phs_base, only: phs_channel_collection_t
    use variables, only: var_list_t
    use model_data, only: model_data_t
    use models, only: syntax_model_file_init, syntax_model_file_final
    use rt_data, only: rt_data_t

    use dispatch_phase_space, only: dispatch_sf_channels
    use dispatch_beams, only: sf_prop_t, dispatch_qcd
    use dispatch_beams, only: dispatch_sf_config, dispatch_sf_data
    use dispatch_me_methods, only: dispatch_core_def, dispatch_core
    use dispatch_me_methods, only: dispatch_core_update, dispatch_core_restore

    use sf_base_ut, only: sf_test_data_t

    <Standard module head>

    <Dispatch: public test auxiliary>

    <Dispatch: test declarations>

contains

    <Dispatch: tests>

```

<Dispatch: test auxiliary>

end module dispatch_uti

API: driver for the unit tests below.

<Dispatch: public test>≡

public :: dispatch_test

<Dispatch: test driver>≡

subroutine dispatch_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Dispatch: execute tests>

end subroutine dispatch_test

Select type: process definition

<Dispatch: execute tests>≡

call test (dispatch_1, "dispatch_1", &
"process configuration method", &
u, results)

<Dispatch: test declarations>≡

public :: dispatch_1

<Dispatch: tests>≡

subroutine dispatch_1 (u)

integer, intent(in) :: u

type(string_t), dimension(2) :: prt_in, prt_out

type(rt_data_t), target :: global

class(prc_core_def_t), allocatable :: core_def

write (u, "(A)") "* Test output: dispatch_1"

write (u, "(A)") "* Purpose: select process configuration method"

write (u, "(A)")

call global%global_init ()

call global%set_log (var_str ("?omega_openmp"), &
.false., is_known = .true.)

prt_in = [var_str ("a"), var_str ("b")]

prt_out = [var_str ("c"), var_str ("d")]

write (u, "(A)") "* Allocate core_def as prc_test_def"

call global%set_string (var_str ("method"), &

var_str ("unit_test"), is_known = .true.)

call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)

select type (core_def)

type is (prc_test_def_t)

call core_def%write (u)

end select

```

deallocate (core_def)

write (u, "(A)")
write (u, "(A)")  "* Allocate core_def as omega_def"
write (u, "(A)")

call global%set_string (var_str ("$method"), &
    var_str ("omega"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)
select type (core_def)
type is (omega_def_t)
    call core_def%write (u)
end select

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_1"

end subroutine dispatch_1

```

Select type: process core

```

<Dispatch: execute tests>+≡
    call test (dispatch_2, "dispatch_2", &
        "process core", &
        u, results)

<Dispatch: test declarations>+≡
    public :: dispatch_2

<Dispatch: tests>+≡
    subroutine dispatch_2 (u)
        integer, intent(in) :: u
        type(string_t), dimension(2) :: prt_in, prt_out
        type(rt_data_t), target :: global
        class(prc_core_def_t), allocatable :: core_def
        class(prc_core_t), allocatable :: core

        write (u, "(A)")  "* Test output: dispatch_2"
        write (u, "(A)")  "* Purpose: select process configuration method"
        write (u, "(A)")  "           and allocate process core"
        write (u, "(A)")

        call syntax_model_file_init ()
        call global%global_init ()

        prt_in = [var_str ("a"), var_str ("b")]
        prt_out = [var_str ("c"), var_str ("d")]

        write (u, "(A)")  "* Allocate core as test_t"
        write (u, "(A)")
    end subroutine dispatch_2

```

```

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)
call dispatch_core (core, core_def)
select type (core)
type is (test_t)
    call core%write (u)
end select

deallocate (core)
deallocate (core_def)

write (u, "(A)")
write (u, "(A)")  "* Allocate core as prc_omega_t"
write (u, "(A)")

call global%set_string (var_str ("$method"), &
    var_str ("omega"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)

call global%select_model (var_str ("Test"))

call global%set_log (&
    var_str ("?helicity_selection_active"), &
    .true., is_known = .true.)
call global%set_real (&
    var_str ("helicity_selection_threshold"), &
    1e9_default, is_known = .true.)
call global%set_int (&
    var_str ("helicity_selection_cutoff"), &
    10, is_known = .true.)

call dispatch_core (core, core_def, &
    global%model, &
    global%get_helicity_selection ())
call core_def%allocate_driver (core%driver, var_str (""))

select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_2"

end subroutine dispatch_2

```

Select type: structure-function data

This is an extra dispatcher that enables the test structure functions. This procedure should be assigned to the `dispatch_sf_data_extra` hook before any tests are executed.

<Dispatch: public test auxiliary>≡

```
public :: dispatch_sf_data_test
```

<Dispatch: test auxiliary>≡

```
subroutine dispatch_sf_data_test (data, sf_method, i_beam, sf_prop, &
    var_list, var_list_global, model, os_data, sqrts, pdg_in, pdg_prc, polarized)
    class(sf_data_t), allocatable, intent(inout) :: data
    type(string_t), intent(in) :: sf_method
    integer, dimension(:), intent(in) :: i_beam
    type(var_list_t), intent(in) :: var_list
    type(var_list_t), intent(inout) :: var_list_global
    class(model_data_t), target, intent(in) :: model
    type(os_data_t), intent(in) :: os_data
    real(default), intent(in) :: sqrts
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_in
    type(pdg_array_t), dimension(:, :), intent(in) :: pdg_prc
    type(sf_prop_t), intent(inout) :: sf_prop
    logical, intent(in) :: polarized
    select case (char (sf_method))
    case ("sf_test_0", "sf_test_1")
        allocate (sf_test_data_t :: data)
        select type (data)
        type is (sf_test_data_t)
            select case (char (sf_method))
            case ("sf_test_0"); call data%init (model, pdg_in(i_beam(1)))
            case ("sf_test_1"); call data%init (model, pdg_in(i_beam(1)), &
                mode = 1)
            end select
        end select
    end select
end subroutine dispatch_sf_data_test
```

The actual test. We can't move this to `beams` as it depends on `model_features` for the `model_list_t`.

<Dispatch: execute tests>+≡

```
call test (dispatch_7, "dispatch_7", &
    "structure-function data", &
    u, results)
```

<Dispatch: test declarations>+≡

```
public :: dispatch_7
```

<Dispatch: tests>+≡

```
subroutine dispatch_7 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global
    type(os_data_t) :: os_data
    type(string_t) :: prt, sf_method
    type(sf_prop_t) :: sf_prop
    class(sf_data_t), allocatable :: data
```

```

type(pdg_array_t), dimension(1) :: pdg_in
type(pdg_array_t), dimension(1,1) :: pdg_prc
type(pdg_array_t), dimension(1) :: pdg_out
integer, dimension(:), allocatable :: pdg1

write (u, "(A)")  "* Test output: dispatch_7"
write (u, "(A)")  "* Purpose: select and configure &
                  &structure function data"
write (u, "(A)")

call global%global_init ()

call os_data%init ()
call syntax_model_file_init ()
call global%select_model (var_str ("QCD"))

call reset_interaction_counter ()
call global%set_real (var_str ("sqrts"), &
                    14000._default, is_known = .true.)
prt = "p"
call global%beam_structure%init_sf ([prt, prt], [1])
pdg_in = 2212

write (u, "(A)")  "* Allocate data as sf_pdf_builtin_t"
write (u, "(A)")

sf_method = "pdf_builtin"
call dispatch_sf_data (data, sf_method, [1], sf_prop, &
                    global%get_var_list_ptr (), global%var_list, &
                    global%model, global%os_data, global%get_sqrts (), &
                    pdg_in, pdg_prc, .false.)
call data%write (u)

call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(A)")
write (u, "(1x,A,99(1x,I0))") "PDG(out) = ", pdg1

deallocate (data)

write (u, "(A)")
write (u, "(A)")  "* Allocate data for different PDF set"
write (u, "(A)")

pdg_in = 2212

call global%set_string (var_str ("pdf_builtin_set"), &
                    var_str ("CTEQ6M"), is_known = .true.)
sf_method = "pdf_builtin"
call dispatch_sf_data (data, sf_method, [1], sf_prop, &
                    global%get_var_list_ptr (), global%var_list, &
                    global%model, global%os_data, global%get_sqrts (), &
                    pdg_in, pdg_prc, .false.)
call data%write (u)

```



```

call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(A)")
write (u, "(1x,A,99(1x,I0))") "PDG(out) = ", pdg1

deallocate (data)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_7"

end subroutine dispatch_7

```

Beam structure

The actual test. We can't move this to beams as it depends on model_features for the model_list_t.

```

<Dispatch: execute tests>+≡
  call test (dispatch_8, "dispatch_8", &
    "beam structure", &
    u, results)

<Dispatch: test declarations>+≡
  public :: dispatch_8

<Dispatch: tests>+≡
  subroutine dispatch_8 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global
    type(os_data_t) :: os_data
    type(flavor_t), dimension(2) :: flv
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_prop_t) :: sf_prop
    type(sf_channel_t), dimension(:), allocatable :: sf_channel
    type(phs_channel_collection_t) :: coll
    type(string_t) :: sf_string
    integer :: i
    type(pdg_array_t), dimension (2,1) :: pdg_prc

    write (u, "(A)")  "* Test output: dispatch_8"
    write (u, "(A)")  "* Purpose: configure a structure-function chain"
    write (u, "(A)")

    call global%global_init ()

    call os_data%init ()
    call syntax_model_file_init ()
    call global%select_model (var_str ("QCD"))

    write (u, "(A)")  "* Allocate LHC beams with PDF builtin"

```

```

write (u, "(A)")

call flv(1)%init (PROTON, global%model)
call flv(2)%init (PROTON, global%model)

call reset_interaction_counter ()
call global%set_real (var_str ("sqrts"), &
    14000._default, is_known = .true.)

call global%beam_structure%init_sf (flv%get_name (), [1])
call global%beam_structure%set_sf (1, 1, var_str ("pdf_builtin"))

call dispatch_sf_config (sf_config, sf_prop, global%beam_structure, &
    global%get_var_list_ptr (), global%var_list, &
    global%model, global%os_data, global%get_sqrts (), pdg_prc)
do i = 1, size (sf_config)
    call sf_config(i)%write (u)
end do

call dispatch_sf_channels (sf_channel, sf_string, sf_prop, coll, &
    global%var_list, global%get_sqrts(), global%beam_structure)
write (u, "(1x,A)") "Mapping configuration:"
do i = 1, size (sf_channel)
    write (u, "(2x)", advance = "no")
    call sf_channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Allocate ILC beams with CIRCE1"
write (u, "(A)")

call global%select_model (var_str ("QED"))
call flv(1)%init ( ELECTRON, global%model)
call flv(2)%init (-ELECTRON, global%model)

call reset_interaction_counter ()
call global%set_real (var_str ("sqrts"), &
    500._default, is_known = .true.)
call global%set_log (var_str ("?circe1_generate"), &
    .false., is_known = .true.)

call global%beam_structure%init_sf (flv%get_name (), [1])
call global%beam_structure%set_sf (1, 1, var_str ("circe1"))

call dispatch_sf_config (sf_config, sf_prop, global%beam_structure, &
    global%get_var_list_ptr (), global%var_list, &
    global%model, global%os_data, global%get_sqrts (), pdg_prc)
do i = 1, size (sf_config)
    call sf_config(i)%write (u)
end do

call dispatch_sf_channels (sf_channel, sf_string, sf_prop, coll, &
    global%var_list, global%get_sqrts(), global%beam_structure)
write (u, "(1x,A)") "Mapping configuration:"

```

```

do i = 1, size (sf_channel)
  write (u, "(2x)", advance = "no")
  call sf_channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_8"

end subroutine dispatch_8

```

Update process core parameters

This test dispatches a process core, temporarily modifies parameters, then restores the original.

```

<Dispatch: execute tests>+≡
  call test (dispatch_10, "dispatch_10", &
    "process core update", &
    u, results)

<Dispatch: test declarations>+≡
  public :: dispatch_10

<Dispatch: tests>+≡
  subroutine dispatch_10 (u)
    integer, intent(in) :: u
    type(string_t), dimension(2) :: prt_in, prt_out
    type(rt_data_t), target :: global
    class(prc_core_def_t), allocatable :: core_def
    class(prc_core_t), allocatable :: core, saved_core
    type(var_list_t), pointer :: model_vars

    write (u, "(A)")  "* Test output: dispatch_10"
    write (u, "(A)")  "* Purpose: select process configuration method,"
    write (u, "(A)")  "          allocate process core,"
    write (u, "(A)")  "          temporarily reset parameters"
    write (u, "(A)")

    call syntax_model_file_init ()
    call global%global_init ()

    prt_in = [var_str ("a"), var_str ("b")]
    prt_out = [var_str ("c"), var_str ("d")]

    write (u, "(A)")  "* Allocate core as prc_omega_t"
    write (u, "(A)")

    call global%set_string (var_str ("method"), &

```

```

        var_str ("omega"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)

call global%select_model (var_str ("Test"))

call dispatch_core (core, core_def, global%model)
call core_def%allocate_driver (core%driver, var_str (""))

select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Update core with modified model and helicity selection"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%set_real (var_str ("gy"), 2._default, &
    is_known = .true.)
call global%model%update_parameters ()

call global%set_log (&
    var_str ("?helicity_selection_active"), &
    .true., is_known = .true.)
call global%set_real (&
    var_str ("helicity_selection_threshold"), &
    2e10_default, is_known = .true.)
call global%set_int (&
    var_str ("helicity_selection_cutoff"), &
    5, is_known = .true.)

call dispatch_core_update (core, &
    global%model, &
    global%get_helicity_selection (), &
    saved_core = saved_core)
select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Restore core from save"
write (u, "(A)")

call dispatch_core_restore (core, saved_core)
select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

call global%final ()
call syntax_model_file_final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_10"

end subroutine dispatch_10

```

QCD Coupling

This test dispatches an `qcd` object, which is used to compute the (running) coupling by one of several possible methods.

We can't move this to `beams` as it depends on `model_features` for the `model_list_t`.

```

<Dispatch: execute tests>+≡
  call test (dispatch_11, "dispatch_11", &
    "QCD coupling", &
    u, results)

<Dispatch: test declarations>+≡
  public :: dispatch_11

<Dispatch: tests>+≡
  subroutine dispatch_11 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global
    type(var_list_t), pointer :: model_vars
    type(qcd_t) :: qcd

    write (u, "(A)")  "* Test output: dispatch_11"
    write (u, "(A)")  "* Purpose: select QCD coupling formula"
    write (u, "(A)")

    call syntax_model_file_init ()
    call global%global_init ()
    call global%select_model (var_str ("SM"))
    model_vars => global%get_var_list_ptr ()

    write (u, "(A)")  "* Allocate alpha_s as fixed"
    write (u, "(A)")

    call global%set_log (var_str ("?alphas_is_fixed"), &
      .true., is_known = .true.)
    call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
    call qcd%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Allocate alpha_s as running (built-in)"
    write (u, "(A)")

    call global%set_log (var_str ("?alphas_is_fixed"), &
      .false., is_known = .true.)
    call global%set_log (var_str ("?alphas_from_mz"), &
      .true., is_known = .true.)
    call global%set_int &

```

```

        (var_str ("alphas_order"), 1, is_known = .true.)
call model_vars%set_real (var_str ("alphas"), 0.1234_default, &
    is_known=.true.)
call model_vars%set_real (var_str ("mZ"), 91.234_default, &
    is_known=.true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate alpha_s as running (built-in, Lambda defined)"
write (u, "(A)")

call global%set_log (var_str ("?alphas_from_mz"), &
    .false., is_known = .true.)
call global%set_log (&
    var_str ("?alphas_from_lambda_qcd"), &
    .true., is_known = .true.)
call global%set_real &
    (var_str ("lambda_qcd"), 250.e-3_default, &
    is_known=.true.)
call global%set_int &
    (var_str ("alphas_order"), 2, is_known = .true.)
call global%set_int &
    (var_str ("alphas_nf"), 4, is_known = .true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate alpha_s as running (using builtin PDF set)"
write (u, "(A)")

call global%set_log (&
    var_str ("?alphas_from_lambda_qcd"), &
    .false., is_known = .true.)
call global%set_log &
    (var_str ("?alphas_from_pdf_builtin"), &
    .true., is_known = .true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_11"

end subroutine dispatch_11

```

33.4 Process Configuration

This module communicates between the toplevel command structure with its runtime data set and the process-library handling modules which collect the definition of individual processes. Its primary purpose is to select from the available matrix-element generating methods and configure the entry in the process library accordingly.

```
<process_configurations.f90>≡
  <File header>

  module process_configurations

    <Use strings>
    use models
    use particle_specifiers
    use process_libraries
    use rt_data
    use variables, only: var_list_t

    <Standard module head>

    <Process configurations: public>

    <Process configurations: types>

    interface
    <Process configurations: sub interfaces>
    end interface

  end module process_configurations

<process_configurations_sub.f90>≡
  <File header>

  submodule (process_configurations) process_configurations_s

    <Use debug>
    use diagnostics
    use io_units
    use physics_defs, only: BORN, NLO_VIRTUAL, NLO_REAL, NLO_DGLAP, &
      NLO_SUBTRACTION, NLO_MISMATCH
    use prc_core_def
    use dispatch_me_methods, only: dispatch_core_def
    use prc_external, only: prc_external_def_t

    implicit none

  contains

    <Process configurations: procedures>

  end submodule process_configurations_s
```

33.4.1 Data Type

```

<Process configurations: public>≡
    public :: process_configuration_t

<Process configurations: types>≡
    type :: process_configuration_t
        type(process_def_entry_t), pointer :: entry => null ()
        type(string_t) :: id
        integer :: num_id = 0
    contains
        <Process configurations: process configuration: TBP>
    end type process_configuration_t

```

Output (for unit tests).

```

<Process configurations: process configuration: TBP>≡
    procedure :: write => process_configuration_write

<Process configurations: sub interfaces>≡
    module subroutine process_configuration_write (config, unit)
        class(process_configuration_t), intent(in) :: config
        integer, intent(in), optional :: unit
    end subroutine process_configuration_write

<Process configurations: procedures>≡
    module subroutine process_configuration_write (config, unit)
        class(process_configuration_t), intent(in) :: config
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A)") "Process configuration:"
        if (associated (config%entry)) then
            call config%entry%write (u)
        else
            write (u, "(1x,3A)") "ID      = '", char (config%id), "'"
            write (u, "(1x,A,1x,IO)") "num ID =", config%num_id
            write (u, "(2x,A)") "[no entry]"
        end if
    end subroutine process_configuration_write

```

Initialize a process. We only need the name, the number of incoming particles, and the number of components.

```

<Process configurations: process configuration: TBP>+≡
    procedure :: init => process_configuration_init

<Process configurations: sub interfaces>+≡
    module subroutine process_configuration_init &
        (config, prc_name, n_in, n_components, model, var_list, &
         nlo_process, negative_sf)
        class(process_configuration_t), intent(out) :: config
        type(string_t), intent(in) :: prc_name
        integer, intent(in) :: n_in
        integer, intent(in) :: n_components
        type(model_t), intent(in), pointer :: model
        type(var_list_t), intent(in) :: var_list
    end subroutine process_configuration_init

```



```

        logical, intent(in), optional :: nlo_process, negative_sf
    end subroutine process_configuration_init
(Process configurations: procedures)+≡
module subroutine process_configuration_init &
    (config, prc_name, n_in, n_components, model, var_list, &
    nlo_process, negative_sf)
class(process_configuration_t), intent(out) :: config
type(string_t), intent(in) :: prc_name
integer, intent(in) :: n_in
integer, intent(in) :: n_components
type(model_t), intent(in), pointer :: model
type(var_list_t), intent(in) :: var_list
logical, intent(in), optional :: nlo_process, negative_sf
logical :: nlo_proc, neg_sf
logical :: requires_resonances
if (debug_on) call msg_debug (D_CORE, "process_configuration_init")
config%id = prc_name
if (present (nlo_process)) then
    nlo_proc = nlo_process
else
    nlo_proc = .false.
end if
if (present (negative_sf)) then
    neg_sf = negative_sf
else
    neg_sf = .false.
end if
requires_resonances = var_list%get_lval (var_str ("?resonance_history"))

if (debug_on) call msg_debug (D_CORE, "nlo_process", nlo_proc)
allocate (config%entry)
if (var_list%is_known (var_str ("process_num_id"))) then
    config%num_id = &
        var_list%get_ival (var_str ("process_num_id"))
    call config%entry%init (prc_name, &
        model = model, n_in = n_in, n_components = n_components, &
        num_id = config%num_id, &
        nlo_process = nlo_proc, &
        negative_sf = neg_sf, &
        requires_resonances = requires_resonances)
else
    call config%entry%init (prc_name, &
        model = model, n_in = n_in, n_components = n_components, &
        nlo_process = nlo_proc, &
        negative_sf = neg_sf, &
        requires_resonances = requires_resonances)
end if
end subroutine process_configuration_init

```

Initialize a process component. The details depend on the process method, which determines the type of the process component core. We set the incoming and outgoing particles (as strings, to be interpreted by the process driver). All other information is taken from the variable list.

The dispatcher gets only the names of the particles. The process component definition gets the complete specifiers which contains a polarization flag and names of decay processes, where applicable.

```

(Process configurations: process configuration: TBP)+≡
  procedure :: setup_component => process_configuration_setup_component

(Process configurations: sub interfaces)+≡
  module subroutine process_configuration_setup_component &
    (config, i_component, prt_in, prt_out, model, var_list, &
     nlo_type, can_be_integrated)
    class(process_configuration_t), intent(inout) :: config
    integer, intent(in) :: i_component
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(model_t), pointer, intent(in) :: model
    type(var_list_t), intent(in) :: var_list
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: can_be_integrated
  end subroutine process_configuration_setup_component

(Process configurations: procedures)+≡
  module subroutine process_configuration_setup_component &
    (config, i_component, prt_in, prt_out, model, var_list, &
     nlo_type, can_be_integrated)
    class(process_configuration_t), intent(inout) :: config
    integer, intent(in) :: i_component
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(model_t), pointer, intent(in) :: model
    type(var_list_t), intent(in) :: var_list
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: can_be_integrated
    type(string_t), dimension(:), allocatable :: prt_str_in
    type(string_t), dimension(:), allocatable :: prt_str_out
    class(prc_core_def_t), allocatable :: core_def
    type(string_t) :: method
    type(string_t) :: born_me_method
    type(string_t) :: real_tree_me_method
    type(string_t) :: loop_me_method
    type(string_t) :: correlation_me_method
    type(string_t) :: dglap_me_method
    integer :: i
    if (debug_on) call msg_debug2 &
      (D_CORE, "process_configuration_setup_component")
    allocate (prt_str_in (size (prt_in)))
    allocate (prt_str_out (size (prt_out)))
    forall (i = 1:size (prt_in)) prt_str_in(i) = prt_in(i)%get_name ()
    forall (i = 1:size (prt_out)) prt_str_out(i) = prt_out(i)%get_name ()

    method = var_list%get_sval (var_str ("method"))
    if (present (nlo_type)) then
      select case (nlo_type)
      case (BORN)
        born_me_method = var_list%get_sval (var_str ("born_me_method"))
        if (born_me_method /= var_str ("")) then

```

```

        method = born_me_method
    end if
case (NLO_VIRTUAL)
    loop_me_method = var_list%get_sval (var_str ("$_loop_me_method"))
    if (loop_me_method /= var_str ("")) then
        method = loop_me_method
    end if
case (NLO_REAL)
    real_tree_me_method = &
        var_list%get_sval (var_str ("$_real_tree_me_method"))
    if (real_tree_me_method /= var_str ("")) then
        method = real_tree_me_method
    end if
case (NLO_DGLAP)
    dglap_me_method = &
        var_list%get_sval (var_str ("$_dglap_me_method"))
    if (dglap_me_method /= var_str ("")) then
        method = dglap_me_method
    end if
case (NLO_SUBTRACTION,NLO_MISMATCH)
    correlation_me_method = &
        var_list%get_sval (var_str ("$_correlation_me_method"))
    if (correlation_me_method /= var_str ("")) then
        method = correlation_me_method
    end if
case default
end select
end if
call dispatch_core_def (core_def, prt_str_in, prt_str_out, &
    model, var_list, config%id, nlo_type, method)
select type (core_def)
class is (prc_external_def_t)
    if (present (can_be_integrated)) then
        call core_def%set_active_writer (can_be_integrated)
    else
        call msg_fatal ("Cannot decide if external core is integrated!")
    end if
end select

if (debug_on) call msg_debug2 &
    (D_CORE, "import_component with method ", method)
call config%entry%import_component (i_component, &
    n_out = size (prt_out), &
    prt_in = prt_in, &
    prt_out = prt_out, &
    method = method, &
    variant = core_def, &
    nlo_type = nlo_type, &
    can_be_integrated = can_be_integrated)
end subroutine process_configuration_setup_component

```

(Process configurations: process configuration: TBP)+=
 procedure :: set_fixed_emitter => process_configuration_set_fixed_emitter

```

(Process configurations: sub interfaces)+≡
    module subroutine process_configuration_set_fixed_emitter &
        (config, i, emitter)
        class(process_configuration_t), intent(inout) :: config
        integer, intent(in) :: i, emitter
    end subroutine process_configuration_set_fixed_emitter

(Process configurations: procedures)+≡
    module subroutine process_configuration_set_fixed_emitter (config, i, emitter)
        class(process_configuration_t), intent(inout) :: config
        integer, intent(in) :: i, emitter
        call config%entry%set_fixed_emitter (i, emitter)
    end subroutine process_configuration_set_fixed_emitter

(Process configurations: process configuration: TBP)+≡
    procedure :: set_coupling_powers => process_configuration_set_coupling_powers

(Process configurations: sub interfaces)+≡
    module subroutine process_configuration_set_coupling_powers &
        (config, alpha_power, alphas_power)
        class(process_configuration_t), intent(inout) :: config
        integer, intent(in) :: alpha_power, alphas_power
    end subroutine process_configuration_set_coupling_powers

(Process configurations: procedures)+≡
    module subroutine process_configuration_set_coupling_powers &
        (config, alpha_power, alphas_power)
        class(process_configuration_t), intent(inout) :: config
        integer, intent(in) :: alpha_power, alphas_power
        call config%entry%set_coupling_powers (alpha_power, alphas_power)
    end subroutine process_configuration_set_coupling_powers

(Process configurations: process configuration: TBP)+≡
    procedure :: set_component_associations => &
        process_configuration_set_component_associations

(Process configurations: sub interfaces)+≡
    module subroutine process_configuration_set_component_associations &
        (config, i_list, remnant, use_real_finite, mismatch)
        class(process_configuration_t), intent(inout) :: config
        integer, dimension(:), intent(in) :: i_list
        logical, intent(in) :: remnant, use_real_finite, mismatch
    end subroutine process_configuration_set_component_associations

(Process configurations: procedures)+≡
    module subroutine process_configuration_set_component_associations &
        (config, i_list, remnant, use_real_finite, mismatch)
        class(process_configuration_t), intent(inout) :: config
        integer, dimension(:), intent(in) :: i_list
        logical, intent(in) :: remnant, use_real_finite, mismatch
        integer :: i_component
        do i_component = 1, config%entry%get_n_components ()
            if (any (i_list == i_component)) then
                call config%entry%set_associated_components (i_component, &
                    i_list, remnant, use_real_finite, mismatch)
            end if
        end do
    end subroutine process_configuration_set_component_associations

```

```

end do
end subroutine process_configuration_set_component_associations

```

Record a process configuration: append it to the currently selected process definition library.

```

<Process configurations: process configuration: TBP>+≡
  procedure :: record => process_configuration_record

<Process configurations: sub interfaces>+≡
  module subroutine process_configuration_record (config, global)
    class(process_configuration_t), intent(inout) :: config
    type(rt_data_t), intent(inout) :: global
  end subroutine process_configuration_record

<Process configurations: procedures>+≡
  module subroutine process_configuration_record (config, global)
    class(process_configuration_t), intent(inout) :: config
    type(rt_data_t), intent(inout) :: global
    if (associated (global%prclib)) then
      call global%prclib%open ()
      call global%prclib%append (config%entry)
      if (config%num_id /= 0) then
        write (msg_buffer, "(5A,I0,A)") "Process library '", &
          char (global%prclib%get_name ()), &
          "' : recorded process '", char (config%id), "' (" , &
          config%num_id, ")"
      else
        write (msg_buffer, "(5A)") "Process library '", &
          char (global%prclib%get_name ()), &
          "' : recorded process '", char (config%id), "'"
      end if
      call msg_message ()
    else
      call msg_fatal ("Recording process '" // char (config%id) &
        // "' : active process library undefined")
    end if
  end subroutine process_configuration_record

```

33.4.2 Unit Tests

Test module, followed by the corresponding implementation module.

```

<process_configurations_ut.f90>≡
  <File header>

  module process_configurations_ut
    use unit_tests
    use process_configurations_uti

  <Standard module head>

  <Process configurations: public test>

  <Process configurations: public test auxiliary>

```

```

contains

  <Process configurations: test driver>

end module process_configurations_ut

<process_configurations_util.f90>≡
  <File header>

module process_configurations_util

  <Use strings>
  use particle_specifiers, only: new_prt_spec
  use prclib_stacks
  use models
  use rt_data

  use process_configurations

  <Standard module head>

  <Process configurations: test declarations>

  <Process configurations: public test auxiliary>

contains

  <Process configurations: test auxiliary>

  <Process configurations: tests>

end module process_configurations_util

```

API: driver for the unit tests below.

```

<Process configurations: public test>≡
  public :: process_configurations_test

<Process configurations: test driver>≡
  subroutine process_configurations_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Process configurations: execute tests>
  end subroutine process_configurations_test

```

Minimal setup

The workflow for setting up a minimal process configuration with the test matrix element method.

We wrap this in a public procedure, so we can reuse it in later modules. The procedure prepares a process definition list for two processes (one `prc_test` and one `omega` type) and appends this to the process library stack in the global data set.

The `mode` argument determines which processes to build.
The `procname` argument replaces the predefined `procname(s)`.
This is re-exported by the UT module.

```

(Process configurations: public test auxiliary)≡
  public :: prepare_test_library

(Process configurations: test auxiliary)≡
  subroutine prepare_test_library (global, libname, mode, procname)
    type(rt_data_t), intent(inout), target :: global
    type(string_t), intent(in) :: libname
    integer, intent(in) :: mode
    type(string_t), intent(in), dimension(:), optional :: procname
    type(prclib_entry_t), pointer :: lib
    type(string_t) :: prc_name
    type(string_t), dimension(:), allocatable :: prt_in, prt_out
    integer :: n_components
    type(process_configuration_t) :: prc_config

    if (.not. associated (global%prclib_stack%get_first_ptr ())) then
      allocate (lib)
      call lib%init (libname)
      call global%add_prclib (lib)
    end if

    if (btest (mode, 0)) then

      call global%select_model (var_str ("Test"))

      if (present (procname)) then
        prc_name = procname(1)
      else
        prc_name = "prc_config_a"
      end if
      n_components = 1
      allocate (prt_in (2), prt_out (2))
      prt_in = [var_str ("s"), var_str ("s")]
      prt_out = [var_str ("s"), var_str ("s")]

      call global%set_string (var_str ("$method"), &
        var_str ("unit_test"), is_known = .true.)

      call prc_config%init (prc_name, &
        size (prt_in), n_components, &
        global%model, global%var_list)
      call prc_config%setup_component (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global%model, global%var_list)
      call prc_config%record (global)

      deallocate (prt_in, prt_out)

    end if

    if (btest (mode, 1)) then

```

```

call global%select_model (var_str ("QED"))

if (present (procname)) then
    prc_name = procname(2)
else
    prc_name = "prc_config_b"
end if
n_components = 1
allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

call global%set_string (var_str ("method"), &
    var_str ("omega"), is_known = .true.)

call prc_config%init (prc_name, &
    size (prt_in), n_components, &
    global%model, global%var_list)
call prc_config%setup_component (1, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), &
    global%model, global%var_list)
call prc_config%record (global)

deallocate (prt_in, prt_out)

end if

if (btest (mode, 2)) then

    call global%select_model (var_str ("Test"))

    if (present (procname)) then
        prc_name = procname(1)
    else
        prc_name = "prc_config_a"
    end if
    n_components = 1
    allocate (prt_in (1), prt_out (2))
    prt_in = [var_str ("s")]
    prt_out = [var_str ("f"), var_str ("fbar")]

    call global%set_string (var_str ("method"), &
        var_str ("unit_test"), is_known = .true.)

    call prc_config%init (prc_name, &
        size (prt_in), n_components, &
        global%model, global%var_list)
    call prc_config%setup_component (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global%model, global%var_list)
    call prc_config%record (global)

    deallocate (prt_in, prt_out)

```



```

end if

end subroutine prepare_test_library

```

The actual test: the previous procedure with some prelude and postlude. In the global variable list, just before printing we reset the variables where the value may depend on the system and run environment.

```

<Process configurations: execute tests>≡
  call test (process_configurations_1, "process_configurations_1", &
    "test processes", &
    u, results)

<Process configurations: test declarations>≡
  public :: process_configurations_1

<Process configurations: tests>≡
  subroutine process_configurations_1 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: process_configurations_1"
    write (u, "(A)")  "* Purpose: configure test processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)

    write (u, "(A)")  "* Configure processes as prc_test, model Test"
    write (u, "(A)")  "*                               and omega, model QED"
    write (u, *)

    call global%set_int (var_str ("process_num_id"), &
      42, is_known = .true.)
    call prepare_test_library (global, var_str ("prc_config_lib_1"), 3)

    global%os_data%fc = "Fortran-compiler"
    global%os_data%fcflags = "Fortran-flags"
    global%os_data%fclibs = "Fortran-libs"

    call global%write_libraries (u)

    call global%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: process_configurations_1"

  end subroutine process_configurations_1

```

O'MEGA options

Slightly extended example where we pass O'MEGA options to the library. The `prepare_test_library` contents are spelled out.

```
(Process configurations: execute tests)+≡
    call test (process_configurations_2, "process_configurations_2", &
              "omega options", &
              u, results)

(Process configurations: test declarations)+≡
    public :: process_configurations_2

(Process configurations: tests)+≡
    subroutine process_configurations_2 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global

        type(string_t) :: libname
        type(prclib_entry_t), pointer :: lib
        type(string_t) :: prc_name
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        integer :: n_components
        type(process_configuration_t) :: prc_config

        write (u, "(A)")  "* Test output: process_configurations_2"
        write (u, "(A)")  "* Purpose: configure test processes with options"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

        write (u, "(A)")  "* Configure processes as omega, model QED"
        write (u, *)

        libname = "prc_config_lib_2"

        allocate (lib)
        call lib%init (libname)
        call global%add_prclib (lib)

        call global%select_model (var_str ("QED"))

        prc_name = "prc_config_c"
        n_components = 2
        allocate (prt_in (2), prt_out (2))
        prt_in = [var_str ("e+"), var_str ("e-")]
        prt_out = [var_str ("m+"), var_str ("m-")]

        call global%set_string (var_str ("method"), &
                               var_str ("omega"), is_known = .true.)
        call global%set_log (var_str ("?omega_openmp"), &
                             .false., is_known = .true.)

        call prc_config%init (prc_name, size (prt_in), n_components, &
```

```

        global%model, global%var_list)

call global%set_log (var_str ("?report_progress"), &
    .true., is_known = .true.)
call prc_config%setup_component (1, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), global%model, global%var_list)

call global%set_log (var_str ("?report_progress"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?omega_omp"), &
    .true., is_known = .true.)
call global%set_string (var_str ("restrictions"), &
    var_str ("3+4~A"), is_known = .true.)
call global%set_string (var_str ("omega_flags"), &
    var_str ("-fusion:progress_file omega_prc_config.log"), &
    is_known = .true.)
call prc_config%setup_component (2, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), global%model, global%var_list)

call prc_config%record (global)

deallocate (prt_in, prt_out)

global%os_data%fc = "Fortran-compiler"
global%os_data%fcflags = "Fortran-flags"
global%os_data%fclibs = "Fortran-libs"

call global%write_vars (u, [ &
    var_str ("model_name"), &
    var_str ("method"), &
    var_str ("?report_progress"), &
    var_str ("restrictions"), &
    var_str ("omega_flags")])
write (u, "(A)")
call global%write_libraries (u)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_configurations_2"

end subroutine process_configurations_2

```

33.5 Compilation

This module manages compilation and loading of process libraries. It is needed as a separate module because integration depends on it.

```
<compilations.f90>≡  
  <File header>  
  
  module compilations  
  
    <Use strings>  
    use os_interface  
    use variables, only: var_list_t  
    use model_data  
    use process_libraries  
    use prclib_stacks  
    use rt_data  
  
    <Standard module head>  
  
    <Compilations: public>  
  
    <Compilations: types>  
  
    <Compilations: parameters>  
  
    interface  
    <Compilations: sub interfaces>  
    end interface  
  
  end module compilations  
  
<compilations_sub.f90>≡  
  <File header>  
  
  submodule (compilations) compilations_s  
  
    use io_units  
    use system_defs, only: TAB  
    use system_dependencies, only: OS_IS_DARWIN  
    use diagnostics  
  
    implicit none  
  
  contains  
  
  <Compilations: procedures>  
  
  end submodule compilations_s
```

33.5.1 The data type

The compilation item handles the compilation and loading of a single process library.

```

<Compilations: public>≡
    public :: compilation_item_t

<Compilations: types>≡
    type :: compilation_item_t
        private
            type(string_t) :: libname
            type(string_t) :: static_external_tag
            type(process_library_t), pointer :: lib => null ()
            logical :: recompile_library = .false.
            logical :: verbose = .false.
            logical :: use_workspace = .false.
            type(string_t) :: workspace
        contains
            <Compilations: compilation item: TBP>
        end type compilation_item_t

```

Initialize.

Set flags and global properties of the library. Establish the workspace name, if defined.

```

<Compilations: compilation item: TBP>≡
    procedure :: init => compilation_item_init

<Compilations: sub interfaces>≡
    module subroutine compilation_item_init (comp, libname, stack, var_list)
        class(compilation_item_t), intent(out) :: comp
        type(string_t), intent(in) :: libname
        type(prclib_stack_t), intent(inout) :: stack
        type(var_list_t), intent(in) :: var_list
    end subroutine compilation_item_init

<Compilations: procedures>≡
    module subroutine compilation_item_init (comp, libname, stack, var_list)
        class(compilation_item_t), intent(out) :: comp
        type(string_t), intent(in) :: libname
        type(prclib_stack_t), intent(inout) :: stack
        type(var_list_t), intent(in) :: var_list
        comp%libname = libname
        comp%lib => stack%get_library_ptr (comp%libname)
        if (.not. associated (comp%lib)) then
            call msg_fatal ("Process library '" // char (comp%libname) &
                // "' has not been declared.")
        end if
        comp%recompile_library = &
            var_list%get_lval (var_str ("?recompile_library"))
        comp%verbose = &
            var_list%get_lval (var_str ("?me_verbose"))
        comp%use_workspace = &
            var_list%is_known (var_str ("$compile_workspace"))
        if (comp%use_workspace) then
            comp%workspace = &
                var_list%get_sval (var_str ("$compile_workspace"))
            if (comp%workspace == "") comp%use_workspace = .false.
        else
            comp%workspace = ""
        end if
    end subroutine compilation_item_init

```

```

        end if
    end subroutine compilation_item_init

```

Compile the current library. The `force` flag has the effect that we first delete any previous files, as far as accessible by the current makefile. It also guarantees that previous files not accessible by a makefile will be overwritten.

```

<Compilations: compilation item: TBP>+≡
    procedure :: compile => compilation_item_compile

<Compilations: sub interfaces>+≡
    module subroutine compilation_item_compile &
        (comp, model, os_data, force, recompile)
        class(compilation_item_t), intent(inout) :: comp
        class(model_data_t), intent(in), target :: model
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: force, recompile
    end subroutine compilation_item_compile

<Compilations: procedures>+≡
    module subroutine compilation_item_compile &
        (comp, model, os_data, force, recompile)
        class(compilation_item_t), intent(inout) :: comp
        class(model_data_t), intent(in), target :: model
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: force, recompile
        if (associated (comp%lib)) then
            if (comp%use_workspace) call setup_workspace (comp%workspace, os_data)
            call msg_message ("Process library '" &
                // char (comp%libname) // "': compiling ...")
            call comp%lib%configure (os_data)
            if (signal_is_pending ()) return
            call comp%lib%compute_md5sum (model)
            call comp%lib%write_makefile &
                (os_data, force, verbose=comp%verbose, workspace=comp%workspace)
            if (signal_is_pending ()) return
            if (force) then
                call comp%lib%clean &
                    (os_data, distclean = .false., workspace=comp%workspace)
                if (signal_is_pending ()) return
            end if
            call comp%lib%write_driver (force, workspace=comp%workspace)
            if (signal_is_pending ()) return
            if (recompile) then
                call comp%lib%load &
                    (os_data, keep_old_source = .true., workspace=comp%workspace)
                if (signal_is_pending ()) return
            end if
            call comp%lib%update_status (os_data, workspace=comp%workspace)
        end if
    end subroutine compilation_item_compile

```

The workspace directory is created if it does not exist. (Applies only if the user has set the workspace directory.)

```

<Compilations: parameters>≡

```

```

character(*), parameter :: ALLOWED_IN_DIRNAME = &
  "abcdefghijklmnopqrstuvwxyz&
  &ABCDEFGHIJKLMNOPQRSTUVWXYZ&
  &1234567890&
  &.,_-= "

```

```

<Compilations: procedures>+≡
subroutine setup_workspace (workspace, os_data)
  type(string_t), intent(in) :: workspace
  type(os_data_t), intent(in) :: os_data
  if (verify (workspace, ALLOWED_IN_DIRNAME) == 0) then
    call msg_message ("Compile: preparing workspace directory '" &
      // char (workspace) // "'")
    call os_system_call ("mkdir -p '" // workspace // "'")
  else
    call msg_fatal ("compile: workspace name '" &
      // char (workspace) // "' contains illegal characters")
  end if
end subroutine setup_workspace

```

Load the current library, just after compiling it.

```

<Compilations: compilation item: TBP>+≡
procedure :: load => compilation_item_load

<Compilations: sub interfaces>+≡
module subroutine compilation_item_load (comp, os_data)
  class(compilation_item_t), intent(inout) :: comp
  type(os_data_t), intent(in) :: os_data
end subroutine compilation_item_load

<Compilations: procedures>+≡
module subroutine compilation_item_load (comp, os_data)
  class(compilation_item_t), intent(inout) :: comp
  type(os_data_t), intent(in) :: os_data
  if (associated (comp%lib)) then
    call comp%lib%load (os_data, workspace=comp%workspace)
  end if
end subroutine compilation_item_load

```

Message as a separate call:

```

<Compilations: compilation item: TBP>+≡
procedure :: success => compilation_item_success

<Compilations: sub interfaces>+≡
module subroutine compilation_item_success (comp)
  class(compilation_item_t), intent(in) :: comp
end subroutine compilation_item_success

<Compilations: procedures>+≡
module subroutine compilation_item_success (comp)
  class(compilation_item_t), intent(in) :: comp
  if (associated (comp%lib)) then
    call msg_message ("Process library '" // char (comp%libname) &
      // "': ... success.")
  else

```

```

        call msg_fatal ("Process library '" // char (comp%libname) &
            // "' : ... failure.")
    end if
end subroutine compilation_item_success

```

33.5.2 API for library compilation and loading

This is a shorthand for compiling and loading a single library. The `compilation_item` object is used only internally.

The `global` data set may actually be local to the caller. The compilation affects the library specified by its name if it is on the stack, but it does not reset the currently selected library.

```

<Compilations: public>+≡
    public :: compile_library

<Compilations: sub interfaces>+≡
    module subroutine compile_library (libname, global)
        type(string_t), intent(in) :: libname
        type(rt_data_t), intent(inout), target :: global
    end subroutine compile_library

<Compilations: procedures>+≡
    module subroutine compile_library (libname, global)
        type(string_t), intent(in) :: libname
        type(rt_data_t), intent(inout), target :: global
        type(compilation_item_t) :: comp
        logical :: force, recompile
        force = &
            global%var_list%get_lval (var_str ("?rebuild_library"))
        recompile = &
            global%var_list%get_lval (var_str ("?recompile_library"))
        if (associated (global%model)) then
            call comp%init (libname, global%prclib_stack, global%var_list)
            call comp%compile (global%model, global%os_data, force, recompile)
            if (signal_is_pending ()) return
            call comp%load (global%os_data)
            if (signal_is_pending ()) return
        else
            call msg_fatal ("Process library compilation: " &
                // " model is undefined.")
        end if
        call comp%success ()
    end subroutine compile_library

```

33.5.3 Compiling static executable

This object handles the creation of a static executable which should contain a set of static process libraries.

```

<Compilations: public>+≡
    public :: compilation_t

```



```

<Compilations: types>+≡
  type :: compilation_t
  private
    type(string_t) :: exe_name
    type(string_t), dimension(:), allocatable :: lib_name
  contains
    <Compilations: compilation: TBP>
  end type compilation_t

```

Output.

```

<Compilations: compilation: TBP>≡
  procedure :: write => compilation_write

<Compilations: sub interfaces>+≡
  module subroutine compilation_write (object, unit)
    class(compilation_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine compilation_write

<Compilations: procedures>+≡
  module subroutine compilation_write (object, unit)
    class(compilation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Compilation object:"
    write (u, "(3x,3A)") "executable      = '", &
      char (object%exe_name), "'"
    write (u, "(3x,A)", advance="no") "process libraries ="
    do i = 1, size (object%lib_name)
      write (u, "(1x,3A)", advance="no") "'", char (object%lib_name(i)), "'"
    end do
    write (u, *)
  end subroutine compilation_write

```

Initialize: we know the names of the executable and of the libraries. Optionally, we may provide a workspace directory.

```

<Compilations: compilation: TBP>+≡
  procedure :: init => compilation_init

<Compilations: sub interfaces>+≡
  module subroutine compilation_init (compilation, exe_name, lib_name)
    class(compilation_t), intent(out) :: compilation
    type(string_t), intent(in) :: exe_name
    type(string_t), dimension(:), intent(in) :: lib_name
  end subroutine compilation_init

<Compilations: procedures>+≡
  module subroutine compilation_init (compilation, exe_name, lib_name)
    class(compilation_t), intent(out) :: compilation
    type(string_t), intent(in) :: exe_name
    type(string_t), dimension(:), intent(in) :: lib_name
    compilation%exe_name = exe_name
    allocate (compilation%lib_name (size (lib_name)))
    compilation%lib_name = lib_name

```

```
end subroutine compilation_init
```

Write the dispatcher subroutine for the compiled libraries. Also write a subroutine which returns the names of the compiled libraries.

```
<Compilations: compilation: TBP>+≡
```

```
procedure :: write_dispatcher => compilation_write_dispatcher
```

```
<Compilations: sub interfaces>+≡
```

```
module subroutine compilation_write_dispatcher (compilation)
  class(compilation_t), intent(in) :: compilation
end subroutine compilation_write_dispatcher
```

```
<Compilations: procedures>+≡
```

```
module subroutine compilation_write_dispatcher (compilation)
  class(compilation_t), intent(in) :: compilation
  type(string_t) :: file
  integer :: u, i
  file = compilation%exe_name // "_prclib_dispatcher.f90"
  call msg_message ("Static executable '" // char (compilation%exe_name) &
    // "' : writing library dispatcher")
  u = free_unit ()
  open (u, file = char (file), status="replace", action="write")
  write (u, "(3A)") " ! Whizard: process libraries for executable '", &
    char (compilation%exe_name), "'"
  write (u, "(A)") " ! Automatically generated file, do not edit"
  write (u, "(A)") " subroutine dispatch_prclib_static " // &
    "(driver, basename, modellibs_ldflags)"
  write (u, "(A)") " use iso_varying_string, string_t => varying_string"
  write (u, "(A)") " use prclib_interfaces"
  do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
      write (u, "(A)") " use " // char (lib_name) // "_driver"
    end associate
  end do
  write (u, "(A)") " implicit none"
  write (u, "(A)") " class(prclib_driver_t), intent(inout), allocatable &
    &:: driver"
  write (u, "(A)") " type(string_t), intent(in) :: basename"
  write (u, "(A)") " logical, intent(in), optional :: " // &
    "modellibs_ldflags"
  write (u, "(A)") " select case (char (basename))"
  do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
      write (u, "(3A)") " case ('', char (lib_name), '')"
      write (u, "(3A)") " allocate (" // char (lib_name), "_driver_t &
        &:: driver)"
    end associate
  end do
  write (u, "(A)") " end select"
  write (u, "(A)") "end subroutine dispatch_prclib_static"
  write (u, *)
  write (u, "(A)") "subroutine get_prclib_static (libname)"
  write (u, "(A)") " use iso_varying_string, string_t => varying_string"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " type(string_t), dimension(:), intent(inout), &
```

```

        &allocatable :: libname"
write (u, "(A,IO,A)") " allocate (libname (" , &
    size (compilation%lib_name), ") )"
do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
        write (u, "(A,IO,A,A,A)") " libname(" , i, ") = '", &
            char (lib_name), "'"
    end associate
end do
write (u, "(A)") "end subroutine get_prclib_static"
close (u)
end subroutine compilation_write_dispatcher

```

Write the Makefile subroutine for the compiled libraries.

<Compilations: compilation: TBP>+≡

```

    procedure :: write_makefile => compilation_write_makefile

```

<Compilations: sub interfaces>+≡

```

    module subroutine compilation_write_makefile &
        (compilation, os_data, ext_libtag, verbose, overwrite_os)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: overwrite_os
    type(string_t), intent(in), optional :: ext_libtag
    end subroutine compilation_write_makefile

```

<Compilations: procedures>+≡

```

    module subroutine compilation_write_makefile &
        (compilation, os_data, ext_libtag, verbose, overwrite_os)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: overwrite_os
    type(string_t), intent(in), optional :: ext_libtag
    logical :: overwrite
    type(string_t) :: file, ext_tag
    integer :: u, i
    overwrite = .false.
    if (present (overwrite_os)) overwrite = overwrite_os
    if (present (ext_libtag)) then
        ext_tag = ext_libtag
    else
        ext_tag = ""
    end if
    file = compilation%exe_name // ".makefile"
    call msg_message ("Static executable '" // char (compilation%exe_name) &
        // "': writing makefile")
    u = free_unit ()
    open (u, file = char (file), status="replace", action="write")
    write (u, "(3A)") "# WHIZARD: Makefile for executable '", &
        char (compilation%exe_name), "'"
    write (u, "(A)") "# Automatically generated file, do not edit"
    write (u, "(A)") ""
    write (u, "(A)") "# Executable name"

```

```

write (u, "(A)") "EXE = " // char (compilation%exe_name)
write (u, "(A)") ""
write (u, "(A)") "# Compiler"
write (u, "(A)") "FC = " // char (os_data%fc)
write (u, "(A)") "CXX = " // char (os_data%cxx)
write (u, "(A)") ""
write (u, "(A)") "# Included libraries"
write (u, "(A)") "FCINCL = " // char (os_data%whizard_includes)
write (u, "(A)") ""
write (u, "(A)") "# Compiler flags"
write (u, "(A)") "FCFLAGS = " // char (os_data%fcflags)
write (u, "(A)") "FCLIBS = " // char (os_data%fclibs)
write (u, "(A)") "CXXFLAGS = " // char (os_data%cxxflags)
write (u, "(A)") "CXXLIBSS = " // char (os_data%cxxlibs)
write (u, "(A)") "LDFLAGS = " // char (os_data%ldflags)
write (u, "(A)") "LDFLAGS_STATIC = " // char (os_data%ldflags_static)
write (u, "(A)") "LDFLAGS_HEPMC = " // char (os_data%ldflags_hePMC)
write (u, "(A)") "LDFLAGS_LCIO = " // char (os_data%ldflags_lcio)
write (u, "(A)") "LDFLAGS_HOPPET = " // char (os_data%ldflags_hoppet)
write (u, "(A)") "LDFLAGS_LOOPTOOLS = " // char (os_data%ldflags_looptools)
write (u, "(A)") "LDWHIZARD = " // char (os_data%whizard_ldflags)
write (u, "(A)") ""
write (u, "(A)") "# Libtool"
write (u, "(A)") "LIBTOOL = " // char (os_data%whizard_libtool)
if (verbose) then
  write (u, "(A)") "FCOMPILE = $(LIBTOOL) -tag=FC -mode=compile"
  if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") "LINK = $(LIBTOOL) -tag=CXX -mode=link"
  else
    write (u, "(A)") "LINK = $(LIBTOOL) -tag=FC -mode=link"
  end if
else
  write (u, "(A)") "FCOMPILE = @$(LIBTOOL) -silent -tag=FC -mode=compile"
  if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") "LINK = @$(LIBTOOL) -silent -tag=CXX -mode=link"
  else
    write (u, "(A)") "LINK = @$(LIBTOOL) -silent -tag=FC -mode=link"
  end if
end if
write (u, "(A)") ""
write (u, "(A)") "# Compile commands (default)"
write (u, "(A)") "LTF_COMPILE = $(FCOMPILE) $(FC) -c $(FCINCL) $(FCFLAGS)"
write (u, "(A)") ""
write (u, "(A)") "# Default target"
write (u, "(A)") "all: link"
write (u, "(A)") ""
write (u, "(A)") "# Libraries"
do i = 1, size (compilation%lib_name)
  associate (lib_name => compilation%lib_name(i))
    write (u, "(A)") "LIBRARIES += " // char (lib_name) // ".la"
    write (u, "(A)") char (lib_name) // ".la:"
    write (u, "(A)") TAB // "$(MAKE) -f " // char (lib_name) // ".makefile"
  end associate
end do

```

```

write (u, "(A)") ""
write (u, "(A)") "# Library dispatcher"
write (u, "(A)") "DISP = $(EXE)_prclib_dispatcher"
write (u, "(A)") "$(DISP).lo: $(DISP).f90 $(LIBRARIES)"
if (.not. verbose) then
    write (u, "(A)") TAB // '@echo " FC          " $@"
end if
write (u, "(A)") TAB // "$(LTF_COMPILE) $<"
write (u, "(A)") ""
write (u, "(A)") "# Executable"
write (u, "(A)") "$(EXE): $(DISP).lo $(LIBRARIES)"
if (.not. verbose) then
    if (OS_IS_DARWIN .and. .not. overwrite) then
        write (u, "(A)") TAB // '@echo " CXXLD          " $@"
    else
        write (u, "(A)") TAB // '@echo " FCLD          " $@"
    end if
end if
if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") TAB // "$(LINK) $(CXX) -static $(CXXFLAGS) \"
else
    write (u, "(A)") TAB // "$(LINK) $(FC) -static $(FCFLAGS) \"
end if
write (u, "(A)") TAB // " $(LDWHIZARD) $(LDFLAGS) \"
write (u, "(A)") TAB // " -o $(EXE) $^ \"
write (u, "(A)") TAB // " $(LDFLAGS_HEPMC) $(LDFLAGS_LCIO) $(LDFLAGS_HOPPET) \"
if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") TAB // " $(LDFLAGS_LOOPTOOLS) $(LDFLAGS_STATIC) \"
    write (u, "(A)") TAB // " $(CXXLIBS) $(FCLIBS)\" // char (ext_tag)
else
    write (u, "(A)") TAB // " $(LDFLAGS_LOOPTOOLS) $(LDFLAGS_STATIC)\" // char (ext_tag)
end if
write (u, "(A)") ""
write (u, "(A)") "# Main targets"
write (u, "(A)") "link: compile $(EXE)"
write (u, "(A)") "compile: $(LIBRARIES) $(DISP).lo"
write (u, "(A)") ".PHONY: link compile"
write (u, "(A)") ""
write (u, "(A)") "# Cleanup targets"
write (u, "(A)") "clean-exe:"
write (u, "(A)") TAB // "rm -f $(EXE)"
write (u, "(A)") "clean-objects:"
write (u, "(A)") TAB // "rm -f $(DISP).lo"
write (u, "(A)") "clean-source:"
write (u, "(A)") TAB // "rm -f $(DISP).f90"
write (u, "(A)") "clean-makefile:"
write (u, "(A)") TAB // "rm -f $(EXE).makefile"
write (u, "(A)") ""
write (u, "(A)") "clean: clean-exe clean-objects clean-source"
write (u, "(A)") "distclean: clean clean-makefile"
write (u, "(A)") ".PHONY: clean distclean"
close (u)
end subroutine compilation_write_makefile

```

Compile the dispatcher source code.

```

<Compilations: compilation: TBP>+=
  procedure :: make_compile => compilation_make_compile

<Compilations: sub interfaces>+=
  module subroutine compilation_make_compile (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
  end subroutine compilation_make_compile

<Compilations: procedures>+=
  module subroutine compilation_make_compile (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    call os_system_call ("make compile " // os_data%makeflags &
      // " -f " // compilation%exe_name // ".makefile")
  end subroutine compilation_make_compile

```

Link the dispatcher together with all matrix-element code and the WHIZARD and O'MEGA main libraries, to generate a static executable.

```

<Compilations: compilation: TBP>+=
  procedure :: make_link => compilation_make_link

<Compilations: sub interfaces>+=
  module subroutine compilation_make_link (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
  end subroutine compilation_make_link

<Compilations: procedures>+=
  module subroutine compilation_make_link (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    call os_system_call ("make link " // os_data%makeflags &
      // " -f " // compilation%exe_name // ".makefile")
  end subroutine compilation_make_link

```

Cleanup.

```

<Compilations: compilation: TBP>+=
  procedure :: make_clean_exe => compilation_make_clean_exe

<Compilations: sub interfaces>+=
  module subroutine compilation_make_clean_exe (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
  end subroutine compilation_make_clean_exe

<Compilations: procedures>+=
  module subroutine compilation_make_clean_exe (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    call os_system_call ("make clean-exe " // os_data%makeflags &
      // " -f " // compilation%exe_name // ".makefile")
  end subroutine compilation_make_clean_exe

```

33.5.4 API for executable compilation

This is a shorthand for compiling and loading an executable, including the enclosed libraries. The `compile` object is used only internally.

The `global` data set may actually be local to the caller. The compilation affects the library specified by its name if it is on the stack, but it does not reset the currently selected library.

<Compilations: public>+≡

```
public :: compile_executable
```

<Compilations: sub interfaces>+≡

```
module subroutine compile_executable (exename, libname, global)
  type(string_t), intent(in) :: exename
  type(string_t), dimension(:), intent(in) :: libname
  type(rt_data_t), intent(inout), target :: global
end subroutine compile_executable
```

<Compilations: procedures>+≡

```
module subroutine compile_executable (exename, libname, global)
  type(string_t), intent(in) :: exename
  type(string_t), dimension(:), intent(in) :: libname
  type(rt_data_t), intent(inout), target :: global
  type(compilation_t) :: compilation
  type(compilation_item_t) :: item
  type(string_t) :: ext_libtag
  logical :: force, recompile, verbose
  integer :: i
  ext_libtag = ""
  force = &
    global%var_list%get_lval (var_str ("?rebuild_library"))
  recompile = &
    global%var_list%get_lval (var_str ("?recompile_library"))
  verbose = &
    global%var_list%get_lval (var_str ("?me_verbose"))
  call compilation%init (exename, [libname])
  if (signal_is_pending ()) return
  call compilation%write_dispatcher ()
  if (signal_is_pending ()) return
  do i = 1, size (libname)
    call item%init (libname(i), global%prclib_stack, global%var_list)
    call item%compile (global%model, global%os_data, &
      force=force, recompile=recompile)
    ext_libtag = "" // item%lib%get_static_modelname (global%os_data)
    if (signal_is_pending ()) return
    call item%success ()
  end do
  call compilation%write_makefile &
    (global%os_data, ext_libtag=ext_libtag, verbose=verbose)
  if (signal_is_pending ()) return
  call compilation%make_compile (global%os_data)
  if (signal_is_pending ()) return
  call compilation%make_link (global%os_data)
end subroutine compile_executable
```

33.5.5 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

```
<compilations_ut.f90>≡  
  <File header>  
  
  module compilations_ut  
    use unit_tests  
    use compilations_uti  
  
    <Standard module head>  
  
    <Compilations: public test>  
  
    contains  
  
    <Compilations: test driver>  
  
  end module compilations_ut  
<compilations_uti.f90>≡  
  <File header>  
  
  module compilations_uti  
  
    <Use strings>  
    use io_units  
    use models  
    use rt_data  
    use process_configurations_ut, only: prepare_test_library  
  
    use compilations  
  
    <Standard module head>  
  
    <Compilations: test declarations>  
  
    contains  
  
    <Compilations: tests>  
  
  end module compilations_uti
```

API: driver for the unit tests below.

```
<Compilations: public test>≡  
  public :: compilations_test  
<Compilations: test driver>≡  
  subroutine compilations_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <Compilations: execute tests>  
  end subroutine compilations_test
```


Intrinsic Matrix Element

Compile an intrinsic test matrix element (`prc_test` type).

Note: In this and the following test, we reset the Fortran compiler and flag variables immediately before they are printed, so the test is portable.

```
<Compilations: execute tests>≡
    call test (compilations_1, "compilations_1", &
               "intrinsic test processes", &
               u, results)

<Compilations: test declarations>≡
    public :: compilations_1

<Compilations: tests>≡
    subroutine compilations_1 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: compilations_1"
        write (u, "(A)")  "*   Purpose: configure and compile test process"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

        libname = "compilation_1"
        procname = "prc_comp_1"
        call prepare_test_library (global, libname, 1, [procname])

        call compile_library (libname, global)

        call global%write_libraries (u)

        call global%final ()
        call syntax_model_file_final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: compilations_1"

    end subroutine compilations_1
```

External Matrix Element

Compile an external test matrix element (`omega` type)

```
<Compilations: execute tests>+≡
    call test (compilations_2, "compilations_2", &
               "external process (omega)", &
               u, results)

<Compilations: test declarations>+≡
    public :: compilations_2
```

```

<Compilations: tests>+≡
subroutine compilations_2 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname
  type(rt_data_t), target :: global

  write (u, "(A)")  "* Test output: compilations_2"
  write (u, "(A)")  "* Purpose: configure and compile test process"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()
  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

  libname = "compilation_2"
  procname = "prc_comp_2"
  call prepare_test_library (global, libname, 2, [procname,procname])

  call compile_library (libname, global)

  call global%write_libraries (u, libpath = .false.)

  call global%final ()
  call syntax_model_file_final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: compilations_2"

end subroutine compilations_2

```

External Matrix Element

Compile an external test matrix element (*omega* type) and create driver files for a static executable.

```

<Compilations: execute tests>+≡
  call test (compilations_3, "compilations_3", &
    "static executable: driver", &
    u, results)

<Compilations: test declarations>+≡
  public :: compilations_3

<Compilations: tests>+≡
subroutine compilations_3 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname, exename
  type(rt_data_t), target :: global
  type(compilation_t) :: compilation
  integer :: u_file
  character(80) :: buffer

```

```

write (u, "(A)")  "* Test output: compilations_3"
write (u, "(A)")  "* Purpose: make static executable"
write (u, "(A)")

write (u, "(A)")  "* Initialize library"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

libname = "compilations_3_lib"
procname = "prc_comp_3"
exename = "compilations_3"

call prepare_test_library (global, libname, 2, [procname,procname])

call compilation%init (exename, [libname])
call compilation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write dispatcher"
write (u, "(A)")

call compilation%write_dispatcher ()

u_file = free_unit ()
open (u_file, file = char (exename) // "_prclib_dispatcher.f90", &
    status = "old", action = "read")
do
    read (u_file, "(A)", end = 1) buffer
    write (u, "(A)") trim (buffer)
end do
1 close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Write Makefile"
write (u, "(A)")

associate (os_data => global%os_data)
    os_data%fc = "fortran-compiler"
    os_data%cxx = "c++-compiler"
    os_data%whizard_includes = "my-includes"
    os_data%fcflags = "my-fcflags"
    os_data%fclibs = "my-fclibs"
    os_data%cxxflags = "my-cxxflags"
    os_data%cxlibs = "my-cxlibs"
    os_data%ldflags = "my-ldflags"
    os_data%ldflags_static = "my-ldflags-static"
    os_data%ldflags_hepmc = "my-ldflags-hepmc"
    os_data%ldflags_lcio = "my-ldflags-lcio"
    os_data%ldflags_hoppet = "my-ldflags-hoppet"

```

```

        os_data%ldflags_looptools = "my-ldflags-looptools"
        os_data%whizard_ldflags = "my-ldwhizard"
        os_data%whizard_libtool = "my-libtool"
    end associate

    call compilation%write_makefile &
        (global%os_data, verbose = .true., overwrite_os = .true.)

    open (u_file, file = char (exename) // ".makefile", &
        status = "old", action = "read")
    do
        read (u_file, "(A)", end = 2) buffer
        write (u, "(A)") trim (buffer)
    end do
2   close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call global%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: compilations_3"

end subroutine compilations_3

```

33.5.6 Test static build

The tests for building a static executable are separate, since they should be skipped if the WHIZARD build itself has static libraries disabled.

```

<Compilations: public test>+≡
    public :: compilations_static_test

<Compilations: test driver>+≡
    subroutine compilations_static_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Compilations: static tests>
    end subroutine compilations_static_test

```

External Matrix Element

Compile an external test matrix element (omega type) and incorporate this in a new static WHIZARD executable.

```

<Compilations: static tests>≡
    call test (compilations_static_1, "compilations_static_1", &
        "static executable: compilation", &
        u, results)

<Compilations: test declarations>+≡
    public :: compilations_static_1

```

```

<Compilations: tests>+=
subroutine compilations_static_1 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname, exename
  type(rt_data_t), target :: global
  type(compilation_item_t) :: item
  type(compilation_t) :: compilation
  logical :: exist

  write (u, "(A)")  "* Test output: compilations_static_1"
  write (u, "(A)")  "* Purpose: make static executable"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize library"

  call syntax_model_file_init ()

  call global%global_init ()
  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

  libname = "compilations_static_1_lib"
  procname = "prc_comp_stat_1"
  exename = "compilations_static_1"

  call prepare_test_library (global, libname, 2, [procname,procname])

  call compilation%init (exename, [libname])

  write (u, "(A)")
  write (u, "(A)")  "* Write dispatcher"

  call compilation%write_dispatcher ()

  write (u, "(A)")
  write (u, "(A)")  "* Write Makefile"

  call compilation%write_makefile (global%os_data, verbose = .true.)

  write (u, "(A)")
  write (u, "(A)")  "* Build libraries"

  call item%init (libname, global%prclib_stack, global%var_list)
  call item%compile &
    (global%model, global%os_data, force=.true., recompile=.false.)
  call item%success ()

  write (u, "(A)")
  write (u, "(A)")  "* Check executable (should be absent)"
  write (u, "(A)")

  call compilation%make_clean_exe (global%os_data)
  inquire (file = char (exename), exist = exist)
  write (u, "(A,A,L1)") char (exename), " exists = ", exist

```

```

write (u, "(A)")
write (u, "(A)")  "* Build executable"
write (u, "(A)")

call compilation%make_compile (global%os_data)
call compilation%make_link (global%os_data)

write (u, "(A)")  "* Check executable (should be present)"
write (u, "(A)")

inquire (file = char (exename), exist = exist)
write (u, "(A,A,L1)") char (exename), " exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call compilation%make_clean_exe (global%os_data)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: compilations_static_1"

end subroutine compilations_static_1

```

External Matrix Element

Compile an external test matrix element (ω type) and incorporate this in a new static WHIZARD executable. In this version, we use the wrapper `compile_executable` procedure.

```

<Compilations: static tests>+≡
  call test (compilations_static_2, "compilations_static_2", &
    "static executable: shortcut", &
    u, results)

<Compilations: test declarations>+≡
  public :: compilations_static_2

<Compilations: tests>+≡
  subroutine compilations_static_2 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname, exename
    type(rt_data_t), target :: global
    logical :: exist
    integer :: u_file

    write (u, "(A)")  "* Test output: compilations_static_2"
    write (u, "(A)")  "* Purpose: make static executable"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize library and compile"

```

```

write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

libname = "compilations_static_2_lib"
procname = "prc_comp_stat_2"
exename = "compilations_static_2"

call prepare_test_library (global, libname, 2, [procname,procname])

call compile_executable (exename, [libname], global)

write (u, "(A)")  "* Check executable (should be present)"
write (u, "(A)")

inquire (file = char (exename), exist = exist)
write (u, "(A,A,L1)") char (exename), " exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

u_file = free_unit ()
open (u_file, file = char (exename), status = "old", action = "write")
close (u_file, status = "delete")

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: compilations_static_2"

end subroutine compilations_static_2

```

33.6 Integration

This module manages phase space setup, matrix-element evaluation and integration, as far as it is not done by lower-level routines, in particular in the `processes` module.

```
<integrations.f90>≡  
  <File header>  
  
  module integrations  
  
    <Use kinds>  
    <Use strings>  
    <Use debug>  
    use diagnostics  
    use prc_core  
    use process  
    use instances  
    use process_stacks  
    use iterations  
    use rt_data  
    use nlo_data  
  
    <Standard module head>  
  
    <Integrations: public>  
  
    <Integrations: types>  
  
    interface  
    <Integrations: sub interfaces>  
    end interface  
  
    contains  
  
    <Integrations: main procedures>  
  
  end module integrations  
<integrations_sub.f90>≡  
  <File header>  
  
  submodule (integrations) integrations_s  
  
    <Use mpi f08>  
    use io_units  
    use cputime  
    use os_interface  
    use physics_defs  
    use model_data  
    use pdg_arrays  
    use variables, only: var_list_t  
    use eval_trees  
    use sf_mappings  
    use sf_base
```



```

use phs_base
use models
use dispatch_me_methods, only: dispatch_core
use dispatch_beams, only: dispatch_qcd, sf_prop_t, dispatch_sf_config
use dispatch_phase_space, only: dispatch_sf_channels
use dispatch_phase_space, only: dispatch_phs
use dispatch_mci, only: dispatch_mci_setup, setup_grid_path
use dispatch_transforms, only: dispatch_evt_shower_hook
use compilations, only: compile_library

implicit none

contains

<Integrations: procedures>

end submodule integrations_s

```

33.6.1 The integration type

This type holds all relevant data, the integration methods operates on this. In contrast to the `simulation_t` introduced later, the `integration_t` applies to a single process.

```

<Integrations: public>≡
    public :: integration_t

<Integrations: types>≡
    type :: integration_t
    private
        type(string_t) :: process_id
        type(string_t) :: run_id
        type(process_t), pointer :: process => null ()
        logical :: rebuild_phs = .false.
        logical :: ignore_phs_mismatch = .false.
        logical :: phs_only = .false.
        logical :: process_has_me = .true.
        integer :: n_calls_test = 0
        logical :: vis_history = .true.
        type(string_t) :: history_filename
        type(string_t) :: log_filename
        type(helicity_selection_t) :: helicity_selection
        logical :: use_color_factors = .false.
        logical :: has_beam_pol = .false.
        logical :: combined_integration = .false.
        type(iteration_multipliers_t) :: iteration_multipliers
        type(nlo_settings_t) :: nlo_settings
    contains
        <Integrations: integration: TBP>
end type integration_t

```

33.6.2 Initialization

Initialization, first part: Create a process entry. Push it on the stack if the global environment is supplied. Gfortran7/8/9 bug, has to remain in the main module:

```

<Integrations: integration: TBP>≡
    procedure :: create_process => integration_create_process

<Integrations: main procedures>≡
    subroutine integration_create_process (intg, process_id, global)
        class(integration_t), intent(out) :: intg
        type(rt_data_t), intent(inout), optional, target :: global
        type(string_t), intent(in) :: process_id
        type(process_entry_t), pointer :: process_entry
        if (debug_on) call msg_debug (D_CORE, "integration_create_process")
        intg%process_id = process_id
        if (present (global)) then
            allocate (process_entry)
            intg%process => process_entry%process_t
            call global%process_stack%push (process_entry)
        else
            allocate (process_t :: intg%process)
        end if
    end subroutine integration_create_process

```

Initialization, second part: Initialize the process object, using the local environment. We allocate a RNG factory and a QCD object. We also fetch a pointer to the model that the process uses. The process initializer will create a snapshot of that model.

This procedure does not modify the local stack directly. The intent(inout) attribute for the local data set is due to the random generator seed which may be incremented during initialization.

NOTE: Changes to model parameters within the current context are respected only if the process model coincides with the current model. This is the usual case. If not, we read the model from the global model library, which has default parameters. To become more flexible, we should implement a local model library which records local changes to currently inactive models.

```

<Integrations: integration: TBP>+≡
    procedure :: init_process => integration_init_process

<Integrations: sub interfaces>≡
    module subroutine integration_init_process (intg, local)
        class(integration_t), intent(inout) :: intg
        type(rt_data_t), intent(inout), target :: local
    end subroutine integration_init_process

<Integrations: procedures>≡
    module subroutine integration_init_process (intg, local)
        class(integration_t), intent(inout) :: intg
        type(rt_data_t), intent(inout), target :: local
        type(string_t) :: model_name
        type(model_t), pointer :: model
        class(model_data_t), pointer :: model_instance
        type(var_list_t), pointer :: var_list

```

```

if (debug_on) call msg_debug (D_CORE, "integration_init_process")
if (.not. local%prclib%contains (intg%process_id)) then
    call msg_fatal ("Process '" // char (intg%process_id) // "' not found" &
        // " in library '" // char (local%prclib%get_name ()) // "'")
    return
end if
model_name = local%prclib%get_model_name (intg%process_id)
if (local%get_sval (var_str ("model_name")) == model_name) then
    model => local%model
else
    model => local%model_list%get_model_ptr (model_name)
end if
var_list => local%get_var_list_ptr ()
call intg%process%init (intg%process_id, &
    local%prclib, &
    local%os_data, &
    model, &
    var_list, &
    local%beam_structure)
intg%run_id = intg%process%get_run_id ()
end subroutine integration_init_process

```

Initialization, third part: complete process configuration.

(Integrations: integration: TBP)+≡

```

procedure :: setup_process => integration_setup_process

```

(Integrations: sub interfaces)+≡

```

module subroutine integration_setup_process &
    (intg, local, verbose, init_only)
    class(integration_t), intent(inout) :: intg
    type(rt_data_t), intent(inout), target :: local
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: init_only
end subroutine integration_setup_process

```

(Integrations: procedures)+≡

```

module subroutine integration_setup_process (intg, local, verbose, init_only)
    class(integration_t), intent(inout) :: intg
    type(rt_data_t), intent(inout), target :: local
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: init_only

    type(var_list_t), pointer :: var_list
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_prop_t) :: sf_prop
    type(sf_channel_t), dimension(:), allocatable :: sf_channel
    type(phs_channel_collection_t) :: phs_channel_collection
    logical :: sf_trace
    logical :: verb, initialize_only
    type(string_t) :: sf_string
    type(string_t) :: workspace
    real(default) :: sqrts

    verb = .true.; if (present (verbose)) verb = verbose

```

```

initialize_only = .false.
if (present (init_only)) initialize_only = init_only

call display_init_message (verb)

var_list => local%get_var_list_ptr ()
call setup_log_and_history ()

associate (process => intg%process)
  call set_intg_parameters (process)

  call process%setup_cores (dispatch_core, &
    intg%helicity_selection, intg%use_color_factors, intg%has_beam_pol)

  call process%init_phs_config ()
  call process%init_components ()

  call process%record_inactive_components ()
  intg%process_has_me = process%has_matrix_element ()
  if (.not. intg%process_has_me) then
    call msg_warning ("Process '" &
      // char (intg%process_id) // "': matrix element vanishes")
  end if

  call setup_beams ()
  call setup_structure_functions ()

  workspace = var_list%get_sval (var_str ("$integrate_workspace"))
  if (workspace == "") then
    call process%configure_phs &
      (intg%rebuild_phs, &
        intg%ignore_phs_mismatch, &
        intg%combined_integration)
  else
    call setup_grid_path (workspace)
    call process%configure_phs &
      (intg%rebuild_phs, &
        intg%ignore_phs_mismatch, &
        intg%combined_integration, &
        workspace)
  end if

  call process%complete_pcm_setup ()

  call process%prepare_blha_cores ()
  call process%create_blha_interface ()
  call process%prepare_any_external_code ()

  call process%setup_terms (with_beams = intg%has_beam_pol)
  call process%check_masses ()
  call process%optimize_nlo_singular_regions ()

  if (verb) then
    call process%write (screen = .true.)
  end if

```

```

        call process%print_phs_startup_message ()
    end if

    if (intg%process_has_me) then
        if (size (sf_config) > 0) then
            call process%collect_channels (phs_channel_collection)
        else if (.not. initialize_only &
            .and. process%contains_trivial_component ()) then
            call msg_fatal ("Integrate: 2 -> 1 process can't be handled &
                &with fixed-energy beams")
        end if
        if (local%beam_structure%asymmetric ()) then
            sqrts = process%get_sqrts ()
        else
            sqrts = local%get_sqrts ()
        end if
        call dispatch_sf_channels &
            (sf_channel, sf_string, sf_prop, phs_channel_collection, &
            local%var_list, sqrts, local%beam_structure)
        if (allocated (sf_channel)) then
            if (size (sf_channel) > 0) then
                call process%set_sf_channel (sf_channel)
            end if
        end if
        call phs_channel_collection%final ()
        if (verb) call process%sf_startup_message (sf_string)
    end if

    call process%setup_mci (dispatch_mci_setup)

    call setup_expressions ()

    call process%compute_md5sum ()
end associate

contains

subroutine setup_log_and_history ()
    if (intg%run_id /= "") then
        intg%history_filename = intg%process_id // "." // intg%run_id &
            // ".history"
        intg%log_filename = intg%process_id // "." // intg%run_id // ".log"
    else
        intg%history_filename = intg%process_id // ".history"
        intg%log_filename = intg%process_id // ".log"
    end if
    intg%vis_history = &
        var_list%get_lval (var_str ("?vis_history"))
end subroutine setup_log_and_history

subroutine set_intg_parameters (process)
    type(process_t), intent(in) :: process
    intg%n_calls_test = &
        var_list%get_ival (var_str ("n_calls_test"))
end subroutine

```

```

    intg%combined_integration = &
        var_list%get_lval (var_str ('?combined_nlo_integration')) &
        .and. process%is_nlo_calculation ()
    intg%use_color_factors = &
        var_list%get_lval (var_str ("?read_color_factors"))
    intg%has_beam_pol = &
        local%beam_structure%has_polarized_beams ()
    intg%helicity_selection = &
        local%get_helicity_selection ()
    intg%rebuild_phs = &
        var_list%get_lval (var_str ("?rebuild_phase_space"))
    intg%ignore_phs_mismatch = &
        .not. var_list%get_lval (var_str ("?check_phs_file"))
    intg%phs_only = &
        var_list%get_lval (var_str ("?phs_only"))
end subroutine set_intg_parameters

subroutine display_init_message (verb)
    logical, intent(in) :: verb
    if (verb) then
        call msg_message ("Initializing integration for process " &
            // char (intg%process_id) // ":")
        if (intg%run_id /= "") &
            call msg_message ("Run ID = " // ' ' // char (intg%run_id) // ' ')
    end if
end subroutine display_init_message

subroutine setup_beams ()
    real(default) :: sqrts
    logical :: decay_rest_frame
    sqrts = local%get_sqrts ()
    decay_rest_frame = &
        var_list%get_lval (var_str ("?decay_rest_frame"))
    if (intg%process_has_me) then
        call intg%process%setup_beams_beam_structure &
            (local%beam_structure, sqrts, decay_rest_frame)
    end if
    if (verb .and. intg%process_has_me) then
        call intg%process%beams_startup_message &
            (beam_structure = local%beam_structure)
    end if
end subroutine setup_beams

subroutine setup_structure_functions ()
    integer :: n_in
    type(pdg_array_t), dimension(:, :), allocatable :: pdg_prc
    type(string_t) :: sf_trace_file
    if (intg%process_has_me) then
        call intg%process%get_pdg_in (pdg_prc)
    else
        n_in = intg%process%get_n_in ()
        allocate (pdg_prc (n_in, intg%process%get_n_components ()))
        pdg_prc = 0
    end if
end if

```

```

call dispatch_sf_config (sf_config, sf_prop, local%beam_structure, &
    local%get_var_list_ptr (), local%var_list, &
    local%model, local%os_data, local%get_sqrts (), pdg_prc)

sf_trace = &
    var_list%get_lval (var_str ("?sf_trace"))
sf_trace_file = &
    var_list%get_sval (var_str ("$sf_trace_file"))
if (sf_trace) then
    call intg%process%init_sf_chain (sf_config, sf_trace_file)
else
    call intg%process%init_sf_chain (sf_config)
end if
end subroutine setup_structure_functions

subroutine setup_expressions ()
type(eval_tree_factory_t) :: expr_factory
if (associated (local%pn%cuts_lexpr)) then
    if (verb) call msg_message ("Applying user-defined cuts.")
    call expr_factory%init (local%pn%cuts_lexpr)
    call intg%process%set_cuts (expr_factory)
else
    if (verb) call msg_warning ("No cuts have been defined.")
end if
if (associated (local%pn%scale_expr)) then
    if (verb) call msg_message ("Using user-defined general scale.")
    call expr_factory%init (local%pn%scale_expr)
    call intg%process%set_scale (expr_factory)
end if
if (associated (local%pn%fac_scale_expr)) then
    if (verb) call msg_message ("Using user-defined factorization scale.")
    call expr_factory%init (local%pn%fac_scale_expr)
    call intg%process%set_fac_scale (expr_factory)
end if
if (associated (local%pn%ren_scale_expr)) then
    if (verb) call msg_message ("Using user-defined renormalization scale.")
    call expr_factory%init (local%pn%ren_scale_expr)
    call intg%process%set_ren_scale (expr_factory)
end if
if (associated (local%pn%weight_expr)) then
    if (verb) call msg_message ("Using user-defined reweighting factor.")
    call expr_factory%init (local%pn%weight_expr)
    call intg%process%set_weight (expr_factory)
end if
end subroutine setup_expressions
end subroutine integration_setup_process

```

33.6.3 Integration

Integrate: do the final integration. Here, we do a multi-iteration integration. Again, we skip iterations that are already on file. Record the results in the global variable list.

```

<Integrations: integration: TBP>+≡
  procedure :: evaluate => integration_evaluate

<Integrations: sub interfaces>+≡
  module subroutine integration_evaluate &
    (intg, process_instance, i_mci, pass, it_list, pacify)
    class(integration_t), intent(inout) :: intg
    type(process_instance_t), intent(inout), target :: process_instance
    integer, intent(in) :: i_mci
    integer, intent(in) :: pass
    type(iterations_list_t), intent(in) :: it_list
    logical, intent(in), optional :: pacify
  end subroutine integration_evaluate

<Integrations: procedures>+≡
  module subroutine integration_evaluate &
    (intg, process_instance, i_mci, pass, it_list, pacify)
    class(integration_t), intent(inout) :: intg
    type(process_instance_t), intent(inout), target :: process_instance
    integer, intent(in) :: i_mci
    integer, intent(in) :: pass
    type(iterations_list_t), intent(in) :: it_list
    logical, intent(in), optional :: pacify
    integer :: n_calls, n_it
    logical :: adapt_grids, adapt_weights, final
    n_it = it_list%get_n_it (pass)
    n_calls = it_list%get_n_calls (pass)
    adapt_grids = it_list%adapt_grids (pass)
    adapt_weights = it_list%adapt_weights (pass)
    final = pass == it_list%get_n_pass ()
    call process_instance%integrate ( &
      i_mci, n_it, n_calls, adapt_grids, adapt_weights, &
      final, pacify)
  end subroutine integration_evaluate

```

In case the user has not provided a list of iterations, make a reasonable default. This can depend on the process. The usual approach is to define two distinct passes, one for adaptation and one for integration.

```

<Integrations: integration: TBP>+≡
  procedure :: make_iterations_list => integration_make_iterations_list

<Integrations: sub interfaces>+≡
  module subroutine integration_make_iterations_list (intg, it_list)
    class(integration_t), intent(in) :: intg
    type(iterations_list_t), intent(out) :: it_list
  end subroutine integration_make_iterations_list

<Integrations: procedures>+≡
  module subroutine integration_make_iterations_list (intg, it_list)
    class(integration_t), intent(in) :: intg
    type(iterations_list_t), intent(out) :: it_list
    integer :: pass, n_pass
    integer, dimension(:), allocatable :: n_it, n_calls
    logical, dimension(:), allocatable :: adapt_grids, adapt_weights
    n_pass = intg%process%get_n_pass_default ()
    allocate (n_it (n_pass), n_calls (n_pass))

```



```

allocate (adapt_grids (n_pass), adapt_weights (n_pass))
do pass = 1, n_pass
  n_it(pass)      = intg%process%get_n_it_default (pass)
  n_calls(pass)   = intg%process%get_n_calls_default (pass)
  adapt_grids(pass) = intg%process%adapt_grids_default (pass)
  adapt_weights(pass) = intg%process%adapt_weights_default (pass)
end do
call it_list%init (n_it, n_calls, &
  adapt_grids = adapt_grids, adapt_weights = adapt_weights)
end subroutine integration_make_iterations_list

```

In NLO calculations, the individual components might scale very differently with the number of calls. This especially applies to the real-subtracted component, which usually fluctuates more than the Born and virtual component, making it a bottleneck of the calculation. Thus, the calculation is throttled twice, first by the number of calls for the real component, second by the number of surplus calls of computation-intense virtual matrix elements. Therefore, we want to set a different number of calls for each component, which is done by the subroutine `integration_apply_call_multipliers`.

(Integrations: integration: TBP)+≡

```

procedure :: init_iteration_multipliers => &
  integration_init_iteration_multipliers

```

(Integrations: sub interfaces)+≡

```

module subroutine integration_init_iteration_multipliers (intg, local)
  class(integration_t), intent(inout) :: intg
  type(rt_data_t), intent(in) :: local
end subroutine integration_init_iteration_multipliers

```

(Integrations: procedures)+≡

```

module subroutine integration_init_iteration_multipliers (intg, local)
  class(integration_t), intent(inout) :: intg
  type(rt_data_t), intent(in) :: local
  integer :: n_pass, pass
  type(iterations_list_t) :: it_list
  n_pass = local%it_list%get_n_pass ()
  if (n_pass == 0) then
    call intg%make_iterations_list (it_list)
    n_pass = it_list%get_n_pass ()
  end if
  associate (it_multipliers => intg%iteration_multipliers)
    allocate (it_multipliers%n_calls0 (n_pass))
    do pass = 1, n_pass
      it_multipliers%n_calls0(pass) = local%it_list%get_n_calls (pass)
    end do
    it_multipliers%mult_real = local%var_list%get_rval &
      (var_str ("mult_call_real"))
    it_multipliers%mult_virt = local%var_list%get_rval &
      (var_str ("mult_call_virt"))
    it_multipliers%mult_dglap = local%var_list%get_rval &
      (var_str ("mult_call_dglap"))
  end associate
end subroutine integration_init_iteration_multipliers

```

```

<Integrations: integration: TBP>+≡
  procedure :: apply_call_multipliers => integration_apply_call_multipliers

<Integrations: sub interfaces>+≡
  module subroutine integration_apply_call_multipliers &
    (intg, n_pass, i_component, it_list)
    class(integration_t), intent(in) :: intg
    integer, intent(in) :: n_pass, i_component
    type(iterations_list_t), intent(inout) :: it_list
  end subroutine integration_apply_call_multipliers

<Integrations: procedures>+≡
  module subroutine integration_apply_call_multipliers &
    (intg, n_pass, i_component, it_list)
    class(integration_t), intent(in) :: intg
    integer, intent(in) :: n_pass, i_component
    type(iterations_list_t), intent(inout) :: it_list
    integer :: nlo_type
    integer :: n_calls0, n_calls
    integer :: pass
    real(default) :: multiplier
    nlo_type = intg%process%get_component_nlo_type (i_component)
    do pass = 1, n_pass
      associate (multipliers => intg%iteration_multipliers)
        select case (nlo_type)
          case (NLO_REAL)
            multiplier = multipliers%mult_real
          case (NLO_VIRTUAL)
            multiplier = multipliers%mult_virt
          case (NLO_DGLAP)
            multiplier = multipliers%mult_dglap
          case default
            return
        end select
      end associate
      if (n_pass <= size (intg%iteration_multipliers%n_calls0)) then
        n_calls0 = intg%iteration_multipliers%n_calls0 (pass)
        n_calls = floor (multiplier * n_calls0)
        call it_list%set_n_calls (pass, n_calls)
      end if
    end do
  end subroutine integration_apply_call_multipliers

```

33.6.4 API for integration objects

This initializer does everything except assigning cuts/scale/weight expressions.

```

<Integrations: integration: TBP>+≡
  procedure :: init => integration_init

<Integrations: sub interfaces>+≡
  module subroutine integration_init &
    (intg, process_id, local, global, local_stack, init_only)
    class(integration_t), intent(out) :: intg
    type(string_t), intent(in) :: process_id

```

```

    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    logical, intent(in), optional :: init_only
    logical, intent(in), optional :: local_stack
end subroutine integration_init

```

<Integrations: procedures>+≡

```

module subroutine integration_init &
    (intg, process_id, local, global, local_stack, init_only)
class(integration_t), intent(out) :: intg
type(string_t), intent(in) :: process_id
type(rt_data_t), intent(inout), target :: local
type(rt_data_t), intent(inout), optional, target :: global
logical, intent(in), optional :: init_only
logical, intent(in), optional :: local_stack
logical :: use_local
use_local = .false.; if (present (local_stack)) use_local = local_stack
if (present (global)) then
    call intg%create_process (process_id, global)
else if (use_local) then
    call intg%create_process (process_id, local)
else
    call intg%create_process (process_id)
end if
call intg%init_process (local)
call intg%setup_process (local, init_only = init_only)
call intg%init_iteration_multipliers (local)
end subroutine integration_init

```

Do the integration for a single process, both warmup and final evaluation. The `eff_reset` flag is to suppress numerical noise in the graphical output of the integration history.

<Integrations: integration: TBP>+≡

```

procedure :: integrate => integration_integrate

```

<Integrations: sub interfaces>+≡

```

module subroutine integration_integrate (intg, local, eff_reset)
class(integration_t), intent(inout) :: intg
type(rt_data_t), intent(in), target :: local
logical, intent(in), optional :: eff_reset
end subroutine integration_integrate

```

<Integrations: procedures>+≡

```

module subroutine integration_integrate (intg, local, eff_reset)
class(integration_t), intent(inout) :: intg
type(rt_data_t), intent(in), target :: local
logical, intent(in), optional :: eff_reset
type(string_t) :: log_filename
type(var_list_t), pointer :: var_list
type(process_instance_t), allocatable, target :: process_instance
type(iterations_list_t) :: it_list
logical :: pacify
integer :: pass, i_mci, n_mci, n_pass
integer :: i_component
integer :: nlo_type

```

```

logical :: display_summed
logical :: nlo_active
type(string_t) :: component_output

allocate (process_instance)
call process_instance%init (intg%process)

var_list => intg%process%get_var_list_ptr ()
call openmp_set_num_threads_verbose &
    (var_list%get_ival (var_str ("openmp_num_threads")), &
    var_list%get_lval (var_str ("?openmp_logging")))
pacify = var_list%get_lval (var_str ("?pacify"))

display_summed = .true.
n_mci = intg%process%get_n_mci ()
if (n_mci == 1) then
    write (msg_buffer, "(A,A,A)") &
        "Starting integration for process '", &
        char (intg%process%get_id ()), "'"
    call msg_message ()
end if

call setup_hooks ()

nlo_active = any (intg%process%get_component_nlo_type &
    ([i_mci, i_mci = 1, n_mci]) /= BORN)
do i_mci = 1, n_mci
    i_component = intg%process%get_master_component (i_mci)
    nlo_type = intg%process%get_component_nlo_type (i_component)
    if (intg%process%component_can_be_integrated (i_component)) then
        if (n_mci > 1) then
            if (nlo_active) then
                if (intg%combined_integration .and. nlo_type == BORN) then
                    component_output = var_str ("Combined")
                else
                    component_output = component_status (nlo_type)
                end if
                write (msg_buffer, "(A,A,A,A,A)") &
                    "Starting integration for process '", &
                    char (intg%process%get_id ()), "' part '", &
                    char (component_output), "'"
            else
                write (msg_buffer, "(A,A,A,I0)") &
                    "Starting integration for process '", &
                    char (intg%process%get_id ()), "' part ", i_mci
            end if
            call msg_message ()
        end if
        n_pass = local%it_list%get_n_pass ()
        if (n_pass == 0) then
            call msg_message ("Integrate: iterations not specified, &
                &using default")
            call intg%make_iterations_list (it_list)
            n_pass = it_list%get_n_pass ()
        end if
    end if
end do

```

```

else
    it_list = local%it_list
end if
call intg%apply_call_multipliers (n_pass, i_mci, it_list)
call msg_message ("Integrate: " // char (it_list%to_string ()))
do pass = 1, n_pass
    call intg%evaluate (process_instance, i_mci, pass, it_list, pacify)
    if (signal_is_pending ()) return
end do
call intg%process%final_integration (i_mci)
if (intg%vis_history) then
    call intg%process%display_integration_history &
        (i_mci, intg%history_filename, local%os_data, eff_reset)
end if
if (local%logfile == intg%log_filename) then
    if (intg%run_id /= "") then
        log_filename = intg%process_id // "." // intg%run_id // &
            ".var.log"
    else
        log_filename = intg%process_id // ".var.log"
    end if
    call msg_message ("Name clash for global logfile and process log: ", &
        arr=[var_str ("| Renaming log file from ") // local%logfile, &
            var_str ("|   to ") // log_filename // var_str (" .")])
else
    log_filename = intg%log_filename
end if
call intg%process%write_logfile (i_mci, log_filename)
end if
end do

if (n_mci > 1 .and. display_summed) then
    call msg_message ("Integrate: sum of all components")
    call intg%process%display_summed_results (pacify)
end if

call process_instance%final ()
deallocate (process_instance)
contains
subroutine setup_hooks ()
    class(process_instance_hook_t), pointer :: hook
    call dispatch_evt_shower_hook (hook, var_list, process_instance, &
        local%beam_structure, intg%process%get_pdf_set())
    if (associated (hook)) then
        call process_instance%append_after_hook (hook)
    end if
end subroutine setup_hooks
end subroutine integration_integrate

```

Do a dummy integration for a process which could not be initialized (e.g., has no matrix element). The result is zero.

(Integrations: integration: TBP)+≡

```

procedure :: integrate_dummy => integration_integrate_dummy

```

```

<Integrations: sub interfaces>+≡
    module subroutine integration_integrate_dummy (intg)
        class(integration_t), intent(inout) :: intg
        end subroutine integration_integrate_dummy

```

```

<Integrations: procedures>+≡
    module subroutine integration_integrate_dummy (intg)
        class(integration_t), intent(inout) :: intg
        call intg%process%integrate_dummy ()
    end subroutine integration_integrate_dummy

```

Just sample the matrix element under realistic conditions (but no cuts); throw away the results.

```

<Integrations: integration: TBP>+≡
    procedure :: sampler_test => integration_sampler_test

```

```

<Integrations: sub interfaces>+≡
    module subroutine integration_sampler_test (intg)
        class(integration_t), intent(inout) :: intg
        end subroutine integration_sampler_test

```

```

<Integrations: procedures>+≡
    module subroutine integration_sampler_test (intg)
        class(integration_t), intent(inout) :: intg
        type(process_instance_t), allocatable, target :: process_instance
        integer :: n_mci, i_mci
        type(timer_t) :: timer_mci, timer_tot
        real(default) :: t_mci, t_tot
        allocate (process_instance)
        call process_instance%init (intg%process)
        n_mci = intg%process%get_n_mci ()
        if (n_mci == 1) then
            write (msg_buffer, "(A,A,A)") &
                "Test: probing process '", &
                char (intg%process%get_id ()), "'"
            call msg_message ()
        end if
        call timer_tot%start ()
        do i_mci = 1, n_mci
            if (n_mci > 1) then
                write (msg_buffer, "(A,A,A,IO)") &
                    "Test: probing process '", &
                    char (intg%process%get_id ()), "' part ", i_mci
                call msg_message ()
            end if
            call timer_mci%start ()
            call process_instance%sampler_test (i_mci, intg%n_calls_test)
            call timer_mci%stop ()
            t_mci = timer_mci
            write (msg_buffer, "(A,ES12.5)") "Test: " &
                // "time in seconds (wallclock): ", t_mci
            call msg_message ()
        end do
        call timer_tot%stop ()
        t_tot = timer_tot
    end subroutine integration_sampler_test

```

```

    if (n_mci > 1) then
        write (msg_buffer, "(A,ES12.5)") "Test: " &
            // "total time      (wallclock): ", t_tot
        call msg_message ()
    end if
    call process_instance%final ()
end subroutine integration_sampler_test

```

Return the process pointer (needed by simulate):

```

<Integrations: integration: TBP>+≡
    procedure :: get_process_ptr => integration_get_process_ptr

<Integrations: sub interfaces>+≡
    module function integration_get_process_ptr (intg) result (ptr)
        class(integration_t), intent(in) :: intg
        type(process_t), pointer :: ptr
    end function integration_get_process_ptr

<Integrations: procedures>+≡
    module function integration_get_process_ptr (intg) result (ptr)
        class(integration_t), intent(in) :: intg
        type(process_t), pointer :: ptr
        ptr => intg%process
    end function integration_get_process_ptr

```

Simply integrate, do a dummy integration if necessary. The `integration` object exists only internally.

If the `global` environment is provided, the process object is appended to the global stack. Otherwise, if `local_stack` is set, we append to the local process stack. If this is unset, the process object is not recorded permanently.

The `init_only` flag can be used to skip the actual integration part. We will end up with a process object that is completely initialized, including phase space configuration.

The `eff_reset` flag is to suppress numerical noise in the visualization of the integration history.

```

<Integrations: public>+≡
    public :: integrate_process

<Integrations: sub interfaces>+≡
    module subroutine integrate_process &
        (process_id, local, global, local_stack, init_only, eff_reset)
        type(string_t), intent(in) :: process_id
        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), optional, target :: global
        logical, intent(in), optional :: local_stack, init_only, eff_reset
    end subroutine integrate_process

<Integrations: procedures>+≡
    module subroutine integrate_process &
        (process_id, local, global, local_stack, init_only, eff_reset)
        type(string_t), intent(in) :: process_id
        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), optional, target :: global
        logical, intent(in), optional :: local_stack, init_only, eff_reset

```

```

type(string_t) :: prclib_name
type(integration_t) :: intg
character(32) :: buffer
<Integrations: integrate process: variables>
<Integrations: integrate process: init>
if (.not. associated (local%prclib)) then
    call msg_fatal ("Integrate: current process library is undefined")
    return
end if

if (.not. local%prclib%is_active ()) then
    call msg_message ("Integrate: current process library needs compilation")
    prclib_name = local%prclib%get_name ()
    call compile_library (prclib_name, local)
    if (signal_is_pending ()) return
    call msg_message ("Integrate: compilation done")
end if

call intg%init (process_id, local, global, local_stack, init_only)
if (signal_is_pending ()) return

if (present (init_only)) then
    if (init_only) return
end if

if (intg%n_calls_test > 0) then
    write (buffer, "(I0)") intg%n_calls_test
    call msg_message ("Integrate: test (" // trim (buffer) // " calls) ...")
    call intg%sampler_test ()
    call msg_message ("Integrate: ... test complete.")
    if (signal_is_pending ()) return
end if
<Integrations: integrate process: end init>

if (intg%phs_only) then
    call msg_message ("Integrate: phase space only, skipping integration")
else
    if (intg%process_has_me) then
        call intg%integrate (local, eff_reset)
    else
        call intg%integrate_dummy ()
    end if
end if
end subroutine integrate_process

```

<Integrations: integrate process: variables>≡

<Integrations: integrate process: init>≡

<Integrations: integrate process: end init>≡

The parallelization leads to undefined behavior while writing simultaneously to one file. The master worker has to initialize single-handed the corresponding library files and the phase space file. The slave worker will wait with a blocking

MPI_BCAST until they receive a logical flag.

```
<MPI: Integrations: integrate process: variables>≡
  type(var_list_t), pointer :: var_list
  logical :: mpi_logging, process_init
  integer :: rank, n_size

<MPI: Integrations: integrate process: init>≡
  if (debug_on) call msg_debug (D_MPI, "integrate_process")
  var_list => local%get_var_list_ptr ()
  process_init = .false.
  call mpi_get_comm_id (n_size, rank)
  mpi_logging = (("vamp2" == char (var_list%get_sval (var_str ("integration_method")))) .and. &
    & (n_size > 1)) .or. var_list%get_lval (var_str ("mpi_logging")))
  if (debug_on) call msg_debug (D_MPI, "n_size", rank)
  if (debug_on) call msg_debug (D_MPI, "rank", rank)
  if (debug_on) call msg_debug (D_MPI, "mpi_logging", mpi_logging)
  if (rank /= 0) then
    if (mpi_logging) then
      call msg_message ("MPI: wait for master to finish process initialization ...")
    end if
    call MPI_bcast (process_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
  else
    process_init = .true.
  end if

  if (process_init) then

<MPI: Integrations: integrate process: end init>≡
    if (rank == 0) then
      if (mpi_logging) then
        call msg_message ("MPI: finish process initialization, load slaves ...")
      end if
      call MPI_bcast (process_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
    end if
  end if
  call MPI_barrier (MPI_COMM_WORLD)
  call mpi_set_logging (mpi_logging)
```

33.6.5 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

```
<integrations_ut.f90>≡
  <File header>

  module integrations_ut
    use unit_tests
    use integrations_uti

    <Standard module head>

    <Integrations: public test>

    contains
```

```

    <Integrations: test driver>

    end module integrations_ut

    <integrations_uti.f90>≡
    <File header>

    module integrations_uti

    <Use kinds>
    <Use strings>
        use io_units
        use ifiles
        use lexers
        use parser
        use flavors
        use interactions, only: reset_interaction_counter
        use phs_forests
        use eval_trees
        use models
        use rt_data
        use process_configurations_ut, only: prepare_test_library
        use compilations, only: compile_library

        use integrations

        use phs_wood_ut, only: write_test_phs_file

    <Standard module head>

    <Integrations: test declarations>

    contains

    <Integrations: tests>

    end module integrations_uti

```

API: driver for the unit tests below.

```

    <Integrations: public test>≡
        public :: integrations_test

    <Integrations: test driver>≡
        subroutine integrations_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <Integrations: execute tests>
        end subroutine integrations_test

    <Integrations: public test>+≡
        public :: integrations_history_test

    <Integrations: test driver>+≡
        subroutine integrations_history_test (u, results)

```

```

integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
<Integrations: execute history tests>
end subroutine integrations_history_test

```

Integration of test process

Compile and integrate an intrinsic test matrix element (`prc_test` type). The phase-space implementation is `phs_single` (single-particle phase space), the integrator is `mci_midpoint`.

The cross section for the $2 \rightarrow 2$ process $ss \rightarrow ss$ with its constant matrix element is given by

$$\sigma = c \times f \times \Phi_2 \times |M|^2. \quad (33.1)$$

c is the conversion constant

$$c = 0.3894 \times 10^{12} \text{ fb GeV}^2. \quad (33.2)$$

f is the flux of the incoming particles with mass $m = 125 \text{ GeV}$ and energy $\sqrt{s} = 1000 \text{ GeV}$

$$f = \frac{(2\pi)^4}{2\lambda^{1/2}(s, m^2, m^2)} = \frac{(2\pi)^4}{2\sqrt{s}\sqrt{s-4m^2}} = 8.048 \times 10^{-4} \text{ GeV}^{-2} \quad (33.3)$$

Φ_2 is the volume of the two-particle phase space

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.5529 \times 10^{-5}. \quad (33.4)$$

The squared matrix element $|M|^2$ is unity. Combining everything, we obtain

$$\sigma = 8000 \text{ fb} \quad (33.5)$$

This number should appear as the final result.

Note: In this and the following test, we reset the Fortran compiler and flag variables immediately before they are printed, so the test is portable.

```

<Integrations: execute tests>≡
  call test (integrations_1, "integrations_1", &
    "intrinsic test process", &
    u, results)

<Integrations: test declarations>≡
  public :: integrations_1

<Integrations: tests>≡
  subroutine integrations_1 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: integrations_1"
    write (u, "(A)")  "* Purpose: integrate test process"
    write (u, "(A)")

```

```

call syntax_model_file_init ()

call global%global_init ()

libname = "integrations_1"
procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [ &
    var_str ("$method"), &
    var_str ("sqrts"), &
    var_str ("$integration_method"), &
    var_str ("$phs_method"), &
    var_str ("$run_id")])

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_1"

end subroutine integrations_1

```

Integration with cuts

Compile and integrate an intrinsic test matrix element (`prc_test` type) with cuts set.

```

<Integrations: execute tests>+≡
    call test (integrations_2, "integrations_2", &
        "intrinsic test process with cut", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_2

<Integrations: tests>+≡
    subroutine integrations_2 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        type(string_t) :: cut_expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: parse_tree

        type(string_t), dimension(0) :: empty_string_array

        write (u, "(A)")  "* Test output: integrations_2"
        write (u, "(A)")  "* Purpose: integrate test process with cut"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

        write (u, "(A)")  "* Prepare a cut expression"
        write (u, "(A)")

        call syntax_pexpr_init ()
        cut_expr_text = "all Pt > 100 [s]"
        call ifile_append (ifile, cut_expr_text)
        call stream_init (stream, ifile)
        call parse_tree_init_lexpr (parse_tree, stream, .true.)
        global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

        write (u, "(A)")  "* Build and initialize a test process"
        write (u, "(A)")

        libname = "integration_3"
        procname = "prc_config_a"

        call prepare_test_library (global, libname, 1)
        call compile_library (libname, global)

        call global%set_string (var_str ("$run_id"), &
            var_str ("integrations1"), is_known = .true.)
        call global%set_string (var_str ("$method"), &
            var_str ("unit_test"), is_known = .true.)
        call global%set_string (var_str ("$phs_method"), &
            var_str ("single"), is_known = .true.)
        call global%set_string (var_str ("$integration_method"),&

```

```

        var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = empty_string_array)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_2"

end subroutine integrations_2

```

Standard phase space

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. We use an explicit phase-space configuration file with a single channel and integrate by `mci_midpoint`.

```

<Integrations: execute tests>+≡
    call test (integrations_3, "integrations_3", &
        "standard phase space", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_3

<Integrations: tests>+≡
    subroutine integrations_3 (u)
    <Use kinds>
    <Use strings>
        use interactions, only: reset_interaction_counter
        use models
        use rt_data
        use process_configurations_ut, only: prepare_test_library
        use compilations, only: compile_library
        use integrations

    implicit none

    integer, intent(in) :: u

```

```

type(string_t) :: libname, procname
type(rt_data_t), target :: global
integer :: u_phs

write (u, "(A)")  "* Test output: integrations_3"
write (u, "(A)")  "* Purpose: integrate test process"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and parameters"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

call global%global_init ()

libname = "integration_3"
procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("default"), is_known = .true.)
call global%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

write (u, "(A)")  "* Create a scratch phase-space file"
write (u, "(A)")

u_phs = free_unit ()
open (u_phs, file = "integrations_3.phs", &
    status = "replace", action = "write")
call write_test_phs_file (u_phs, var_str ("prc_config_a_i1"))
close (u_phs)

call global%set_string (var_str ("$phs_file"), &
    var_str ("integrations_3.phs"), is_known = .true.)

```

```

call global%it_list%init ([1], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [ &
    var_str ("phs_method"), &
    var_str ("phs_file")])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_3"

end subroutine integrations_3

```

VAMP integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`.

```

<Integrations: execute tests>+≡
    call test (integrations_4, "integrations_4", &
        "VAMP integration (one iteration)", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_4

<Integrations: tests>+≡
    subroutine integrations_4 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: integrations_4"
        write (u, "(A)")  "* Purpose: integrate test process using VAMP"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and parameters"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

```



```

libname = "integrations_4_lib"
procname = "integrations_4"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = [var_str ("$_integration_method")], &
    pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_4"

end subroutine integrations_4

```

Multiple iterations integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`. We launch three iterations.

```
<Integrations: execute tests>+≡
    call test (integrations_5, "integrations_5", &
               "VAMP integration (three iterations)", &
               u, results)

<Integrations: test declarations>+≡
    public :: integrations_5

<Integrations: tests>+≡
    subroutine integrations_5 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: integrations_5"
        write (u, "(A)")  "* Purpose: integrate test process using VAMP"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and parameters"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

        libname = "integrations_5_lib"
        procname = "integrations_5"

        call prepare_test_library (global, libname, 1, [procname])
        call compile_library (libname, global)

        call global%append_log (&
                                var_str ("?rebuild_grids"), .true., intrinsic = .true.)

        call global%set_string (var_str ("$run_id"), &
                                var_str ("r1"), is_known = .true.)
        call global%set_string (var_str ("$method"), &
                                var_str ("unit_test"), is_known = .true.)
        call global%set_string (var_str ("$phs_method"), &
                                var_str ("single"), is_known = .true.)
        call global%set_string (var_str ("$integration_method"), &
                                var_str ("vamp"), is_known = .true.)
        call global%set_log (var_str ("?use_vamp_equivalences"), &
                              .false., is_known = .true.)
        call global%set_log (var_str ("?vis_history"), &
                              .false., is_known = .true.)
        call global%set_log (var_str ("?integration_timer"), &
                              .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
                              0, is_known=.true.)
```

```

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([3], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = [var_str ("integration_method")], &
    pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_5"

end subroutine integrations_5

```

Multiple passes integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`. We launch three passes with three iterations each.

```

<Integrations: execute tests>+≡
    call test (integrations_6, "integrations_6", &
        "VAMP integration (three passes)", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_6

<Integrations: tests>+≡
    subroutine integrations_6 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global
        type(string_t), dimension(0) :: no_vars

        write (u, "(A)")  "* Test output: integrations_6"
        write (u, "(A)")  "* Purpose: integrate test process using VAMP"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and parameters"
        write (u, "(A)")

```

```

call syntax_model_file_init ()

call global%global_init ()

libname = "integrations_6_lib"
procname = "integrations_6"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([3, 3, 3], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: integrations_6"

    end subroutine integrations_6

```

VAMP and default phase space

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. The integration method is `vamp`. We launch three passes with three iterations each. We enable channel equivalences and groves.

```

<Integrations: execute tests>+≡
    call test (integrations_7, "integrations_7", &
        "VAMP integration with wood phase space", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_7

<Integrations: tests>+≡
    subroutine integrations_7 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global
        type(string_t), dimension(0) :: no_vars
        integer :: iostat, u_phs
        character(95) :: buffer
        type(string_t) :: phs_file
        logical :: exist

        write (u, "(A)")  "* Test output: integrations_7"
        write (u, "(A)")  "* Purpose: integrate test process using VAMP"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and parameters"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        call global%global_init ()

        libname = "integrations_7_lib"
        procname = "integrations_7"

        call prepare_test_library (global, libname, 1, [procname])
        call compile_library (libname, global)

        call global%append_log (&
            var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
        call global%append_log (&
            var_str ("?rebuild_grids"), .true., intrinsic = .true.)

        call global%set_string (var_str ("$_run_id"), &

```

```

        var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([3, 3, 3], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Generated phase-space file"
write (u, "(A)")

phs_file = procname // ".r1.i1.phs"
inquire (file = char (phs_file), exist = exist)
if (exist) then
    u_phs = free_unit ()
    open (u_phs, file = char (phs_file), action = "read", status = "old")
    iostat = 0
    do while (iostat == 0)
        read (u_phs, "(A)", iostat = iostat)  buffer
        if (iostat == 0) write (u, "(A)")  trim (buffer)
    enddo
enddo

```

```

        end do
        close (u_phs)
    else
        write (u, "(A)") "[file is missing]"
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: integrations_7"

end subroutine integrations_7

```

Structure functions

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. The integration method is `vamp`. There is a structure function of type `unit_test`.

We use a test structure function $f(x) = x$ for both beams. Together with the $1/x_1x_2$ factor from the phase-space flux and a unit matrix element, we should get the same result as previously for the process without structure functions. There is a slight correction due to the m_s mass which we set to zero here.

```

<Integrations: execute tests>+≡
    call test (integrations_8, "integrations_8", &
        "integration with structure function", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_8

<Integrations: tests>+≡
    subroutine integrations_8 (u)
    <Use kinds>
    <Use strings>
        use interactions, only: reset_interaction_counter
        use phs_forests
        use models
        use rt_data
        use process_configurations_ut, only: prepare_test_library
        use compilations, only: compile_library
        use integrations

    implicit none

    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global
    type(flavor_t) :: flv
    type(string_t) :: name

    write (u, "(A)")  "* Test output: integrations_8"
    write (u, "(A)")  "* Purpose: integrate test process using VAMP &
        &with structure function"
    write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize process and parameters"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

call global%global_init ()

libname = "integrations_8_lib"
procname = "integrations_8"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), 0._default)

call reset_interaction_counter ()

call flv%init (25, global%model)

name = flv%get_name ()
call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call global%it_list%init ([1], [1000])

```



```

call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [var_str ("ms")])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_8"

end subroutine integrations_8

```

Integration with sign change

Compile and integrate an intrinsic test matrix element (`prc_test` type). The phase-space implementation is `phs_single` (single-particle phase space), the integrator is `mci_midpoint`. The weight that is applied changes the sign in half of phase space. The weight is -3 and 1 , respectively, so the total result is equal to the original, but negative sign.

The efficiency should (approximately) become the average of 1 and $1/3$, that is $2/3$.

```

<Integrations: execute tests>+≡
  call test (integrations_9, "integrations_9", &
    "handle sign change", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_9

<Integrations: tests>+≡
  subroutine integrations_9 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    type(string_t) :: wgt_expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: parse_tree

    write (u, "(A)")  "* Test output: integrations_9"
    write (u, "(A)")  "* Purpose: integrate test process"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()

    write (u, "(A)")  "* Prepare a weight expression"

```

```

write (u, "(A)")

call syntax_pexpr_init ()
wgt_expr_text = "eval 2 * sgn (Pz) - 1 [s]"
call ifile_append (ifile, wgt_expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (parse_tree, stream, .true.)
global%pn%weight_expr => parse_tree%get_root_ptr ()

write (u, "(A)")  "* Build and evaluate a test process"
write (u, "(A)")

libname = "integration_9"
procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [ &
    var_str ("$method"), &
    var_str ("sqrts"), &
    var_str ("$integration_method"), &
    var_str ("$phs_method"), &
    var_str ("$run_id")])

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_9"

```

```
end subroutine integrations_9
```

Integration history for VAMP integration with default phase space

This test is only run when event analysis can be done.

```

<Integrations: execute history tests>≡
  call test (integrations_history_1, "integrations_history_1", &
    "Test integration history files", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_history_1

<Integrations: tests>+≡
  subroutine integrations_history_1 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global
    type(string_t), dimension(0) :: no_vars
    integer :: iostat, u_his
    character(91) :: buffer
    type(string_t) :: his_file, ps_file, pdf_file
    logical :: exist, exist_ps, exist_pdf

    write (u, "(A)")  "* Test output: integrations_history_1"
    write (u, "(A)")  "* Purpose: test integration history files"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and parameters"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_phs_forest_init ()

    call global%global_init ()

    libname = "integrations_history_1_lib"
    procname = "integrations_history_1"

    call global%set_log (var_str ("?vis_history"), &
      .true., is_known = .true.)
    call global%set_log (var_str ("?integration_timer"),&
      .false., is_known = .true.)
    call global%set_log (var_str ("?phs_s_mapping"),&
      .false., is_known = .true.)

    call prepare_test_library (global, libname, 1, [procname])
    call compile_library (libname, global)

    call global%append_log (&
      var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
    call global%append_log (&
      var_str ("?rebuild_grids"), .true., intrinsic = .true.)

```

```

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_real (var_str ("error_threshold"), &
    5E-6_default, is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([2, 2, 2], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true., &
    eff_reset = .true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Generated history files"
write (u, "(A)")

his_file = procname // ".r1.history.tex"
ps_file  = procname // ".r1.history.ps"
pdf_file = procname // ".r1.history.pdf"
inquire (file = char (his_file), exist = exist)
if (exist) then
    u_his = free_unit ()
    open (u_his, file = char (his_file), action = "read", status = "old")
    iostat = 0
    do while (iostat == 0)
        read (u_his, "(A)", iostat = iostat)  buffer
        if (iostat == 0) write (u, "(A)")  trim (buffer)
    end do
    close (u_his)
else
    write (u, "(A)")  "[History LaTeX file is missing]"
end if
inquire (file = char (ps_file), exist = exist_ps)
if (exist_ps) then

```

```

        write (u, "(A)") "[History Postscript file exists and is nonempty]"
    else
        write (u, "(A)") "[History Postscript file is missing/non-regular]"
    end if
    inquire (file = char (pdf_file), exist = exist_pdf)
    if (exist_pdf) then
        write (u, "(A)") "[History PDF file exists and is nonempty]"
    else
        write (u, "(A)") "[History PDF file is missing/non-regular]"
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call global%final ()
    call syntax_phs_forest_final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: integrations_history_1"

end subroutine integrations_history_1

```

33.7 Event Streams

This module manages I/O from/to multiple concurrent event streams. Usually, there is at most one input stream, but several output streams. For the latter, we set up an array which can hold `eio_t` (event I/O) objects of different dynamic types simultaneously. One of them may be marked as an input channel.

```
(event_streams.f90)≡
  <File header>

  module event_streams

    <Use strings>
    use events
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base
    use rt_data

    use dispatch_transforms, only: dispatch_eio

    <Standard module head>

    <Event streams: public>

    <Event streams: types>

    interface
    <Event streams: sub interfaces>
    end interface

  end module event_streams

(event_streams_sub.f90)≡
  <File header>

  submodule (event_streams) event_streams_s

    use io_units
    use diagnostics

    implicit none

  contains

    <Event streams: procedures>

  end submodule event_streams_s
```

33.7.1 Event Stream Array

Each entry is an `eio_t` object. Since the type is dynamic, we need a wrapper:

```
<Event streams: types>≡
```

```

type :: event_stream_entry_t
  class(eio_t), allocatable :: eio
end type event_stream_entry_t

```

An array of event-stream entry objects. If one of the entries is an input channel, `i_in` is the corresponding index.

```

<Event streams: public>≡
  public :: event_stream_array_t

<Event streams: types>+≡
  type :: event_stream_array_t
    type(event_stream_entry_t), dimension(:), allocatable :: entry
    integer :: i_in = 0
  contains
    <Event streams: event stream array: TBP>
  end type event_stream_array_t

```

Output.

```

<Event streams: event stream array: TBP>≡
  procedure :: write => event_stream_array_write

<Event streams: sub interfaces>≡
  module subroutine event_stream_array_write (object, unit)
    class(event_stream_array_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine event_stream_array_write

<Event streams: procedures>≡
  module subroutine event_stream_array_write (object, unit)
    class(event_stream_array_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event stream array:"
    if (allocated (object%entry)) then
      select case (size (object%entry))
      case (0)
        write (u, "(3x,A)") "[empty]"
      case default
        do i = 1, size (object%entry)
          if (i == object%i_in) write (u, "(1x,A)") "Input stream:"
          call object%entry(i)%eio%write (u)
        end do
      end select
    else
      write (u, "(3x,A)") "[undefined]"
    end if
  end subroutine event_stream_array_write

```

Check if there is content.

```

<Event streams: event stream array: TBP>+≡
  procedure :: is_valid => event_stream_array_is_valid

```

```

<Event streams: sub interfaces>+≡
    module function event_stream_array_is_valid (es_array) result (flag)
        class(event_stream_array_t), intent(in) :: es_array
        logical :: flag
    end function event_stream_array_is_valid

<Event streams: procedures>+≡
    module function event_stream_array_is_valid (es_array) result (flag)
        class(event_stream_array_t), intent(in) :: es_array
        logical :: flag

        flag = allocated (es_array%entry)

    end function event_stream_array_is_valid

```

Finalize all streams.

```

<Event streams: event stream array: TBP>+≡
    procedure :: final => event_stream_array_final

<Event streams: sub interfaces>+≡
    module subroutine event_stream_array_final (es_array)
        class(event_stream_array_t), intent(inout) :: es_array
    end subroutine event_stream_array_final

<Event streams: procedures>+≡
    module subroutine event_stream_array_final (es_array)
        class(event_stream_array_t), intent(inout) :: es_array
        integer :: i
        if (allocated (es_array%entry)) then
            do i = 1, size (es_array%entry)
                call es_array%entry(i)%eio%final ()
            end do
        end if
    end subroutine event_stream_array_final

```

Initialization. We use a generic sample name, open event I/O objects for all provided stream types (using the `dispatch_eio` routine), and initialize for the given list of process pointers. If there is an `input` argument, this channel is initialized as an input channel and appended to the array.

The `input_data` or, if not present, `data` may be modified. This happens if we open a stream for reading and get new information there.

```

<Event streams: event stream array: TBP>+≡
    procedure :: init => event_stream_array_init

<Event streams: sub interfaces>+≡
    module subroutine event_stream_array_init &
        (es_array, sample, stream_fmt, global, &
        data, input, input_sample, input_data, allow_switch, &
        checkpoint, callback, &
        error)
        class(event_stream_array_t), intent(out) :: es_array
        type(string_t), intent(in) :: sample
        type(string_t), dimension(:), intent(in) :: stream_fmt
        type(rt_data_t), intent(in) :: global
    end subroutine event_stream_array_init

```



```

type(event_sample_data_t), intent(inout), optional :: data
type(string_t), intent(in), optional :: input
type(string_t), intent(in), optional :: input_sample
type(event_sample_data_t), intent(inout), optional :: input_data
logical, intent(in), optional :: allow_switch
integer, intent(in), optional :: checkpoint
integer, intent(in), optional :: callback
logical, intent(out), optional :: error
end subroutine event_stream_array_init

```

(Event streams: procedures)+≡

```

module subroutine event_stream_array_init &
  (es_array, sample, stream_fmt, global, &
   data, input, input_sample, input_data, allow_switch, &
   checkpoint, callback, &
   error)
class(event_stream_array_t), intent(out) :: es_array
type(string_t), intent(in) :: sample
type(string_t), dimension(:), intent(in) :: stream_fmt
type(rt_data_t), intent(in) :: global
type(event_sample_data_t), intent(inout), optional :: data
type(string_t), intent(in), optional :: input
type(string_t), intent(in), optional :: input_sample
type(event_sample_data_t), intent(inout), optional :: input_data
logical, intent(in), optional :: allow_switch
integer, intent(in), optional :: checkpoint
integer, intent(in), optional :: callback
logical, intent(out), optional :: error
type(string_t) :: sample_in
integer :: n, i, n_output, i_input, i_checkpoint, i_callback
logical :: success, switch
if (present (input_sample)) then
  sample_in = input_sample
else
  sample_in = sample
end if
if (present (allow_switch)) then
  switch = allow_switch
else
  switch = .true.
end if
if (present (error)) then
  error = .false.
end if
n = size (stream_fmt)
n_output = n
if (present (input)) then
  n = n + 1
  i_input = n
else
  i_input = 0
end if
if (present (checkpoint)) then
  n = n + 1
  i_checkpoint = n

```

```

else
    i_checkpoint = 0
end if
if (present (callback)) then
    n = n + 1
    i_callback = n
else
    i_callback = 0
end if
allocate (es_array%entry (n))
if (i_checkpoint > 0) then
    call dispatch_eio &
        (es_array%entry(i_checkpoint)%eio, var_str ("checkpoint"), &
        global%var_list, global%fallback_model, &
        global%event_callback)
    call es_array%entry(i_checkpoint)%eio%init_out (sample, data)
end if
if (i_callback > 0) then
    call dispatch_eio &
        (es_array%entry(i_callback)%eio, var_str ("callback"), &
        global%var_list, global%fallback_model, &
        global%event_callback)
    call es_array%entry(i_callback)%eio%init_out (sample, data)
end if
if (i_input > 0) then
    call dispatch_eio (es_array%entry(i_input)%eio, input, &
        global%var_list, global%fallback_model, &
        global%event_callback)
    if (present (input_data)) then
        call es_array%entry(i_input)%eio%init_in &
            (sample_in, input_data, success)
    else
        call es_array%entry(i_input)%eio%init_in &
            (sample_in, data, success)
    end if
    if (success) then
        es_array%i_in = i_input
    else if (present (input_sample)) then
        if (present (error)) then
            error = .true.
        else
            call msg_fatal ("Events: &
                &parameter mismatch in input, aborting")
        end if
    else
        call msg_message ("Events: &
            &parameter mismatch, discarding old event set")
        call es_array%entry(i_input)%eio%final ()
        if (switch) then
            call msg_message ("Events: generating new events")
            call es_array%entry(i_input)%eio%init_out (sample, data)
        end if
    end if
end if
end if

```

```

do i = 1, n_output
  call dispatch_eio (es_array%entry(i)%eio, stream_fmt(i), &
    global%var_list, global%fallback_model, &
    global%event_callback)
  call es_array%entry(i)%eio%init_out (sample, data)
end do
end subroutine event_stream_array_init

```

Switch the (only) input channel to an output channel, so further events are appended to the respective stream.

```

<Event streams: event stream array: TBP>+≡
  procedure :: switch_inout => event_stream_array_switch_inout

<Event streams: sub interfaces>+≡
  module subroutine event_stream_array_switch_inout (es_array)
    class(event_stream_array_t), intent(inout) :: es_array
  end subroutine event_stream_array_switch_inout

<Event streams: procedures>+≡
  module subroutine event_stream_array_switch_inout (es_array)
    class(event_stream_array_t), intent(inout) :: es_array
    integer :: n
    if (es_array%has_input ()) then
      n = es_array%i_in
      call es_array%entry(n)%eio%switch_inout ()
      es_array%i_in = 0
    else
      call msg_bug ("Reading events: switch_inout: no input stream selected")
    end if
  end subroutine event_stream_array_switch_inout

```

Output an event (with given process number) to all output streams. If there is no output stream, do nothing.

```

<Event streams: event stream array: TBP>+≡
  procedure :: output => event_stream_array_output

<Event streams: sub interfaces>+≡
  module subroutine event_stream_array_output &
    (es_array, event, i_prc, event_index, passed, pacify, event_handle)
    class(event_stream_array_t), intent(inout) :: es_array
    type(event_t), intent(in), target :: event
    integer, intent(in) :: i_prc, event_index
    logical, intent(in), optional :: passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine event_stream_array_output

<Event streams: procedures>+≡
  module subroutine event_stream_array_output &
    (es_array, event, i_prc, event_index, passed, pacify, event_handle)
    class(event_stream_array_t), intent(inout) :: es_array
    type(event_t), intent(in), target :: event
    integer, intent(in) :: i_prc, event_index
    logical, intent(in), optional :: passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    logical :: increased

```

```

integer :: i
do i = 1, size (es_array%entry)
  if (i /= es_array%i_in) then
    associate (eio => es_array%entry(i)%eio)
      if (eio%split) then
        if (eio%split_n_evt > 0 .and. event_index > 1) then
          if (mod (event_index, eio%split_n_evt) == 1) then
            call eio%split_out ()
          end if
        else if (eio%split_n_kbytes > 0) then
          call eio%update_split_count (increased)
          if (increased) call eio%split_out ()
        end if
      end if
      call eio%output (event, i_prc, reading = es_array%i_in /= 0, &
        passed = passed, &
        pacify = pacify, &
        event_handle = event_handle)
    end associate
  end if
end do
end subroutine event_stream_array_output

```

Input the `i_prc` index which selects the process for the current event. This is separated from reading the event, because it determines which event record to read. `iostat` may indicate an error or an EOF condition, as usual.

(Event streams: event stream array: TBP)+≡

```

procedure :: input_i_prc => event_stream_array_input_i_prc

```

(Event streams: sub interfaces)+≡

```

module subroutine event_stream_array_input_i_prc (es_array, i_prc, iostat)
  class(event_stream_array_t), intent(inout) :: es_array
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
end subroutine event_stream_array_input_i_prc

```

(Event streams: procedures)+≡

```

module subroutine event_stream_array_input_i_prc (es_array, i_prc, iostat)
  class(event_stream_array_t), intent(inout) :: es_array
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
  integer :: n
  if (es_array%has_input ()) then
    n = es_array%i_in
    call es_array%entry(n)%eio%input_i_prc (i_prc, iostat)
  else
    call msg_fatal ("Reading events: no input stream selected")
  end if
end subroutine event_stream_array_input_i_prc

```

Input an event from the selected input stream. `iostat` may indicate an error or an EOF condition, as usual.

(Event streams: event stream array: TBP)+≡

```

procedure :: input_event => event_stream_array_input_event

```

<Event streams: sub interfaces>+≡

```
module subroutine event_stream_array_input_event &
  (es_array, event, iostat, event_handle)
  class(event_stream_array_t), intent(inout) :: es_array
  type(event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
end subroutine event_stream_array_input_event
```

<Event streams: procedures>+≡

```
module subroutine event_stream_array_input_event &
  (es_array, event, iostat, event_handle)
  class(event_stream_array_t), intent(inout) :: es_array
  type(event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  integer :: n
  if (es_array%has_input ()) then
    n = es_array%i_in
    call es_array%entry(n)%eio%input_event (event, iostat, event_handle)
  else
    call msg_fatal ("Reading events: no input stream selected")
  end if
end subroutine event_stream_array_input_event
```

Skip an entry of eio_t. Used to synchronize the event read-in for NLO events.

<Event streams: event stream array: TBP>+≡

```
procedure :: skip_eio_entry => event_stream_array_skip_eio_entry
```

<Event streams: sub interfaces>+≡

```
module subroutine event_stream_array_skip_eio_entry (es_array, iostat)
  class(event_stream_array_t), intent(inout) :: es_array
  integer, intent(out) :: iostat
end subroutine event_stream_array_skip_eio_entry
```

<Event streams: procedures>+≡

```
module subroutine event_stream_array_skip_eio_entry (es_array, iostat)
  class(event_stream_array_t), intent(inout) :: es_array
  integer, intent(out) :: iostat
  integer :: n
  if (es_array%has_input ()) then
    n = es_array%i_in
    call es_array%entry(n)%eio%skip (iostat)
  else
    call msg_fatal ("Reading events: no input stream selected")
  end if
end subroutine event_stream_array_skip_eio_entry
```

Return true if there is an input channel among the event streams.

<Event streams: event stream array: TBP>+≡

```
procedure :: has_input => event_stream_array_has_input
```

<Event streams: sub interfaces>+≡

```
module function event_stream_array_has_input (es_array) result (flag)
  class(event_stream_array_t), intent(in) :: es_array
```

```

        logical :: flag
    end function event_stream_array_has_input
<Event streams: procedures>+≡
    module function event_stream_array_has_input (es_array) result (flag)
        class(event_stream_array_t), intent(in) :: es_array
        logical :: flag
        flag = es_array%i_in /= 0
    end function event_stream_array_has_input

```

33.7.2 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

```

<event_streams_ut.f90>≡
    <File header>

    module event_streams_ut
        use unit_tests
        use event_streams_uti

    <Standard module head>

    <Event streams: public test>

    contains

    <Event streams: test driver>

    end module event_streams_ut
<event_streams_uti.f90>≡
    <File header>

    module event_streams_uti

    <Use kinds>
    <Use strings>
        use model_data
        use eio_data
        use process, only: process_t
        use instances, only: process_instance_t
        use models
        use rt_data
        use events

        use event_streams

    <Standard module head>

    <Event streams: test declarations>

    contains

```

<Event streams: tests>

end module event_streams_util

API: driver for the unit tests below.

<Event streams: public test>≡

public :: event_streams_test

<Event streams: test driver>≡

subroutine event_streams_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Event streams: execute tests>

end subroutine event_streams_test

Empty event stream

This should set up an empty event output stream array, including initialization, output, and finalization (which are all no-ops).

<Event streams: execute tests>≡

call test (event_streams_1, "event_streams_1", &
"empty event stream array", &
u, results)

<Event streams: test declarations>≡

public :: event_streams_1

<Event streams: tests>≡

subroutine event_streams_1 (u)

integer, intent(in) :: u

type(event_stream_array_t) :: es_array

type(rt_data_t) :: global

type(event_t) :: event

type(string_t) :: sample

type(string_t), dimension(0) :: empty_string_array

write (u, "(A)") "* Test output: event_streams_1"

write (u, "(A)") "* Purpose: handle empty event stream array"

write (u, "(A)")

sample = "event_streams_1"

call es_array%init (sample, empty_string_array, global)

call es_array%output (event, 42, 1)

call es_array%write (u)

call es_array%final ()

write (u, "(A)")

write (u, "(A)") "* Test output end: event_streams_1"

end subroutine event_streams_1

Nontrivial event stream

Here we generate a trivial event and choose raw output as an entry in the stream array.

```
(Event streams: execute tests)+≡
    call test (event_streams_2, "event_streams_2", &
        "nontrivial event stream array", &
        u, results)

(Event streams: test declarations)+≡
    public :: event_streams_2

(Event streams: tests)+≡
    subroutine event_streams_2 (u)
        use processes_ut, only: prepare_test_process
        integer, intent(in) :: u
        type(event_stream_array_t) :: es_array
        type(rt_data_t) :: global
        type(model_data_t), target :: model
        type(event_t), allocatable, target :: event
        type(process_t), allocatable, target :: process
        type(process_instance_t), allocatable, target :: process_instance
        type(string_t) :: sample
        type(string_t), dimension(0) :: empty_string_array
        integer :: i_prc, iostat

        write (u, "(A)")  "* Test output: event_streams_2"
        write (u, "(A)")  "* Purpose: handle empty event stream array"
        write (u, "(A)")

        call syntax_model_file_init ()
        call global%global_init ()
        call global%init_fallback_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

        call model%init_test ()

        write (u, "(A)")  "* Generate test process event"
        write (u, "(A)")

        allocate (process)
        allocate (process_instance)
        call prepare_test_process (process, process_instance, model, &
            run_id = var_str ("run_test"))
        call process_instance%setup_event_data ()

        allocate (event)
        call event%basic_init ()
        call event%connect (process_instance, process%get_model_ptr ())
        call event%generate (1, [0.4_default, 0.4_default])
        call event%set_index (42)
        call event%evaluate_expressions ()
        call event%write (u)

        write (u, "(A)")
```



```

write (u, "(A)") "* Allocate raw eio stream and write event to file"
write (u, "(A)")

sample = "event_streams_2"

call es_array%init (sample, [var_str ("raw")], global)
call es_array%output (event, 1, 1)
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

sample = "foo"
call es_array%init (sample, empty_string_array, global, &
    input = var_str ("raw"), input_sample = var_str ("event_streams_2"))
call es_array%write (u)

write (u, "(A)")
write (u, "(A)") "* Reread event"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)

write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call es_array%input_event (event, iostat)
call es_array%final ()

call event%write (u)

call global%final ()

call model%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: event_streams_2"

end subroutine event_streams_2

```

Switch in/out

Here we generate an event file and test switching from writing to reading when the file is exhausted.

```

<Event streams: execute tests>+≡
    call test (event_streams_3, "event_streams_3", &
        "switch input/output", &
        u, results)

<Event streams: test declarations>+≡
    public :: event_streams_3

```

<Event streams: tests>+≡

```

subroutine event_streams_3 (u)
  use processes_ut, only: prepare_test_process
  integer, intent(in) :: u
  type(event_stream_array_t) :: es_array
  type(rt_data_t) :: global
  type(model_data_t), target :: model
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(string_t) :: sample
  type(string_t), dimension(0) :: empty_string_array
  integer :: i_prc, iostat

  write (u, "(A)")  "* Test output: event_streams_3"
  write (u, "(A)")  "* Purpose: handle in/out switching"
  write (u, "(A)")

  call syntax_model_file_init ()
  call global%global_init ()
  call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

  call model%init_test ()

  write (u, "(A)")  "* Generate test process event"
  write (u, "(A)")

  allocate (process)
  allocate (process_instance)
  call prepare_test_process (process, process_instance, model, &
    run_id = var_str ("run_test"))
  call process_instance%setup_event_data ()

  allocate (event)
  call event%basic_init ()
  call event%connect (process_instance, process%get_model_ptr ())
  call event%generate (1, [0.4_default, 0.4_default])
  call event%increment_index ()
  call event%evaluate_expressions ()

  write (u, "(A)")  "* Allocate raw eio stream and write event to file"
  write (u, "(A)")

  sample = "event_streams_3"

  call es_array%init (sample, [var_str ("raw")], global)
  call es_array%output (event, 1, 1)
  call es_array%write (u)
  call es_array%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Reallocate raw eio stream for reading"
  write (u, "(A)")

```

```

call es_array%init (sample, empty_string_array, global, &
    input = var_str ("raw"))
call es_array%write (u)

write (u, "(A)")
write (u, "(A)") "* Reread event"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)
call es_array%input_event (event, iostat)

write (u, "(A)") "* Attempt to read another event (fail), then generate"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)
if (iostat < 0) then
    call es_array%switch_inout ()
    call event%generate (1, [0.3_default, 0.3_default])
    call event%increment_index ()
    call event%evaluate_expressions ()
    call es_array%output (event, 1, 2)
end if
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
call event%write (u)

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

call es_array%init (sample, empty_string_array, global, &
    input = var_str ("raw"))
call es_array%write (u)

write (u, "(A)")
write (u, "(A)") "* Reread two events and display 2nd event"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)
call es_array%input_event (event, iostat)
call es_array%input_i_prc (i_prc, iostat)

call es_array%input_event (event, iostat)
call es_array%final ()

call event%write (u)

call global%final ()

call model%final ()
call syntax_model_file_final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: event_streams_3"

end subroutine event_streams_3

```

Checksum

Here we generate an event file and repeat twice, once with identical parameters and once with modified parameters.

```

<Event streams: execute tests>+≡
  call test (event_streams_4, "event_streams_4", &
    "check MD5 sum", &
    u, results)

<Event streams: test declarations>+≡
  public :: event_streams_4

<Event streams: tests>+≡
  subroutine event_streams_4 (u)
    integer, intent(in) :: u
    type(event_stream_array_t) :: es_array
    type(rt_data_t) :: global
    type(process_t), allocatable, target :: process
    type(string_t) :: sample
    type(string_t), dimension(0) :: empty_string_array
    type(event_sample_data_t) :: data

    write (u, "(A)")  "* Test output: event_streams_4"
    write (u, "(A)")  "* Purpose: handle in/out switching"
    write (u, "(A)")

    write (u, "(A)")  "* Generate test process event"
    write (u, "(A)")

    call syntax_model_file_init ()
    call global%global_init ()
    call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

    call global%set_log (var_str ("?check_event_file"), &
      .true., is_known = .true.)

    allocate (process)

    write (u, "(A)")  "* Allocate raw eio stream for writing"
    write (u, "(A)")

    sample = "event_streams_4"
    data%md5sum_cfg = "1234567890abcdef1234567890abcdef"

    call es_array%init (sample, [var_str ("raw")], global, data)
    call es_array%write (u)

```

```

call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate modified raw eio stream for reading (fail)"
write (u, "(A)")

data%md5sum_cfg = "1234567890_____1234567890_____"
call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Repeat ignoring checksum"
write (u, "(A)")

call global%set_log (var_str ("?check_event_file"), &
    .false., is_known = .true.)
call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: event_streams_4"

end subroutine event_streams_4

```

33.8 Restricted Subprocesses

This module provides an automatic means to construct restricted subprocesses of a current process object. A restricted subprocess has the same initial and final state as the current process, but a restricted set of Feynman graphs.

The actual application extracts the set of resonance histories that apply to the process and uses this to construct subprocesses that are restricted to one of those histories, respectively. The resonance histories are derived from the phase-space setup. This implies that the method is tied to the OMega matrix element generator and to the wood phase space method.

The processes are collected in a new process library that is generated on-the-fly.

The `resonant_subprocess_t` object is intended as a component of the event record, which manages all operations regarding resonance handling.

The run-time calculations are delegated to an event transform (`evt_resonance_t`), as a part of the event transform chain. The transform selects one (or none) of the resonance histories, given the momentum configuration, computes matrix elements and inserts resonances into the particle set.

```
<restricted_subprocesses.f90>≡  
  <File header>
```

```
module restricted_subprocesses
```

```
  <Use kinds>
```

```
  <Use strings>
```

```
  use particle_specifiers, only: prt_spec_t  
  use resonances, only: resonance_history_t, resonance_history_set_t  
  use variables, only: var_list_t  
  use models, only: model_t  
  use event_transforms, only: evt_t  
  use resonance_insertion, only: evt_resonance_t  
  use rt_data, only: rt_data_t  
  use process_configurations, only: process_configuration_t  
  use process, only: process_t, process_ptr_t  
  use instances, only: process_instance_t, process_instance_ptr_t
```

```
  <Standard module head>
```

```
  <Restricted subprocesses: public>
```

```
  <Restricted subprocesses: types>
```

```
  <Restricted subprocesses: interfaces>
```

```
    interface
```

```
  <Restricted subprocesses: sub interfaces>
```

```
    end interface
```

```
end module restricted_subprocesses
```

```
<restricted_subprocesses_sub.f90>≡  
  <File header>
```

```

submodule (restricted_subprocesses) restricted_subprocesses_s

  use diagnostics, only: msg_message, msg_fatal, msg_bug
  use diagnostics, only: signal_is_pending
  use io_units, only: given_output_unit
  use format_defs, only: FMT_14, FMT_19
  use string_utils, only: str
  use process_libraries, only: process_component_def_t
  use process_libraries, only: process_library_t
  use process_libraries, only: STAT_ACTIVE
  use prclib_stacks, only: prclib_entry_t
  use compilations, only: compile_library
  use integrations, only: integrate_process

  implicit none

contains

  <Restricted subprocesses: procedures>

end submodule restricted_subprocesses_s

```

33.8.1 Process configuration

We extend the `process_configuration_t` by another method for initialization that takes into account a resonance history.

```

<Restricted subprocesses: public>≡
  public :: restricted_process_configuration_t

<Restricted subprocesses: types>≡
  type, extends (process_configuration_t) :: restricted_process_configuration_t
  private
  contains
  <Restricted subprocesses: restricted process configuration: TBP>
  end type restricted_process_configuration_t

```

Resonance history as an argument. We use it to override the `restrictions` setting in a local variable list. Since we can construct the restricted process only by using OMega, we enforce it as the ME method. Other settings are taken from the variable list. The model will most likely be set, but we insert a safeguard just in case.

Also, the resonant subprocess should not itself spawn resonant subprocesses, so we unset `?resonance_history`.

We have to create a local copy of the model here, via pointer allocation. The reason is that the model as stored (via pointer) in the base type will be finalized and deallocated.

The current implementation will generate a LO process, the optional `nlo_process` is unset. (It is not obvious whether the construction makes sense beyond LO.)

```

<Restricted subprocesses: restricted process configuration: TBP>≡
  procedure :: init_resonant_process

```

```

<Restricted subprocesses: sub interfaces>≡
module subroutine init_resonant_process &
    (prc_config, prc_name, prt_in, prt_out, res_history, model, var_list)
    class(restricted_process_configuration_t), intent(out) :: prc_config
    type(string_t), intent(in) :: prc_name
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(resonance_history_t), intent(in) :: res_history
    type(model_t), intent(in), target :: model
    type(var_list_t), intent(in), target :: var_list
end subroutine init_resonant_process

<Restricted subprocesses: procedures>≡
module subroutine init_resonant_process &
    (prc_config, prc_name, prt_in, prt_out, res_history, model, var_list)
    class(restricted_process_configuration_t), intent(out) :: prc_config
    type(string_t), intent(in) :: prc_name
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(resonance_history_t), intent(in) :: res_history
    type(model_t), intent(in), target :: model
    type(var_list_t), intent(in), target :: var_list
    type(model_t), pointer :: local_model
    type(var_list_t) :: local_var_list
    allocate (local_model)
    call local_model%init_instance (model)
    call local_var_list%link (var_list)
    call local_var_list%append_string (var_str ("$model_name"), &
        sval = local_model%get_name (), &
        intrinsic=.true.)
    call local_var_list%append_string (var_str ("method"), &
        sval = var_str ("omega"), &
        intrinsic=.true.)
    call local_var_list%append_string (var_str ("restrictions"), &
        sval = res_history%as_omega_string (size (prt_in)), &
        intrinsic = .true.)
    call local_var_list%append_log (var_str ("?resonance_history"), &
        lval = .false., &
        intrinsic = .true.)
    call prc_config%init (prc_name, size (prt_in), 1, &
        local_model, local_var_list)
    call prc_config%setup_component (1, &
        prt_in, prt_out, &
        local_model, local_var_list)
end subroutine init_resonant_process

```

33.8.2 Resonant-subprocess set manager

This data type enables generation of a library of resonant subprocesses for a given master process, and it allows for convenient access. The matrix elements from the subprocesses can be used as channel weights to activate a selector, which then returns a preferred channel via some random number generator.

```

<Restricted subprocesses: public>+≡

```



```

public :: resonant_subprocess_set_t
<Restricted subprocesses: types>+≡
type :: resonant_subprocess_set_t
private
integer, dimension(:), allocatable :: n_history
type(resonance_history_set_t), dimension(:), allocatable :: res_history_set
logical :: lib_active = .false.
type(string_t) :: libname
type(string_t), dimension(:), allocatable :: proc_id
type(process_ptr_t), dimension(:), allocatable :: subprocess
type(process_instance_ptr_t), dimension(:), allocatable :: instance
logical :: filled = .false.
type(evt_resonance_t), pointer :: evt => null ()
contains
<Restricted subprocesses: resonant subprocess set: TBP>
end type resonant_subprocess_set_t

```

Output

```

<Restricted subprocesses: resonant subprocess set: TBP>≡
procedure :: write => resonant_subprocess_set_write

<Restricted subprocesses: sub interfaces>+≡
module subroutine resonant_subprocess_set_write (prc_set, unit, testflag)
class(resonant_subprocess_set_t), intent(in) :: prc_set
integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
end subroutine resonant_subprocess_set_write

<Restricted subprocesses: procedures>+≡
module subroutine resonant_subprocess_set_write (prc_set, unit, testflag)
class(resonant_subprocess_set_t), intent(in) :: prc_set
integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
logical :: truncate
integer :: u, i
u = given_output_unit (unit)
truncate = .false.; if (present (testflag)) truncate = testflag
write (u, "(1x,A)") "Resonant subprocess set:"
if (allocated (prc_set%n_history)) then
if (any (prc_set%n_history > 0)) then
do i = 1, size (prc_set%n_history)
if (prc_set%n_history(i) > 0) then
write (u, "(1x,A,I0)") "Component #", i
call prc_set%res_history_set(i)%write (u, indent=1)
end if
end do
if (prc_set%lib_active) then
write (u, "(3x,A,A,A)") "Process library = ', &
char (prc_set%libname), "'"
else
write (u, "(3x,A)") "Process library: [inactive]"
end if
if (associated (prc_set%evt)) then
if (truncate) then

```

```

        write (u, "(3x,A,1x," // FMT_14 // ")") &
            "Process sqme =", prc_set%get_master_sqme ()
    else
        write (u, "(3x,A,1x," // FMT_19 // ")") &
            "Process sqme =", prc_set%get_master_sqme ()
    end if
end if
if (associated (prc_set%evt)) then
    write (u, "(3x,A)") "Event transform: associated"
    write (u, "(2x)", advance="no")
    call prc_set%evt%write_selector (u, testflag)
else
    write (u, "(3x,A)") "Event transform: not associated"
end if
else
    write (u, "(2x,A)") "[empty]"
end if
else
    write (u, "(3x,A)") "[not allocated]"
end if
end subroutine resonant_subprocess_set_write

```

33.8.3 Resonance history set

Initialize subprocess set with an array of pre-created resonance history sets.

Safeguard: if there are no resonances in the input, initialize the local set as empty, but complete.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: init => resonant_subprocess_set_init
    procedure :: fill_resonances => resonant_subprocess_set_fill_resonances

<Restricted subprocesses: sub interfaces>+≡
    module subroutine resonant_subprocess_set_init (prc_set, n_component)
        class(resonant_subprocess_set_t), intent(out) :: prc_set
        integer, intent(in) :: n_component
    end subroutine resonant_subprocess_set_init
    module subroutine resonant_subprocess_set_fill_resonances (prc_set, &
        res_history_set, i_component)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        type(resonance_history_set_t), intent(in) :: res_history_set
        integer, intent(in) :: i_component
    end subroutine resonant_subprocess_set_fill_resonances

<Restricted subprocesses: procedures>+≡
    module subroutine resonant_subprocess_set_init (prc_set, n_component)
        class(resonant_subprocess_set_t), intent(out) :: prc_set
        integer, intent(in) :: n_component
        allocate (prc_set%res_history_set (n_component))
        allocate (prc_set%n_history (n_component), source = 0)
    end subroutine resonant_subprocess_set_init

    module subroutine resonant_subprocess_set_fill_resonances (prc_set, &
        res_history_set, i_component)

```

```

class(resonant_subprocess_set_t), intent(inout) :: prc_set
type(resonance_history_set_t), intent(in) :: res_history_set
integer, intent(in) :: i_component
prc_set%n_history(i_component) = res_history_set%get_n_history ()
if (prc_set%n_history(i_component) > 0) then
    prc_set%res_history_set(i_component) = res_history_set
else
    call prc_set%res_history_set(i_component)%init (initial_size = 0)
    call prc_set%res_history_set(i_component)%freeze ()
end if
end subroutine resonant_subprocess_set_fill_resonances

```

Return the resonance history set.

<Restricted subprocesses: resonant subprocess set: TBP>+≡

```

procedure :: get_resonance_history_set &
=> resonant_subprocess_set_get_resonance_history_set

```

<Restricted subprocesses: sub interfaces>+≡

```

module function resonant_subprocess_set_get_resonance_history_set &
    (prc_set) result (res_history_set)
class(resonant_subprocess_set_t), intent(in) :: prc_set
type(resonance_history_set_t), dimension(:), allocatable :: &
    res_history_set
end function resonant_subprocess_set_get_resonance_history_set

```

<Restricted subprocesses: procedures>+≡

```

module function resonant_subprocess_set_get_resonance_history_set &
    (prc_set) result (res_history_set)
class(resonant_subprocess_set_t), intent(in) :: prc_set
type(resonance_history_set_t), dimension(:), allocatable :: &
    res_history_set
res_history_set = prc_set%res_history_set
end function resonant_subprocess_set_get_resonance_history_set

```

33.8.4 Library for the resonance history set

The recommended library name: append `_R` to the process name.

<Restricted subprocesses: public>+≡

```

public :: get_libname_res

```

<Restricted subprocesses: sub interfaces>+≡

```

elemental module function get_libname_res (proc_id) result (libname)
type(string_t), intent(in) :: proc_id
type(string_t) :: libname
end function get_libname_res

```

<Restricted subprocesses: procedures>+≡

```

elemental module function get_libname_res (proc_id) result (libname)
type(string_t), intent(in) :: proc_id
type(string_t) :: libname
libname = proc_id // "_R"
end function get_libname_res

```

Here we scan the global process library whether any processes require resonant subprocesses to be constructed. If yes, create process objects with phase space and construct the process libraries as usual. Then append the library names to the array.

The temporary integration objects should carry the `phs_only` flag. We set this in the local environment.

Once a process object with resonance histories (derived from phase space) has been created, we extract the resonance histories and use them, together with the process definition, to create the new library.

Finally, compile the library.

```

<Restricted subprocesses: public>+≡
    public :: spawn_resonant_subprocess_libraries

<Restricted subprocesses: sub interfaces>+≡
    module subroutine spawn_resonant_subprocess_libraries &
        (libname, local, global, libname_res)
        type(string_t), intent(in) :: libname
        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), target :: global
        type(string_t), dimension(:), allocatable, intent(inout) :: libname_res
    end subroutine spawn_resonant_subprocess_libraries

<Restricted subprocesses: procedures>+≡
    module subroutine spawn_resonant_subprocess_libraries &
        (libname, local, global, libname_res)
        type(string_t), intent(in) :: libname
        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), target :: global
        type(string_t), dimension(:), allocatable, intent(inout) :: libname_res
        type(process_library_t), pointer :: lib
        type(string_t), dimension(:), allocatable :: process_id_res
        type(process_t), pointer :: process
        type(resonance_history_set_t) :: res_history_set
        type(process_component_def_t), pointer :: process_component_def
        logical :: phs_only_saved, exist
        integer :: i_proc, i_component
        lib => global%prclib_stack%get_library_ptr (libname)
        call lib%get_process_id_req_resonant (process_id_res)
        if (size (process_id_res) > 0) then
            call msg_message ("Creating resonant-subprocess libraries &
                &for library '" // char (libname) // "'")
            libname_res = get_libname_res (process_id_res)
            phs_only_saved = local%var_list%get_lval (var_str ("?phs_only"))
            call local%var_list%set_log &
                (var_str ("?phs_only"), .true., is_known=.true.)
            do i_proc = 1, size (process_id_res)
                associate (proc_id => process_id_res (i_proc))
                    call msg_message ("Process '" // char (proc_id) // "': &
                        &constructing phase space for resonance structure")
                    call integrate_process (proc_id, local, global)
                    process => global%process_stack%get_process_ptr (proc_id)
                    call create_library (libname_res(i_proc), global, exist)
                    if (.not. exist) then
                        do i_component = 1, process%get_n_components ()

```

```

        call process%extract_resonance_history_set &
            (res_history_set, i_component = i_component)
        process_component_def &
            => process%get_component_def_ptr (i_component)
        call add_to_library (libname_res(i_proc), &
            res_history_set, &
            process_component_def%get_prt_spec_in (), &
            process_component_def%get_prt_spec_out (), &
            global)
    end do
    call msg_message ("Process library '" &
        // char (libname_res(i_proc)) &
        // ": created")
    end if
    call global%update_prclib (lib)
end associate
end do
call local%var_list%set_log &
    (var_str ("?phs_only"), phs_only_saved, is_known=.true.)
end if
end subroutine spawn_resonant_subprocess_libraries

```

This is another version of the library constructor, bound to a restricted-subprocess set object. Create the appropriate process library, add processes, and close the library.

(Restricted subprocesses: resonant subprocess set: TBP)+≡

```

procedure :: create_library => resonant_subprocess_set_create_library
procedure :: add_to_library => resonant_subprocess_set_add_to_library
procedure :: freeze_library => resonant_subprocess_set_freeze_library

```

(Restricted subprocesses: sub interfaces)+≡

```

module subroutine resonant_subprocess_set_create_library (prc_set, &
    libname, global, exist)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(string_t), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: global
    logical, intent(out) :: exist
end subroutine resonant_subprocess_set_create_library
module subroutine resonant_subprocess_set_add_to_library (prc_set, &
    i_component, prt_in, prt_out, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer, intent(in) :: i_component
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(rt_data_t), intent(inout), target :: global
end subroutine resonant_subprocess_set_add_to_library
module subroutine resonant_subprocess_set_freeze_library (prc_set, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(inout), target :: global
end subroutine resonant_subprocess_set_freeze_library

```

(Restricted subprocesses: procedures)+≡

```

module subroutine resonant_subprocess_set_create_library (prc_set, &
    libname, global, exist)

```

```

class(resonant_subprocess_set_t), intent(inout) :: prc_set
type(string_t), intent(in) :: libname
type(rt_data_t), intent(inout), target :: global
logical, intent(out) :: exist
prc_set%libname = libname
call create_library (prc_set%libname, global, exist)
end subroutine resonant_subprocess_set_create_library

module subroutine resonant_subprocess_set_add_to_library (prc_set, &
    i_component, prt_in, prt_out, global)
class(resonant_subprocess_set_t), intent(inout) :: prc_set
integer, intent(in) :: i_component
type(prt_spec_t), dimension(:), intent(in) :: prt_in
type(prt_spec_t), dimension(:), intent(in) :: prt_out
type(rt_data_t), intent(inout), target :: global
call add_to_library (prc_set%libname, &
    prc_set%res_history_set(i_component), &
    prt_in, prt_out, global)
end subroutine resonant_subprocess_set_add_to_library

module subroutine resonant_subprocess_set_freeze_library (prc_set, global)
class(resonant_subprocess_set_t), intent(inout) :: prc_set
type(rt_data_t), intent(inout), target :: global
type(prclib_entry_t), pointer :: lib_entry
type(process_library_t), pointer :: lib
lib => global%prclib_stack%get_library_ptr (prc_set%libname)
call lib%get_process_id_list (prc_set%proc_id)
prc_set%lib_active = .true.
end subroutine resonant_subprocess_set_freeze_library

```

The common parts of the procedures above: (i) create a new process library or recover it, (ii) for each history, create a process configuration and record it.

<Restricted subprocesses: procedures>+≡

```

subroutine create_library (libname, global, exist)
type(string_t), intent(in) :: libname
type(rt_data_t), intent(inout), target :: global
logical, intent(out) :: exist
type(prclib_entry_t), pointer :: lib_entry
type(process_library_t), pointer :: lib
type(resonance_history_t) :: res_history
type(string_t), dimension(:), allocatable :: proc_id
type(restricted_process_configuration_t) :: prc_config
integer :: i
lib => global%prclib_stack%get_library_ptr (libname)
exist = associated (lib)
if (.not. exist) then
    call msg_message ("Creating library for resonant subprocesses '" &
        // char (libname) // "'")
    allocate (lib_entry)
    call lib_entry%init (libname)
    lib => lib_entry%process_library_t
    call global%add_prclib (lib_entry)
else

```

```

        call msg_message ("Using library for resonant subprocesses '" &
            // char (libname) // "'")
        call global%update_prclib (lib)
    end if
end subroutine create_library

subroutine add_to_library (libname, res_history_set, prt_in, prt_out, global)
    type(string_t), intent(in) :: libname
    type(resonance_history_set_t), intent(in) :: res_history_set
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(rt_data_t), intent(inout), target :: global
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    type(resonance_history_t) :: res_history
    type(string_t), dimension(:), allocatable :: proc_id
    type(restricted_process_configuration_t) :: prc_config
    integer :: n0, i
    lib => global%prclib_stack%get_library_ptr (libname)
    if (associated (lib)) then
        n0 = lib%get_n_processes ()
        allocate (proc_id (res_history_set%get_n_history ()))
        do i = 1, size (proc_id)
            proc_id(i) = libname // str (n0 + i)
            res_history = res_history_set%get_history(i)
            call prc_config%init_resonant_process (proc_id(i), &
                prt_in, prt_out, &
                res_history, &
                global%model, global%var_list)
            call msg_message ("Resonant subprocess #" &
                // char (str(n0+i)) // ": " &
                // char (res_history%as_omega_string (size (prt_in))))
            call prc_config%record (global)
            if (signal_is_pending ()) return
        end do
    else
        call msg_bug ("Adding subprocesses: library '" &
            // char (libname) // "' not found")
    end if
end subroutine add_to_library

```

Compile the generated library, required settings taken from the `global` data set.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: compile_library => resonant_subprocess_set_compile_library

<Restricted subprocesses: sub interfaces>+≡
    module subroutine resonant_subprocess_set_compile_library (prc_set, global)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        type(rt_data_t), intent(inout), target :: global
    end subroutine resonant_subprocess_set_compile_library

<Restricted subprocesses: procedures>+≡
    module subroutine resonant_subprocess_set_compile_library (prc_set, global)
        class(resonant_subprocess_set_t), intent(in) :: prc_set

```

```

type(rt_data_t), intent(inout), target :: global
type(process_library_t), pointer :: lib
lib => global%prclib_stack%get_library_ptr (prc_set%libname)
if (lib%get_status () < STAT_ACTIVE) then
    call compile_library (prc_set%libname, global)
end if
end subroutine resonant_subprocess_set_compile_library

```

Check if the library has been created / the process has been evaluated.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: is_active => resonant_subprocess_set_is_active

<Restricted subprocesses: sub interfaces>+≡
    module function resonant_subprocess_set_is_active (prc_set) result (flag)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        logical :: flag
    end function resonant_subprocess_set_is_active

<Restricted subprocesses: procedures>+≡
    module function resonant_subprocess_set_is_active (prc_set) result (flag)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        logical :: flag
        flag = prc_set%lib_active
    end function resonant_subprocess_set_is_active

```

Return number of generated process objects, library, and process IDs.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: get_n_process => resonant_subprocess_set_get_n_process
    procedure :: get_libname => resonant_subprocess_set_get_libname
    procedure :: get_proc_id => resonant_subprocess_set_get_proc_id

<Restricted subprocesses: sub interfaces>+≡
    module function resonant_subprocess_set_get_n_process (prc_set) result (n)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        integer :: n
    end function resonant_subprocess_set_get_n_process
    module function resonant_subprocess_set_get_libname &
        (prc_set) result (libname)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        type(string_t) :: libname
    end function resonant_subprocess_set_get_libname
    module function resonant_subprocess_set_get_proc_id &
        (prc_set, i) result (proc_id)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        integer, intent(in) :: i
        type(string_t) :: proc_id
    end function resonant_subprocess_set_get_proc_id

<Restricted subprocesses: procedures>+≡
    module function resonant_subprocess_set_get_n_process (prc_set) result (n)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        integer :: n
        if (prc_set%lib_active) then
            n = size (prc_set%proc_id)
        else

```



```

        n = 0
    end if
end function resonant_subprocess_set_get_n_process

module function resonant_subprocess_set_get_libname (prc_set) result (libname)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    type(string_t) :: libname
    if (prc_set%lib_active) then
        libname = prc_set%libname
    else
        libname = ""
    end if
end function resonant_subprocess_set_get_libname

module function resonant_subprocess_set_get_proc_id &
    (prc_set, i) result (proc_id)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    integer, intent(in) :: i
    type(string_t) :: proc_id
    if (allocated (prc_set%proc_id)) then
        proc_id = prc_set%proc_id(i)
    else
        proc_id = ""
    end if
end function resonant_subprocess_set_get_proc_id

```

33.8.5 Process objects and instances

Prepare process objects for all entries in the resonant-subprocesses library. The process objects are appended to the global process stack. A local environment can be used where we place temporary variable settings that affect process-object generation. We initialize the processes, such that we can evaluate matrix elements, but we do not need to integrate them.

The internal procedure `prepare_process` is an abridged version of the procedure with this name in the `simulations` module.

(Restricted subprocesses: resonant subprocess set: TBP)+≡

```

procedure :: prepare_process_objects &
=> resonant_subprocess_set_prepare_process_objects

```

(Restricted subprocesses: sub interfaces)+≡

```

module subroutine resonant_subprocess_set_prepare_process_objects &
    (prc_set, local, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
end subroutine resonant_subprocess_set_prepare_process_objects

```

(Restricted subprocesses: procedures)+≡

```

module subroutine resonant_subprocess_set_prepare_process_objects &
    (prc_set, local, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global

```

```

type(rt_data_t), pointer :: current
type(process_library_t), pointer :: lib
type(string_t) :: phs_method_saved, integration_method_saved
type(string_t) :: proc_id, libname_cur, libname_res
integer :: i, n
if (.not. prc_set%is_active ()) return
if (present (global)) then
    current => global
else
    current => local
end if
libname_cur = current%prclib%get_name ()
libname_res = prc_set%get_libname ()
lib => current%prclib_stack%get_library_ptr (libname_res)
if (associated (lib)) call current%update_prclib (lib)
phs_method_saved = local%get_sval (var_str ("phs_method"))
integration_method_saved = local%get_sval (var_str ("integration_method"))
call local%set_string (var_str ("phs_method"), &
    var_str ("none"), is_known = .true.)
call local%set_string (var_str ("integration_method"), &
    var_str ("none"), is_known = .true.)
n = prc_set%get_n_process ()
allocate (prc_set%subprocess (n))
do i = 1, n
    proc_id = prc_set%get_proc_id (i)
    call prepare_process (prc_set%subprocess(i)%p, proc_id)
    if (signal_is_pending ()) return
end do
call local%set_string (var_str ("phs_method"), &
    phs_method_saved, is_known = .true.)
call local%set_string (var_str ("integration_method"), &
    integration_method_saved, is_known = .true.)
lib => current%prclib_stack%get_library_ptr (libname_cur)
if (associated (lib)) call current%update_prclib (lib)
contains
subroutine prepare_process (process, process_id)
    type(process_t), pointer, intent(out) :: process
    type(string_t), intent(in) :: process_id
    call msg_message ("Simulate: initializing resonant subprocess '" &
        // char (process_id) // "'")
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .true.)
    else
        call integrate_process (process_id, local, local_stack = .true., &
            init_only = .true.)
    end if
    process => current%process_stack%get_process_ptr (process_id)
    if (.not. associated (process)) then
        call msg_fatal ("Simulate: resonant subprocess '" &
            // char (process_id) // "' could not be initialized: aborting")
    end if
end subroutine prepare_process
end subroutine resonant_subprocess_set_prepare_process_objects

```

Workspace for the resonant subprocesses.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: prepare_process_instances &
    => resonant_subprocess_set_prepare_process_instances

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_prepare_process_instances &
    (prc_set, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(in), target :: global
  end subroutine resonant_subprocess_set_prepare_process_instances

<Restricted subprocesses: procedures>+≡
  module subroutine resonant_subprocess_set_prepare_process_instances &
    (prc_set, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(in), target :: global
    integer :: i, n
    if (.not. prc_set%is_active ()) return
    n = size (prc_set%subprocess)
    allocate (prc_set%instance (n))
    do i = 1, n
      allocate (prc_set%instance(i)%p)
      call prc_set%instance(i)%p%init (prc_set%subprocess(i)%p)
      call prc_set%instance(i)%p%setup_event_data (global%model)
    end do
  end subroutine resonant_subprocess_set_prepare_process_instances

```

33.8.6 Event transform connection

The idea is that the resonance-insertion event transform has been allocated somewhere (namely, in the standard event-transform chain), but we maintain a link such that we can inject matrix-element results event by event. The event transform holds a selector, to choose one of the resonance histories (or none), and it manages resonance insertion for the particle set.

The data that the event transform requires can be provided here. The resonance history set has already been assigned with the `dispatch` initializer. Here, we supply the set of subprocess instances that we have generated (see above). The master-process instance is set when we `connect` the transform by the standard method.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: connect_transform => &
    resonant_subprocess_set_connect_transform

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_connect_transform (prc_set, evt)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    class(evt_t), intent(in), target :: evt
  end subroutine resonant_subprocess_set_connect_transform

```

```

<Restricted subprocesses: procedures>+≡
module subroutine resonant_subprocess_set_connect_transform (prc_set, evt)
  class(resonant_subprocess_set_t), intent(inout) :: prc_set
  class(evt_t), intent(in), target :: evt
  select type (evt)
  type is (evt_resonance_t)
    prc_set%evt => evt
    call prc_set%evt%set_subprocess_instances (prc_set%instance)
  class default
    call msg_bug ("Resonant subprocess set: event transform has wrong type")
  end select
end subroutine resonant_subprocess_set_connect_transform

```

Set the on-shell limit value in the connected transform.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
procedure :: set_on_shell_limit => resonant_subprocess_set_on_shell_limit

```

```

<Restricted subprocesses: sub interfaces>+≡
module subroutine resonant_subprocess_set_on_shell_limit &
  (prc_set, on_shell_limit)
  class(resonant_subprocess_set_t), intent(inout) :: prc_set
  real(default), intent(in) :: on_shell_limit
end subroutine resonant_subprocess_set_on_shell_limit

```

```

<Restricted subprocesses: procedures>+≡
module subroutine resonant_subprocess_set_on_shell_limit &
  (prc_set, on_shell_limit)
  class(resonant_subprocess_set_t), intent(inout) :: prc_set
  real(default), intent(in) :: on_shell_limit
  call prc_set%evt%set_on_shell_limit (on_shell_limit)
end subroutine resonant_subprocess_set_on_shell_limit

```

Set the Gaussian turnoff parameter in the connected transform.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
procedure :: set_on_shell_turnoff => resonant_subprocess_set_on_shell_turnoff

```

```

<Restricted subprocesses: sub interfaces>+≡
module subroutine resonant_subprocess_set_on_shell_turnoff &
  (prc_set, on_shell_turnoff)
  class(resonant_subprocess_set_t), intent(inout) :: prc_set
  real(default), intent(in) :: on_shell_turnoff
end subroutine resonant_subprocess_set_on_shell_turnoff

```

```

<Restricted subprocesses: procedures>+≡
module subroutine resonant_subprocess_set_on_shell_turnoff &
  (prc_set, on_shell_turnoff)
  class(resonant_subprocess_set_t), intent(inout) :: prc_set
  real(default), intent(in) :: on_shell_turnoff
  call prc_set%evt%set_on_shell_turnoff (on_shell_turnoff)
end subroutine resonant_subprocess_set_on_shell_turnoff

```

Reweight (suppress) the background contribution probability, for the kinematics where a resonance history is active.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡

```

```

    procedure :: set_background_factor &
        => resonant_subprocess_set_background_factor
    <Restricted subprocesses: sub interfaces>+≡
        module subroutine resonant_subprocess_set_background_factor &
            (prc_set, background_factor)
            class(resonant_subprocess_set_t), intent(inout) :: prc_set
            real(default), intent(in) :: background_factor
            end subroutine resonant_subprocess_set_background_factor
    <Restricted subprocesses: procedures>+≡
        module subroutine resonant_subprocess_set_background_factor &
            (prc_set, background_factor)
            class(resonant_subprocess_set_t), intent(inout) :: prc_set
            real(default), intent(in) :: background_factor
            call prc_set%evt%set_background_factor (background_factor)
            end subroutine resonant_subprocess_set_background_factor

```

33.8.7 Wrappers for runtime calculations

All runtime calculations are delegated to the event transform. The following procedures are essentially redundant wrappers. We retain them for a unit test below.

Debugging aid:

```

    <Restricted subprocesses: resonant subprocess set: TBP>+≡
        procedure :: dump_instances => resonant_subprocess_set_dump_instances
    <Restricted subprocesses: sub interfaces>+≡
        module subroutine resonant_subprocess_set_dump_instances &
            (prc_set, unit, testflag)
            class(resonant_subprocess_set_t), intent(inout) :: prc_set
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: testflag
            end subroutine resonant_subprocess_set_dump_instances
    <Restricted subprocesses: procedures>+≡
        module subroutine resonant_subprocess_set_dump_instances &
            (prc_set, unit, testflag)
            class(resonant_subprocess_set_t), intent(inout) :: prc_set
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: testflag
            integer :: i, n, u
            u = given_output_unit (unit)
            write (u, "(A)")  "*** Process instances of resonant subprocesses"
            write (u, *)
            n = size (prc_set%subprocess)
            do i = 1, n
                associate (instance => prc_set%instance(i)%p)
                    call instance%write (u, testflag)
                    write (u, *)
                    write (u, *)
                end associate
            end do
            end subroutine resonant_subprocess_set_dump_instances

```

Inject the current kinematics configuration, reading from the previous event transform or from the process instance.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: fill_momenta => resonant_subprocess_set_fill_momenta

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_fill_momenta (prc_set)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
  end subroutine resonant_subprocess_set_fill_momenta

<Restricted subprocesses: procedures>+≡
  module subroutine resonant_subprocess_set_fill_momenta (prc_set)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer :: i, n
    call prc_set%evt%fill_momenta ()
  end subroutine resonant_subprocess_set_fill_momenta

```

Determine the indices of the resonance histories that can be considered on-shell for the current kinematics.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: determine_on_shell_histories &
    => resonant_subprocess_set_determine_on_shell_histories

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_determine_on_shell_histories &
    (prc_set, i_component, index_array)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    integer, intent(in) :: i_component
    integer, dimension(:), allocatable, intent(out) :: index_array
  end subroutine resonant_subprocess_set_determine_on_shell_histories

<Restricted subprocesses: procedures>+≡
  module subroutine resonant_subprocess_set_determine_on_shell_histories &
    (prc_set, i_component, index_array)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    integer, intent(in) :: i_component
    integer, dimension(:), allocatable, intent(out) :: index_array
    call prc_set%evt%determine_on_shell_histories (index_array)
  end subroutine resonant_subprocess_set_determine_on_shell_histories

```

Evaluate selected subprocesses. (In actual operation, the ones that have been tagged as on-shell.)

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: evaluate_subprocess &
    => resonant_subprocess_set_evaluate_subprocess

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_evaluate_subprocess &
    (prc_set, index_array)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer, dimension(:), intent(in) :: index_array
  end subroutine resonant_subprocess_set_evaluate_subprocess

```

```

<Restricted subprocesses: procedures>+≡
  module subroutine resonant_subprocess_set_evaluate_subprocess &
    (prc_set, index_array)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer, dimension(:), intent(in) :: index_array
    call prc_set%evt%evaluate_subprocess (index_array)
  end subroutine resonant_subprocess_set_evaluate_subprocess

```

Extract the matrix elements of the master process / the resonant subprocesses.
After the previous routine has been executed, they should be available and stored in the corresponding process instances.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: get_master_sqme &
    => resonant_subprocess_set_get_master_sqme
  procedure :: get_subprocess_sqme &
    => resonant_subprocess_set_get_subprocess_sqme

```

```

<Restricted subprocesses: sub interfaces>+≡
  module function resonant_subprocess_set_get_master_sqme &
    (prc_set) result (sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default) :: sqme
  end function resonant_subprocess_set_get_master_sqme
  module subroutine resonant_subprocess_set_get_subprocess_sqme &
    (prc_set, sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default), dimension(:), intent(inout) :: sqme
  end subroutine resonant_subprocess_set_get_subprocess_sqme

```

```

<Restricted subprocesses: procedures>+≡
  module function resonant_subprocess_set_get_master_sqme &
    (prc_set) result (sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default) :: sqme
    sqme = prc_set%evt%get_master_sqme ()
  end function resonant_subprocess_set_get_master_sqme

  module subroutine resonant_subprocess_set_get_subprocess_sqme (prc_set, sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default), dimension(:), intent(inout) :: sqme
    integer :: i
    call prc_set%evt%get_subprocess_sqme (sqme)
  end subroutine resonant_subprocess_set_get_subprocess_sqme

```

We use the calculations of resonant matrix elements to determine probabilities for all resonance configurations.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: compute_probabilities &
    => resonant_subprocess_set_compute_probabilities

<Restricted subprocesses: sub interfaces>+≡
  module subroutine resonant_subprocess_set_compute_probabilities &
    (prc_set, prob_array)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set

```

```

        real(default), dimension(:), allocatable, intent(out) :: prob_array
    end subroutine resonant_subprocess_set_compute_probabilities
<Restricted subprocesses: procedures>+≡
    module subroutine resonant_subprocess_set_compute_probabilities &
        (prc_set, prob_array)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        real(default), dimension(:), allocatable, intent(out) :: prob_array
        integer, dimension(:), allocatable :: index_array
        real(default) :: sqme, sqme_sum, sqme_bg
        real(default), dimension(:), allocatable :: sqme_res
        integer :: n
        n = size (prc_set%subprocess)
        allocate (prob_array (0:n), source = 0._default)
        call prc_set%evt%compute_probabilities ()
        call prc_set%evt%get_selector_weights (prob_array)
    end subroutine resonant_subprocess_set_compute_probabilities

```

33.8.8 Unit tests

Test module, followed by the stand-alone unit-test procedures.

```

<restricted_subprocesses_ut.f90>≡
    <File header>

    module restricted_subprocesses_ut
        use unit_tests
        use restricted_subprocesses_uti

    <Standard module head>

    <Restricted subprocesses: public test>

    contains

    <Restricted subprocesses: test driver>

    end module restricted_subprocesses_ut
<restricted_subprocesses_uti.f90>≡
    <File header>

    module restricted_subprocesses_uti

    <Use kinds>
    <Use strings>
        use io_units, only: free_unit
        use format_defs, only: FMT_10, FMT_12
        use lorentz, only: vector4_t, vector3_moving, vector4_moving
        use particle_specifiers, only: new_prt_spec
        use process_libraries, only: process_library_t
        use resonances, only: resonance_info_t
        use resonances, only: resonance_history_t
        use resonances, only: resonance_history_set_t

```



```

use state_matrices, only: FM_IGNORE_HELICITY
use particles, only: particle_set_t
use model_data, only: model_data_t
use models, only: syntax_model_file_init, syntax_model_file_final
use models, only: model_t
use rng_base_ut, only: rng_test_factory_t
use mci_base, only: mci_t
use phs_base, only: phs_config_t
use phs_forests, only: syntax_phs_forest_init, syntax_phs_forest_final
use phs_wood, only: phs_wood_config_t
use process_libraries, only: process_def_entry_t
use process_libraries, only: process_component_def_t
use prclib_stacks, only: prclib_entry_t
use prc_core_def, only: prc_core_def_t
use prc_omega, only: omega_def_t
use process, only: process_t
use instances, only: process_instance_t
use process_stacks, only: process_entry_t
use event_transforms, only: evt_trivial_t
use resonance_insertion, only: evt_resonance_t
use integrations, only: integrate_process
use rt_data, only: rt_data_t

```

```

use restricted_subprocesses

```

⟨Standard module head⟩

⟨Restricted subprocesses: test declarations⟩

⟨Restricted subprocesses: test auxiliary types⟩

⟨Restricted subprocesses: public test auxiliary⟩

contains

⟨Restricted subprocesses: tests⟩

⟨Restricted subprocesses: test auxiliary⟩

end module restricted_subprocesses_util

API: driver for the unit tests below.

⟨Restricted subprocesses: public test⟩≡

```

public :: restricted_subprocesses_test

```

⟨Restricted subprocesses: test driver⟩≡

```

subroutine restricted_subprocesses_test (u, results)

```

```

    integer, intent(in) :: u

```

```

    type(test_results_t), intent(inout) :: results

```

⟨Restricted subprocesses: execute tests⟩

```

end subroutine restricted_subprocesses_test

```

subprocess configuration

Initialize a `restricted_subprocess_configuration_t` object which represents a given process with a defined resonance history.

```
(Restricted subprocesses: execute tests)≡
    call test (restricted_subprocesses_1, "restricted_subprocesses_1", &
              "single subprocess", &
              u, results)

(Restricted subprocesses: test declarations)≡
    public :: restricted_subprocesses_1

(Restricted subprocesses: tests)≡
    subroutine restricted_subprocesses_1 (u)
        integer, intent(in) :: u
        type(rt_data_t) :: global
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(string_t) :: prc_name
        type(string_t), dimension(2) :: prt_in
        type(string_t), dimension(3) :: prt_out
        type(restricted_process_configuration_t) :: prc_config

        write (u, "(A)")  "* Test output: restricted_subprocesses_1"
        write (u, "(A)")  "* Purpose: create subprocess list from resonances"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
                           .false., is_known = .true.)
        call global%select_model (var_str ("SM"))

        write (u, "(A)")  "* Create resonance history"
        write (u, "(A)")

        call res_info%init (3, -24, global%model, 5)
        call res_history%add_resonance (res_info)
        call res_history%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Create process configuration"
        write (u, "(A)")

        prc_name = "restricted_subprocesses_1_p"
        prt_in(1) = "e-"
        prt_in(2) = "e+"
        prt_out(1) = "d"
        prt_out(2) = "u"
        prt_out(3) = "W+"

        call prc_config%init_resonant_process (prc_name, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        res_history, global%model, global%var_list)
```

```

call prc_config%write (u)

write (u, *)
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_1"

end subroutine restricted_subprocesses_1

```

Subprocess library configuration

Create a process library that represents restricted subprocesses for a given set of resonance histories

```

<Restricted subprocesses: execute tests>+≡
  call test (restricted_subprocesses_2, "restricted_subprocesses_2", &
    "subprocess library", &
    u, results)

<Restricted subprocesses: test declarations>+≡
  public :: restricted_subprocesses_2

<Restricted subprocesses: tests>+≡
  subroutine restricted_subprocesses_2 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global
    type(resonance_info_t) :: res_info
    type(resonance_history_t), dimension(2) :: res_history
    type(resonance_history_set_t) :: res_history_set
    type(string_t) :: libname
    type(string_t), dimension(2) :: prt_in
    type(string_t), dimension(3) :: prt_out
    type(resonant_subprocess_set_t) :: prc_set
    type(process_library_t), pointer :: lib
    logical :: exist

    write (u, "(A)")  "* Test output: restricted_subprocesses_2"
    write (u, "(A)")  "* Purpose: create subprocess library from resonances"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%select_model (var_str ("SM"))

    write (u, "(A)")  "* Create resonance histories"
    write (u, "(A)")

```

```

call res_info%init (3, -24, global%model, 5)
call res_history(1)%add_resonance (res_info)
call res_history(1)%write (u)

call res_info%init (7, 23, global%model, 5)
call res_history(2)%add_resonance (res_info)
call res_history(2)%write (u)

call res_history_set%init ()
call res_history_set%enter (res_history(1))
call res_history_set%enter (res_history(2))
call res_history_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "* Empty restricted subprocess set"
write (u, "(A)")

write (u, "(A,1x,L1)")  "active =", prc_set%is_active ()
write (u, "(A)")

call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill restricted subprocess set"
write (u, "(A)")

libname = "restricted_subprocesses_2_p_R"
prt_in(1) = "e-"
prt_in(2) = "e+"
prt_out(1) = "d"
prt_out(2) = "u"
prt_out(3) = "W+"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set, 1)
call prc_set%create_library (libname, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global)
end if
call prc_set%freeze_library (global)

write (u, "(A,1x,L1)")  "active =", prc_set%is_active ()
write (u, "(A)")

call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Queries"
write (u, "(A)")

write (u, "(A,1x,I0)")  "n_process =", prc_set%get_n_process ()

```

```

write (u, "(A)")
write (u, "(A,A,A)") "libname = '", char (prc_set%get_libname ()), "'"
write (u, "(A)")
write (u, "(A,A,A)") "proc_id(1) = '", char (prc_set%get_proc_id (1)), "'"
write (u, "(A,A,A)") "proc_id(2) = '", char (prc_set%get_proc_id (2)), "'"

write (u, "(A)")
write (u, "(A)")  "* Process library"
write (u, "(A)")

call prc_set%compile_library (global)

lib => global%prclib_stack%get_library_ptr (libname)
if (associated (lib)) call lib%write (u, libpath=.false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_2"

end subroutine restricted_subprocesses_2

```

Auxiliary: Test processes

Auxiliary subroutine that constructs the process library for the above test. This parallels a similar subroutine in `processes_util`, but this time we want an O'MEGA process.

```

<Restricted subprocesses: public test auxiliary>≡
  public :: prepare_resonance_test_library

<Restricted subprocesses: test auxiliary>≡
  subroutine prepare_resonance_test_library &
    (lib, libname, procname, model, global, u)
    type(process_library_t), target, intent(out) :: lib
    type(string_t), intent(in) :: libname
    type(string_t), intent(in) :: procname
    class(model_data_t), intent(in), pointer :: model
    type(rt_data_t), intent(in), target :: global
    integer, intent(in) :: u
    type(string_t), dimension(:), allocatable :: prt_in, prt_out
    class(prc_core_def_t), allocatable :: def
    type(process_def_entry_t), pointer :: entry

    call lib%init (libname)

    allocate (prt_in (2), prt_out (3))
    prt_in = [var_str ("e+"), var_str ("e-")]
    prt_out = [var_str ("d"), var_str ("ubar"), var_str ("W+")]

```

```

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model%get_name (), prt_in, prt_out, &
        ovm=.false., ufo=.false.)
end select
allocate (entry)
call entry%init (procname, &
    model_name = model%get_name (), &
    n_in = 2, n_components = 1, &
    requires_resonances = .true.)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call entry%write (u)

call lib%append (entry)

call lib%configure (global%os_data)
call lib%write_makefile (global%os_data, force = .true., verbose = .false.)
call lib%clean (global%os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (global%os_data)

end subroutine prepare_resonance_test_library

```

Kinematics and resonance selection

Prepare an actual process with resonant subprocesses. Insert kinematics and apply the resonance selector in an associated event transform.

```

<Restricted subprocesses: execute tests>+≡
    call test (restricted_subprocesses_3, "restricted_subprocesses_3", &
        "resonance kinematics and probability", &
        u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_3

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_3 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist

```

```

type(process_t), pointer :: process
type(process_instance_t), target :: process_instance
type(resonance_history_set_t), dimension(1) :: res_history_set
type(resonant_subprocess_set_t) :: prc_set
type(particle_set_t) :: pset
real(default) :: sqrts, mw, pp
real(default), dimension(3) :: p3
type(vector4_t), dimension(:), allocatable :: p
real(default), dimension(:), allocatable :: m
integer, dimension(:), allocatable :: pdg
real(default), dimension(:), allocatable :: sqme
logical, dimension(:), allocatable :: mask
real(default) :: on_shell_limit
integer, dimension(:), allocatable :: i_array
real(default), dimension(:), allocatable :: prob_array
type(evt_resonance_t), target :: evt_resonance
integer :: i, u_dump

write (u, "(A)")  "* Test output: restricted_subprocesses_3"
write (u, "(A)")  "* Purpose: handle process and resonance kinematics"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_3_lib"
libname_res = "restricted_subprocesses_3_lib_res"
procname = "restricted_subprocesses_3_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

```

```

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
    local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call process%extract_resonance_history_set &
    (res_history_set(1), include_trivial=.true., i_component=1)
call res_history_set(1)%write (u)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"
write (u, "(A)")

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        process_component_def%get_prt_spec_in (), &
        process_component_def%get_prt_spec_out (), &
        global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)
call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2, -sqrts/2, 3)
m(2) = 0
pdg(3) = 1

```



```

p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)
call pset%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill process instance"

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
    (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonant subprocesses"

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%connect (process_instance, model)

call prc_set%fill_momenta ()

write (u, "(A)")
write (u, "(A)")  "* Show squared matrix element of master process,"
write (u, "(A)")  "  should coincide with 2nd subprocess sqme"
write (u, "(A)")

write (u, "(1x,I0,1x," // FMT_12 // ")")  0, prc_set%get_master_sqme ()

write (u, "(A)")
write (u, "(A)")  "* Compute squared matrix elements &
    &of selected resonant subprocesses [1,2]"
write (u, "(A)")

call prc_set%evaluate_subprocess ([1,2])

```

```

allocate (sqme (3), source = 0._default)
call prc_set%get_subprocess_sqme (sqme)
do i = 1, size (sqme)
    write (u, "(1x,I0,1x," // FMT_12 // ")") i, sqme(i)
end do
deallocate (sqme)

write (u, "(A)")
write (u, "(A)")  "* Compute squared matrix elements &
    &of all resonant subprocesses"
write (u, "(A)")

call prc_set%evaluate_subprocess ([1,2,3])

allocate (sqme (3), source = 0._default)
call prc_set%get_subprocess_sqme (sqme)
do i = 1, size (sqme)
    write (u, "(1x,I0,1x," // FMT_12 // ")") i, sqme(i)
end do
deallocate (sqme)

write (u, "(A)")
write (u, "(A)")  "* Write process instances to file &
    &restricted_subprocesses_3_lib_res.dat"

u_dump = free_unit ()
open (unit = u_dump, file = "restricted_subprocesses_3_lib_res.dat", &
    action = "write", status = "replace")
call prc_set%dump_instances (u_dump)
close (u_dump)

write (u, "(A)")
write (u, "(A)")  "* Determine on-shell resonant subprocesses"
write (u, "(A)")

on_shell_limit = 0
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 0.1_default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 10000._default

```

```

write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")  " (The first number is the probability for background)"
write (u, "(A)")

on_shell_limit = 0
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
call prc_set%write (u, testflag=.true.)
write (u, *)

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
call prc_set%write (u, testflag=.true.)
write (u, *)

on_shell_limit = 10000._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
write (u, *)
call prc_set%write (u, testflag=.true.)
write (u, *)

write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_3"

end subroutine restricted_subprocesses_3

```

Event transform

Prepare an actual process with resonant subprocesses. Prepare the resonance selector for a fixed event and apply the resonance-insertion event transform.

```
(Restricted subprocesses: execute tests)+≡
    call test (restricted_subprocesses_4, "restricted_subprocesses_4", &
               "event transform", &
               u, results)

(Restricted subprocesses: test declarations)+≡
    public :: restricted_subprocesses_4

(Restricted subprocesses: tests)+≡
    subroutine restricted_subprocesses_4 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist
        type(process_t), pointer :: process
        type(process_instance_t), target :: process_instance
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(resonant_subprocess_set_t) :: prc_set
        type(particle_set_t) :: pset
        real(default) :: sqrts, mw, pp
        real(default), dimension(3) :: p3
        type(vector4_t), dimension(:), allocatable :: p
        real(default), dimension(:), allocatable :: m
        integer, dimension(:), allocatable :: pdg
        real(default) :: on_shell_limit
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: restricted_subprocesses_4"
        write (u, "(A)")  "*   Purpose: employ event transform"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        call global%global_init ()
        call global%append_log (&
                                var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
        call global%set_log (var_str ("?omega_openmp"), &
                             .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
                             0, is_known = .true.)
        call global%set_real (var_str ("sqrts"),&
```

```

        1000._default, is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_4_lib"
libname_res = "restricted_subprocesses_4_lib_res"
procname = "restricted_subprocesses_4_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
    local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
    (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        process_component_def%get_prt_spec_in (), &
        process_component_def%get_prt_spec_out (), &
        global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

```

```

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
(1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"
write (u, "(A)")

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)

```

```

call evt_trivial%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  "  and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_4"

end subroutine restricted_subprocesses_4

```

Gaussian turnoff

Identical to the previous process, except that we apply a Gaussian turnoff to the resonance kinematics, which affects the subprocess selector.

```

(Restricted subprocesses: execute tests)+≡
  call test (restricted_subprocesses_5, "restricted_subprocesses_5", &

```

```

        "event transform with gaussian turnoff", &
        u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_5

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_5 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist
        type(process_t), pointer :: process
        type(process_instance_t), target :: process_instance
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(resonant_subprocess_set_t) :: prc_set
        type(particle_set_t) :: pset
        real(default) :: sqrts, mw, pp
        real(default), dimension(3) :: p3
        type(vector4_t), dimension(:), allocatable :: p
        real(default), dimension(:), allocatable :: m
        integer, dimension(:), allocatable :: pdg
        real(default) :: on_shell_limit
        real(default) :: on_shell_turnoff
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: restricted_subprocesses_5"
        write (u, "(A)")  "* Purpose: employ event transform &
            &with gaussian turnoff"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        call global%global_init ()
        call global%append_log (&
            var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
            0, is_known = .true.)
        call global%set_real (var_str ("sqrts"), &
            1000._default, is_known = .true.)
        call global%set_log (var_str ("?resonance_history"), &
            .true., is_known = .true.)

```



```

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_5_lib"
libname_res = "restricted_subprocesses_5_lib_res"
procname = "restricted_subprocesses_5_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
      (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
      local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
      (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
  call prc_set%add_to_library (1, &
    process_component_def%get_prt_spec_in (), &
    process_component_def%get_prt_spec_out (), &
    global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

```

```

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
    (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"
write (u, "(A)")

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"

```

```

write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit  =", &
    on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

on_shell_turnoff = 1._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_turnoff =", &
    on_shell_turnoff
call evt_resonance%set_on_shell_turnoff (on_shell_turnoff)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_5"

end subroutine restricted_subprocesses_5

```

Event transform

The same process and event again. This time, switch off the background contribution, so the selector becomes trivial.

```

<Restricted subprocesses: execute tests>+≡
    call test (restricted_subprocesses_6, "restricted_subprocesses_6", &
        "event transform with background switched off", &
        u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_6

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_6 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist
        type(process_t), pointer :: process
        type(process_instance_t), target :: process_instance
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(resonant_subprocess_set_t) :: prc_set
        type(particle_set_t) :: pset
        real(default) :: sqrts, mw, pp
        real(default), dimension(3) :: p3
        type(vector4_t), dimension(:), allocatable :: p
        real(default), dimension(:), allocatable :: m
        integer, dimension(:), allocatable :: pdg
        real(default) :: on_shell_limit
        real(default) :: background_factor
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: restricted_subprocesses_6"
        write (u, "(A)")  "*   Purpose: employ event transform &
            &with background switched off"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        call global%global_init ()
        call global%append_log (&
            var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
            0, is_known = .true.)
        call global%set_real (var_str ("sqrts"), &
            1000._default, is_known = .true.)
        call global%set_log (var_str ("?resonance_history"), &

```

```

        .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_6_lib"
libname_res = "restricted_subprocesses_6_lib_res"
procname = "restricted_subprocesses_6_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
      (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
      local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
      (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        process_component_def%get_prt_spec_in (), &
        process_component_def%get_prt_spec_out (), &
        global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

write (u, "(A)")

```

```

write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default    ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
    (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"
write (u, "(A)")

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") &
    "on_shell_limit    =", on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

background_factor = 0
write (u, "(1x,A,1x," // FMT_10 // ")") &
    "background_factor =", background_factor
call evt_resonance%set_background_factor (background_factor)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_6"

end subroutine restricted_subprocesses_6

```

33.9 Simulation

This module manages simulation: event generation and reading/writing of event files. The `simulation` object is intended to be used (via a pointer) outside of WHIZARD, if events are generated individually by an external driver.

```
<simulations.f90>≡
  <File header>

  module simulations

    <Use mpi f08>
    <Use kinds>
    <Use strings>
    use sm_qcd
    use model_data
    use particles
    use rng_base
    use selectors
    use process_libraries, only: process_library_t
    use process_libraries, only: process_component_def_t
    use prc_core
    use process
    use event_base
    use event_handles, only: event_handle_t
    use events
    use event_transforms
    use eio_data
    use eio_base
    use rt_data

    use event_streams
    use restricted_subprocesses, only: resonant_subprocess_set_t
    use restricted_subprocesses, only: get_libname_res

    <Standard module head>

    <Simulations: public>

    <Simulations: types>

    <Simulations: interfaces>

    interface
    <Simulations: sub interfaces>
    end interface

  end module simulations

<simulations_sub.f90>≡
  <File header>

  submodule (simulations) simulations_s
```



```

<Use mpi f08>
<Use debug>
  use io_units
  use format_utils, only: write_separator
  use format_defs, only: FMT_15, FMT_19
  use numeric_utils
  use string_utils, only: str
  use diagnostics
  use os_interface
  use md5
  use variables, only: var_list_t
  use eval_trees
  use flavors
  use state_matrices, only: FM_IGNORE_HELICITY
  use beam_structures, only: beam_structure_t
  use beams
  use rng_stream, only: rng_stream_t
  use resonances, only: resonance_history_set_t
  ! TODO: (bcn 2016-09-13) should be ideally only pcm_base
  use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t
  ! TODO: (bcn 2016-09-13) details of process config should not be necessary here
  use process_config, only: COMP_REAL_FIN, COMP_MASTER, COMP_REAL, &
    COMP_REAL_SING
  use instances
  use shower
  use evt_nlo

  use dispatch_beams, only: dispatch_qcd
  use dispatch_rng, only: dispatch_rng_factory
  use dispatch_rng, only: update_rng_seed_in_var_list
  use dispatch_me_methods, only: dispatch_core_update, dispatch_core_restore
  use dispatch_transforms, only: dispatch_evt_isr_epa_handler
  use dispatch_transforms, only: dispatch_evt_resonance
  use dispatch_transforms, only: dispatch_evt_decay
  use dispatch_transforms, only: dispatch_evt_shower
  use dispatch_transforms, only: dispatch_evt_hadrons
  use dispatch_transforms, only: dispatch_evt_nlo

  use integrations

  implicit none

contains

<Simulations: procedures>

end submodule simulations_s

```

33.9.1 Event counting

In this object we collect statistical information about an event sample or sub-sample.

```

<Simulations: types>≡
type :: counter_t
  integer :: total = 0
  integer :: generated = 0
  integer :: read = 0
  integer :: positive = 0
  integer :: negative = 0
  integer :: zero = 0
  integer :: excess = 0
  integer :: dropped = 0
  real(default) :: max_excess = 0
  real(default) :: sum_excess = 0
  logical :: reproduce_xsection = .false.
  real(default) :: mean = 0
  real(default) :: varsq = 0
  integer :: nlo_weight_counter = 0
contains
  <Simulations: counter: TBP>
end type counter_t

```

Output.

```

<Simulations: counter: TBP>≡
  procedure :: write => counter_write

<Simulations: sub interfaces>≡
  module subroutine counter_write (counter, unit)
    class(counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
  end subroutine counter_write

<Simulations: procedures>≡
  module subroutine counter_write (counter, unit)
    class(counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
1   format (3x,A,I0)
2   format (5x,A,I0)
3   format (5x,A,ES19.12)
    write (u, 1) "Events total      = ", counter%total
    write (u, 2) "generated        = ", counter%generated
    write (u, 2) "read              = ", counter%read
    write (u, 2) "positive weight = ", counter%positive
    write (u, 2) "negative weight = ", counter%negative
    write (u, 2) "zero weight      = ", counter%zero
    write (u, 2) "excess weight   = ", counter%excess
    if (counter%excess /= 0) then
      write (u, 3) "max excess      = ", counter%max_excess
      write (u, 3) "avg excess      = ", counter%sum_excess / counter%total
    end if
    write (u, 1) "Events dropped    = ", counter%dropped
  end subroutine counter_write

```

This is a screen message: if there was an excess, display statistics.

```

<Simulations: counter: TBP>+≡
  procedure :: show_excess => counter_show_excess

<Simulations: sub interfaces>+≡
  module subroutine counter_show_excess (counter)
    class(counter_t), intent(in) :: counter
    end subroutine counter_show_excess

<Simulations: procedures>+≡
  module subroutine counter_show_excess (counter)
    class(counter_t), intent(in) :: counter
    if (counter%excess > 0) then
      write (msg_buffer, "(A,1x,I0,1x,A,1x,'(,F7.3,' %)'") &
        "Encountered events with excess weight:", counter%excess, &
        "events", 100 * counter%excess / real (counter%total)
      call msg_warning ()
      write (msg_buffer, "(A,ES10.3)") &
        "Maximum excess weight =", counter%max_excess
      call msg_message ()
      write (msg_buffer, "(A,ES10.3)") &
        "Average excess weight =", counter%sum_excess / counter%total
      call msg_message ()
    end if
  end subroutine counter_show_excess

```

If events have been dropped during simulation of weighted events, issue a message here. If a fraction `n_dropped / n_total` of the events fail the cuts, we keep generating new ones until we have `n_total` events with `weight > 0`. Thus, the total sum of weights will be a fraction of `n_dropped / n_total` too large. However, we do not know how many events will pass or fail the cuts prior to generating them so we leave it to the user to correct for this factor.

```

<Simulations: counter: TBP>+≡
  procedure :: show_dropped => counter_show_dropped

<Simulations: sub interfaces>+≡
  module subroutine counter_show_dropped (counter)
    class(counter_t), intent(in) :: counter
    end subroutine counter_show_dropped

<Simulations: procedures>+≡
  module subroutine counter_show_dropped (counter)
    class(counter_t), intent(in) :: counter
    if (counter%dropped > 0) then
      write (msg_buffer, "(A,1x,I0,1x,'(,A,1x,I0,')'") &
        "Dropped events (weight zero) =", &
        counter%dropped, "total", counter%dropped + counter%total
      call msg_message ()
      write (msg_buffer, "(A,ES15.8)") &
        "All event weights must be rescaled by f =", &
        real (counter%total, default) &
        / real (counter%dropped + counter%total, default)
      call msg_warning ()
    end if
  end subroutine counter_show_dropped

```

```

<Simulations: counter: TBP>+≡
  procedure :: show_mean_and_variance => counter_show_mean_and_variance

<Simulations: sub interfaces>+≡
  module subroutine counter_show_mean_and_variance (counter)
    class(counter_t), intent(in) :: counter
  end subroutine counter_show_mean_and_variance

<Simulations: procedures>+≡
  module subroutine counter_show_mean_and_variance (counter)
    class(counter_t), intent(in) :: counter
    if (counter%reproduce_xsection .and. counter%nlo_weight_counter > 1) then
      print *, "Reconstructed cross-section from event weights: "
      print *, counter%mean, '+-', &
        sqrt (counter%varsq / (counter%nlo_weight_counter - 1))
    end if
  end subroutine counter_show_mean_and_variance

```

Count an event. The weight and event source are optional; by default we assume that the event has been generated and has positive weight.

The optional integer `n_dropped` counts weighted events with weight zero that were encountered while generating the current event, but dropped (because of their zero weight). Accumulating this number allows for renormalizing event weight sums in histograms, after the generation step has been completed.

```

<Simulations: counter: TBP>+≡
  procedure :: record => counter_record

<Simulations: sub interfaces>+≡
  module subroutine counter_record &
    (counter, weight, excess, n_dropped, from_file)
    class(counter_t), intent(inout) :: counter
    real(default), intent(in), optional :: weight, excess
    integer, intent(in), optional :: n_dropped
    logical, intent(in), optional :: from_file
  end subroutine counter_record

<Simulations: procedures>+≡
  module subroutine counter_record &
    (counter, weight, excess, n_dropped, from_file)
    class(counter_t), intent(inout) :: counter
    real(default), intent(in), optional :: weight, excess
    integer, intent(in), optional :: n_dropped
    logical, intent(in), optional :: from_file
    counter%total = counter%total + 1
    if (present (from_file)) then
      if (from_file) then
        counter%read = counter%read + 1
      else
        counter%generated = counter%generated + 1
      end if
    else
      counter%generated = counter%generated + 1
    end if
    if (present (weight)) then
      if (weight > 0) then

```

```

        counter%positive = counter%positive + 1
    else if (weight < 0) then
        counter%negative = counter%negative + 1
    else
        counter%zero = counter%zero + 1
    end if
else
    counter%positive = counter%positive + 1
end if
if (present (excess)) then
    if (excess > 0) then
        counter%excess = counter%excess + 1
        counter%max_excess = max (counter%max_excess, excess)
        counter%sum_excess = counter%sum_excess + excess
    end if
end if
if (present (n_dropped)) then
    counter%dropped = counter%dropped + n_dropped
end if
end subroutine counter_record

```

<MPI: Simulations: counter: TBP>≡

```

    procedure :: allreduce_record => counter_allreduce_record

```

<MPI: Simulations: sub interfaces>≡

```

    module subroutine counter_allreduce_record (counter)
        class(counter_t), intent(inout) :: counter
    end subroutine counter_allreduce_record

```

<MPI: Simulations: procedures>≡

```

    module subroutine counter_allreduce_record (counter)
        class(counter_t), intent(inout) :: counter
        integer :: read, generated
        integer :: positive, negative, zero, excess, dropped
        real(default) :: max_excess, sum_excess
        read = counter%read
        generated = counter%generated
        positive = counter%positive
        negative = counter%negative
        zero = counter%zero
        excess = counter%excess
        max_excess = counter%max_excess
        sum_excess = counter%sum_excess
        dropped = counter%dropped
        call MPI_ALLREDUCE (read, counter%read, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (generated, counter%generated, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (positive, counter%positive, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (negative, counter%negative, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (zero, counter%zero, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (excess, counter%excess, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (max_excess, counter%max_excess, 1, MPI_DOUBLE_PRECISION, MPI_MAX, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (sum_excess, counter%sum_excess, 1, MPI_DOUBLE_PRECISION, MPI_SUM, MPI_COMM_WORLD)
        call MPI_ALLREDUCE (dropped, counter%dropped, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
        !! \todo{sbrass - Implement allreduce of mean and variance, relevant for weighted events.}
    end subroutine counter_allreduce_record

```

```

<Simulations: counter: TBP>+≡
    procedure :: record_mean_and_variance => &
        counter_record_mean_and_variance

<Simulations: sub interfaces>+≡
    module subroutine counter_record_mean_and_variance (counter, weight, i_nlo)
        class(counter_t), intent(inout) :: counter
        real(default), intent(in) :: weight
        integer, intent(in) :: i_nlo
    end subroutine counter_record_mean_and_variance

<Simulations: procedures>+≡
    module subroutine counter_record_mean_and_variance (counter, weight, i_nlo)
        class(counter_t), intent(inout) :: counter
        real(default), intent(in) :: weight
        integer, intent(in) :: i_nlo
        real(default), save :: weight_buffer = 0._default
        integer, save :: nlo_count = 1
        if (.not. counter%reproduce_xsection) return
        if (i_nlo == 1) then
            call flush_weight_buffer (weight_buffer, nlo_count)
            weight_buffer = weight
            nlo_count = 1
        else
            weight_buffer = weight_buffer + weight
            nlo_count = nlo_count + 1
        end if
    contains
        subroutine flush_weight_buffer (w, n_nlo)
            real(default), intent(in) :: w
            integer, intent(in) :: n_nlo
            integer :: n
            real(default) :: mean_new
            counter%nlo_weight_counter = counter%nlo_weight_counter + 1
            !!! Minus 1 to take into account offset from initialization
            n = counter%nlo_weight_counter - 1
            if (n > 0) then
                mean_new = counter%mean + (w / n_nlo - counter%mean) / n
                if (n > 1) &
                    counter%varsq = counter%varsq - counter%varsq / (n - 1) + &
                        n * (mean_new - counter%mean)**2
                counter%mean = mean_new
            end if
        end subroutine flush_weight_buffer
    end subroutine counter_record_mean_and_variance

```

33.9.2 Simulation: component sets

For each set of process components that share a MCI entry in the process configuration, we keep a separate event record.

```

<Simulations: types>+≡
    type :: mci_set_t

```

```

private
integer :: n_components = 0
integer, dimension(:), allocatable :: i_component
type(string_t), dimension(:), allocatable :: component_id
logical :: has_integral = .false.
real(default) :: integral = 0
real(default) :: error = 0
real(default) :: weight_mci = 0
type(counter_t) :: counter
contains
<Simulations: mci set: TBP>
end type mci_set_t

```

Output.

```

<Simulations: mci set: TBP>≡
procedure :: write => mci_set_write

<Simulations: sub interfaces>+≡
module subroutine mci_set_write (object, unit, pacified)
class(mci_set_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: pacified
end subroutine mci_set_write

<Simulations: procedures>+≡
module subroutine mci_set_write (object, unit, pacified)
class(mci_set_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: pacified
logical :: pacify
integer :: u, i
u = given_output_unit (unit)
pacify = .false.; if (present (pacified)) pacify = pacified
write (u, "(3x,A)") "Components:"
do i = 1, object%n_components
write (u, "(5x,I0,A,A,A)") object%i_component(i), &
": ", char (object%component_id(i)), ""
end do
if (object%has_integral) then
if (pacify) then
write (u, "(3x,A," // FMT_15 // ")") "Integral = ", object%integral
write (u, "(3x,A," // FMT_15 // ")") "Error = ", object%error
write (u, "(3x,A,F9.6)") "Weight = ", object%weight_mci
else
write (u, "(3x,A," // FMT_19 // ")") "Integral = ", object%integral
write (u, "(3x,A," // FMT_19 // ")") "Error = ", object%error
write (u, "(3x,A,F13.10)") "Weight = ", object%weight_mci
end if
else
write (u, "(3x,A)") "Integral = [undefined]"
end if
call object%counter%write (u)
end subroutine mci_set_write

```

Initialize: Get the indices and names for the process components that will contribute to this set.

```

<Simulations: mci set: TBP>+=
  procedure :: init => mci_set_init

<Simulations: sub interfaces>+=
  module subroutine mci_set_init (object, i_mci, process)
    class(mci_set_t), intent(out) :: object
    integer, intent(in) :: i_mci
    type(process_t), intent(in), target :: process
  end subroutine mci_set_init

<Simulations: procedures>+=
  module subroutine mci_set_init (object, i_mci, process)
    class(mci_set_t), intent(out) :: object
    integer, intent(in) :: i_mci
    type(process_t), intent(in), target :: process
    integer :: i
    call process%get_i_component (i_mci, object%i_component)
    object%n_components = size (object%i_component)
    allocate (object%component_id (object%n_components))
    do i = 1, size (object%component_id)
      object%component_id(i) = &
        process%get_component_id (object%i_component(i))
    end do
    if (process%has_integral (i_mci)) then
      object%integral = process%get_integral (i_mci)
      object%error = process%get_error (i_mci)
      object%has_integral = .true.
    end if
  end subroutine mci_set_init

```

33.9.3 Process-core Safe

This is an object that temporarily holds a process core object. We need this while rescanning a process with modified parameters. After the rescan, we want to restore the original state.

```

<Simulations: types>+=
  type :: core_safe_t
    class(prc_core_t), allocatable :: core
  end type core_safe_t

```

33.9.4 Process Object

The simulation works on process objects. This subroutine makes a process object available for simulation. The process is in the process stack. `use_process` implies that the process should already exist as an object in the process stack. If integration is not yet done, do it. Any generated process object should be put on the global stack, if it is separate from the local one.

```

<Simulations: procedures>+=
  subroutine prepare_process &

```



```

        (process, process_id, use_process, integrate, local, global)
type(process_t), pointer, intent(out) :: process
type(string_t), intent(in) :: process_id
logical, intent(in) :: use_process, integrate
type(rt_data_t), intent(inout), target :: local
type(rt_data_t), intent(inout), optional, target :: global
type(rt_data_t), pointer :: current
if (debug_on) call msg_debug (D_CORE, "prepare_process")
if (debug_on) call msg_debug (D_CORE, "global present", present (global))
if (present (global)) then
    current => global
else
    current => local
end if
process => current%process_stack%get_process_ptr (process_id)
if (debug_on) call msg_debug (D_CORE, "use_process", use_process)
if (debug_on) call msg_debug (D_CORE, "associated process", associated (process))
if (use_process .and. .not. associated (process)) then
    if (integrate) then
        call msg_message ("Simulate: process '" &
            // char (process_id) // "' needs integration")
    else
        call msg_message ("Simulate: process '" &
            // char (process_id) // "' needs initialization")
    end if
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .not. integrate)
    else
        call integrate_process (process_id, local, &
            local_stack = .true., init_only = .not. integrate)
    end if
    if (signal_is_pending ()) return
    process => current%process_stack%get_process_ptr (process_id)
    if (associated (process)) then
        if (integrate) then
            call msg_message ("Simulate: integration done")
            call current%process_stack%fill_result_vars (process_id)
        else
            call msg_message ("Simulate: process initialization done")
        end if
    else
        call msg_fatal ("Simulate: process '" &
            // char (process_id) // "' could not be initialized: aborting")
    end if
else if (.not. associated (process)) then
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .true.)
    else
        call integrate_process (process_id, local, &
            local_stack = .true., init_only = .true.)
    end if
    process => current%process_stack%get_process_ptr (process_id)

```

```

        call msg_message &
            ("Simulate: process '" &
             // char (process_id) // "' : enabled for rescan only")
    end if
end subroutine prepare_process

```

33.9.5 Simulation-entry object

For each process that we consider for event generation, we need a separate entry. The entry separately records the process ID and run ID. The `weight_mci` array is used for selecting a component set (which shares an MCI record inside the process container) when generating an event for the current process.

The simulation entry is an extension of the `event_t` event record. This core object contains configuration data, pointers to the process and process instance, the expressions, flags and values that are evaluated at runtime, and the resulting particle set.

The entry explicitly allocates the `process_instance`, which becomes the process-specific workspace for the event record.

If entries with differing environments are present simultaneously, we may need to switch QCD parameters and/or the model event by event. In this case, the `qcd` and/or `model` components are present.

For the purpose of NLO events, `entry_t` contains a pointer list to other simulation-entries. This is due to the fact that we have to associate an event for each component of the fixed order simulation, i.e. one N -particle event and N_{phs} $N + 1$ -particle events. However, all entries share the same event transforms.

(Simulations: types)+≡

```

type, extends (event_t) :: entry_t
private
type(string_t) :: process_id
type(string_t) :: library
type(string_t) :: run_id
logical :: has_integral = .false.
real(default) :: integral = 0
real(default) :: error = 0
real(default) :: process_weight = 0
logical :: valid = .false.
type(counter_t) :: counter
integer :: n_in = 0
integer :: n_mci = 0
type(mci_set_t), dimension(:), allocatable :: mci_sets
type(selector_t) :: mci_selector
logical :: has_resonant_subprocess_set = .false.
type(resonant_subprocess_set_t) :: resonant_subprocess_set
type(core_safe_t), dimension(:), allocatable :: core_safe
class(model_data_t), pointer :: model => null ()
type(qcd_t) :: qcd
type(entry_t), pointer :: first => null ()
type(entry_t), pointer :: next => null ()
class(evt_t), pointer :: evt_powheg => null ()
contains
(Simulations: entry: TBP)

```

```
end type entry_t
```

Output. Write just the configuration, the event is written by a separate routine.

The `verbose` option is unused, it is required by the interface of the base-object method.

```
<Simulations: entry: TBP>≡
  procedure :: write_config => entry_write_config

<Simulations: sub interfaces>+≡
  module subroutine entry_write_config (object, unit, pacified)
    class(entry_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacified
  end subroutine entry_write_config

<Simulations: procedures>+≡
  module subroutine entry_write_config (object, unit, pacified)
    class(entry_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacified
    logical :: pacify
    integer :: u, i
    u = given_output_unit (unit)
    pacify = .false.; if (present (pacified)) pacify = pacified
    write (u, "(3x,A,A,A)") "Process   = ', char (object%process_id), "'
    write (u, "(3x,A,A,A)") "Library   = ', char (object%library), "'
    write (u, "(3x,A,A,A)") "Run       = ', char (object%run_id), "'
    write (u, "(3x,A,L1)")  "is valid  = ", object%valid
    if (object%has_integral) then
      if (pacify) then
        write (u, "(3x,A," // FMT_15 // ")") "Integral = ", object%integral
        write (u, "(3x,A," // FMT_15 // ")") "Error     = ", object%error
        write (u, "(3x,A,F9.6)") "Weight    = ", object%process_weight
      else
        write (u, "(3x,A," // FMT_19 // ")") "Integral = ", object%integral
        write (u, "(3x,A," // FMT_19 // ")") "Error     = ", object%error
        write (u, "(3x,A,F13.10)") "Weight    = ", object%process_weight
      end if
    else
      write (u, "(3x,A)") "Integral = [undefined]"
    end if
    write (u, "(3x,A,I0)") "MCI sets = ", object%n_mci
    call object%counter%write (u)
    do i = 1, size (object%mc_i_sets)
      write (u, "(A)")
      write (u, "(1x,A,I0,A)") "MCI set #", i, ":"
      call object%mc_i_sets(i)%write (u, pacified)
    end do
    if (object%resonant_subprocess_set%is_active ()) then
      write (u, "(A)")
      call object%write_resonant_subprocess_data (u)
    end if
    if (allocated (object%core_safe)) then
      do i = 1, size (object%core_safe)
        write (u, "(1x,A,I0,A)") "Saved process-component core #", i, ":"
```

```

        call object%core_safe(i)%core%write (u)
    end do
end if
end subroutine entry_write_config

```

Finalizer. The `instance` pointer component of the `event_t` base type points to a target which we did explicitly allocate in the `entry_init` procedure. Therefore, we finalize and explicitly deallocate it here. Then we call the finalizer of the base type.

```

<Simulations: entry: TBP>+≡
    procedure :: final => entry_final

<Simulations: sub interfaces>+≡
    module subroutine entry_final (object)
        class(entry_t), intent(inout) :: object
    end subroutine entry_final

<Simulations: procedures>+≡
    module subroutine entry_final (object)
        class(entry_t), intent(inout) :: object
        integer :: i
        if (associated (object%instance)) then
            do i = 1, object%n_mci
                call object%instance%final_simulation (i)
            end do
            call object%instance%final ()
            deallocate (object%instance)
        end if
        call object%event_t%final ()
    end subroutine entry_final

```

Copy the content of an entry into another one, except for the next-pointer

```

<Simulations: entry: TBP>+≡
    procedure :: copy_entry => entry_copy_entry

<Simulations: sub interfaces>+≡
    module subroutine entry_copy_entry (entry1, entry2)
        class(entry_t), intent(in), target :: entry1
        type(entry_t), intent(inout), target :: entry2
    end subroutine entry_copy_entry

<Simulations: procedures>+≡
    module subroutine entry_copy_entry (entry1, entry2)
        class(entry_t), intent(in), target :: entry1
        type(entry_t), intent(inout), target :: entry2
        call entry1%event_t%clone (entry2%event_t)
        entry2%process_id = entry1%process_id
        entry2%library = entry1%library
        entry2%run_id = entry1%run_id
        entry2%has_integral = entry1%has_integral
        entry2%integral = entry1%integral
        entry2%error = entry1%error
        entry2%process_weight = entry1%process_weight
        entry2%valid = entry1%valid
        entry2%counter = entry1%counter
    end subroutine entry_copy_entry

```

```

entry2%n_in = entry1%n_in
entry2%n_mci = entry1%n_mci
if (allocated (entry1%mci_sets)) then
    allocate (entry2%mci_sets (size (entry1%mci_sets)))
    entry2%mci_sets = entry1%mci_sets
end if
entry2%mci_selector = entry1%mci_selector
if (allocated (entry1%core_safe)) then
    allocate (entry2%core_safe (size (entry1%core_safe)))
    entry2%core_safe = entry1%core_safe
end if
entry2%model => entry1%model
entry2%qcd = entry1%qcd
end subroutine entry_copy_entry

```

Simulation-entry initialization

Search for a process entry and allocate a process instance as an anonymous object, temporarily accessible via the `process_instance` pointer. Assign data by looking at the process object and at the environment.

If `n_alt` is set, we prepare for additional alternate sqme and weight entries.

The `compile` flag is only false if we do not need the Whizard process at all, just its definition. In that case, we skip process initialization.

Otherwise, and if the process object is not found initially: if `integrate` is set, attempt an integration pass and try again. Otherwise, just initialize the object.

If `generate` is set, prepare the MCI objects for generating new events. For pure rescanning, this is not necessary.

If `resonance_history` is set, we create a separate process library which contains all possible restricted subprocesses with distinct resonance histories. These processes will not be integrated, but their matrix element codes are used for determining probabilities of resonance histories. Note that this can work only if the process method is `OMega`, and the phase-space method is 'wood'.

When done, we assign the `instance` and `process` pointers of the base type by the `connect` method, so we can reference them later.

TODO: In case of NLO event generation, copying the configuration from the master process is rather intransparent. For instance, we override the process var list by the global var list.

```

<Simulations: entry: TBP>+≡
    procedure :: init => entry_init

<Simulations: sub interfaces>+≡
    module subroutine entry_init &
        (entry, process_id, &
         use_process, integrate, generate, update_sqme, &
         support_resonance_history, &
         local, global, n_alt)
        class(entry_t), intent(inout), target :: entry
        type(string_t), intent(in) :: process_id
        logical, intent(in) :: use_process, integrate, generate, update_sqme
        logical, intent(in) :: support_resonance_history
    end module

```

```

        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), optional, target :: global
        integer, intent(in), optional :: n_alt
    end subroutine entry_init
<Simulations: procedures>+≡
module subroutine entry_init &
    (entry, process_id, &
     use_process, integrate, generate, update_sqme, &
     support_resonance_history, &
     local, global, n_alt)
class(entry_t), intent(inout), target :: entry
type(string_t), intent(in) :: process_id
logical, intent(in) :: use_process, integrate, generate, update_sqme
logical, intent(in) :: support_resonance_history
type(rt_data_t), intent(inout), target :: local
type(rt_data_t), intent(inout), optional, target :: global
integer, intent(in), optional :: n_alt
type(process_t), pointer :: process, master_process
type(process_instance_t), pointer :: process_instance
type(process_library_t), pointer :: prclib_saved
integer :: i
logical :: res_include_trivial
logical :: combined_integration
integer :: selected_mci
selected_mci = 0
if (debug_on) call msg_debug (D_CORE, "entry_init")
if (debug_on) call msg_debug (D_CORE, "process_id", process_id)
call prepare_process &
    (master_process, process_id, use_process, integrate, local, global)
if (signal_is_pending ()) return

if (associated (master_process)) then
    if (.not. master_process%has_matrix_element ()) then
        entry%has_integral = .true.
        entry%process_id = process_id
        entry%valid = .false.
        return
    end if
else
    call entry%basic_init (local%var_list)
    entry%has_integral = .false.
    entry%process_id = process_id
    call entry%import_process_def_characteristics (local%prclib, process_id)
    entry%valid = .true.
    return
end if

call entry%basic_init (local%var_list, n_alt)

entry%process_id = process_id
if (generate .or. integrate) then
    entry%run_id = master_process%get_run_id ()
    process => master_process
else

```

```

call local%set_log (var_str ("?rebuild_phase_space"), &
    .false., is_known = .true.)
call local%set_log (var_str ("?check_phs_file"), &
    .false., is_known = .true.)
call local%set_log (var_str ("?rebuild_grids"), &
    .false., is_known = .true.)
entry%run_id = &
    local%var_list%get_sval (var_str ("$run_id"))
if (update_sqme) then
    call prepare_local_process (process, process_id, local)
else
    process => master_process
end if
end if

call entry%import_process_characteristics (process)

allocate (entry%mci_sets (entry%n_mci))
do i = 1, size (entry%mci_sets)
    call entry%mci_sets(i)%init (i, master_process)
end do

call entry%import_process_results (master_process)
call entry%prepare_expressions (local)

if (process%is_nlo_calculation ()) then
    call process%init_nlo_settings (global%var_list)
end if
combined_integration = local%get_lval (var_str ("?combined_nlo_integration"))
if (.not. combined_integration) &
    selected_mci = process%extract_active_component_mci ()
call prepare_process_instance (process_instance, process, local%model, &
    local = local)

if (generate) then
    if (selected_mci > 0) then
        call process%prepare_simulation (selected_mci)
        call process_instance%init_simulation (selected_mci, entry%config%safety_factor, &
            local%get_lval (var_str ("?keep_failed_events")))
    else
        do i = 1, entry%n_mci
            call process%prepare_simulation (i)
            call process_instance%init_simulation (i, entry%config%safety_factor, &
                local%get_lval (var_str ("?keep_failed_events")))
        end do
    end if
end if

if (support_resonance_history) then
    prclib_saved => local%prclib
    call entry%setup_resonant_subprocesses (local, process)
    if (entry%has_resonant_subprocess_set) then
        if (signal_is_pending ()) return
        call entry%compile_resonant_subprocesses (local)
    end if
end if

```

```

        if (signal_is_pending ()) return
        call entry%prepare_resonant_subprocesses (local, global)
        if (signal_is_pending ()) return
        call entry%prepare_resonant_subprocess_instances (local)
    end if
    if (signal_is_pending ()) return
    if (associated (prclib_saved)) call local%update_prclib (prclib_saved)
end if

call entry%setup_event_transforms (process, local)

call dispatch_qcd (entry%qcd, local%get_var_list_ptr (), local%os_data)

call entry%connect_qcd ()

if (present (global)) then
    call entry%connect (process_instance, local%model, global%process_stack)
else
    call entry%connect (process_instance, local%model, local%process_stack)
end if
call entry%setup_expressions ()

entry%model => process%get_model_ptr ()

entry%valid = .true.

end subroutine entry_init

```

<Simulations: entry: TBP>+≡

```

    procedure :: set_active_real_components => entry_set_active_real_components

```

<Simulations: sub interfaces>+≡

```

    module subroutine entry_set_active_real_components (entry)
        class(entry_t), intent(inout) :: entry
    end subroutine entry_set_active_real_components

```

<Simulations: procedures>+≡

```

    module subroutine entry_set_active_real_components (entry)
        class(entry_t), intent(inout) :: entry
        integer :: i_active_real
        select type (pcm => entry%instance%pcm)
        class is (pcm_nlo_t)
            i_active_real = entry%instance%get_real_of_mci ()
            if (debug_on) call msg_debug2 (D_CORE, "i_active_real", i_active_real)
            if (associated (entry%evt_powheg)) then
                select type (evt => entry%evt_powheg)
                type is (evt_shower_t)
                    if (entry%process%get_component_type(i_active_real) == &
                        COMP_REAL_FIN) then
                        if (debug_on) call msg_debug &
                            (D_CORE, "Disabling Powheg matching for ", i_active_real)
                        call evt%disable_powheg_matching ()
                    else
                        if (debug_on) call msg_debug &
                            (D_CORE, "Enabling Powheg matching for ", i_active_real)

```



```

        call evt%enable_powheg_matching ()
    end if
    class default
        call msg_fatal ("powheg-evt should be evt_shower_t!")
    end select
end if
end select
end subroutine entry_set_active_real_components

```

Part of simulation-entry initialization: set up a process object for local use.

(Simulations: procedures)+≡

```

subroutine prepare_local_process (process, process_id, local)
    type(process_t), pointer, intent(inout) :: process
    type(string_t), intent(in) :: process_id
    type(rt_data_t), intent(inout), target :: local
    type(integration_t) :: intg
    call intg%create_process (process_id)
    call intg%init_process (local)
    call intg%setup_process (local, verbose=.false.)
    process => intg%get_process_ptr ()
end subroutine prepare_local_process

```

Part of simulation-entry initialization: set up a process instance matching the selected process object.

The model that we can provide as an extra argument can modify particle settings (polarization) in the density matrices that will be constructed. It does not affect parameters.

(Restricted subprocesses: sub interfaces)+≡

(Simulations: procedures)+≡

```

subroutine prepare_process_instance &
    (process_instance, process, model, local)
    type(process_instance_t), pointer, intent(inout) :: process_instance
    type(process_t), intent(inout), target :: process
    class(model_data_t), intent(in), optional :: model
    type(rt_data_t), intent(in), optional, target :: local
    allocate (process_instance)
    call process_instance%init (process)
    if (process%is_nlo_calculation ()) then
        select type (pcm_work => process_instance%pcm_work)
        type is (pcm_nlo_workspace_t)
            select type (pcm => process_instance%pcm)
            type is (pcm_nlo_t)
                if (.not. pcm%settings%combined_integration) &
                    call pcm_work%set_radiation_event ()
                if (pcm%settings%fixed_order_nlo) &
                    call pcm_work%set_fixed_order_event_mode ()
            end select
        end select
    end select
    call process%prepare_any_external_code ()
end if
call process_instance%setup_event_data (model)
end subroutine prepare_process_instance

```

Part of simulation-entry initialization: query the process for basic information.

```

<Simulations: entry: TBP>+≡
    procedure, private :: import_process_characteristics &
        => entry_import_process_characteristics

<Simulations: sub interfaces>+≡
    module subroutine entry_import_process_characteristics (entry, process)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(in), target :: process
    end subroutine entry_import_process_characteristics

<Simulations: procedures>+≡
    module subroutine entry_import_process_characteristics (entry, process)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(in), target :: process
        entry%library = process%get_library_name ()
        entry%n_in = process%get_n_in ()
        entry%n_mci = process%get_n_mci ()
    end subroutine entry_import_process_characteristics

```

This is the alternative form which applies if there is no process entry, but just a process definition which we take from the provided prclib definition library.

```

<Simulations: entry: TBP>+≡
    procedure, private :: import_process_def_characteristics &
        => entry_import_process_def_characteristics

<Simulations: sub interfaces>+≡
    module subroutine entry_import_process_def_characteristics &
        (entry, prclib, id)
        class(entry_t), intent(inout) :: entry
        type(process_library_t), intent(in), target :: prclib
        type(string_t), intent(in) :: id
    end subroutine entry_import_process_def_characteristics

<Simulations: procedures>+≡
    module subroutine entry_import_process_def_characteristics (entry, prclib, id)
        class(entry_t), intent(inout) :: entry
        type(process_library_t), intent(in), target :: prclib
        type(string_t), intent(in) :: id
        entry%library = prclib%get_name ()
        entry%n_in = prclib%get_n_in (id)
    end subroutine entry_import_process_def_characteristics

```

Part of simulation-entry initialization: query the process for integration results.

```

<Simulations: entry: TBP>+≡
    procedure, private :: import_process_results &
        => entry_import_process_results

<Simulations: sub interfaces>+≡
    module subroutine entry_import_process_results (entry, process)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(in), target :: process
    end subroutine entry_import_process_results

```

```

<Simulations: procedures>+≡
module subroutine entry_import_process_results (entry, process)
  class(entry_t), intent(inout) :: entry
  type(process_t), intent(in), target :: process
  if (process%has_integral ()) then
    entry%integral = process%get_integral ()
    entry%error = process%get_error ()
    call entry%set_sigma (entry%integral)
    entry%has_integral = .true.
  end if
end subroutine entry_import_process_results

```

Part of simulation-entry initialization: create expression factory objects and store them.

```

<Simulations: entry: TBP>+≡
  procedure, private :: prepare_expressions &
    => entry_prepare_expressions

<Simulations: sub interfaces>+≡
  module subroutine entry_prepare_expressions (entry, local)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(in), target :: local
  end subroutine entry_prepare_expressions

<Simulations: procedures>+≡
module subroutine entry_prepare_expressions (entry, local)
  class(entry_t), intent(inout) :: entry
  type(rt_data_t), intent(in), target :: local
  type(eval_tree_factory_t) :: expr_factory
  call expr_factory%init (local%pn%selection_lexpr)
  call entry%set_selection (expr_factory)
  call expr_factory%init (local%pn%reweight_expr)
  call entry%set_reweight (expr_factory)
  call expr_factory%init (local%pn%analysis_lexpr)
  call entry%set_analysis (expr_factory)
end subroutine entry_prepare_expressions

```

Extra (NLO) entries

Initializes the list of additional NLO entries. The routine gets the information about how many entries to associate from `region_data`.

```

<Simulations: entry: TBP>+≡
  procedure :: setup_additional_entries => entry_setup_additional_entries

<Simulations: sub interfaces>+≡
  module subroutine entry_setup_additional_entries (entry)
    class(entry_t), intent(inout), target :: entry
  end subroutine entry_setup_additional_entries

<Simulations: procedures>+≡
module subroutine entry_setup_additional_entries (entry)
  class(entry_t), intent(inout), target :: entry
  type(entry_t), pointer :: current_entry
  integer :: i, n_phs

```

```

type(evt_nlo_t), pointer :: evt
integer :: mode
evt => null ()
select type (pcm => entry%instance%pcm)
type is (pcm_nlo_t)
    n_phs = pcm%region_data%n_phs
end select
select type (entry)
type is (entry_t)
    current_entry => entry
    current_entry%first => entry
    call get_nlo_evt_ptr (current_entry, evt, mode)
    if (mode > EVT_NLO_SEPARATE_BORNLIKE) then
        allocate (evt%particle_set_nlo (n_phs + 1))
        evt%event_deps%n_phs = n_phs
        evt%qcd = entry%qcd
        do i = 1, n_phs
            allocate (current_entry%next)
            current_entry%next%first => current_entry%first
            current_entry => current_entry%next
            call entry%copy_entry (current_entry)
            current_entry%i_event = i
        end do
    else
        allocate (evt%particle_set_nlo (1))
    end if
end select
contains
subroutine get_nlo_evt_ptr (entry, evt, mode)
    type(entry_t), intent(in), target :: entry
    type(evt_nlo_t), intent(out), pointer :: evt
    integer, intent(out) :: mode
    class(evt_t), pointer :: current_evt
    evt => null ()
    current_evt => entry%transform_first
    do
        select type (current_evt)
        type is (evt_nlo_t)
            evt => current_evt
            mode = evt%mode
            exit
        end select
        if (associated (current_evt%next)) then
            current_evt => current_evt%next
        else
            call msg_fatal ("evt_nlo not in list of event transforms")
        end if
    end do
end subroutine get_nlo_evt_ptr
end subroutine entry_setup_additional_entries

```

<Simulations: entry: TBP>+≡
 procedure :: get_first => entry_get_first

```

⟨Simulations: sub interfaces⟩+≡
    module function entry_get_first (entry) result (entry_out)
        class(entry_t), intent(in), target :: entry
        type(entry_t), pointer :: entry_out
    end function entry_get_first

⟨Simulations: procedures⟩+≡
    module function entry_get_first (entry) result (entry_out)
        class(entry_t), intent(in), target :: entry
        type(entry_t), pointer :: entry_out
        entry_out => null ()
        select type (entry)
        type is (entry_t)
            if (entry%is_nlo ()) then
                entry_out => entry%first
            else
                entry_out => entry
            end if
        end select
    end function entry_get_first

⟨Simulations: entry: TBP⟩+≡
    procedure :: get_next => entry_get_next

⟨Simulations: sub interfaces⟩+≡
    module function entry_get_next (entry) result (next_entry)
        class(entry_t), intent(in) :: entry
        type(entry_t), pointer :: next_entry
    end function entry_get_next

⟨Simulations: procedures⟩+≡
    module function entry_get_next (entry) result (next_entry)
        class(entry_t), intent(in) :: entry
        type(entry_t), pointer :: next_entry
        next_entry => null ()
        if (associated (entry%next)) then
            next_entry => entry%next
        else
            call msg_fatal ("Get next entry: No next entry")
        end if
    end function entry_get_next

⟨Simulations: entry: TBP⟩+≡
    procedure :: count_nlo_entries => entry_count_nlo_entries

⟨Simulations: sub interfaces⟩+≡
    module function entry_count_nlo_entries (entry) result (n)
        class(entry_t), intent(in), target :: entry
        integer :: n
    end function entry_count_nlo_entries

⟨Simulations: procedures⟩+≡
    module function entry_count_nlo_entries (entry) result (n)
        class(entry_t), intent(in), target :: entry
        integer :: n
        type(entry_t), pointer :: current_entry

```

```

n = 1
if (.not. associated (entry%next)) then
  return
else
  current_entry => entry%next
  do
    n = n + 1
    if (.not. associated (current_entry%next)) exit
    current_entry => current_entry%next
  end do
end if
end function entry_count_nlo_entries

```

<Simulations: entry: TBP>+≡
 procedure :: reset_nlo_counter => entry_reset_nlo_counter

<Simulations: sub interfaces>+≡
 module subroutine entry_reset_nlo_counter (entry)
 class(entry_t), intent(inout) :: entry
 end subroutine entry_reset_nlo_counter

<Simulations: procedures>+≡
 module subroutine entry_reset_nlo_counter (entry)
 class(entry_t), intent(inout) :: entry
 class(evt_t), pointer :: evt
 evt => entry%transform_first
 do
 select type (evt)
 type is (evt_nlo_t)
 evt%i_evaluation = 0
 exit
 end select
 if (associated (evt%next)) evt => evt%next
 end do
end subroutine entry_reset_nlo_counter

<Simulations: entry: TBP>+≡
 procedure :: determine_if_powheg_matching => &
 entry_determine_if_powheg_matching

<Simulations: sub interfaces>+≡
 module subroutine entry_determine_if_powheg_matching (entry)
 class(entry_t), intent(inout) :: entry
 end subroutine entry_determine_if_powheg_matching

<Simulations: procedures>+≡
 module subroutine entry_determine_if_powheg_matching (entry)
 class(entry_t), intent(inout) :: entry
 class(evt_t), pointer :: current_transform
 if (associated (entry%transform_first)) then
 current_transform => entry%transform_first
 do
 select type (current_transform)
 type is (evt_shower_t)
 if (current_transform%contains_powheg_matching ()) &

```

        entry%evt_powheg => current_transform
    exit
end select
if (associated (current_transform%next)) then
    current_transform => current_transform%next
else
    exit
end if
end do
end if
end subroutine entry_determine_if_powheg_matching

```

Event-transform initialization

Part of simulation-entry initialization: dispatch event transforms (decay, shower) as requested. If a transform is not applicable or switched off via some variable, it will be skipped.

Regarding resonances/decays: these two transforms are currently mutually exclusive. Resonance insertion will not be applied if there is an unstable particle in the game.

The initial particle set is the output of the trivial transform; this has already been applied when the transforms listed here are encountered. Each transform takes a particle set and produces a new one, with one exception: the decay module takes its input from the process object, ignoring the trivial transform. (Reason: spin correlations.) Therefore, the decay module must be first in line.

Settings that we don't or can't support (yet) are rejected by the embedded call to `event_transforms_check`.

```

<Simulations: entry: TBP>+≡
    procedure, private :: setup_event_transforms &
        => entry_setup_event_transforms

<Simulations: sub interfaces>+≡
    module subroutine entry_setup_event_transforms (entry, process, local)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(inout), target :: process
        type(rt_data_t), intent(in), target :: local
    end subroutine entry_setup_event_transforms

<Simulations: procedures>+≡
    module subroutine entry_setup_event_transforms (entry, process, local)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(inout), target :: process
        type(rt_data_t), intent(in), target :: local
        class(evt_t), pointer :: evt
        type(var_list_t), pointer :: var_list
        logical :: enable_isr_handler
        logical :: enable_epa_handler
        logical :: enable_fixed_order
        logical :: enable_shower
        character(len=7) :: sample_normalization

        call event_transforms_check (entry, process, local)
    end subroutine entry_setup_event_transforms

```

```

var_list => local%get_var_list_ptr ()

if (process%contains_unstable (local%model)) then
  call dispatch_evt_decay (evt, local%var_list)
  if (associated (evt)) call entry%import_transform (evt)
end if

if (entry%resonant_subprocess_set%is_active ()) then
  call dispatch_evt_resonance (evt, local%var_list, &
    entry%resonant_subprocess_set%get_resonance_history_set (), &
    entry%resonant_subprocess_set%get_libname ())
  if (associated (evt)) then
    call entry%resonant_subprocess_set%connect_transform (evt)
    call entry%resonant_subprocess_set%set_on_shell_limit &
      (local%get_rval (var_str ("resonance_on_shell_limit")))
    call entry%resonant_subprocess_set%set_on_shell_turnoff &
      (local%get_rval (var_str ("resonance_on_shell_turnoff")))
    call entry%resonant_subprocess_set%set_background_factor &
      (local%get_rval (var_str ("resonance_background_factor")))
    call entry%import_transform (evt)
  end if
end if

enable_fixed_order = local%get_lval (var_str ("?fixed_order_nlo_events"))
if (enable_fixed_order) then
  call dispatch_evt_nlo &
    (evt, local%get_lval (var_str ("?keep_failed_events")))
  call entry%import_transform (evt)
end if

enable_isr_handler = local%get_lval (var_str ("?isr_handler"))
enable_epa_handler = local%get_lval (var_str ("?epa_handler"))
if (enable_isr_handler .or. enable_epa_handler) then
  call dispatch_evt_isr_epa_handler (evt, local%var_list)
  if (associated (evt)) call entry%import_transform (evt)
end if

enable_shower = local%get_lval (var_str ("?allow_shower")) .and. &
  (local%get_lval (var_str ("?ps_isr_active")) &
  .or. local%get_lval (var_str ("?ps_fsr_active")) &
  .or. local%get_lval (var_str ("?muli_active")) &
  .or. local%get_lval (var_str ("?mlm_matching")) &
  .or. local%get_lval (var_str ("?ckkw_matching")) &
  .or. local%get_lval (var_str ("?powheg_matching")))
if (enable_shower) then
  call dispatch_evt_shower (evt, var_list, local%model, &
    local%fallback_model, local%os_data, local%beam_structure, &
    process)
  call entry%import_transform (evt)
end if

if (local%get_lval (var_str ("?hadronization_active"))) then
  call dispatch_evt_hadrons (evt, var_list, local%fallback_model)
  call entry%import_transform (evt)

```



```

end if

end subroutine entry_setup_event_transforms

```

This routine rejects all event-transform settings which we don't support at present.

```

<Simulations: procedures>+≡
subroutine event_transforms_check (entry, process, local)
  class(entry_t), intent(in) :: entry
  type(process_t), intent(in), target :: process
  type(rt_data_t), intent(in), target :: local

  if (local%get_lval (var_str ("?fixed_order_nlo_events"))) then
    if (local%get_lval (var_str ("?unweighted"))) then
      call msg_fatal ("NLO fixed-order events have to be generated with &
        &?unweighted = false")
    end if
    select case (char (local%get_sval (var_str ("sample_normalization"))))
    case ("sigma", "auto")
    case default
      call msg_fatal ("NLO fixed-order events: only &
        &sample_normalization = 'sigma' is supported.")
    end select
    if (process%contains_unstable (local%model)) then
      call msg_fatal ("NLO fixed-order events: unstable final-state &
        &particles not supported yet")
    end if
    if (entry%resonant_subprocess_set%is_active ()) then
      call msg_fatal ("NLO fixed-order events: resonant subprocess &
        &insertion not supported")
    end if
    if (local%get_lval (var_str ("?isr_handler")) &
      .or. local%get_lval (var_str ("?epa_handler"))) then
      call msg_fatal ("NLO fixed-order events: ISR handler for &
        &photon-pT generation not supported yet")
    end if
  end if

  if (process%contains_unstable (local%model) &
    .and. entry%resonant_subprocess_set%is_active ()) then
    call msg_fatal ("Simulation: resonant subprocess insertion with &
      &unstable final-state particles not supported")
  end if

end subroutine event_transforms_check

```

Process/MCI selector

Compute weights. The integral in the argument is the sum of integrals for all processes in the sample. After computing the process weights, we repeat the normalization procedure for the process components.

```

<Simulations: entry: TBP>+≡

```

```

        procedure :: init_mci_selector => entry_init_mci_selector

<Simulations: sub interfaces>+≡
        module subroutine entry_init_mci_selector (entry, negative_weights)
            class(entry_t), intent(inout), target :: entry
            logical, intent(in), optional :: negative_weights
            end subroutine entry_init_mci_selector

<Simulations: procedures>+≡
        module subroutine entry_init_mci_selector (entry, negative_weights)
            class(entry_t), intent(inout), target :: entry
            logical, intent(in), optional :: negative_weights
            type(entry_t), pointer :: current_entry
            integer :: i, j, k
            if (debug_on) call msg_debug (D_CORE, "entry_init_mci_selector")
            if (entry%has_integral) then
                select type (entry)
                type is (entry_t)
                    current_entry => entry
                    do j = 1, current_entry%count_nlo_entries ()
                        if (j > 1) current_entry => current_entry%get_next ()
                        do k = 1, size(current_entry%mci_sets%integral)
                            if (debug_on) call msg_debug &
                                (D_CORE, "current_entry%mci_sets(k)%integral", &
                                current_entry%mci_sets(k)%integral)
                        end do
                        call current_entry%mci_selector%init &
                            (current_entry%mci_sets%integral, negative_weights)
                        do i = 1, current_entry%n_mci
                            current_entry%mci_sets(i)%weight_mci = &
                                current_entry%mci_selector%get_weight (i)
                        end do
                    end do
                end select
            end if
        end subroutine entry_init_mci_selector

```

Select a MCI entry, using the embedded random-number generator.

```

<Simulations: entry: TBP>+≡
        procedure :: select_mci => entry_select_mci

<Simulations: sub interfaces>+≡
        module function entry_select_mci (entry) result (i_mci)
            class(entry_t), intent(inout) :: entry
            integer :: i_mci
            end function entry_select_mci

<Simulations: procedures>+≡
        module function entry_select_mci (entry) result (i_mci)
            class(entry_t), intent(inout) :: entry
            integer :: i_mci
            if (debug_on) call msg_debug2 (D_CORE, "entry_select_mci")
            i_mci = entry%process%extract_active_component_mci ()
            if (i_mci == 0) call entry%mci_selector%generate (entry%rng, i_mci)
            if (debug_on) call msg_debug2 (D_CORE, "i_mci", i_mci)
        end function entry_select_mci

```

Entries: event-wise updates

Record an event for this entry, i.e., increment the appropriate counters.

<Simulations: entry: TBP>+≡

```
procedure :: record => entry_record
```

<Simulations: sub interfaces>+≡

```
module subroutine entry_record (entry, i_mci, from_file)
  class(entry_t), intent(inout) :: entry
  integer, intent(in) :: i_mci
  logical, intent(in), optional :: from_file
end subroutine entry_record
```

<Simulations: procedures>+≡

```
module subroutine entry_record (entry, i_mci, from_file)
  class(entry_t), intent(inout) :: entry
  integer, intent(in) :: i_mci
  logical, intent(in), optional :: from_file
  real(default) :: weight, excess
  integer :: n_dropped
  weight = entry%get_weight_prc ()
  excess = entry%get_excess_prc ()
  n_dropped = entry%get_n_dropped ()
  call entry%counter%record (weight, excess, n_dropped, from_file)
  if (i_mci > 0) then
    call entry%mc_i_sets(i_mci)%counter%record (weight, excess)
  end if
end subroutine entry_record
```

Update and restore the process core that this entry accesses, when parameters change. If explicit arguments `model`, `qcd`, or `helicity_selection` are provided, use those. Otherwise use the parameters stored in the process object.

These two procedures come with a caching mechanism which guarantees that the current core object is saved when calling `update_process`, and restored by calling `restore_process`. If the flag `saved` is unset, saving is skipped, and the `restore` procedure should not be called.

<Simulations: entry: TBP>+≡

```
procedure :: update_process => entry_update_process
procedure :: restore_process => entry_restore_process
```

<Simulations: sub interfaces>+≡

```
module subroutine entry_update_process &
  (entry, model, qcd, helicity_selection, saved)
  class(entry_t), intent(inout) :: entry
  class(model_data_t), intent(in), optional, target :: model
  type(qcd_t), intent(in), optional :: qcd
  type(helicity_selection_t), intent(in), optional :: helicity_selection
  logical, intent(in), optional :: saved
end subroutine entry_update_process
module subroutine entry_restore_process (entry)
  class(entry_t), intent(inout) :: entry
end subroutine entry_restore_process
```

(Simulations: procedures)+≡

```

module subroutine entry_update_process &
  (entry, model, qcd, helicity_selection, saved)
  class(entry_t), intent(inout) :: entry
  class(model_data_t), intent(in), optional, target :: model
  type(qcd_t), intent(in), optional :: qcd
  type(helicity_selection_t), intent(in), optional :: helicity_selection
  logical, intent(in), optional :: saved
  type(process_t), pointer :: process
  class(prc_core_t), allocatable :: core
  integer :: i, n_terms
  class(model_data_t), pointer :: model_local
  type(qcd_t) :: qcd_local
  logical :: use_saved
  if (present (model)) then
    model_local => model
  else
    model_local => entry%model
  end if
  if (present (qcd)) then
    qcd_local = qcd
  else
    qcd_local = entry%qcd
  end if
  use_saved = .true.; if (present (saved)) use_saved = saved
  process => entry%get_process_ptr ()
  n_terms = process%get_n_terms ()
  if (use_saved) allocate (entry%core_safe (n_terms))
  do i = 1, n_terms
    if (process%has_matrix_element (i, is_term_index = .true.)) then
      call process%extract_core (i, core)
      if (use_saved) then
        call dispatch_core_update (core, &
          model_local, helicity_selection, qcd_local, &
          entry%core_safe(i)%core)
      else
        call dispatch_core_update (core, &
          model_local, helicity_selection, qcd_local)
      end if
      call process%restore_core (i, core)
    end if
  end do
end subroutine entry_update_process

module subroutine entry_restore_process (entry)
  class(entry_t), intent(inout) :: entry
  type(process_t), pointer :: process
  class(prc_core_t), allocatable :: core
  integer :: i, n_terms
  process => entry%get_process_ptr ()
  n_terms = process%get_n_terms ()
  do i = 1, n_terms
    if (process%has_matrix_element (i, is_term_index = .true.)) then
      call process%extract_core (i, core)
    end if
  end do
end subroutine entry_restore_process

```

```

        call dispatch_core_restore (core, entry%core_safe(i)%core)
        call process%restore_core (i, core)
    end if
end do
deallocate (entry%core_safe)
end subroutine entry_restore_process

<Simulations: entry: TBP>+≡
    procedure :: connect_qcd => entry_connect_qcd

<Simulations: sub interfaces>+≡
    module subroutine entry_connect_qcd (entry)
        class(entry_t), intent(inout), target :: entry
    end subroutine entry_connect_qcd

<Simulations: procedures>+≡
    module subroutine entry_connect_qcd (entry)
        class(entry_t), intent(inout), target :: entry
        class(evt_t), pointer :: evt
        evt => entry%transform_first
        do while (associated (evt))
            select type (evt)
            type is (evt_shower_t)
                evt%qcd = entry%qcd
                if (allocated (evt%matching)) then
                    evt%matching%qcd = entry%qcd
                end if
            end select
            evt => evt%next
        end do
    end subroutine entry_connect_qcd

```

33.9.6 Handling resonant subprocesses

Resonant subprocesses are required if we want to determine resonance histories when generating events. The feature is optional, to be switched on by the user.

This procedure initializes a new, separate process library that contains copies of the current process, restricted to the relevant resonance histories. (If this library exists already, it is just kept.) The histories can be extracted from the process object.

The code has to match the assignments in `create_resonant_subprocess_library`. The library may already exist – in that case, here it will be recovered without recompilation.

```

<Simulations: entry: TBP>+≡
    procedure :: setup_resonant_subprocesses &
        => entry_setup_resonant_subprocesses

<Simulations: sub interfaces>+≡
    module subroutine entry_setup_resonant_subprocesses (entry, global, process)
        class(entry_t), intent(inout) :: entry
        type(rt_data_t), intent(inout), target :: global
        type(process_t), intent(in), target :: process
    end subroutine entry_setup_resonant_subprocesses

```

<Simulations: procedures>+≡

```

module subroutine entry_setup_resonant_subprocesses (entry, global, process)
  class(entry_t), intent(inout) :: entry
  type(rt_data_t), intent(inout), target :: global
  type(process_t), intent(in), target :: process
  type(string_t) :: libname
  type(resonance_history_set_t) :: res_history_set
  type(process_library_t), pointer :: lib
  type(process_component_def_t), pointer :: process_component_def
  logical :: req_resonant, library_exist
  integer :: i_component
  libname = process%get_library_name ()
  lib => global%prclib_stack%get_library_ptr (libname)
  entry%has_resonant_subprocess_set = lib%req_resonant (process%get_id ())
  if (entry%has_resonant_subprocess_set) then
    libname = get_libname_res (process%get_id ())
    call entry%resonant_subprocess_set%init (process%get_n_components ())
    call entry%resonant_subprocess_set%create_library &
      (libname, global, library_exist)
    do i_component = 1, process%get_n_components ()
      select case (process%get_component_type (i_component))
      case (COMP_MASTER, COMP_REAL_FIN, COMP_REAL_SING, COMP_REAL)
        call process%extract_resonance_history_set &
          (res_history_set, i_component = i_component)
        call entry%resonant_subprocess_set%fill_resonances &
          (res_history_set, i_component)
        if (.not. library_exist) then
          process_component_def &
            => process%get_component_def_ptr (i_component)
          call entry%resonant_subprocess_set%add_to_library &
            (i_component, &
              process_component_def%get_prt_spec_in (), &
              process_component_def%get_prt_spec_out (), &
              global)
        end if
      end select
    end do
    call entry%resonant_subprocess_set%freeze_library (global)
  end if
end subroutine entry_setup_resonant_subprocesses

```

Compile the resonant-subprocesses library. The library is assumed to be the current library in the global object. This is a simple wrapper.

<Simulations: entry: TBP>+≡

```

procedure :: compile_resonant_subprocesses &
  => entry_compile_resonant_subprocesses

```

<Simulations: sub interfaces>+≡

```

module subroutine entry_compile_resonant_subprocesses (entry, global)
  class(entry_t), intent(inout) :: entry
  type(rt_data_t), intent(inout), target :: global
end subroutine entry_compile_resonant_subprocesses

```

<Simulations: procedures>+≡

```

module subroutine entry_compile_resonant_subprocesses (entry, global)

```

```

class(entry_t), intent(inout) :: entry
type(rt_data_t), intent(inout), target :: global
call entry%resonant_subprocess_set%compile_library (global)
end subroutine entry_compile_resonant_subprocesses

```

Prepare process objects for the resonant-subprocesses library. The process objects are appended to the global process stack. We initialize the processes, such that we can evaluate matrix elements, but we do not need to integrate them.

```

<Simulations: entry: TBP>+≡
  procedure :: prepare_resonant_subprocesses &
    => entry_prepare_resonant_subprocesses

<Simulations: sub interfaces>+≡
  module subroutine entry_prepare_resonant_subprocesses (entry, local, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
  end subroutine entry_prepare_resonant_subprocesses

<Simulations: procedures>+≡
  module subroutine entry_prepare_resonant_subprocesses (entry, local, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    call entry%resonant_subprocess_set%prepare_process_objects (local, global)
  end subroutine entry_prepare_resonant_subprocesses

```

Prepare process instances. They are linked to their corresponding process objects. Both, process and instance objects, are allocated as anonymous targets inside the `resonant_subprocess_set` component.

NOTE: those anonymous object are likely forgotten during finalization of the parent `event_t` (extended as `entry_t`) object. This should be checked! The memory leak is probably harmless as long as the event object is created once per run, not once per event.

```

<Simulations: entry: TBP>+≡
  procedure :: prepare_resonant_subprocess_instances &
    => entry_prepare_resonant_subprocess_instances

<Simulations: sub interfaces>+≡
  module subroutine entry_prepare_resonant_subprocess_instances &
    (entry, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(in), target :: global
  end subroutine entry_prepare_resonant_subprocess_instances

<Simulations: procedures>+≡
  module subroutine entry_prepare_resonant_subprocess_instances (entry, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(in), target :: global
    call entry%resonant_subprocess_set%prepare_process_instances (global)
  end subroutine entry_prepare_resonant_subprocess_instances

```

Display the resonant subprocesses. This includes, upon request, the resonance set that defines those subprocess, and a short or long account of the process objects themselves.

```

<Simulations: entry: TBP>+≡
  procedure :: write_resonant_subprocess_data &
    => entry_write_resonant_subprocess_data

<Simulations: sub interfaces>+≡
  module subroutine entry_write_resonant_subprocess_data (entry, unit)
    class(entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
  end subroutine entry_write_resonant_subprocess_data

<Simulations: procedures>+≡
  module subroutine entry_write_resonant_subprocess_data (entry, unit)
    class(entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    call entry%resonant_subprocess_set%write (unit)
    write (u, "(1x,A,I0)") "Resonant subprocesses refer to &
      &process component #", 1
  end subroutine entry_write_resonant_subprocess_data

```

Display of the master process for the current event, for diagnostics.

```

<Simulations: entry: TBP>+≡
  procedure :: write_process_data => entry_write_process_data

<Simulations: sub interfaces>+≡
  module subroutine entry_write_process_data &
    (entry, unit, show_process, show_instance, verbose)
    class(entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_process
    logical, intent(in), optional :: show_instance
    logical, intent(in), optional :: verbose
  end subroutine entry_write_process_data

<Simulations: procedures>+≡
  module subroutine entry_write_process_data &
    (entry, unit, show_process, show_instance, verbose)
    class(entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_process
    logical, intent(in), optional :: show_instance
    logical, intent(in), optional :: verbose
    integer :: u, i
    logical :: s_proc, s_inst, verb
    type(process_t), pointer :: process
    type(process_instance_t), pointer :: instance
    u = given_output_unit (unit)
    s_proc = .false.; if (present (show_process)) s_proc = show_process
    s_inst = .false.; if (present (show_instance)) s_inst = show_instance
    verb = .false.; if (present (verbose)) verb = verbose
    if (s_proc .or. s_inst) then

```



```

write (u, "(1x,A,':')") "Process data"
if (s_proc) then
  process => entry%process
  if (associated (process)) then
    if (verb) then
      call write_separator (u, 2)
      call process%write (.false., u)
    else
      call process%show (u, verbose=.false.)
    end if
  else
    write (u, "(3x,A)") "[not associated]"
  end if
end if
if (s_inst) then
  instance => entry%instance
  if (associated (instance)) then
    if (verb) then
      call instance%write (u)
    else
      call instance%write_header (u)
    end if
  else
    write (u, "(3x,A)") "Process instance: [not associated]"
  end if
end if
end if
end subroutine entry_write_process_data

```

33.9.7 Entries for alternative environment

Entries for alternate environments. [No additional components anymore, so somewhat redundant.]

```

<Simulations: types>+≡
  type, extends (entry_t) :: alt_entry_t
    contains
      <Simulations: alt entry: TBP>
    end type alt_entry_t

```

The alternative entries are there to re-evaluate the event, given momenta, in a different context.

Therefore, we allocate a local process object and use this as the reference for the local process instance, when initializing the entry. We temporarily import the `process` object into an `integration_t` wrapper, to take advantage of the associated methods. The local process object is built in the context of the current environment, here called `global`. Then, we initialize the process instance.

The `master_process` object contains the integration results to which we refer when recalculating an event. Therefore, we use this object instead of the locally built `process` when we extract the integration results.

The locally built `process` object should be finalized when done. It remains accessible via the `event_t` base object of `entry`, which contains pointers to the process and instance.

```

<Simulations: alt entry: TBP>≡
  procedure :: init_alt => alt_entry_init

<Simulations: sub interfaces>+≡
  module subroutine alt_entry_init (entry, process_id, master_process, local)
    class<alt_entry_t>, intent(inout), target :: entry
    type<string_t>, intent(in) :: process_id
    type<process_t>, intent(in), target :: master_process
    type<rt_data_t>, intent(inout), target :: local
  end subroutine alt_entry_init

<Simulations: procedures>+≡
  module subroutine alt_entry_init (entry, process_id, master_process, local)
    class<alt_entry_t>, intent(inout), target :: entry
    type<string_t>, intent(in) :: process_id
    type<process_t>, intent(in), target :: master_process
    type<rt_data_t>, intent(inout), target :: local
    type<process_t>, pointer :: process
    type<process_instance_t>, pointer :: process_instance
    type<string_t> :: run_id
    integer :: i

    call msg_message ("Simulate: initializing alternate process setup ...")

    run_id = &
      local%var_list%get_sval (var_str ("$_run_id"))
    call local%set_log (var_str ("?rebuild_phase_space"), &
      .false., is_known = .true.)
    call local%set_log (var_str ("?check_phs_file"), &
      .false., is_known = .true.)
    call local%set_log (var_str ("?rebuild_grids"), &
      .false., is_known = .true.)

    call entry%basic_init (local%var_list)

    call prepare_local_process (process, process_id, local)
    entry%process_id = process_id
    entry%run_id = run_id

    call entry%import_process_characteristics (process)

    allocate (entry%mci_sets (entry%n_mci))
    do i = 1, size (entry%mci_sets)
      call entry%mci_sets(i)%init (i, master_process)
    end do

    call entry%import_process_results (master_process)
    call entry%prepare_expressions (local)

    call prepare_process_instance (process_instance, process, local%model)
    call entry%setup_event_transforms (process, local)

```

```

call entry%connect (process_instance, local%model, local%process_stack)
call entry%setup_expressions ()

entry%model => process%get_model_ptr ()

call msg_message ("... alternate process setup complete.")

end subroutine alt_entry_init

```

Copy the particle set from the master entry to the alternate entry. This is the particle set of the hard process.

```

<Simulations: alt_entry: TBP>+≡
  procedure :: fill_particle_set => entry_fill_particle_set

<Simulations: sub interfaces>+≡
  module subroutine entry_fill_particle_set (alt_entry, entry)
    class(alt_entry_t), intent(inout) :: alt_entry
    class(entry_t), intent(in), target :: entry
  end subroutine entry_fill_particle_set

<Simulations: procedures>+≡
  module subroutine entry_fill_particle_set (alt_entry, entry)
    class(alt_entry_t), intent(inout) :: alt_entry
    class(entry_t), intent(in), target :: entry
    type(particle_set_t) :: pset
    call entry%get_hard_particle_set (pset)
    call alt_entry%set_hard_particle_set (pset)
    call pset%final ()
  end subroutine entry_fill_particle_set

```

33.9.8 The simulation object

Each simulation object corresponds to an event sample, identified by the **sample_id**.

The simulation may cover several processes simultaneously. All process-specific data, including the event records, are stored in the **entry** subobjects. The **current** index indicates which record was selected last. **version** is foreseen to contain a tag on the WHIZARD event file version. It can be

```

<Simulations: public>≡
  public :: simulation_t

<Simulations: types>+≡
  type :: simulation_t
    private
    type(rt_data_t), pointer :: local => null ()
    type(string_t) :: sample_id
    logical :: unweighted = .true.
    logical :: negative_weights = .false.
    logical :: support_resonance_history = .false.
    logical :: respect_selection = .true.
    integer :: norm_mode = NORM_UNDEFINED
    logical :: update_sqme = .false.
    logical :: update_weight = .false.
    logical :: update_event = .false.

```

```

logical :: recover_beams = .false.
logical :: pacify = .false.
integer :: n_max_tries = 10000
integer :: n_prc = 0
integer :: n_alt = 0
logical :: has_integral = .false.
logical :: valid = .false.
real(default) :: integral = 0
real(default) :: error = 0
integer :: version = 1
character(32) :: md5sum_prc = ""
character(32) :: md5sum_cfg = ""
character(32), dimension(:), allocatable :: md5sum_alt
type(entry_t), dimension(:), allocatable :: entry
type(alt_entry_t), dimension(:,:), allocatable :: alt_entry
type(selector_t) :: process_selector
integer :: n_evt_requested = 0
integer :: event_index_offset = 0
logical :: event_index_set = .false.
integer :: event_index = 0
integer :: split_n_evt = 0
integer :: split_n_kbytes = 0
integer :: split_index = 0
type(counter_t) :: counter
class(rng_t), allocatable :: rng
integer :: i_prc = 0
integer :: i_mci = 0
real(default) :: weight = 0
real(default) :: excess = 0
integer :: n_dropped = 0
contains
  <Simulations: simulation: TBP>
end type simulation_t

```

Output of the simulation data

`write_config` writes just the configuration. `write` as a method of the base type `event_t` writes the current event and process instance, depending on options.

<Simulations: simulation: TBP>≡

```
procedure :: write => simulation_write
```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_write (object, unit, testflag)
  class(simulation_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
end subroutine simulation_write

```

<Simulations: procedures>+≡

```

module subroutine simulation_write (object, unit, testflag)
  class(simulation_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag

```

```

logical :: pacified
integer :: u, i
u = given_output_unit (unit)
pacified = object%pacify; if (present (testflag)) pacified = testflag
call write_separator (u, 2)
write (u, "(1x,A,A,A)") "Event sample: '", char (object%sample_id), "'"
write (u, "(3x,A,I0)") "Processes      = ", object%n_prc
if (object%n_alt > 0) then
  write (u, "(3x,A,I0)") "Alt.wgts      = ", object%n_alt
end if
write (u, "(3x,A,L1)") "Unweighted    = ", object%unweighted
write (u, "(3x,A,A)") "Event norm    = ", &
  char (event_normalization_string (object%norm_mode))
write (u, "(3x,A,L1)") "Neg. weights = ", object%negative_weights
write (u, "(3x,A,L1)") "Res. history = ", object%support_resonance_history
write (u, "(3x,A,L1)") "Respect sel. = ", object%respect_selection
write (u, "(3x,A,L1)") "Update sqme  = ", object%update_sqme
write (u, "(3x,A,L1)") "Update wgt   = ", object%update_weight
write (u, "(3x,A,L1)") "Update event = ", object%update_event
write (u, "(3x,A,L1)") "Recov. beams = ", object%recover_beams
write (u, "(3x,A,L1)") "Pacify      = ", object%pacify
write (u, "(3x,A,I0)") "Max. tries   = ", object%n_max_tries
if (object%has_integral) then
  if (pacified) then
    write (u, "(3x,A," // FMT_15 // ")") &
      "Integral      = ", object%integral
    write (u, "(3x,A," // FMT_15 // ")") &
      "Error         = ", object%error
  else
    write (u, "(3x,A," // FMT_19 // ")") &
      "Integral      = ", object%integral
    write (u, "(3x,A," // FMT_19 // ")") &
      "Error         = ", object%error
  end if
else
  write (u, "(3x,A)") "Integral      = [undefined]"
end if
write (u, "(3x,A,L1)") "Sim. valid    = ", object%valid
write (u, "(3x,A,I0)") "Ev.file ver. = ", object%version
if (object%md5sum_prc /= "") then
  write (u, "(3x,A,A,A)") "MD5 sum (proc) = '", object%md5sum_prc, "'"
end if
if (object%md5sum_cfg /= "") then
  write (u, "(3x,A,A,A)") "MD5 sum (config) = '", object%md5sum_cfg, "'"
end if
write (u, "(3x,A,I0)") "Events requested = ", object%n_evt_requested
if (object%event_index_offset /= 0) then
  write (u, "(3x,A,I0)") "Event index offset= ", object%event_index_offset
end if
if (object%event_index_set) then
  write (u, "(3x,A,I0)") "Event index      = ", object%event_index
end if
if (object%split_n_evt > 0 .or. object%split_n_kbytes > 0) then
  write (u, "(3x,A,I0)") "Events per file  = ", object%split_n_evt

```

```

        write (u, "(3x,A,I0)") "KBytes per file  = ", object%split_n_kbytes
        write (u, "(3x,A,I0)") "First file index = ", object%split_index
    end if
    call object%counter%write (u)
    call write_separator (u)
    if (object%i_prc /= 0) then
        write (u, "(1x,A)") "Current event:"
        write (u, "(3x,A,I0,A,A)") "Process #", &
            object%i_prc, ": ", &
            char (object%entry(object%i_prc)%process_id)
        write (u, "(3x,A,I0)") "MCI set #", object%i_mci
        write (u, "(3x,A," // FMT_19 // ")") "Weight  = ", object%weight
        if (.not. vanishes (object%excess)) &
            write (u, "(3x,A," // FMT_19 // ")") "Excess  = ", object%excess
        write (u, "(3x,A,I0)") "Zero-weight events dropped = ", object%n_dropped
    else
        write (u, "(1x,A,I0,A,A)") "Current event: [undefined]"
    end if
    call write_separator (u)
    if (allocated (object%rng)) then
        call object%rng%write (u)
    else
        write (u, "(3x,A)") "Random-number generator: [undefined]"
    end if
    if (allocated (object%entry)) then
        do i = 1, size (object%entry)
            if (i == 1) then
                call write_separator (u, 2)
            else
                call write_separator (u)
            end if
            write (u, "(1x,A,I0,A)") "Process #", i, ":"
            call object%entry(i)%write_config (u, pacified)
        end do
    end if
    call write_separator (u, 2)
end subroutine simulation_write

```

Write the current event record. If an explicit index is given, write that event record.

We implement writing to unit (event contents / debugging format) and writing to an eio event stream (storage). We include a testflag in order to suppress numerical noise in the testsuite.

<Simulations: simulation: TBP>+≡

```

generic :: write_event => write_event_unit
procedure :: write_event_unit => simulation_write_event_unit

```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_write_event_unit &
    (object, unit, i_prc, verbose, testflag)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer, intent(in), optional :: i_prc

```

```

        logical, intent(in), optional :: testflag
    end subroutine simulation_write_event_unit

<Simulations: procedures>+≡
module subroutine simulation_write_event_unit &
    (object, unit, i_prc, verbose, testflag)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: testflag
    logical :: pacified
    integer :: current
    pacified = .false.; if (present(testflag)) pacified = testflag
    pacified = pacified .or. object%pacify
    if (present (i_prc)) then
        current = i_prc
    else
        current = object%i_prc
    end if
    if (current > 0) then
        call object%entry(current)%write (unit, verbose = verbose, &
            testflag = pacified)
    else
        call msg_fatal ("Simulation: write event: no process selected")
    end if
end subroutine simulation_write_event_unit

```

This writes one of the alternate events, if allocated.

```

<Simulations: simulation: TBP>+≡
    procedure :: write_alt_event => simulation_write_alt_event

<Simulations: sub interfaces>+≡
    module subroutine simulation_write_alt_event (object, unit, j_alt, i_prc, &
        verbose, testflag)
        class(simulation_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: j_alt
        integer, intent(in), optional :: i_prc
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: testflag
    end subroutine simulation_write_alt_event

<Simulations: procedures>+≡
    module subroutine simulation_write_alt_event (object, unit, j_alt, i_prc, &
        verbose, testflag)
        class(simulation_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: j_alt
        integer, intent(in), optional :: i_prc
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: testflag
        integer :: i, j
        if (present (j_alt)) then
            j = j_alt

```

```

else
    j = 1
end if
if (present (i_prc)) then
    i = i_prc
else
    i = object%i_prc
end if
if (i > 0) then
    if (j > 0 .and. j <= object%n_alt) then
        call object%alt_entry(i,j)%write (unit, verbose = verbose, &
            testflag = testflag)
    else
        call msg_fatal ("Simulation: write alternate event: out of range")
    end if
else
    call msg_fatal ("Simulation: write alternate event: no process selected")
end if
end subroutine simulation_write_alt_event

```

This writes the contents of the resonant subprocess set in the current event record.

```

<Simulations: simulation: TBP>+≡
    procedure :: write_resonant_subprocess_data &
        => simulation_write_resonant_subprocess_data

<Simulations: sub interfaces>+≡
    module subroutine simulation_write_resonant_subprocess_data &
        (object, unit, i_prc)
        class(simulation_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: i_prc
    end subroutine simulation_write_resonant_subprocess_data

<Simulations: procedures>+≡
    module subroutine simulation_write_resonant_subprocess_data &
        (object, unit, i_prc)
        class(simulation_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: i_prc
        integer :: i
        if (present (i_prc)) then
            i = i_prc
        else
            i = object%i_prc
        end if
        call object%entry(i)%write_resonant_subprocess_data (unit)
    end subroutine simulation_write_resonant_subprocess_data

```

The same for the master process, as an additional debugging aid.

```

<Simulations: simulation: TBP>+≡
    procedure :: write_process_data &
        => simulation_write_process_data

```



```

<Simulations: sub interfaces>+≡
  module subroutine simulation_write_process_data &
    (object, unit, i_prc, &
      show_process, show_instance, verbose)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: show_process
    logical, intent(in), optional :: show_instance
    logical, intent(in), optional :: verbose
  end subroutine simulation_write_process_data

```

```

<Simulations: procedures>+≡
  module subroutine simulation_write_process_data &
    (object, unit, i_prc, &
      show_process, show_instance, verbose)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: show_process
    logical, intent(in), optional :: show_instance
    logical, intent(in), optional :: verbose
    integer :: i
    if (present (i_prc)) then
      i = i_prc
    else
      i = object%i_prc
    end if
    call object%entry(i)%write_process_data &
      (unit, show_process, show_instance, verbose)
  end subroutine simulation_write_process_data

```

Write the actual efficiency of the simulation run. We get the total number of events stored in the simulation counter and compare this with the total number of calls stored in the event entries.

In order not to miscount samples that are partly read from file, use the **generated** counter, not the **total** counter.

```

<Simulations: simulation: TBP>+≡
  procedure :: show_efficiency => simulation_show_efficiency

<Simulations: sub interfaces>+≡
  module subroutine simulation_show_efficiency (simulation)
    class(simulation_t), intent(inout) :: simulation
  end subroutine simulation_show_efficiency

```

```

<Simulations: procedures>+≡
  module subroutine simulation_show_efficiency (simulation)
    class(simulation_t), intent(inout) :: simulation
    integer :: n_events, n_calls
    real(default) :: eff
    n_events = simulation%counter%generated
    n_calls = sum (simulation%entry%get_actual_calls_total ())
    if (n_calls > 0) then
      eff = real (n_events, kind=default) / n_calls
      write (msg_buffer, "(A,1x,F6.2,1x,A)") &

```

```

        "Events: actual unweighting efficiency =", 100 * eff, "%"
        call msg_message ()
    end if
end subroutine simulation_show_efficiency

```

Compute the checksum of the process set. We retrieve the MD5 sums of all processes. This depends only on the process definitions, while parameters are not considered. The configuration checksum is retrieved from the MCI records in the process objects and furthermore includes beams, parameters, integration results, etc., so matching the latter should guarantee identical physics.

```

<Simulations: simulation: TBP>+=
    procedure :: compute_md5sum => simulation_compute_md5sum

<Simulations: sub interfaces>+=
    module subroutine simulation_compute_md5sum (simulation)
        class(simulation_t), intent(inout) :: simulation
    end subroutine simulation_compute_md5sum

<Simulations: procedures>+=
    module subroutine simulation_compute_md5sum (simulation)
        class(simulation_t), intent(inout) :: simulation
        type(process_t), pointer :: process
        type(string_t) :: buffer
        integer :: j, i, n_mci, i_mci, n_component, i_component
        if (simulation%md5sum_prc == "") then
            buffer = ""
            do i = 1, simulation%n_prc
                if (.not. simulation%entry(i)%valid) cycle
                process => simulation%entry(i)%get_process_ptr ()
                if (associated (process)) then
                    n_component = process%get_n_components ()
                    do i_component = 1, n_component
                        if (process%has_matrix_element (i_component)) then
                            buffer = buffer // process%get_md5sum_prc (i_component)
                        end if
                    end do
                end if
            end do
            simulation%md5sum_prc = md5sum (char (buffer))
        end if
        if (simulation%md5sum_cfg == "") then
            buffer = ""
            do i = 1, simulation%n_prc
                if (.not. simulation%entry(i)%valid) cycle
                process => simulation%entry(i)%get_process_ptr ()
                if (associated (process)) then
                    n_mci = process%get_n_mci ()
                    do i_mci = 1, n_mci
                        buffer = buffer // process%get_md5sum_mci (i_mci)
                    end do
                end if
            end do
            simulation%md5sum_cfg = md5sum (char (buffer))
        end if
    end if
end if

```

```

do j = 1, simulation%n_alt
  if (simulation%md5sum_alt(j) == "") then
    buffer = ""
    do i = 1, simulation%n_prc
      process => simulation%alt_entry(i,j)%get_process_ptr ()
      if (associated (process)) then
        buffer = buffer // process%get_md5sum_cfg ()
      end if
    end do
    simulation%md5sum_alt(j) = md5sum (char (buffer))
  end if
end do
end subroutine simulation_compute_md5sum

```

Simulation-object finalizer

```

<Simulations: simulation: TBP>+≡
  procedure :: final => simulation_final

<Simulations: sub interfaces>+≡
  module subroutine simulation_final (object)
    class(simulation_t), intent(inout) :: object
  end subroutine simulation_final

<Simulations: procedures>+≡
  module subroutine simulation_final (object)
    class(simulation_t), intent(inout) :: object
    integer :: i, j
    if (allocated (object%entry)) then
      do i = 1, size (object%entry)
        call object%entry(i)%final ()
      end do
    end if
    if (allocated (object%alt_entry)) then
      do j = 1, size (object%alt_entry, 2)
        do i = 1, size (object%alt_entry, 1)
          call object%alt_entry(i,j)%final ()
        end do
      end do
    end if
    if (allocated (object%rng)) call object%rng%final ()
  end subroutine simulation_final

```

Simulation-object initialization

We can deduce all data from the given list of process IDs and the global data set. The process objects are taken from the stack. Once the individual integrals are known, we add them (and the errors), to get the sample integral.

If there are alternative environments, we suspend initialization for setting up alternative process objects, then restore the master process and its parameters. The generator or rescanner can then switch rapidly between processes.

If `integrate` is set, we make sure that all affected processes are integrated before simulation. This is necessary if we want to actually generate events. If `integrate` is unset, we do not need the integral because we just rescan existing events. In that case, we just need compiled matrix elements.

If `generate` is set, we prepare for actually generating events. Otherwise, we may only read and rescan events.

```

<Simulations: simulation: TBP>+≡
  procedure :: init => simulation_init

<Simulations: sub interfaces>+≡
  module subroutine simulation_init (simulation, &
    process_id, integrate, generate, local, global, alt_env)
    class(simulation_t), intent(out), target :: simulation
    type(string_t), dimension(:), intent(in) :: process_id
    logical, intent(in) :: integrate, generate
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    type(rt_data_t), dimension(:), intent(inout), optional, target :: alt_env
  end subroutine simulation_init

<Simulations: procedures>+≡
  module subroutine simulation_init (simulation, &
    process_id, integrate, generate, local, global, alt_env)
    class(simulation_t), intent(out), target :: simulation
    type(string_t), dimension(:), intent(in) :: process_id
    logical, intent(in) :: integrate, generate
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    type(rt_data_t), dimension(:), intent(inout), optional, target :: alt_env
    class(rng_factory_t), allocatable :: rng_factory
    integer :: next_rng_seed
    type(string_t) :: norm_string, version_string
    logical :: use_process
    integer :: i, j
    type(string_t) :: sample_suffix
  <Simulations: simulation init: extra variables>
    sample_suffix = ""
  <Simulations: simulation init: extra init>
    simulation%local => local
    simulation%sample_id = &
      local%get_sval (var_str ("sample"))
    simulation%unweighted = &
      local%get_lval (var_str ("unweighted"))
    simulation%negative_weights = &
      local%get_lval (var_str ("negative_weights"))
    simulation%support_resonance_history = &
      local%get_lval (var_str ("resonance_history"))
    simulation%respect_selection = &
      local%get_lval (var_str ("sample_select"))
    version_string = &
      local%get_sval (var_str ("event_file_version"))
    norm_string = &
      local%get_sval (var_str ("sample_normalization"))
    simulation%norm_mode = &
      event_normalization_mode (norm_string, simulation%unweighted)

```

```

simulation%pacify = &
    local%get_lval (var_str ("?sample_pacify"))
simulation%event_index_offset = &
    local%get_ival (var_str ("event_index_offset"))
simulation%n_max_tries = &
    local%get_ival (var_str ("sample_max_tries"))
simulation%split_n_evt = &
    local%get_ival (var_str ("sample_split_n_evt"))
simulation%split_n_kbytes = &
    local%get_ival (var_str ("sample_split_n_kbytes"))
simulation%split_index = &
    local%get_ival (var_str ("sample_split_index"))
simulation%update_sqme = &
    local%get_lval (var_str ("?update_sqme"))
simulation%update_weight = &
    local%get_lval (var_str ("?update_weight"))
simulation%update_event = &
    local%get_lval (var_str ("?update_event"))
simulation%recover_beams = &
    local%get_lval (var_str ("?recover_beams"))
simulation%counter%reproduce_xsection = &
    local%get_lval (var_str ("?check_event_weights_against_xsection"))
use_process = &
    integrate .or. generate &
    .or. simulation%update_sqme &
    .or. simulation%update_weight &
    .or. simulation%update_event &
    .or. present (alt_env)
select case (size (process_id))
case (0)
    call msg_error ("Simulation: no process selected")
case (1)
    write (msg_buffer, "(A,A,A)") &
        "Starting simulation for process '", &
        char (process_id(1)), "'"
    call msg_message ()
case default
    write (msg_buffer, "(A,A,A)") &
        "Starting simulation for processes '", &
        char (process_id(1)), "' etc."
    call msg_message ()
end select
select case (char (version_string))
case ("", "2.2.4")
    simulation%version = 2
case ("2.2")
    simulation%version = 1
case default
    simulation%version = 0
end select
if (simulation%version == 0) then
    call msg_fatal ("Event file format '" &
        // char (version_string) &
        // "' is not compatible with this version.")

```

```

end if
simulation%n_prc = size (process_id)
allocate (simulation%entry (simulation%n_prc))
if (present (alt_env)) then
  simulation%n_alt = size (alt_env)
  do i = 1, simulation%n_prc
    call simulation%entry(i)%init (process_id(i), &
      use_process, integrate, generate, &
      simulation%update_sqme, &
      simulation%support_resonance_history, &
      local, global, simulation%n_alt)
    if (signal_is_pending ()) return
  end do
  simulation%valid = any (simulation%entry%valid)
  if (.not. simulation%valid) then
    call msg_error ("Simulate: no process has a valid matrix element.")
    return
  end if
  call simulation%update_processes ()
  allocate (simulation%alt_entry (simulation%n_prc, simulation%n_alt))
  allocate (simulation%md5sum_alt (simulation%n_alt))
  simulation%md5sum_alt = ""
  do j = 1, simulation%n_alt
    do i = 1, simulation%n_prc
      call simulation%alt_entry(i,j)%init_alt (process_id(i), &
        simulation%entry(i)%get_process_ptr (), alt_env(j))
      if (signal_is_pending ()) return
    end do
  end do
  call simulation%restore_processes ()
else
  do i = 1, simulation%n_prc
    call simulation%entry(i)%init &
      (process_id(i), &
      use_process, integrate, generate, &
      simulation%update_sqme, &
      simulation%support_resonance_history, &
      local, global)
    call simulation%entry(i)%determine_if_powheg_matching ()
    if (signal_is_pending ()) return
    if (simulation%entry(i)%is_nlo ()) &
      call simulation%entry(i)%setup_additional_entries ()
  end do
  simulation%valid = any (simulation%entry%valid)
  if (.not. simulation%valid) then
    call msg_error ("Simulate: " &
      // "no process has a valid matrix element.")
    return
  end if
end if
!!! if this becomes conditional, some ref files will need update (seed change)
!   if (generate) then
    call dispatch_rng_factory (rng_factory, local%var_list, next_rng_seed)
    call update_rng_seed_in_var_list (local%var_list, next_rng_seed)

```

```

        call rng_factory%make (simulation%rng)
        <Simulations: simulation init: extra RNG init>
!    end if
    if (all (simulation%entry%has_integral)) then
        simulation%integral = sum (simulation%entry%integral)
        simulation%error = sqrt (sum (simulation%entry%error ** 2))
        simulation%has_integral = .true.
        if (integrate .and. generate) then
            do i = 1, simulation%n_prc
                if (simulation%entry(i)%integral < 0 .and. .not. &
                    simulation%negative_weights) then
                    call msg_fatal ("Integral of process '" // &
                        char (process_id (i)) // "'is negative.")
                end if
            end do
        end if
    else
        if (integrate .and. generate) &
            call msg_error ("Simulation contains undefined integrals.")
        end if
        if (simulation%integral > 0 .or. &
            (simulation%integral < 0 .and. simulation%negative_weights)) then
            simulation%valid = .true.
        else if (generate) then
            call msg_error ("Simulate: " &
                // "sum of process integrals must be positive; skipping.")
            simulation%valid = .false.
        else
            simulation%valid = .true.
        end if
        if (simulation%sample_id == "") then
            simulation%sample_id = simulation%get_default_sample_name ()
        end if
        simulation%sample_id = simulation%sample_id // sample_suffix
        if (simulation%valid) call simulation%compute_md5sum ()
    end subroutine simulation_init

```

The RNG initialization depends on serial/MPI mode.

<Simulations: simulation init: extra variables>≡

<MPI: Simulations: simulation init: extra variables>≡

```
integer :: rank, n_size
```

<Simulations: simulation init: extra init>≡

<MPI: Simulations: simulation init: extra init>≡

```
call mpi_get_comm_id (n_size, rank)
if (n_size > 1) then
    sample_suffix = var_str ("-") // str (rank)
end if

```

<Simulations: simulation init: extra RNG init>≡

<MPI: Simulations: simulation init: extra RNG init>≡

```
do i = 2, rank + 1
    select type (rng => simulation%rng)

```

```

type is (rng_stream_t)
  call rng%next_substream ()
  if (i == rank) &
    call msg_message ("Simulate: Advance RNG for parallel event generation")
class default
  call rng%write ()
  call msg_bug ("Parallel event generation: random-number generator &
    &must be 'rng_stream'.")
end select
end do

```

The number of events that we want to simulate is determined by the settings of `n_events`, `luminosity`, and `?unweighted`. For weighted events, we take `n_events` at face value as the number of matrix element calls. For unweighted events, if the process is a decay, `n_events` is the number of unweighted events. In these cases, the `luminosity` setting is ignored.

For unweighted events with a scattering process, we calculate the event number that corresponds to the `luminosity`, given the current value of the integral. We then compare this with `n_events` and choose the larger number.

```

<Simulations: simulation: TBP>+≡
  procedure :: compute_n_events => simulation_compute_n_events

<Simulations: sub interfaces>+≡
  module subroutine simulation_compute_n_events (simulation, n_events)
    class(simulation_t), intent(in) :: simulation
    integer, intent(out) :: n_events
  end subroutine simulation_compute_n_events

<Simulations: procedures>+≡
  module subroutine simulation_compute_n_events (simulation, n_events)
    class(simulation_t), intent(in) :: simulation
    integer, intent(out) :: n_events
    real(default) :: lumi, x_events_lumi
    integer :: n_events_lumi
    logical :: is_scattering
    n_events = &
      simulation%local%get_ival (var_str ("n_events"))
    lumi = &
      simulation%local%get_rval (var_str ("luminosity"))
    if (simulation%unweighted) then
      is_scattering = simulation%entry(1)%n_in == 2
      if (is_scattering) then
        x_events_lumi = abs (simulation%integral * lumi)
        if (x_events_lumi < huge (n_events)) then
          n_events_lumi = nint (x_events_lumi)
        else
          call msg_message ("Simulation: luminosity too large, &
            &limiting number of events")
          n_events_lumi = huge (n_events)
        end if
      if (n_events_lumi > n_events) then
        call msg_message ("Simulation: using n_events as computed from &
          &luminosity value")
        n_events = n_events_lumi
      else

```



```

        write (msg_buffer, "(A,1x,I0)") &
            "Simulation: requested number of events =", n_events
        call msg_message ()
        if (.not. vanishes (simulation%integral)) then
            write (msg_buffer, "(A,1x,ES11.4)") &
                "            corr. to luminosity [fb-1] = ", &
                n_events / simulation%integral
            call msg_message ()
        end if
    end if
end if
end if
end subroutine simulation_compute_n_events

```

Configuration of the OpenMP parameters, in case OpenMP is active. We use the settings accessible via the local environment.

```

<Simulations: simulation: TBP>+≡
    procedure :: setup_openmp => simulation_setup_openmp

<Simulations: sub interfaces>+≡
    module subroutine simulation_setup_openmp (simulation)
        class(simulation_t), intent(inout) :: simulation
    end subroutine simulation_setup_openmp

<Simulations: procedures>+≡
    module subroutine simulation_setup_openmp (simulation)
        class(simulation_t), intent(inout) :: simulation

        call openmp_set_num_threads_verbose &
            (simulation%local%get_ival (var_str ("openmp_num_threads")), &
            simulation%local%get_lval (var_str ("?openmp_logging")))

    end subroutine simulation_setup_openmp

```

Configuration of the event-stream array – i.e., the setup of output file formats.

```

<Simulations: simulation: TBP>+≡
    procedure :: prepare_event_streams => simulation_prepare_event_streams

<Simulations: sub interfaces>+≡
    module subroutine simulation_prepare_event_streams (sim, es_array)
        class(simulation_t), intent(inout) :: sim
        type(event_stream_array_t), intent(out) :: es_array
    end subroutine simulation_prepare_event_streams

<Simulations: procedures>+≡
    module subroutine simulation_prepare_event_streams (sim, es_array)
        class(simulation_t), intent(inout) :: sim
        type(event_stream_array_t), intent(out) :: es_array

        integer :: n_events
        logical :: rebuild_events, read_raw, write_raw
        integer :: checkpoint, callback
        integer :: n_fmt
        type(event_sample_data_t) :: data
        type(string_t), dimension(:), allocatable :: sample_fmt

```

```

n_events = &
    sim%n_evt_requested
rebuild_events = &
    sim%local%get_lval (var_str ("?rebuild_events"))
read_raw = &
    sim%local%get_lval (var_str ("?read_raw")) .and. .not. rebuild_events
write_raw = &
    sim%local%get_lval (var_str ("?write_raw"))
checkpoint = &
    sim%local%get_ival (var_str ("checkpoint"))
callback = &
    sim%local%get_ival (var_str ("event_callback_interval"))
if (read_raw) then
    inquire (file = char (sim%sample_id) // ".evx", exist = read_raw)
end if
if (allocated (sim%local%sample_fmt)) then
    n_fmt = size (sim%local%sample_fmt)
else
    n_fmt = 0
end if
data = sim%get_data ()
data%n_evt = n_events
data%nlo_multiplier = sim%get_n_nlo_entries (1)
if (read_raw) then
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = sim%local%sample_fmt
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        input = var_str ("raw"), &
        allow_switch = write_raw, &
        checkpoint = checkpoint, &
        callback = callback)
else if (write_raw) then
    allocate (sample_fmt (n_fmt + 1))
    if (n_fmt > 0) sample_fmt(:n_fmt) = sim%local%sample_fmt
    sample_fmt(n_fmt+1) = var_str ("raw")
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        checkpoint = checkpoint, &
        callback = callback)
else if (allocated (sim%local%sample_fmt) &
    .or. checkpoint > 0 &
    .or. callback > 0) then
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = sim%local%sample_fmt
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        checkpoint = checkpoint, &
        callback = callback)
end if

```

```
end subroutine simulation_prepare_event_streams
```

<Simulations: simulation: TBP>+≡

```
procedure :: get_n_nlo_entries => simulation_get_n_nlo_entries
```

<Simulations: sub interfaces>+≡

```
module function simulation_get_n_nlo_entries &
  (simulation, i_prc) result (n_extra)
  class(simulation_t), intent(in) :: simulation
  integer, intent(in) :: i_prc
  integer :: n_extra
end function simulation_get_n_nlo_entries
```

<Simulations: procedures>+≡

```
module function simulation_get_n_nlo_entries &
  (simulation, i_prc) result (n_extra)
  class(simulation_t), intent(in) :: simulation
  integer, intent(in) :: i_prc
  integer :: n_extra
  n_extra = simulation%entry(i_prc)%count_nlo_entries ()
end function simulation_get_n_nlo_entries
```

Initialize the process selector, using the entry integrals as process weights.

<Simulations: simulation: TBP>+≡

```
procedure :: init_process_selector => simulation_init_process_selector
```

<Simulations: sub interfaces>+≡

```
module subroutine simulation_init_process_selector (simulation)
  class(simulation_t), intent(inout) :: simulation
end subroutine simulation_init_process_selector
```

<Simulations: procedures>+≡

```
module subroutine simulation_init_process_selector (simulation)
  class(simulation_t), intent(inout) :: simulation
  integer :: i
  if (simulation%has_integral) then
    call simulation%process_selector%init (simulation%entry%integral, &
      negative_weights = simulation%negative_weights)
    do i = 1, simulation%n_prc
      associate (entry => simulation%entry(i))
        if (.not. entry%valid) then
          call msg_warning ("Process '" // char (entry%process_id) // &
            "' : matrix element vanishes, no events can be generated.")
          cycle
        end if
        call entry%init_mci_selector (simulation%negative_weights)
        entry%process_weight = simulation%process_selector%get_weight (i)
      end associate
    end do
  end if
end subroutine simulation_init_process_selector
```

Select a process, using the random-number generator.

<Simulations: simulation: TBP>+≡

```
procedure :: select_prc => simulation_select_prc
```

```

<Simulations: sub interfaces>+≡
    module function simulation_select_prc (simulation) result (i_prc)
        class(simulation_t), intent(inout) :: simulation
        integer :: i_prc
    end function simulation_select_prc

```

```

<Simulations: procedures>+≡
    module function simulation_select_prc (simulation) result (i_prc)
        class(simulation_t), intent(inout) :: simulation
        integer :: i_prc
        call simulation%process_selector%generate (simulation%rng, i_prc)
    end function simulation_select_prc

```

Select a MCI set for the selected process.

```

<Simulations: simulation: TBP>+≡
    procedure :: select_mci => simulation_select_mci

```

```

<Simulations: sub interfaces>+≡
    module function simulation_select_mci (simulation) result (i_mci)
        class(simulation_t), intent(inout) :: simulation
        integer :: i_mci
    end function simulation_select_mci

```

```

<Simulations: procedures>+≡
    module function simulation_select_mci (simulation) result (i_mci)
        class(simulation_t), intent(inout) :: simulation
        integer :: i_mci
        i_mci = 0
        if (simulation%i_prc /= 0) then
            i_mci = simulation%entry(simulation%i_prc)%select_mci ()
        end if
    end function simulation_select_mci

```

Generate-event loop

The requested number of events should be set by this, in time for the event-array initializers that may use this number.

```

<Simulations: simulation: TBP>+≡
    procedure :: set_n_events_requested => simulation_set_n_events_requested
    procedure :: get_n_events_requested => simulation_get_n_events_requested

```

```

<Simulations: sub interfaces>+≡
    module subroutine simulation_set_n_events_requested (simulation, n)
        class(simulation_t), intent(inout) :: simulation
        integer, intent(in) :: n
    end subroutine simulation_set_n_events_requested
    module function simulation_get_n_events_requested (simulation) result (n)
        class(simulation_t), intent(in) :: simulation
        integer :: n
    end function simulation_get_n_events_requested

```

```

<Simulations: procedures>+≡
    module subroutine simulation_set_n_events_requested (simulation, n)
        class(simulation_t), intent(inout) :: simulation

```

```

integer, intent(in) :: n

simulation%n_evt_requested = n

end subroutine simulation_set_n_events_requested

module function simulation_get_n_events_requested (simulation) result (n)
  class(simulation_t), intent(in) :: simulation
  integer :: n

  n = simulation%n_evt_requested

end function simulation_get_n_events_requested

```

Generate the number of events that has been set by `simulation_set_n_events_requested`. First select a process and a component set, then generate an event for that process and factorize the quantum state. The pair of random numbers can be used for factorization.

When generating events, we drop all configurations where the event is marked as incomplete. This happens if the event fails cuts. In fact, such events are dropped already by the sampler if unweighting is in effect, so this can happen only for weighted events. By setting a limit given by `sample_max_tries` (user parameter), we can avoid an endless loop.

The `begin_it` and `end_it` limits are equal to 1 and the number of events, respectively, in serial mode, but differ for MPI mode.

TODO: When reading from file, event transforms cannot be applied because the process instance will not be complete. (?)

```

<Simulations: simulation: TBP>+≡
  procedure :: generate => simulation_generate

<Simulations: sub interfaces>+≡
  module subroutine simulation_generate (simulation, es_array)
    class(simulation_t), intent(inout), target :: simulation
    type(event_stream_array_t), intent(inout), optional :: es_array
  end subroutine simulation_generate

<Simulations: procedures>+≡
  module subroutine simulation_generate (simulation, es_array)
    class(simulation_t), intent(inout), target :: simulation
    type(event_stream_array_t), intent(inout), optional :: es_array

    integer :: begin_it, end_it
    integer :: i, j, k

    call simulation%before_first_event (begin_it, end_it, es_array)
    do i = begin_it, end_it
      call simulation%next_event (es_array)
    end do
    call simulation%after_last_event (begin_it, end_it)

  end subroutine simulation_generate

```

The header of the event loop: with all necessary information present in the `simulation` and `es_array` objects, and given a number of events `n` to generate, we prepare for actually generating/reading/writing events.

The procedure returns the real iteration bounds `begin_it` and `end_it` for the event loop. This is nontrivial only for MPI; in serial mode those are equal to 1 and to `n_events`, respectively.

```

<Simulations: simulation: TBP>+≡
    procedure :: before_first_event => simulation_before_first_event

<Simulations: sub interfaces>+≡
    module subroutine simulation_before_first_event (simulation, &
        begin_it, end_it, es_array)
        class(simulation_t), intent(inout), target :: simulation
        integer, intent(out) :: begin_it
        integer, intent(out) :: end_it
        type(event_stream_array_t), intent(inout), optional :: es_array
    end subroutine simulation_before_first_event

<Simulations: procedures>+≡
    module subroutine simulation_before_first_event (simulation, &
        begin_it, end_it, es_array)
        class(simulation_t), intent(inout), target :: simulation
        integer, intent(out) :: begin_it
        integer, intent(out) :: end_it
        type(event_stream_array_t), intent(inout), optional :: es_array

        integer :: n_evt_requested
        logical :: has_input
        integer :: n_events_print
        logical :: is_leading_order
        logical :: is_weighted
        logical :: is_polarized

        n_evt_requested = simulation%n_evt_requested
        n_events_print = n_evt_requested * simulation%get_n_nlo_entries (1)
        is_leading_order = (n_events_print == n_evt_requested)

        has_input = .false.
        if (present (es_array)) has_input = es_array%has_input ()

        is_weighted = .not. simulation%entry(1)%config%unweighted
        is_polarized = simulation%entry(1)%config%factorization_mode &
            /= FM_IGNORE_HELICITY

        call simulation%startup_message_generate ( &
            has_input = has_input, &
            is_weighted = is_weighted, &
            is_polarized = is_polarized, &
            is_leading_order = is_leading_order, &
            n_events = n_events_print)

        call simulation%entry%set_n (n_evt_requested)
        if (simulation%n_alt > 0) call simulation%alt_entry%set_n (n_evt_requested)
        call simulation%init_event_index ()

```

```

begin_it = 1
end_it = n_evt_requested
<Simulations: simulation generate: extra init>

end subroutine simulation_before_first_event

```

Keep the user informed:

```

<Simulations: simulation: TBP>+≡
  procedure, private :: startup_message_generate &
    => simulation_startup_message_generate
<Simulations: sub interfaces>+≡
  module subroutine simulation_startup_message_generate (simulation, &
    has_input, is_weighted, is_polarized, is_leading_order, n_events)
    class(simulation_t), intent(in) :: simulation
    logical, intent(in) :: has_input
    logical, intent(in) :: is_weighted
    logical, intent(in) :: is_polarized
    logical, intent(in) :: is_leading_order
    integer, intent(in) :: n_events
  end subroutine simulation_startup_message_generate
<Simulations: procedures>+≡
  module subroutine simulation_startup_message_generate (simulation, &
    has_input, is_weighted, is_polarized, is_leading_order, n_events)
    class(simulation_t), intent(in) :: simulation
    logical, intent(in) :: has_input
    logical, intent(in) :: is_weighted
    logical, intent(in) :: is_polarized
    logical, intent(in) :: is_leading_order
    integer, intent(in) :: n_events

    type(string_t) :: str1, str2, str3, str4

    if (has_input) then
      str1 = "Events: reading"
    else
      str1 = "Events: generating"
    end if
    if (is_weighted) then
      str2 = "weighted"
    else
      str2 = "unweighted"
    end if
    if (is_polarized) then
      str3 = ", polarized"
    else
      str3 = ", unpolarized"
    end if
    str4 = ""
    if (.not. is_leading_order) str4 = " NLO"

    write (msg_buffer, "(A,1X,I0,1X,A,1X,A)") char (str1), n_events, &
      char (str2) // char(str3) // char(str4), "events ..."
    call msg_message ()
  end subroutine simulation_startup_message_generate

```

```

write (msg_buffer, "(A,1x,A)") "Events: event normalization mode", &
char (event_normalization_string (simulation%norm_mode))
call msg_message ()

end subroutine simulation_startup_message_generate

```

The body of the event loop: generate and process a single event.

Optionally transfer the current event to one of the provided event handles, for in and/or output streams. This works for any stream for which the I/O stream type matches the event-handle type.

```

<Simulations: simulation: TBP>+≡
  procedure :: next_event => simulation_next_event

<Simulations: sub interfaces>+≡
  module subroutine simulation_next_event &
    (simulation, es_array, event_handle_out, event_handle_in)
    class(simulation_t), intent(inout) :: simulation
    type(event_stream_array_t), intent(inout), optional :: es_array
    class(event_handle_t), intent(inout), optional :: event_handle_out
    class(event_handle_t), intent(inout), optional :: event_handle_in
  end subroutine simulation_next_event

<Simulations: procedures>+≡
  module subroutine simulation_next_event &
    (simulation, es_array, event_handle_out, event_handle_in)
    class(simulation_t), intent(inout) :: simulation
    type(event_stream_array_t), intent(inout), optional :: es_array
    class(event_handle_t), intent(inout), optional :: event_handle_out
    class(event_handle_t), intent(inout), optional :: event_handle_in

    type(entry_t), pointer :: current_entry
    logical :: generate_new
    logical :: passed
    integer :: j, k

    call simulation%increment_event_index ()

    if (present (es_array)) then
      call simulation%read_event &
        (es_array,.true., generate_new, event_handle_in)
    else
      generate_new = .true.
    end if

    if (generate_new) then
      simulation%i_prc = simulation%select_prc ()
      simulation%i_mci = simulation%select_mci ()

      associate (entry => simulation%entry(simulation%i_prc))

        entry%instance%i_mci = simulation%i_mci
        call entry%set_active_real_components ()
        current_entry => entry%get_first ()

```



```

do k = 1, current_entry%count_nlo_entries ()
  if (k > 1) then
    current_entry => current_entry%get_next ()
    current_entry%particle_set => current_entry%first%particle_set
    current_entry%particle_set_is_valid &
      = current_entry%first%particle_set_is_valid
  end if
  do j = 1, simulation%n_max_tries
    if (.not. current_entry%valid) call msg_warning &
      ("Process '" // char (current_entry%process_id) // "': " // &
      "matrix element vanishes, no events can be generated.")
    call current_entry%generate (simulation%i_mci, i_nlo = k)
    if (signal_is_pending ()) return
    call simulation%counter%record_mean_and_variance &
      (current_entry%weight_prc, k)
    if (current_entry%has_valid_particle_set ()) exit
  end do
end do
if (entry%is_nlo ()) call entry%reset_nlo_counter ()

if (.not. entry%has_valid_particle_set ()) then
  write (msg_buffer, "(A,I0,A)") "Simulation: failed to &
    &generate valid event after ", &
    simulation%n_max_tries, " tries (sample_max_tries)"
  call msg_fatal ()
end if

current_entry => entry%get_first ()
do k = 1, current_entry%count_nlo_entries ()
  if (k > 1) current_entry => current_entry%get_next ()
  call current_entry%set_index (simulation%get_event_index ())
  call current_entry%evaluate_expressions ()
end do
if (signal_is_pending ()) return

simulation%n_dropped = entry%get_n_dropped ()
if (entry%passed_selection ()) then
  simulation%weight = entry%get_weight_ref ()
  simulation%excess = entry%get_excess_prc ()
end if
call simulation%counter%record &
  (simulation%weight, simulation%excess, simulation%n_dropped)
call entry%record (simulation%i_mci)

end associate

else

  associate (entry => simulation%entry(simulation%i_prc))

    call simulation%set_event_index (entry%get_index ())
    call entry%accept_sqme_ref ()
    call entry%accept_weight_ref ()

```

```

        call entry%check ()
        call entry%evaluate_expressions ()
        if (signal_is_pending ()) return

        simulation%n_dropped = entry%get_n_dropped ()
        if (entry%passed_selection ()) then
            simulation%weight = entry%get_weight_ref ()
            simulation%excess = entry%get_excess_prc ()
        end if
        call simulation%counter%record &
            (simulation%weight, simulation%excess, simulation%n_dropped, &
             from_file=.true.)
        call entry%record (simulation%i_mci, from_file=.true.)

    end associate

end if

call simulation%calculate_alt_entries ()
if (simulation%pacify) call pacify (simulation)
if (signal_is_pending ()) return

if (simulation%respect_selection) then
    passed = simulation%entry(simulation%i_prc)%passed_selection ()
else
    passed = .true.
end if
if (present (es_array)) then
    call simulation%write_event (es_array, passed, event_handle_out)
end if

end subroutine simulation_next_event

```

Cleanup after last event: compute and show summary information.

<Simulations: simulation: TBP>+≡

```
procedure :: after_last_event => simulation_after_last_event
```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_after_last_event (simulation, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: begin_it, end_it
end subroutine simulation_after_last_event

```

<Simulations: procedures>+≡

```

module subroutine simulation_after_last_event (simulation, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: begin_it, end_it

```

```

        call msg_message ("          ... event sample complete.")

```

<Simulations: simulation generate: extra finalize>

```

        if (simulation%unweighted) call simulation%show_efficiency ()
        call simulation%counter%show_excess ()
        call simulation%counter%show_dropped ()
        call simulation%counter%show_mean_and_variance ()

```

```
end subroutine simulation_after_last_event
```

MPI additions

Below, we define code chunks that differ between the serial and MPI versions.

Extra logging for MPI only.

```
<Simulations: simulation: TBP>+≡
  procedure :: activate_extra_logging => simulation_activate_extra_logging

<Simulations: sub interfaces>+≡
  module subroutine simulation_activate_extra_logging (simulation)
    class(simulation_t), intent(in) :: simulation
    end subroutine simulation_activate_extra_logging

<Simulations: procedures>+≡
  module subroutine simulation_activate_extra_logging (simulation)
    class(simulation_t), intent(in) :: simulation
    <Simulations: activate extra logging>
    end subroutine simulation_activate_extra_logging

<Simulations: activate extra logging>≡
<MPI: Simulations: activate extra logging>≡
  logical :: mpi_logging
  integer :: rank, n_size
  call mpi_get_comm_id (n_size, rank)
  mpi_logging = &
    (simulation%local%get_sval (var_str ("%integration_method")) == "vamp2" &
    .and. n_size > 1) &
    .or. simulation%local%get_lval (var_str ("%mpi_logging")))
  call mpi_set_logging (mpi_logging)
```

Extra subroutine to be called before the first event:

```
<Simulations: simulation generate: extra init>≡
<MPI: Simulations: simulation generate: extra init>≡
  call simulation%init_event_loop_mpi (n_evt_requested, begin_it, end_it)
```

Extra subroutine to be called after the last event:

```
<Simulations: simulation generate: extra finalize>≡
<MPI: Simulations: simulation generate: extra finalize>≡
  call simulation%final_event_loop_mpi (begin_it, end_it)
```

For MPI event generation, the event-loop interval (1...n) is split up into intervals of `n_workers`.

```
<MPI: Simulations: simulation: TBP>≡
  procedure, private :: init_event_loop_mpi => simulation_init_event_loop_mpi

<MPI: Simulations: sub interfaces>+≡
  module subroutine simulation_init_event_loop_mpi &
    (simulation, n_events, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: n_events
    integer, intent(out) :: begin_it, end_it
    end subroutine simulation_init_event_loop_mpi
```

(MPI: Simulations: procedures)+≡

```

module subroutine simulation_init_event_loop_mpi &
  (simulation, n_events, begin_it, end_it)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: n_events
  integer, intent(out) :: begin_it, end_it

  integer :: rank, n_workers

  call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
  if (n_workers < 2) then
    begin_it = 1; end_it = n_events
    return
  end if
  call MPI_COMM_RANK (MPI_COMM_WORLD, rank)
  if (rank == 0) then
    call compute_and_scatter_intervals (n_events, begin_it, end_it)
  else
    call retrieve_intervals (begin_it, end_it)
  end if

  !! Event index starts by 0 (before incrementing when the first event gets generated/read in).
  !! Proof: event_index_offset in [0, N], start_it in [1, N].
  simulation%event_index_offset = simulation%event_index_offset + (begin_it - 1)
  call simulation%init_event_index ()
  write (msg_buffer, "(A,IO,A,IO,A)") &
    & "MPI: generate events [", begin_it, ":", end_it, "]"
  call msg_message ()

contains

  subroutine compute_and_scatter_intervals (n_events, begin_it, end_it)
    integer, intent(in) :: n_events
    integer, intent(out) :: begin_it, end_it

    integer, dimension(:), allocatable :: all_begin_it, all_end_it
    integer :: rank, n_workers, n_events_per_worker

    call MPI_COMM_RANK (MPI_COMM_WORLD, rank)
    call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
    allocate (all_begin_it (n_workers), source = 1)
    allocate (all_end_it (n_workers), source = n_events)
    n_events_per_worker = floor (real (n_events, default) / n_workers)
    all_begin_it = [(1 + rank * n_events_per_worker, rank = 0, n_workers - 1)]
    all_end_it = [(rank * n_events_per_worker, rank = 1, n_workers)]
    all_end_it(n_workers) = n_events
    call MPI_SCATTER (all_begin_it, 1, MPI_INTEGER, begin_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)
    call MPI_SCATTER (all_end_it, 1, MPI_INTEGER, end_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)

  end subroutine compute_and_scatter_intervals

  subroutine retrieve_intervals (begin_it, end_it)
    integer, intent(out) :: begin_it, end_it

```

```

integer :: local_begin_it, local_end_it

call MPI_SCATTER (local_begin_it, 1, MPI_INTEGER, begin_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)
call MPI_SCATTER (local_end_it, 1, MPI_INTEGER, end_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)

end subroutine retrieve_intervals

end subroutine simulation_init_event_loop_mpi

```

Synchronize, reduce and collect stuff after the event loop has completed.

```

<MPI: Simulations: simulation: TBP>+≡
  procedure, private :: final_event_loop_mpi => simulation_final_event_loop_mpi

<MPI: Simulations: sub interfaces>+≡
  module subroutine simulation_final_event_loop_mpi &
    (simulation, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: begin_it, end_it
  end subroutine simulation_final_event_loop_mpi

<MPI: Simulations: procedures>+≡
  module subroutine simulation_final_event_loop_mpi &
    (simulation, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: begin_it, end_it

    integer :: n_workers, n_events_local, n_events_global

    call MPI_Barrier (MPI_COMM_WORLD)
    call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
    if (n_workers < 2) return
    n_events_local = end_it - begin_it + 1
    call MPI_ALLREDUCE (n_events_local, n_events_global, 1, &
      MPI_INTEGER, MPI_SUM, &
      & MPI_COMM_WORLD)
    write (msg_buffer, "(2(A,1X,I0))") &
      "MPI: Number of generated events locally", n_events_local, &
      " and in world", n_events_global
    call msg_message ()
    call simulation%counter%allreduce_record ()

  end subroutine simulation_final_event_loop_mpi

```

Alternate environments

Compute the event matrix element and weight for all alternative environments, given the current event and selected process. We first copy the particle set, then temporarily update the process core with local parameters, recalculate everything, and restore the process core.

The event weight is obtained by rescaling the original event weight with the ratio of the new and old `sqme` values. (In particular, if the old value was zero, the weight will stay zero.)

Note: this may turn out to be inefficient because we always replace all parameters and recalculate everything, once for each event and environment. However, a more fine-grained control requires more code. In any case, while we may keep multiple process cores (which stay constant for a simulation run), we still have to update the external matrix element parameters event by event. The matrix element “object” is present only once.

```

<Simulations: simulation: TBP>+≡
    procedure :: calculate_alt_entries => simulation_calculate_alt_entries

<Simulations: sub interfaces>+≡
    module subroutine simulation_calculate_alt_entries (simulation)
        class(simulation_t), intent(inout) :: simulation
        end subroutine simulation_calculate_alt_entries

<Simulations: procedures>+≡
    module subroutine simulation_calculate_alt_entries (simulation)
        class(simulation_t), intent(inout) :: simulation
        real(default) :: sqme_prc, weight_prc, factor
        real(default), dimension(:), allocatable :: sqme_alt, weight_alt
        integer :: n_alt, i, j
        i = simulation%i_prc
        n_alt = simulation%n_alt
        if (n_alt == 0) return
        allocate (sqme_alt (n_alt), weight_alt (n_alt))
        associate (entry => simulation%entry(i))
            do j = 1, n_alt
                if (signal_is_pending ()) return
                if (simulation%update_weight) then
                    factor = entry%get_kinematical_weight ()
                else
                    sqme_prc = entry%get_sqme_prc ()
                    weight_prc = entry%get_weight_prc ()
                    if (sqme_prc /= 0) then
                        factor = weight_prc / sqme_prc
                    else
                        factor = 0
                    end if
                end if
            end do
            associate (alt_entry => simulation%alt_entry(i,j))
                call alt_entry%update_process (saved=.false.)
                call alt_entry%select &
                    (entry%get_i_mci (), entry%get_i_term (), entry%get_channel ())
                call alt_entry%fill_particle_set (entry)
                call alt_entry%recalculate &
                    (update_sqme = .true., &
                     recover_beams = simulation%recover_beams, &
                     weight_factor = factor)
                if (signal_is_pending ()) return
                call alt_entry%accept_sqme_prc ()
                call alt_entry%update_normalization ()
                call alt_entry%accept_weight_prc ()
                call alt_entry%check ()
                call alt_entry%set_index (simulation%get_event_index ())
                call alt_entry%evaluate_expressions ()
                if (signal_is_pending ()) return
            end associate
        end associate
    end subroutine simulation_calculate_alt_entries

```

```

        sqme_alt(j) = alt_entry%get_sqme_ref ()
        if (alt_entry%passed_selection ()) then
            weight_alt(j) = alt_entry%get_weight_ref ()
        end if
    end associate
end do
call entry%update_process (saved=.false.)
call entry%set (sqme_alt = sqme_alt, weight_alt = weight_alt)
call entry%check ()
call entry%store_alt_values ()
end associate
end subroutine simulation_calculate_alt_entries

```

These routines take care of temporary parameter redefinitions that we want to take effect while recalculating the matrix elements. We extract the core(s) of the processes that we are simulating, apply the changes, and make sure that the changes are actually used. This is the duty of `dispatch_core_update`. When done, we restore the original versions using `dispatch_core_restore`.

(Simulations: simulation: TBP)+≡

```

    procedure :: update_processes => simulation_update_processes
    procedure :: restore_processes => simulation_restore_processes

```

(Simulations: sub interfaces)+≡

```

    module subroutine simulation_update_processes (simulation, &
        model, qcd, helicity_selection)
        class(simulation_t), intent(inout) :: simulation
        class(model_data_t), intent(in), optional, target :: model
        type(qcd_t), intent(in), optional :: qcd
        type(helicity_selection_t), intent(in), optional :: helicity_selection
    end subroutine simulation_update_processes
    module subroutine simulation_restore_processes (simulation)
        class(simulation_t), intent(inout) :: simulation
    end subroutine simulation_restore_processes

```

(Simulations: procedures)+≡

```

    module subroutine simulation_update_processes (simulation, &
        model, qcd, helicity_selection)
        class(simulation_t), intent(inout) :: simulation
        class(model_data_t), intent(in), optional, target :: model
        type(qcd_t), intent(in), optional :: qcd
        type(helicity_selection_t), intent(in), optional :: helicity_selection
        integer :: i
        do i = 1, simulation%n_prc
            call simulation%entry(i)%update_process &
                (model, qcd, helicity_selection)
        end do
    end subroutine simulation_update_processes

    module subroutine simulation_restore_processes (simulation)
        class(simulation_t), intent(inout) :: simulation
        integer :: i
        do i = 1, simulation%n_prc
            call simulation%entry(i)%restore_process ()
        end do
    end subroutine simulation_restore_processes

```

```
end subroutine simulation_restore_processes
```

Rescan-Events Loop

Rescan an undefined number of events.

If `update_event` or `update_sqme` is set, we have to recalculate the event, starting from the particle set. If the latter is set, this includes the squared matrix element (i.e., the amplitude is evaluated). Otherwise, only kinematics and observables derived from it are recovered.

If any of the update flags is set, we will come up with separate `sqme_prc` and `weight_prc` values. (The latter is only distinct if `update_weight` is set.) Otherwise, we accept the reference values.

(Simulations: simulation: TBP)+≡

```
procedure :: rescan => simulation_rescan
```

(Simulations: sub interfaces)+≡

```
module subroutine simulation_rescan (simulation, n, es_array, global)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: n
  type(event_stream_array_t), intent(inout) :: es_array
  type(rt_data_t), intent(inout) :: global
end subroutine simulation_rescan
```

(Simulations: procedures)+≡

```
module subroutine simulation_rescan (simulation, n, es_array, global)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: n
  type(event_stream_array_t), intent(inout) :: es_array
  type(rt_data_t), intent(inout) :: global
  type(qcd_t) :: qcd
  type(string_t) :: str1, str2, str3
  logical :: complete, check_match
  str1 = "Rescanning"
  if (simulation%entry(1)%config%unweighted) then
    str2 = "unweighted"
  else
    str2 = "weighted"
  end if
  simulation%n_evt_requested = n
  call simulation%entry%set_n (n)
  if (simulation%update_sqme .or. simulation%update_weight) then
    call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
    call simulation%update_processes &
      (global%model, qcd, global%get_helicity_selection ())
    str3 = "(process parameters updated) "
  else
    str3 = ""
  end if
  write (msg_buffer, "(A,1x,A,1x,A,A,A)") char (str1), char (str2), &
    "events ", char (str3), "..."
  call msg_message ()
  call simulation%init_event_index ()
  check_match = .not. global%var_list%get_lval (var_str ("?rescan_force"))
```



```

do
  call simulation%increment_event_index ()
  call simulation%read_event (es_array, .false., complete)
  if (complete) exit
  if (simulation%update_event &
      .or. simulation%update_sqme &
      .or. simulation%update_weight) then
    call simulation%recalculate (check_match = check_match)
    if (signal_is_pending ()) return
    associate (entry => simulation%entry(simulation%i_prc))
      call entry%update_normalization ()
      if (simulation%update_event) then
        call entry%evaluate_transforms ()
      end if
      call entry%check ()
      call entry%evaluate_expressions ()
      if (signal_is_pending ()) return
      simulation%n_dropped = entry%get_n_dropped ()
      simulation%weight = entry%get_weight_prc ()
      call simulation%counter%record &
        (simulation%weight, n_dropped=simulation%n_dropped, from_file=.true.)
      call entry%record (simulation%i_mci, from_file=.true.)
    end associate
  else
    associate (entry => simulation%entry(simulation%i_prc))
      call entry%accept_sqme_ref ()
      call entry%accept_weight_ref ()
      call entry%check ()
      call entry%evaluate_expressions ()
      if (signal_is_pending ()) return
      simulation%n_dropped = entry%get_n_dropped ()
      simulation%weight = entry%get_weight_ref ()
      call simulation%counter%record &
        (simulation%weight, n_dropped=simulation%n_dropped, from_file=.true.)
      call entry%record (simulation%i_mci, from_file=.true.)
    end associate
  end if
  call simulation%calculate_alt_entries ()
  if (signal_is_pending ()) return
  call simulation%write_event (es_array)
end do
call simulation%counter%show_dropped ()
if (simulation%update_sqme .or. simulation%update_weight) then
  call simulation%restore_processes ()
end if
end subroutine simulation_rescan

```

Event index

Here we handle the event index that is kept in the simulation record. The event index is valid for the current sample. When generating or reading events, we initialize the index with the offset that the user provides (if any) and increment

it for each event that is generated or read from file. The event index is stored in the event-entry that is current for the event. If an event on file comes with its own index, that index overwrites the predefined one and also resets the index within the simulation record.

The event index is not connected to the `counter` object. The counter is supposed to collect statistical information. The event index is a user-level object that is visible in event records and analysis expressions.

(Simulations: simulation: TBP)+≡

```
procedure :: init_event_index => simulation_init_event_index
procedure :: increment_event_index => simulation_increment_event_index
procedure :: set_event_index => simulation_set_event_index
procedure :: get_event_index => simulation_get_event_index
```

(Simulations: sub interfaces)+≡

```
module subroutine simulation_init_event_index (simulation)
  class(simulation_t), intent(inout) :: simulation
end subroutine simulation_init_event_index
module subroutine simulation_increment_event_index (simulation)
  class(simulation_t), intent(inout) :: simulation
end subroutine simulation_increment_event_index
module subroutine simulation_set_event_index (simulation, i)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: i
end subroutine simulation_set_event_index
module function simulation_get_event_index (simulation) result (i)
  class(simulation_t), intent(in) :: simulation
  integer :: i
end function simulation_get_event_index
```

(Simulations: procedures)+≡

```
module subroutine simulation_init_event_index (simulation)
  class(simulation_t), intent(inout) :: simulation
  call simulation%set_event_index (simulation%event_index_offset)
end subroutine simulation_init_event_index

module subroutine simulation_increment_event_index (simulation)
  class(simulation_t), intent(inout) :: simulation
  if (simulation%event_index_set) then
    simulation%event_index = simulation%event_index + 1
  end if
end subroutine simulation_increment_event_index

module subroutine simulation_set_event_index (simulation, i)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: i
  simulation%event_index = i
  simulation%event_index_set = .true.
end subroutine simulation_set_event_index

module function simulation_get_event_index (simulation) result (i)
  class(simulation_t), intent(in) :: simulation
  integer :: i
  if (simulation%event_index_set) then
    i = simulation%event_index
  else
```

```

        i = 0
    end if
end function simulation_get_event_index

```

33.9.9 Direct event access

If we want to retrieve event information, we should expose the currently selected event `entry` within the simulation object. We recall that this is an extension of the (generic) `event` type. Assuming that we will restrict this to read access, we return a pointer.

```

<Simulations: simulation: TBP>+≡
    procedure :: get_process_index => simulation_get_process_index
    procedure :: get_event_ptr => simulation_get_event_ptr

<Simulations: sub interfaces>+≡
    module function simulation_get_process_index (simulation) result (i_prc)
        class(simulation_t), intent(in), target :: simulation
        integer :: i_prc
    end function simulation_get_process_index
    module function simulation_get_event_ptr (simulation) result (event)
        class(simulation_t), intent(in), target :: simulation
        class(event_t), pointer :: event
    end function simulation_get_event_ptr

<Simulations: procedures>+≡
    module function simulation_get_process_index (simulation) result (i_prc)
        class(simulation_t), intent(in), target :: simulation
        integer :: i_prc

        i_prc = simulation%i_prc

    end function simulation_get_process_index

    module function simulation_get_event_ptr (simulation) result (event)
        class(simulation_t), intent(in), target :: simulation
        class(event_t), pointer :: event

        event => simulation%entry(simulation%i_prc)

    end function simulation_get_event_ptr

```

33.9.10 Event Stream I/O

Write an event to a generic `eio` event stream. The process index must be selected, or the current index must be available.

```

<Simulations: simulation: TBP>+≡
    generic :: write_event => write_event_eio
    procedure :: write_event_eio => simulation_write_event_eio

```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_write_event_eio (object, eio, i_prc)
  class(simulation_t), intent(in) :: object
  class(eio_t), intent(inout) :: eio
  integer, intent(in), optional :: i_prc
end subroutine simulation_write_event_eio

```

<Simulations: procedures>+≡

```

module subroutine simulation_write_event_eio (object, eio, i_prc)
  class(simulation_t), intent(in) :: object
  class(eio_t), intent(inout) :: eio
  integer, intent(in), optional :: i_prc
  logical :: increased
  integer :: current
  if (present (i_prc)) then
    current = i_prc
  else
    current = object%i_prc
  end if
  if (current > 0) then
    if (object%split_n_evt > 0 .and. object%counter%total > 1) then
      if (mod (object%counter%total, object%split_n_evt) == 1) then
        call eio%split_out ()
      end if
    else if (object%split_n_kbytes > 0) then
      call eio%update_split_count (increased)
      if (increased) call eio%split_out ()
    end if
    call eio%output (object%entry(current)%event_t, current, pacify = object%pacify)
  else
    call msg_fatal ("Simulation: write event: no process selected")
  end if
end subroutine simulation_write_event_eio

```

Read an event from a generic `eio` event stream. The event stream element must specify the process within the sample (`i_prc`), the MC group for this process (`i_mci`), the selected term (`i_term`), the selected MC integration `channel`, and the particle set of the event.

We may encounter EOF, which we indicate by storing 0 for the process index `i_prc`. An I/O error will be reported, and we also abort reading.

<Simulations: simulation: TBP>+≡

```

generic :: read_event => read_event_eio
procedure :: read_event_eio => simulation_read_event_eio

```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_read_event_eio (object, eio)
  class(simulation_t), intent(inout) :: object
  class(eio_t), intent(inout) :: eio
end subroutine simulation_read_event_eio

```

<Simulations: procedures>+≡

```

module subroutine simulation_read_event_eio (object, eio)
  class(simulation_t), intent(inout) :: object
  class(eio_t), intent(inout) :: eio
  integer :: iostat, current

```

```

call eio%input_i_prc (current, iostat)
select case (iostat)
case (0)
    object%i_prc = current
    call eio%input_event (object%entry(current)%event_t, iostat)
end select
select case (iostat)
case (:-1)
    object%i_prc = 0
    object%i_mci = 0
case (1:)
    call msg_error ("Reading events: I/O error, aborting read")
    object%i_prc = 0
    object%i_mci = 0
case default
    object%i_mci = object%entry(current)%get_i_mci ()
end select
end subroutine simulation_read_event_eio

```

33.9.11 Event Stream Array

Write an event using an array of event I/O streams. The process index must be selected, or the current index must be available.

<Simulations: simulation: TBP>+≡

```

generic :: write_event => write_event_es_array
procedure :: write_event_es_array => simulation_write_event_es_array

```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_write_event_es_array &
    (object, es_array, passed, event_handle)
    class(simulation_t), intent(in), target :: object
    class(event_stream_array_t), intent(inout) :: es_array
    logical, intent(in), optional :: passed
    class(event_handle_t), intent(inout), optional :: event_handle
end subroutine simulation_write_event_es_array

```

<Simulations: procedures>+≡

```

module subroutine simulation_write_event_es_array &
    (object, es_array, passed, event_handle)
    class(simulation_t), intent(in), target :: object
    class(event_stream_array_t), intent(inout) :: es_array
    logical, intent(in), optional :: passed
    class(event_handle_t), intent(inout), optional :: event_handle
    integer :: i_prc, event_index
    integer :: i
    type(entry_t), pointer :: current_entry
    i_prc = object%i_prc
    if (i_prc > 0) then
        event_index = object%counter%total
        current_entry => object%entry(i_prc)%get_first ()
        do i = 1, current_entry%count_nlo_entries ()
            if (i > 1) current_entry => current_entry%get_next ()
            call es_array%output (current_entry%event_t, i_prc, &

```

```

        event_index, &
        passed = passed, &
        pacify = object%pacify, &
        event_handle = event_handle)
    end do
else
    call msg_fatal ("Simulation: write event: no process selected")
end if
end subroutine simulation_write_event_es_array

```

Read an event using an array of event I/O streams. Reading is successful if there is an input stream within the array, and if a valid event can be read from that stream. If there is a stream, but EOF is passed when reading the first item, we switch the channel to output and return failure but no error message, such that new events can be appended to that stream.

<Simulations: simulation: TBP>+≡

```

generic :: read_event => read_event_es_array
procedure :: read_event_es_array => simulation_read_event_es_array

```

<Simulations: sub interfaces>+≡

```

module subroutine simulation_read_event_es_array &
    (object, es_array, enable_switch, fail, event_handle)
    class(simulation_t), intent(inout), target :: object
    class(event_stream_array_t), intent(inout), target :: es_array
    logical, intent(in) :: enable_switch
    logical, intent(out) :: fail
    class(event_handle_t), intent(inout), optional :: event_handle
end subroutine simulation_read_event_es_array

```

<Simulations: procedures>+≡

```

module subroutine simulation_read_event_es_array &
    (object, es_array, enable_switch, fail, event_handle)
    class(simulation_t), intent(inout), target :: object
    class(event_stream_array_t), intent(inout), target :: es_array
    logical, intent(in) :: enable_switch
    logical, intent(out) :: fail
    class(event_handle_t), intent(inout), optional :: event_handle
    integer :: iostat, i_prc
    type(entry_t), pointer :: current_entry => null ()
    integer :: i
    if (es_array%has_input ()) then
        fail = .false.
        call es_array%input_i_prc (i_prc, iostat)
        select case (iostat)
        case (0)
            object%i_prc = i_prc
            current_entry => object%entry(i_prc)
            do i = 1, current_entry%count_nlo_entries ()
                if (i > 1) then
                    call es_array%skip_eio_entry (iostat)
                    current_entry => current_entry%get_next ()
                end if
                call current_entry%set_index (object%get_event_index ())
                call es_array%input_event &

```

```

        (current_entry%event_t, iostat, event_handle)
    end do
    case (:-1)
        write (msg_buffer, "(A,1x,I0,1x,A)" &
            "... event file terminates after", &
            object%counter%read, "events."
        call msg_message ()
        if (enable_switch) then
            call es_array%switch_inout ()
            write (msg_buffer, "(A,1x,I0,1x,A)" &
                "Generating remaining ", &
                object%n_evt_requested - object%counter%read, "events ..."
            call msg_message ()
        end if
        fail = .true.
        return
    end select
    select case (iostat)
    case (0)
        object%i_mci = object%entry(i_prc)%get_i_mci ()
    case default
        write (msg_buffer, "(A,1x,I0,1x,A)" &
            "Reading events: I/O error, aborting read after", &
            object%counter%read, "events."
        call msg_error ()
        object%i_prc = 0
        object%i_mci = 0
        fail = .true.
    end select
else
    fail = .true.
end if
end subroutine simulation_read_event_es_array

```

33.9.12 Recover event

Recalculate the process instance contents, given an event with known particle set. The indices for MC, term, and channel must be already set. The `recalculate` method of the selected entry will import the result into `sqme_prc` and `weight_prc`.

If `recover_phs` is set (and false), do not attempt any phase-space calculation. Useful if we need only matrix elements (esp. testing); this flag is not stored in the simulation record.

```

<Simulations: simulation: TBP>+≡
    procedure :: recalculate => simulation_recalculate

<Simulations: sub interfaces>+≡
    module subroutine simulation_recalculate &
        (simulation, recover_phs, check_match)
        class(simulation_t), intent(inout) :: simulation
        logical, intent(in), optional :: recover_phs
        logical, intent(in), optional :: check_match
    end subroutine simulation_recalculate

```

<Simulations: procedures>+≡

```

module subroutine simulation_recalculate &
  (simulation, recover_phs, check_match)
  class(simulation_t), intent(inout) :: simulation
  logical, intent(in), optional :: recover_phs
  logical, intent(in), optional :: check_match
  integer :: i_prc, i_comp, i_term, k
  integer :: i_mci, i_mci0, i_mci1
  integer, dimension(:), allocatable :: i_terms
  logical :: success
  i_prc = simulation%i_prc
  associate (entry => simulation%entry(i_prc))
    if (entry%selected_i_mci /= 0) then
      i_mci0 = entry%selected_i_mci
      i_mci1 = i_mci0
    else
      i_mci0 = 1
      i_mci1 = entry%process%get_n_mci ()
    end if
    SCAN_COMP: do i_mci = i_mci0, i_mci1
      i_comp = entry%process%get_master_component (i_mci)
      call entry%process%reset_selected_cores ()
      call entry%process%select_components ([i_comp])
      i_terms = entry%process%get_component_i_terms (i_comp)
      SCAN_TERM: do k = 1, size (i_terms)
        i_term = i_terms(k)
        call entry%select (i_mci, i_term, entry%selected_channel)
        if (entry%selected_i_term /= 0 &
          .and. entry%selected_i_term /= i_term) cycle SCAN_TERM
        call entry%select (i_mci, i_term, entry%selected_channel)
        if (simulation%update_weight) then
          call entry%recalculate &
            (update_sqme = simulation%update_sqme, &
             recover_beams = simulation%recover_beams, &
             recover_phs = recover_phs, &
             weight_factor = entry%get_kinematical_weight (), &
             check_match = check_match, &
             success = success)
        else
          call entry%recalculate &
            (update_sqme = simulation%update_sqme, &
             recover_beams = simulation%recover_beams, &
             recover_phs = recover_phs, &
             check_match = check_match, &
             success = success)
        end if
        if (success) exit SCAN_COMP
      end do SCAN_TERM
    deallocate (i_terms)
  end do SCAN_COMP
  if (.not. success) then
    call entry%write ()
    call msg_fatal ("Simulation/recalculate: &
      &event could not be matched to the specified process")
  end if
end associate
end module

```



```

        end if
    end associate
end subroutine simulation_recalculate

```

33.9.13 Extract contents of the simulation object

Return the MD5 sum that summarizes configuration and integration (but not the event file). Used for initializing the event streams.

```

<Simulations: simulation: TBP>+≡
    procedure :: get_md5sum_prc => simulation_get_md5sum_prc
    procedure :: get_md5sum_cfg => simulation_get_md5sum_cfg
    procedure :: get_md5sum_alt => simulation_get_md5sum_alt

<Simulations: sub interfaces>+≡
    module function simulation_get_md5sum_prc (simulation) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        character(32) :: md5sum
    end function simulation_get_md5sum_prc
    module function simulation_get_md5sum_cfg (simulation) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        character(32) :: md5sum
    end function simulation_get_md5sum_cfg
    module function simulation_get_md5sum_alt (simulation, i) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        integer, intent(in) :: i
        character(32) :: md5sum
    end function simulation_get_md5sum_alt

<Simulations: procedures>+≡
    module function simulation_get_md5sum_prc (simulation) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        character(32) :: md5sum
        md5sum = simulation%md5sum_prc
    end function simulation_get_md5sum_prc

    module function simulation_get_md5sum_cfg (simulation) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        character(32) :: md5sum
        md5sum = simulation%md5sum_cfg
    end function simulation_get_md5sum_cfg

    module function simulation_get_md5sum_alt (simulation, i) result (md5sum)
        class(simulation_t), intent(in) :: simulation
        integer, intent(in) :: i
        character(32) :: md5sum
        md5sum = simulation%md5sum_alt(i)
    end function simulation_get_md5sum_alt

```

Return data that may be useful for writing event files.

Usually we can refer to a previously integrated process, for which we can fetch a process pointer. Occasionally, we do not have this because we are just rescanning an externally generated file without calculation. For that situation,

we generate our local beam data object using the current environment, or, in simple cases, just fetch the necessary data from the process definition and environment.

```

<Simulations: simulation: TBP>+=
  procedure :: get_data => simulation_get_data

<Simulations: sub interfaces>+=
  module function simulation_get_data (simulation, alt) result (sdata)
    class(simulation_t), intent(in) :: simulation
    logical, intent(in), optional :: alt
    type(event_sample_data_t) :: sdata
  end function simulation_get_data

<Simulations: procedures>+=
  module function simulation_get_data (simulation, alt) result (sdata)
    class(simulation_t), intent(in) :: simulation
    logical, intent(in), optional :: alt
    type(event_sample_data_t) :: sdata
    type(process_t), pointer :: process
    type(beam_data_t), pointer :: beam_data
    type(beam_structure_t), pointer :: beam_structure
    type(flavor_t), dimension(:), allocatable :: flv
    integer :: n, i
    logical :: enable_alt, construct_beam_data
    real(default) :: sqrts
    class(model_data_t), pointer :: model
    logical :: decay_rest_frame
    type(string_t) :: process_id
    enable_alt = .true.; if (present (alt)) enable_alt = alt
    if (debug_on) call msg_debug (D_CORE, "simulation_get_data")
    if (debug_on) call msg_debug (D_CORE, "alternative setup", enable_alt)
    if (enable_alt) then
      call sdata%init (simulation%n_prc, simulation%n_alt)
      do i = 1, simulation%n_alt
        sdata%md5sum_alt(i) = simulation%get_md5sum_alt (i)
      end do
    else
      call sdata%init (simulation%n_prc)
    end if
    sdata%unweighted = simulation%unweighted
    sdata%negative_weights = simulation%negative_weights
    sdata%norm_mode = simulation%norm_mode
    process => simulation%entry(1)%get_process_ptr ()
    if (associated (process)) then
      beam_data => process%get_beam_data_ptr ()
      construct_beam_data = .false.
    else
      n = simulation%entry(1)%n_in
      sqrts = simulation%local%get_sqrts ()
      beam_structure => simulation%local%beam_structure
      call beam_structure%check_against_n_in (n, construct_beam_data)
      if (construct_beam_data) then
        allocate (beam_data)
        model => simulation%local%model
        decay_rest_frame = &

```

```

        simulation%local%get_lval (var_str ("?decay_rest_frame"))
        call beam_data%init_structure (beam_structure, &
            sqrts, model, decay_rest_frame)
    else
        beam_data => null ()
    end if
end if
if (associated (beam_data)) then
    n = beam_data%get_n_in ()
    sdata%n_beam = n
    allocate (flv (n))
    flv = beam_data%get_flavor ()
    sdata%pdg_beam(:n) = flv%get_pdg ()
    sdata%energy_beam(:n) = beam_data%get_energy ()
    if (construct_beam_data) deallocate (beam_data)
else
    n = simulation%entry(1)%n_in
    sdata%n_beam = n
    process_id = simulation%entry(1)%process_id
    call simulation%local%prclib%get_pdg_in_1 &
        (process_id, sdata%pdg_beam(:n))
    sdata%energy_beam(:n) = sqrts / n
end if
do i = 1, simulation%n_prc
    if (.not. simulation%entry(i)%valid) cycle
    process => simulation%entry(i)%get_process_ptr ()
    if (associated (process)) then
        sdata%proc_num_id(i) = process%get_num_id ()
    else
        process_id = simulation%entry(i)%process_id
        sdata%proc_num_id(i) = simulation%local%prclib%get_num_id (process_id)
    end if
    if (sdata%proc_num_id(i) == 0) sdata%proc_num_id(i) = i
    if (simulation%entry(i)%has_integral) then
        sdata%cross_section(i) = simulation%entry(i)%integral
        sdata%error(i) = simulation%entry(i)%error
    end if
end do
sdata%total_cross_section = sum (sdata%cross_section)
sdata%md5sum_prc = simulation%get_md5sum_prc ()
sdata%md5sum_cfg = simulation%get_md5sum_cfg ()
if (simulation%split_n_evt > 0 .or. simulation%split_n_kbytes > 0) then
    sdata%split_n_evt = simulation%split_n_evt
    sdata%split_n_kbytes = simulation%split_n_kbytes
    sdata%split_index = simulation%split_index
end if
end function simulation_get_data

```

Return a default name for the current event sample. This is the process ID of the first process.

<Simulations: simulation: TBP>+≡

procedure :: get_default_sample_name => simulation_get_default_sample_name

<Simulations: sub interfaces>+≡

```

module function simulation_get_default_sample_name &
  (simulation) result (sample)
  class(simulation_t), intent(in) :: simulation
  type(string_t) :: sample
end function simulation_get_default_sample_name

<Simulations: procedures>+≡
module function simulation_get_default_sample_name &
  (simulation) result (sample)
  class(simulation_t), intent(in) :: simulation
  type(string_t) :: sample
  type(process_t), pointer :: process
  sample = "whizard"
  if (simulation%n_prc > 0) then
    process => simulation%entry(1)%get_process_ptr ()
    if (associated (process)) then
      sample = process%get_id ()
    end if
  end if
end function simulation_get_default_sample_name

<Simulations: simulation: TBP>+≡
procedure :: is_valid => simulation_is_valid

<Simulations: sub interfaces>+≡
module function simulation_is_valid (simulation) result (valid)
  class(simulation_t), intent(inout) :: simulation
  logical :: valid
end function simulation_is_valid

<Simulations: procedures>+≡
module function simulation_is_valid (simulation) result (valid)
  class(simulation_t), intent(inout) :: simulation
  logical :: valid
  valid = simulation%valid
end function simulation_is_valid

```

Return the hard-interaction particle set for event entry i_prc.

```

<Simulations: simulation: TBP>+≡
procedure :: get_hard_particle_set => simulation_get_hard_particle_set

<Simulations: sub interfaces>+≡
module function simulation_get_hard_particle_set &
  (simulation, i_prc) result (pset)
  class(simulation_t), intent(in) :: simulation
  integer, intent(in) :: i_prc
  type(particle_set_t) :: pset
end function simulation_get_hard_particle_set

<Simulations: procedures>+≡
module function simulation_get_hard_particle_set &
  (simulation, i_prc) result (pset)
  class(simulation_t), intent(in) :: simulation
  integer, intent(in) :: i_prc
  type(particle_set_t) :: pset
  call simulation%entry(i_prc)%get_hard_particle_set (pset)

```

```
end function simulation_get_hard_particle_set
```

33.9.14 Auxiliary

Call pacify: eliminate numerical noise.

```
<Simulations: public>+≡
    public :: pacify

<Simulations: interfaces>≡
    interface pacify
        module procedure pacify_simulation
    end interface

<Simulations: sub interfaces>+≡
    module subroutine pacify_simulation (simulation)
        class(simulation_t), intent(inout) :: simulation
    end subroutine pacify_simulation

<Simulations: procedures>+≡
    module subroutine pacify_simulation (simulation)
        class(simulation_t), intent(inout) :: simulation
        integer :: i, j
        i = simulation%i_prc
        if (i > 0) then
            call pacify (simulation%entry(i))
            do j = 1, simulation%n_alt
                call pacify (simulation%alt_entry(i,j))
            end do
        end if
    end subroutine pacify_simulation
```

Manually evaluate expressions for the currently selected process. This is used only in the unit tests.

```
<Simulations: simulation: TBP>+≡
    procedure :: evaluate_expressions => simulation_evaluate_expressions

<Simulations: sub interfaces>+≡
    module subroutine simulation_evaluate_expressions (simulation)
        class(simulation_t), intent(inout) :: simulation
    end subroutine simulation_evaluate_expressions

<Simulations: procedures>+≡
    module subroutine simulation_evaluate_expressions (simulation)
        class(simulation_t), intent(inout) :: simulation
        call simulation%entry(simulation%i_prc)%evaluate_expressions ()
    end subroutine simulation_evaluate_expressions
```

Manually evaluate event transforms for the currently selected process. This is used only in the unit tests.

```
<Simulations: simulation: TBP>+≡
    procedure :: evaluate_transforms => simulation_evaluate_transforms
```

```

<Simulations: sub interfaces>+≡
    module subroutine simulation_evaluate_transforms (simulation)
        class(simulation_t), intent(inout) :: simulation
        end subroutine simulation_evaluate_transforms

<Simulations: procedures>+≡
    module subroutine simulation_evaluate_transforms (simulation)
        class(simulation_t), intent(inout) :: simulation
        associate (entry => simulation%entry(simulation%i_prc))
            call entry%evaluate_transforms ()
        end associate
    end subroutine simulation_evaluate_transforms

```

33.9.15 Unit tests

Test module, followed by the stand-alone unit-test procedures.

```

<simulations_ut.f90>≡
    <File header>

    module simulations_ut
        use unit_tests
        use simulations_uti

    <Standard module head>

    <Simulations: public test>

    contains

    <Simulations: test driver>

    end module simulations_ut

<simulations_uti.f90>≡
    <File header>

    module simulations_uti

    <Use kinds>
        use kinds, only: i64
    <Use strings>
        use io_units
        use format_defs, only: FMT_10, FMT_12
        use ifiles
        use lexers
        use parser
        use lorentz
        use flavors
        use interactions, only: reset_interaction_counter
        use process_libraries, only: process_library_t
        use prclib_stacks
        use phs_forests
        use event_base, only: generic_event_t

```

```

    use event_base, only: event_callback_t
    use particles, only: particle_set_t
    use eio_data
    use eio_base
    use eio_direct, only: eio_direct_t
    use eio_raw
    use eio_ascii
    use eio_dump
    use eio_callback
    use eval_trees
    use model_data, only: model_data_t
    use models
    use rt_data
    use event_streams
    use decays_ut, only: prepare_testbed
    use process, only: process_t
    use process_stacks, only: process_entry_t
    use process_configurations_ut, only: prepare_test_library
    use compilations, only: compile_library
    use integrations, only: integrate_process

    use simulations

    use restricted_subprocesses_util, only: prepare_resonance_test_library

    <Standard module head>

    <Simulations: test declarations>

    <Simulations: test auxiliary types>

contains

    <Simulations: tests>

    <Simulations: test auxiliary>

end module simulations_util

```

API: driver for the unit tests below.

```

<Simulations: public test>≡
    public :: simulations_test

<Simulations: test driver>≡
    subroutine simulations_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Simulations: execute tests>
    end subroutine simulations_test

```

Initialization

Initialize a `simulation_t` object, including the embedded event records.

```

<Simulations: execute tests>≡
  call test (simulations_1, "simulations_1", &
    "initialization", &
    u, results)

<Simulations: test declarations>≡
  public :: simulations_1

<Simulations: tests>≡
  subroutine simulations_1 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, procname2
    type(rt_data_t), target :: global
    type(simulation_t), target :: simulation

    write (u, "(A)")  "* Test output: simulations_1"
    write (u, "(A)")  "* Purpose: initialize simulation"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_omp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_1a"
    procname1 = "simulation_1p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

    call global%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known = .true.)
    call global%set_string (var_str ("$phs_method"), &
      var_str ("single"), is_known = .true.)
    call global%set_string (var_str ("$integration_method"), &
      var_str ("midpoint"), is_known = .true.)
    call global%set_log (var_str ("?vis_history"), &
      .false., is_known = .true.)
    call global%set_log (var_str ("?integration_timer"), &
      .false., is_known = .true.)
    call global%set_log (var_str ("?recover_beams"), &
      .false., is_known = .true.)

    call global%set_real (var_str ("sqrts"), &
      1000._default, is_known = .true.)

    call global%it_list%init ([1], [1000])

    call global%set_string (var_str ("$run_id"), &

```



```

        var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

procname2 = "sim_extra"

call prepare_test_library (global, libname, 1, [procname2])
call compile_library (libname, global)
call global%set_string (var_str ("$run_id"), &
    var_str ("simulations2"), is_known = .true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_string (var_str ("$sample"), &
    var_str ("sim1"), is_known = .true.)
call integrate_process (procname2, global, local_stack=.true.)

call simulation%init ([procname1, procname2], .false., .true., global)
call simulation%init_process_selector ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the first process"
write (u, "(A)")

call simulation%write_event (u, i_prc = 1)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_1"

end subroutine simulations_1

```

Weighted events

Generate events for a single process.

```

<Simulations: execute tests>+≡
    call test (simulations_2, "simulations_2", &
        "weighted events", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_2

<Simulations: tests>+≡
    subroutine simulations_2 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1

```

```

type(rt_data_t), target :: global
type(simulation_t), target :: simulation
type(event_sample_data_t) :: data

write (u, "(A)")  "* Test output: simulations_2"
write (u, "(A)")  "* Purpose: generate events for a single process"
write (u, "(A)")

write (u, "(A)")  "* Initialize processes"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_omp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_2a"
procname1 = "simulation_2p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &

```

```

        .false., is_known = .true.)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_2"

end subroutine simulations_2

```

Unweighted events

Generate events for a single process.

```

<Simulations: execute tests>+≡
call test (simulations_3, "simulations_3", &
    "unweighted events", &
    u, results)

<Simulations: test declarations>+≡
public :: simulations_3

<Simulations: tests>+≡
subroutine simulations_3 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1
    type(rt_data_t), target :: global
    type(simulation_t), target :: simulation
    type(event_sample_data_t) :: data

    write (u, "(A)")  "* Test output: simulations_3"
    write (u, "(A)")  "* Purpose: generate unweighted events &
        &for a single process"

```

```

write (u, "(A)")

write (u, "(A)")  "* Initialize processes"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_3a"
procname1 = "simulation_3p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_3"

end subroutine simulations_3

```

Simulating process with structure functions

Generate events for a single process.

```

<Simulations: execute tests>+≡
call test (simulations_4, "simulations_4", &
  "process with structure functions", &
  u, results)

<Simulations: test declarations>+≡
public :: simulations_4

<Simulations: tests>+≡
subroutine simulations_4 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1
  type(rt_data_t), target :: global
  type(flavor_t) :: flv
  type(string_t) :: name
  type(simulation_t), target :: simulation
  type(event_sample_data_t) :: data

  write (u, "(A)")  "* Test output: simulations_4"
  write (u, "(A)")  "* Purpose: generate events for a single process &
    &with structure functions"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize processes"
  write (u, "(A)")

  call syntax_model_file_init ()

```

```

call syntax_phs_forest_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_4a"
procname1 = "simulation_4p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call reset_interaction_counter ()

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call global%it_list%init ([1], [1000])

```

```

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
call global%set_string (var_str ("$_sample"), &
    var_str ("simulations4"), is_known = .true.)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_4"

end subroutine simulations_4

```

Event I/O

Generate event for a test process, write to file and reread.

<Simulations: execute tests>+≡

```

call test (simulations_5, "simulations_5", &
    "raw event I/O", &
    u, results)

```

<Simulations: test declarations>+≡

```

public :: simulations_5

```

<Simulations: tests>+≡

```

subroutine simulations_5 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1, sample
  type(rt_data_t), target :: global
  class(eio_t), allocatable :: eio
  type(simulation_t), allocatable, target :: simulation

  write (u, "(A)")  "* Test output: simulations_5"
  write (u, "(A)")  "* Purpose: generate events for a single process"
  write (u, "(A)")  "*           write to file and reread"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize processes"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()
  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

  libname = "simulation_5a"
  procname1 = "simulation_5p"

  call prepare_test_library (global, libname, 1, [procname1])
  call compile_library (libname, global)

  call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

  call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
  call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
  call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
  call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

  call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

  call global%it_list%init ([1], [1000])

  call global%set_string (var_str ("$run_id"), &
    var_str ("simulations5"), is_known = .true.)
  call integrate_process (procname1, global, local_stack=.true.)

```



```

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations5"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

allocate (eio_raw_t :: eio)
call eio%init_out (sample)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write_event (u)
call simulation%write_event (eio)

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()
allocate (eio_raw_t :: eio)
call eio%init_in (sample)

call simulation%read_event (eio)
call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Recalculate process instance"

```

```

write (u, "(A)")

call simulation%recalculate ()
call simulation%evaluate_expressions ()
call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_5"

end subroutine simulations_5

```

Event I/O

Generate event for a real process with structure functions, write to file and reread.

```

<Simulations: execute tests>+≡
  call test (simulations_6, "simulations_6", &
    "raw event I/O with structure functions", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_6

<Simulations: tests>+≡
  subroutine simulations_6 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, sample
    type(rt_data_t), target :: global
    class(eio_t), allocatable :: eio
    type(simulation_t), allocatable, target :: simulation
    type(flavor_t) :: flv
    type(string_t) :: name

    write (u, "(A)")  "* Test output: simulations_6"
    write (u, "(A)")  "*   Purpose: generate events for a single process"
    write (u, "(A)")  "*               write to file and reread"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and integrate"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)

```

```

call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_6"
procname1 = "simulation_6p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &

```

```

        .false., is_known = .true.)
sample = "simulations6"
call global%set_string (var_str ("sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

allocate (eio_raw_t :: eio)
call eio%init_out (sample)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)
call simulation%write_event (eio)

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()
allocate (eio_raw_t :: eio)
call eio%init_in (sample)

call simulation%read_event (eio)
call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Recalculate process instance"
write (u, "(A)")

call simulation%recalculate ()
call simulation%evaluate_expressions ()

```

```

call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_6"

end subroutine simulations_6

```

Automatic Event I/O

Generate events with raw-format event file as cache: generate, reread, append.

```

<Simulations: execute tests>+≡
call test (simulations_7, "simulations_7", &
  "automatic raw event I/O", &
  u, results)

<Simulations: test declarations>+≡
public :: simulations_7

<Simulations: tests>+≡
subroutine simulations_7 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1, sample
  type(rt_data_t), target :: global
  type(string_t), dimension(0) :: empty_string_array
  type(event_sample_data_t) :: data
  type(event_stream_array_t) :: es_array
  type(simulation_t), allocatable, target :: simulation
  type(flavor_t) :: flv
  type(string_t) :: name

  write (u, "(A)")  "* Test output: simulations_7"
  write (u, "(A)")  "*   Purpose: generate events for a single process"
  write (u, "(A)")  "*               write to file and reread"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize process and integrate"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()
  call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &

```

```

0, is_known = .true.)

libname = "simulation_7"
procname1 = "simulation_7p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)

```

```

sample = "simulations7"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, [var_str ("raw")], global, data)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")  "* Re-read the event from file and generate another one"
write (u, "(A)")

call global%set_log (&
    var_str ("?rebuild_events"), .false., is_known = .true.)

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"))

call simulation%set_n_events_requested (2)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read both events from file"

```

```

write (u, "(A)")

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"))

call simulation%set_n_events_requested (2)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_7"

end subroutine simulations_7

```

Rescanning Events

Generate events and rescan the resulting raw event file.

```

<Simulations: execute tests>+≡
    call test (simulations_8, "simulations_8", &
        "rescan raw event file", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_8

<Simulations: tests>+≡
    subroutine simulations_8 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1, sample
        type(rt_data_t), target :: global
        type(string_t), dimension(0) :: empty_string_array
        type(event_sample_data_t) :: data
        type(event_stream_array_t) :: es_array
        type(simulation_t), allocatable, target :: simulation
        type(flavor_t) :: flv
        type(string_t) :: name

```



```

write (u, "(A)")  "* Test output: simulations_8"
write (u, "(A)")  "* Purpose: generate events for a single process"
write (u, "(A)")  "*           write to file and rescan"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and integrate"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

libname = "simulation_8"
procname1 = "simulation_8p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
      var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
      var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
      var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
      var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
      var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
      .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
      .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
      .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
      .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
      1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
      0._default)

call flv%init (25, global%model)
name = flv%get_name ()

```

```

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations8"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
write (u, "(1x,A,A,A)")  "MD5 sum (proc)  = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)")  "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, [var_str ("raw")], global, &
    data)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call reset_interaction_counter ()

```

```

allocate (simulation)
call simulation%init ([procname1], .false., .false., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)") "MD5 sum (proc) = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"), input_sample = sample, allow_switch = .false.)

call simulation%rescan (1, es_array, global = global)

write (u, "(A)")

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read again and recalculate"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &
    .true., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .false., .false., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)") "MD5 sum (proc) = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"), input_sample = sample, allow_switch = .false.)

call simulation%rescan (1, es_array, global = global)

write (u, "(A)")

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: simulations_8"

end subroutine simulations_8

```

Rescanning Check

Generate events and rescan with process mismatch.

```

<Simulations: execute tests>+≡
call test (simulations_9, "simulations_9", &
  "rescan mismatch", &
  u, results)

<Simulations: test declarations>+≡
public :: simulations_9

<Simulations: tests>+≡
subroutine simulations_9 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1, sample
  type(rt_data_t), target :: global
  type(string_t), dimension(0) :: empty_string_array
  type(event_sample_data_t) :: data
  type(event_stream_array_t) :: es_array
  type(simulation_t), allocatable, target :: simulation
  type(flavor_t) :: flv
  type(string_t) :: name
  logical :: error

  write (u, "(A)")  "** Test output: simulations_9"
  write (u, "(A)")  "** Purpose: generate events for a single process"
  write (u, "(A)")  "**           write to file and rescan"
  write (u, "(A)")

  write (u, "(A)")  "** Initialize process and integrate"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()
  call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

  libname = "simulation_9"
  procname1 = "simulation_9p"

```

```

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations9"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
allocate (simulation)

```

```

call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
write (u, "(1x,A,A,A)") "MD5 sum (proc)  = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, [var_str ("raw")], global, &
    data)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")  "* Initialize event generation for different parameters"
write (u, "(A)")

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1, procname1], .false., .false., global)
call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Attempt to re-read the events (should fail)"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)") "MD5 sum (proc)  = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"), input_sample = sample, &
    allow_switch = .false., error = error)

write (u, "(1x,A,L1)") "error = ", error

call simulation%rescan (1, es_array, global = global)

```

```

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_9"

end subroutine simulations_9

```

Alternative weights

Generate an event for a single process and reweight it in a simultaneous calculation.

```

<Simulations: execute tests>+≡
  call test (simulations_10, "simulations_10", &
    "alternative weight", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_10

<Simulations: tests>+≡
  subroutine simulations_10 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, expr_text
    type(rt_data_t), target :: global
    type(rt_data_t), dimension(1), target :: alt_env
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: pt_weight
    type(simulation_t), target :: simulation
    type(event_sample_data_t) :: data

    write (u, "(A)")  "* Test output: simulations_10"
    write (u, "(A)")  "* Purpose: reweight event"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_pexpr_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_10a"
    procname1 = "simulation_10p"

    call prepare_test_library (global, libname, 1, [procname1])

```

```

call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize alternative environment with custom weight"
write (u, "(A)")

call alt_env(1)%local_init (global)
call alt_env(1)%activate ()

expr_text = "2"
write (u, "(A,A)")  "weight = ", char (expr_text)
write (u, *)

call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)
alt_env(1)%pn%weight_expr => pt_weight%get_root_ptr ()
call alt_env(1)%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &

```



```

        .false., is_known = .true.)
call simulation%init ([procname1], .true., .true., global, alt_env=alt_env)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the alternative setup"
write (u, "(A)")

call simulation%write_alt_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

call syntax_model_file_final ()
call syntax_pexpr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_10"

end subroutine simulations_10

```

Decays

Generate an event with subsequent partonic decays.

```

<Simulations: execute tests>+≡
    call test (simulations_11, "simulations_11", &
        "decay", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_11

<Simulations: tests>+≡
    subroutine simulations_11 (u)

```

```

integer, intent(in) :: u
type(rt_data_t), target :: global
type(prclib_entry_t), pointer :: lib
type(string_t) :: prefix, procname1, procname2
type(simulation_t), target :: simulation

write (u, "(A)")  "* Test output: simulations_11"
write (u, "(A)")  "* Purpose: apply decay"
write (u, "(A)")

write (u, "(A)")  "* Initialize processes"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
allocate (lib)
call global%add_prclib (lib)

call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

prefix = "simulation_11"
procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
    (global%prclib, global%process_stack, &
    prefix, global%os_data, &
    scattering=.true., decay=.true.)

call global%select_model (var_str ("Test"))
call global%model%set_par (var_str ("ff"), 0.4_default)
call global%model%set_par (var_str ("mf"), &
    global%model%get_real (var_str ("ff")) &
    * global%model%get_real (var_str ("ms")))
call global%model%set_unstable (25, [procname2])

write (u, "(A)")  "* Initialize simulation object"
write (u, "(A)")

call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Generate event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write (u)

write (u, *)

```

```

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call simulation%final ()
call global%final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_11"

end subroutine simulations_11

```

Split Event Files

Generate event for a real process with structure functions and write to file, accepting a limit for the number of events per file.

```

<Simulations: execute tests>+≡
call test (simulations_12, "simulations_12", &
    "split event files", &
    u, results)

<Simulations: test declarations>+≡
public :: simulations_12

<Simulations: tests>+≡
subroutine simulations_12 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, sample
    type(rt_data_t), target :: global
    class(eio_t), allocatable :: eio
    type(simulation_t), allocatable, target :: simulation
    type(flavor_t) :: flv
    integer :: i_evt

    write (u, "(A)")  "* Test output: simulations_12"
    write (u, "(A)")  "*   Purpose: generate events for a single process"
    write (u, "(A)")  "*               and write to split event files"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and integrate"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
        .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
        0, is_known = .true.)

```

```

libname = "simulation_12"
procname1 = "simulation_12p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations_12"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
call global%set_int (var_str ("sample_split_n_evt"), &
    2, is_known = .true.)
call global%set_int (var_str ("sample_split_index"), &
    42, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)

```

```

call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize ASCII event file"
write (u, "(A)")

allocate (eio_ascii_short_t :: eio)
select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data = simulation%get_data ())

write (u, "(A)")  "* Generate 5 events, distributed among three files"

do i_evt = 1, 5
    call simulation%set_n_events_requested (1)
    call simulation%generate ()
    call simulation%write_event (eio)
end do

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, *)
call display_file ("simulations_12.42.short.evt", u)
write (u, *)
call display_file ("simulations_12.43.short.evt", u)
write (u, *)
call display_file ("simulations_12.44.short.evt", u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_12"

end subroutine simulations_12

```

Auxiliary: display file contents.

<Simulations: public test auxiliary>≡
public :: display_file

<Simulations: test auxiliary>≡
subroutine display_file (file, u)
use io_units, only: free_unit
character(*), intent(in) :: file
integer, intent(in) :: u
character(256) :: buffer

```

integer :: u_file
write (u, "(3A)")  "* Contents of file '", file, "':"
write (u, *)
u_file = free_unit ()
open (u_file, file = file, action = "read", status = "old")
do
    read (u_file, "(A)", end = 1)  buffer
    write (u, "(A)")  trim (buffer)
end do
1  continue
end subroutine display_file

```

Callback

Generate events and execute a callback in place of event I/O.

```

<Simulations: execute tests>+≡
    call test (simulations_13, "simulations_13", &
        "callback", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_13

<Simulations: tests>+≡
    subroutine simulations_13 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1, sample
        type(rt_data_t), target :: global
        class(eio_t), allocatable :: eio
        type(simulation_t), allocatable, target :: simulation
        type(flavor_t) :: flv
        integer :: i_evt
        type(simulations_13_callback_t) :: event_callback

        write (u, "(A)")  "* Test output: simulations_13"
        write (u, "(A)")  "*   Purpose: generate events for a single process"
        write (u, "(A)")  "*                   and execute callback"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and integrate"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
            0, is_known = .true.)

        libname = "simulation_13"
        procname1 = "simulation_13p"

        call prepare_test_library (global, libname, 1, [procname1])

```

```

call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call flv%init (25, global%model)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations_13"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Prepare callback object"
write (u, "(A)")

event_callback%u = u
call global%set_event_callback (event_callback)

write (u, "(A)")  "* Initialize callback I/O object"
write (u, "(A)")

```

```

allocate (eio_callback_t :: eio)
select type (eio)
class is (eio_callback_t)
    call eio%set_parameters (callback = event_callback, &
        count_interval = 3)
end select
call eio%init_out (sample, data = simulation%get_data ())

write (u, "(A)")  "* Generate 7 events, with callback every 3 events"
write (u, "(A)")

do i_evt = 1, 7
    call simulation%set_n_events_requested (1)
    call simulation%generate ()
    call simulation%write_event (eio)
end do

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_13"

end subroutine simulations_13

```

The callback object and procedure. In the type extension, we can store the output channel `u` so we know where to write into.

<Simulations: test auxiliary types>≡

```

type, extends (event_callback_t) :: simulations_13_callback_t
    integer :: u
contains
    procedure :: write => simulations_13_callback_write
    procedure :: proc => simulations_13_callback
end type simulations_13_callback_t

```

<Simulations: test auxiliary>+≡

```

subroutine simulations_13_callback_write (event_callback, unit)
    class(simulations_13_callback_t), intent(in) :: event_callback
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Hello"
end subroutine simulations_13_callback_write

subroutine simulations_13_callback (event_callback, i, event)

```



```

class(simulations_13_callback_t), intent(in) :: event_callback
integer(i64), intent(in) :: i
class(generic_event_t), intent(in) :: event
write (event_callback%u, "(A,I0)") "hello event #", i
end subroutine simulations_13_callback

```

Resonant subprocess setup

Prepare a process with resonances and enter resonant subprocesses in the simulation object. Select a kinematics configuration and compute probabilities for resonant subprocesses.

The process and its initialization is taken from `processes_18`, but we need a complete O'MEGA matrix element here.

```

<Simulations: execute tests>+≡
  call test (simulations_14, "simulations_14", &
    "resonant subprocesses evaluation", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_14

<Simulations: tests>+≡
  subroutine simulations_14 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, libname_generated
    type(string_t) :: procname
    type(string_t) :: model_name
    type(rt_data_t), target :: global
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    class(model_t), pointer :: model
    class(model_data_t), pointer :: model_data
    type(simulation_t), target :: simulation
    type(particle_set_t) :: pset
    type(eio_direct_t) :: eio_in
    type(eio_dump_t) :: eio_out
    real(default) :: sqrts, mw, pp
    real(default), dimension(3) :: p3
    type(vector4_t), dimension(:), allocatable :: p
    real(default), dimension(:), allocatable :: m
    integer :: u_verbose, i
    real(default) :: sqme_proc
    real(default), dimension(:), allocatable :: sqme
    real(default) :: on_shell_limit
    integer, dimension(:), allocatable :: i_array
    real(default), dimension(:), allocatable :: prob_array

    write (u, "(A)")  "* Test output: simulations_14"
    write (u, "(A)")  "* Purpose: construct resonant subprocesses &
      &in the simulation object"
    write (u, "(A)")

    write (u, "(A)")  "* Build and load a test library with one process"

```

```

write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

libname = "simulations_14_lib"
procname = "simulations_14_p"

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &
    .true., is_known = .true.)

model_name = "SM"
call global%select_model (model_name)
allocate (model)
call model%init_instance (global%model)
model_data => model

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

write (u, "(A)")
write (u, "(A)")  "* Initialize simulation object &
    &with resonant subprocesses"
write (u, "(A)")

call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

```

```

call global%set_real (var_str ("resonance_on_shell_limit"), &
    10._default, is_known = .true.)

call simulation%init ([procname], &
    integrate=.false., generate=.false., local=global)

call simulation%write_resonant_subprocess_data (u, 1)

write (u, "(A)")
write (u, "(A)")  "* Resonant subprocesses: generated library"
write (u, "(A)")

libname_generated = procname // "_R"
lib => global%prclib_stack%get_library_ptr (libname_generated)
if (associated (lib)) call lib%write (u, libpath=.false.)

write (u, "(A)")
write (u, "(A)")  "* Generated process stack"
write (u, "(A)")

call global%process_stack%show (u)

write (u, "(A)")
write (u, "(A)")  "* Particle set"
write (u, "(A)")

pset = simulation%get_hard_particle_set (1)
call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize object for direct access"
write (u, "(A)")

call eio_in%init_direct &
    (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
    pdg = [-11, 11, 1, -2, 24], model=global%model)
call eio_in%set_selection_indices (1, 1, 1, 1)

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (p (5), m (5))
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))

```

```

m(4) = 0
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw
call eio_in%set_momentum (p, m**2)

call eio_in%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer and show particle set"
write (u, "(A)")

call simulation%read_event (eio_in)
pset = simulation%get_hard_particle_set (1)
call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "* (Re)calculate matrix element"
write (u, "(A)")

call simulation%recalculate (recover_phs = .false.)
call simulation%evaluate_transforms ()

write (u, "(A)")  "* Show event with sqme"
write (u, "(A)")

call eio_out%set_parameters (unit = u, &
    weights = .true., pacify = .true., compressed = .true.)
call eio_out%init_out (var_str (""))
call simulation%write_event (eio_out)

write (u, "(A)")
write (u, "(A)")  "* Write event to separate file &
    &'simulations_14_event_verbose.log'"

u_verbose = free_unit ()
open (unit = u_verbose, file = "simulations_14_event_verbose.log", &
    status = "replace", action = "write")
call simulation%write (u_verbose)
write (u_verbose, *)
call simulation%write_event (u_verbose, verbose = .true., testflag = .true.)
close (u_verbose)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_14"

end subroutine simulations_14

```

Resonant subprocess simulation

Prepare a process with resonances and enter resonant subprocesses in the simulation object. Simulate events with selection of resonance histories.

The process and its initialization is taken from `processes_18`, but we need a complete O'MEGA matrix element here.

```
<Simulations: execute tests>+≡
    call test (simulations_15, "simulations_15", &
               "resonant subprocesses in simulation", &
               u, results)

<Simulations: test declarations>+≡
    public :: simulations_15

<Simulations: tests>+≡
    subroutine simulations_15 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, libname_generated
        type(string_t) :: procname
        type(string_t) :: model_name
        type(rt_data_t), target :: global
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(simulation_t), target :: simulation
        real(default) :: sqrts
        type(eio_dump_t) :: eio_out
        integer :: u_verbose

        write (u, "(A)")  "* Test output: simulations_15"
        write (u, "(A)")  "* Purpose: generate event with resonant subprocess"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a test library with one process"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        libname = "simulations_15_lib"
        procname = "simulations_15_p"

        call global%global_init ()
        call global%append_log (&
                                var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
        call global%append_log (&
                                var_str ("?rebuild_grids"), .true., intrinsic = .true.)
        call global%append_log (&
                                var_str ("?rebuild_events"), .true., intrinsic = .true.)
        call global%set_log (var_str ("?omega_openmp"), &
                             .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
                             0, is_known = .true.)
        call global%set_real (var_str ("sqrts"), &
```

```

1000._default, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
.false., is_known = .true.)
call global%set_log (var_str ("?update_sqme"), &
.true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
.true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &
.true., is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
.true., is_known = .true.)
call global%set_real (var_str ("resonance_on_shell_limit"), &
10._default, is_known = .true.)

model_name = "SM"
call global%select_model (model_name)
allocate (model)
call model%init_instance (global%model)
model_data => model

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
(lib, libname, procname, model_data, global, u)

write (u, "(A)")
write (u, "(A)")  "* Initialize simulation object &
&with resonant subprocesses"
write (u, "(A)")

call global%it_list%init ([1], [1000])
call simulation%init ([procname], &
integrate=.true., generate=.true., local=global)

call simulation%write_resonant_subprocess_data (u, 1)

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call simulation%init_process_selector ()
call simulation%set_n_events_requested (1)
call simulation%generate ()

call eio_out%set_parameters (unit = u, &
weights = .true., pacify = .true., compressed = .true.)
call eio_out%init_out (var_str (""))
call simulation%write_event (eio_out)

```

```

write (u, "(A)")
write (u, "(A)")  "* Write event to separate file &
                  &'simulations_15_event_verbose.log'"

u_verbose = free_unit ()
open (unit = u_verbose, file = "simulations_15_event_verbose.log", &
      status = "replace", action = "write")
call simulation%write (u_verbose)
write (u_verbose, *)
call simulation%write_event (u_verbose, verbose =.true., testflag = .true.)
close (u_verbose)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_15"

end subroutine simulations_15

```

Chapter 34

More Unit Tests

This chapter collects some procedures for testing that can't be provided at the point where the corresponding modules are defined, because they use other modules of a different level.

(We should move them back, collecting the high-level functionality in `init`/`final` hooks that we can set at runtime.)

34.1 Expression Testing

Expression objects are part of process and event objects, but the process and event object modules should not depend on the implementation of expressions. Here, we collect unit tests that depend on expression implementation.

```
(expr_tests_ut.f90)≡
  <File header>
  module expr_tests_ut

    use unit_tests
    use expr_tests_util

    <Standard module head>

    <Expr tests: public test>

    contains

    <Expr tests: test driver>

  end module expr_tests_ut
(expr_tests_util.f90)≡
  <File header>

  module expr_tests_util

    <Use kinds>
    <Use strings>
    use format_defs, only: FMT_12
    use format_utils, only: write_separator
```



```

    use os_interface
    use sm_qcd
    use lorentz
    use ifiles
    use lexers
    use parser
    use model_data
    use interactions, only: reset_interaction_counter
    use process_libraries
    use subevents
    use subvt_expr
    use rng_base
    use mci_base
    use phs_base
    use variables, only: var_list_t
    use eval_trees
    use models
    use prc_core
    use prc_test
    use process, only: process_t
    use instances, only: process_instance_t
    use events

    use rng_base_ut, only: rng_test_factory_t
    use phs_base_ut, only: phs_test_config_t

    <Standard module head>

    <Expr tests: test declarations>

contains

    <Expr tests: tests>

    <Expr tests: test auxiliary>

end module expr_tests_util

```

34.1.1 Test

This is the master for calling self-test procedures.

```

    <Expr tests: public test>≡
        public :: subvt_expr_test

    <Expr tests: test driver>≡
        subroutine subvt_expr_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
            <Expr tests: execute tests>
        end subroutine subvt_expr_test

```

Parton-event expressions

```
<Expr tests: execute tests>≡
    call test (subevt_expr_1, "subevt_expr_1", &
        "parton-event expressions", &
        u, results)

<Expr tests: test declarations>≡
    public :: subevt_expr_1

<Expr tests: tests>≡
    subroutine subevt_expr_1 (u)
        integer, intent(in) :: u
        type(string_t) :: expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: pt_cuts, pt_scale, pt_fac_scale, pt_ren_scale
        type(parse_tree_t) :: pt_weight
        type(parse_node_t), pointer :: pn_cuts, pn_scale, pn_fac_scale, pn_ren_scale
        type(parse_node_t), pointer :: pn_weight
        type(eval_tree_factory_t) :: expr_factory
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(parton_expr_t), target :: expr
        real(default) :: E, Ex, m
        type(vector4_t), dimension(6) :: p
        integer :: i, pdg
        logical :: passed
        real(default) :: scale, weight
        real(default), allocatable :: fac_scale, ren_scale

        write (u, "(A)")  "* Test output: subevt_expr_1"
        write (u, "(A)")  "* Purpose: Set up a subevt and associated &
            &process-specific expressions"
        write (u, "(A)")

        call syntax_pexpr_init ()

        call syntax_model_file_init ()
        call os_data%init ()
        call model%read (var_str ("Test.mdl"), os_data)

        write (u, "(A)")  "* Expression texts"
        write (u, "(A)")

        expr_text = "all Pt > 100 [s]"
        write (u, "(A,A)")  "cuts = ", char (expr_text)
        call ifile_clear (ifile)
        call ifile_append (ifile, expr_text)
        call stream_init (stream, ifile)
        call parse_tree_init_lexpr (pt_cuts, stream, .true.)
        call stream_final (stream)
        pn_cuts => pt_cuts%get_root_ptr ()

        expr_text = "sqrt{s}"
```

```

write (u, "(A,A)") "scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_scale, stream, .true.)
call stream_final (stream)
pn_scale => pt_scale%get_root_ptr ()

expr_text = "sqrts_hat"
write (u, "(A,A)") "fac_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_fac_scale, stream, .true.)
call stream_final (stream)
pn_fac_scale => pt_fac_scale%get_root_ptr ()

expr_text = "100"
write (u, "(A,A)") "ren_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_ren_scale, stream, .true.)
call stream_final (stream)
pn_ren_scale => pt_ren_scale%get_root_ptr ()

expr_text = "n_tot - n_in - n_out"
write (u, "(A,A)") "weight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)
pn_weight => pt_weight%get_root_ptr ()

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)") "* Initialize process expr"
write (u, "(A)")

call expr%setup_vars (1000._default)
call expr%var_list%append_real (var_str ("tolerance"), 0._default)
call expr%link_var_list (model%get_var_list_ptr ())

call expr_factory%init (pn_cuts)
call expr%setup_selection (expr_factory)
call expr_factory%init (pn_scale)
call expr%setup_scale (expr_factory)
call expr_factory%init (pn_fac_scale)
call expr%setup_fac_scale (expr_factory)
call expr_factory%init (pn_ren_scale)
call expr%setup_ren_scale (expr_factory)
call expr_factory%init (pn_weight)

```

```

call expr%setup_weight (expr_factory)

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Fill subevt and evaluate expressions"
write (u, "(A)")

call subevt_init (expr%subevt_t, 6)
E = 500._default
Ex = 400._default
m = 125._default
pdg = 25
p(1) = vector4_moving (E, sqrt (E**2 - m**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - m**2), 3)
p(3) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 3)
p(4) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 3)
p(5) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 1)
p(6) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 1)

call expr%reset_contents ()
do i = 1, 2
  call expr%set_beam (i, pdg, p(i), m**2)
end do
do i = 3, 4
  call expr%set_incoming (i, pdg, p(i), m**2)
end do
do i = 5, 6
  call expr%set_outgoing (i, pdg, p(i), m**2)
end do
expr%sqrts_hat = expr%get_sqrts_hat ()
expr%n_in = 2
expr%n_out = 2
expr%n_tot = 4
expr%subevt_filled = .true.

call expr%evaluate (passed, scale, fac_scale, ren_scale, weight)

write (u, "(A,L1)")      "Event has passed      = ", passed
write (u, "(A," // FMT_12 // ")")  "Scale          = ", scale
write (u, "(A," // FMT_12 // ")")  "Factorization scale = ", fac_scale
write (u, "(A," // FMT_12 // ")")  "Renormalization scale = ", ren_scale
write (u, "(A," // FMT_12 // ")")  "Weight          = ", weight
write (u, "(A)")

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call expr%final ()

call model%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: subevt_expr_1"

end subroutine subevt_expr_1

```

Parton-event expressions

```

<Expr tests: execute tests>+≡
call test (subevt_expr_2, "subevt_expr_2", &
  "parton-event expressions", &
  u, results)

<Expr tests: test declarations>+≡
public :: subevt_expr_2

<Expr tests: tests>+≡
subroutine subevt_expr_2 (u)
  integer, intent(in) :: u
  type(string_t) :: expr_text
  type(ifile_t) :: ifile
  type(stream_t) :: stream
  type(parse_tree_t) :: pt_selection
  type(parse_tree_t) :: pt_reweight, pt_analysis
  type(parse_node_t), pointer :: pn_selection
  type(parse_node_t), pointer :: pn_reweight, pn_analysis
  type(os_data_t) :: os_data
  type(model_t), target :: model
  type(eval_tree_factory_t) :: expr_factory
  type(event_expr_t), target :: expr
  real(default) :: E, Ex, m
  type(vector4_t), dimension(6) :: p
  integer :: i, pdg
  logical :: passed
  real(default) :: reweight
  logical :: analysis_flag

  write (u, "(A)")  "* Test output: subevt_expr_2"
  write (u, "(A)")  "* Purpose: Set up a subevt and associated &
    &process-specific expressions"
  write (u, "(A)")

  call syntax_pexpr_init ()

  call syntax_model_file_init ()
  call os_data%init ()
  call model%read (var_str ("Test.mdl"), os_data)

  write (u, "(A)")  "* Expression texts"
  write (u, "(A)")

```

```

expr_text = "all Pt > 100 [s]"
write (u, "(A,A)") "selection = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_selection, stream, .true.)
call stream_final (stream)
pn_selection => pt_selection%get_root_ptr ()

expr_text = "n_tot - n_in - n_out"
write (u, "(A,A)") "reweight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_reweight, stream, .true.)
call stream_final (stream)
pn_reweight => pt_reweight%get_root_ptr ()

expr_text = "true"
write (u, "(A,A)") "analysis = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_analysis, stream, .true.)
call stream_final (stream)
pn_analysis => pt_analysis%get_root_ptr ()

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Initialize process expr"
write (u, "(A)")

call expr%setup_vars (1000._default)
call expr%link_var_list (model%get_var_list_ptr ())
call expr%var_list%append_real (var_str ("tolerance"), 0._default)

call expr_factory%init (pn_selection)
call expr%setup_selection (expr_factory)
call expr_factory%init (pn_analysis)
call expr%setup_analysis (expr_factory)
call expr_factory%init (pn_reweight)
call expr%setup_reweight (expr_factory)

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Fill subevt and evaluate expressions"
write (u, "(A)")

```

```

call subevt_init (expr%subevt_t, 6)
E = 500._default
Ex = 400._default
m = 125._default
pdg = 25
p(1) = vector4_moving (E, sqrt (E**2 - m**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - m**2), 3)
p(3) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 3)
p(4) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 3)
p(5) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 1)
p(6) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 1)

call expr%reset_contents ()
do i = 1, 2
  call expr%set_beam (i, pdg, p(i), m**2)
end do
do i = 3, 4
  call expr%set_incoming (i, pdg, p(i), m**2)
end do
do i = 5, 6
  call expr%set_outgoing (i, pdg, p(i), m**2)
end do
expr%sqrts_hat = expr%get_sqrts_hat ()
expr%n_in = 2
expr%n_out = 2
expr%n_tot = 4
expr%subevt_filled = .true.

call expr%evaluate (passed, reweight, analysis_flag)

write (u, "(A,L1)")      "Event has passed      = ", passed
write (u, "(A," // FMT_12 // ")") "Reweighting factor = ", reweight
write (u, "(A,L1)")      "Analysis flag      = ", analysis_flag
write (u, "(A)")

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call expr%final ()

call model%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: subevt_expr_2"

end subroutine subevt_expr_2

```

Processes: handle partonic cuts

Initialize a process and process instance, choose a sampling point and fill the process instance, evaluating a given cut configuration.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```
(Expr tests: execute tests)+≡
  call test (processes_5, "processes_5", &
    "handle cuts (partonic event)", &
    u, results)

(Expr tests: test declarations)+≡
  public :: processes_5

(Expr tests: tests)+≡
  subroutine processes_5 (u)
    integer, intent(in) :: u
    type(string_t) :: cut_expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: parse_tree
    type(eval_tree_factory_t) :: expr_factory
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), pointer :: model_tmp
    type(model_t), pointer :: model
    type(var_list_t), target :: var_list
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t), allocatable, target :: process_instance

    write (u, "(A)")  "* Test output: processes_5"
    write (u, "(A)")  "* Purpose: create a process &
      &and fill a process instance"
    write (u, "(A)")

    write (u, "(A)")  "* Prepare a cut expression"
    write (u, "(A)")

    call syntax_pexpr_init ()
    cut_expr_text = "all Pt > 100 [s]"
    call ifile_append (ifile, cut_expr_text)
    call stream_init (stream, ifile)
    call parse_tree_init_lexpr (parse_tree, stream, .true.)

    write (u, "(A)")  "* Build and initialize a test process"
    write (u, "(A)")

    libname = "processes5"
    procname = libname

    call os_data%init ()
```



```

call prc_test_create_library (libname, lib)

call syntax_model_file_init ()
allocate (model_tmp)
call model_tmp%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model_tmp%get_var_list_ptr ())
model => model_tmp

call reset_interaction_counter ()

call var_list%append_real (var_str ("tolerance"), 0._default)
call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

allocate (process)
call process%init (procname, lib, os_data, model, var_list)

call var_list%final ()

allocate (phs_test_config_t :: phs_config_template)
call process%setup_test_cores ()
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization and set cuts"
write (u, "(A)")

call process%setup_terms ()
call expr_factory%init (parse_tree%get_root_ptr ())
call process%set_cuts (expr_factory)
call process%write (.false., u, &
    show_var_list=.true., show_expressions=.true., show_os_data=.false.)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpair ([0._default, 0._default])

```

```

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics and subvt, check cuts (should fail)"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set (should succeed)"
write (u, "(A)")

call process_instance%reset ()
call process_instance%set_mcpair ([0.5_default, 0.125_default])
call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set using convenience procedure &
                  &(failure)"
write (u, "(A)")

call process_instance%evaluate_sqme (1, [0.0_default, 0.2_default])

call process_instance%write_header (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set using convenience procedure &
                  &(success)"
write (u, "(A)")

call process_instance%evaluate_sqme (1, [0.1_default, 0.2_default])

call process_instance%write_header (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()

```

```

deallocate (process)

call parse_tree_final (parse_tree)
call stream_final (stream)
call ifile_final (ifile)
call syntax_pexpr_final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_5"

end subroutine processes_5

```

Trivial for testing: do not allocate the MCI record.

```

<Expr tests: test auxiliary>≡
subroutine dispatch_mci_empty (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
end subroutine dispatch_mci_empty

```

Processes: scales and such

Initialize a process and process instance, choose a sampling point and fill the process instance, evaluating a given cut configuration.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Expr tests: execute tests>+≡
  call test (processes_6, "processes_6", &
    "handle scales and weight (partonic event)", &
    u, results)

<Expr tests: test declarations>+≡
  public :: processes_6

<Expr tests: tests>+≡
subroutine processes_6 (u)
  integer, intent(in) :: u
  type(string_t) :: expr_text
  type(ifile_t) :: ifile
  type(stream_t) :: stream
  type(parse_tree_t) :: pt_scale, pt_fac_scale, pt_ren_scale, pt_weight
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), pointer :: model_tmp
  type(model_t), pointer :: model
  type(var_list_t), target :: var_list
  type(process_t), allocatable, target :: process
  class(phs_config_t), allocatable :: phs_config_template

```

```

real(default) :: sqrts
type(process_instance_t), allocatable, target :: process_instance
type(eval_tree_factory_t) :: expr_factory

write (u, "(A)")  "* Test output: processes_6"
write (u, "(A)")  "* Purpose: create a process &
                  &and fill a process instance"
write (u, "(A)")

write (u, "(A)")  "* Prepare expressions"
write (u, "(A)")

call syntax_pexpr_init ()

expr_text = "sqrts - 100 GeV"
write (u, "(A,A)") "scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_scale, stream, .true.)
call stream_final (stream)

expr_text = "sqrts_hat"
write (u, "(A,A)") "fac_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_fac_scale, stream, .true.)
call stream_final (stream)

expr_text = "eval sqrt (M2) [collect [s]]"
write (u, "(A,A)") "ren_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_ren_scale, stream, .true.)
call stream_final (stream)

expr_text = "n_tot * n_in * n_out * (eval Phi / pi [s])"
write (u, "(A,A)") "weight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Build and initialize a test process"
write (u, "(A)")

libname = "processes4"
procname = libname

```

```

call os_data%init ()
call prc_test_create_library (libname, lib)

call syntax_model_file_init ()
allocate (model_tmp)
call model_tmp%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model_tmp%get_var_list_ptr ())
model => model_tmp

call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

call reset_interaction_counter ()

allocate (process)
call process%init (procname, lib, os_data, model, var_list)

call var_list%final ()

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization and set cuts"
write (u, "(A)")

call process%setup_terms ()
call expr_factory%init (pt_scale%get_root_ptr ())
call process%set_scale (expr_factory)
call expr_factory%init (pt_fac_scale%get_root_ptr ())
call process%set_fac_scale (expr_factory)
call expr_factory%init (pt_ren_scale%get_root_ptr ())
call process%set_ren_scale (expr_factory)
call expr_factory%init (pt_weight%get_root_ptr ())
call process%set_weight (expr_factory)
call process%write (.false., u, show_expressions=.true.)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance and evaluate"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, [0.5_default, 0.125_default])

```

```

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call parse_tree_final (pt_scale)
call parse_tree_final (pt_fac_scale)
call parse_tree_final (pt_ren_scale)
call parse_tree_final (pt_weight)
call syntax_pexpr_final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_6"

end subroutine processes_6

```

Event expressions

After generating an event, fill the `subevt` and evaluate expressions for selection, reweighting, and analysis.

```

<Expr tests: execute tests>+≡
  call test (events_3, "events_3", &
    "expression evaluation", &
    u, results)

<Expr tests: test declarations>+≡
  public :: events_3

<Expr tests: tests>+≡
  subroutine events_3 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(string_t) :: expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: pt_selection, pt_reweight, pt_analysis
    type(eval_tree_factory_t) :: expr_factory
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(os_data_t) :: os_data
    type(model_t), pointer :: model
    type(var_list_t), target :: var_list

```

```

write (u, "(A)")  "* Test output: events_3"
write (u, "(A)")  "* Purpose: generate an event and evaluate expressions"
write (u, "(A)")

call syntax_pexpr_init ()

write (u, "(A)")  "* Expression texts"
write (u, "(A)")

expr_text = "all Pt > 100 [s]"
write (u, "(A,A)") "selection = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_selection, stream, .true.)
call stream_final (stream)

expr_text = "1 + sqrts_hat / sqrts"
write (u, "(A,A)") "reweight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_reweight, stream, .true.)
call stream_final (stream)

expr_text = "true"
write (u, "(A,A)") "analysis = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_analysis, stream, .true.)
call stream_final (stream)

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Initialize test process event"

call os_data%init ()

call syntax_model_file_init ()
allocate (model)
call model%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model%get_var_list_ptr ())

call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model, var_list)

call var_list%final ()

```

```

call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Initialize event object and set expressions"

allocate (event)
call event%basic_init ()

call expr_factory%init (pt_selection%get_root_ptr ())
call event%set_selection (expr_factory)
call expr_factory%init (pt_reweight%get_root_ptr ())
call event%set_reweight (expr_factory)
call expr_factory%init (pt_analysis%get_root_ptr ())
call event%set_analysis (expr_factory)

call event%connect (process_instance, process%get_model_ptr ())
call event%expr%var_list%append_real (var_str ("tolerance"), 0._default)
call event%setup_expressions ()

write (u, "(A)")
write (u, "(A)")  "* Generate test process event"

call process_instance%generate_weighted_event (1)

write (u, "(A)")
write (u, "(A)")  "* Fill event object and evaluate expressions"
write (u, "(A)")

call event%generate (1, [0.4_default, 0.4_default])
call event%set_index (42)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_3"

end subroutine events_3

```


Chapter 35

Top Level

The top level consists of

commands Defines generic command-list and command objects, and all specific implementations. Each command type provides a specific functionality. Together with the modules that provide expressions and variables, this module defines the Sindarin language.

whizard This module interprets streams of various kind in terms of the command language. It also contains the unit-test feature. We also define the externally visible procedures here, for the **WHIZARD** as a library.

main The driver for **WHIZARD** as a stand-alone program. Contains the command-line interpreter.

whizard_c_interface Alternative top-level procedures, for use in the context of a C-compatible caller program.

35.1 Commands

This module defines the command language of the main input file.

```
<commands.f90>≡
  <File header>

  module commands

    <Use kinds>
    <Use strings>
    <Use debug>
    use diagnostics
    use lexers
    use syntax_rules
    use parser
    use variables, only: var_list_t, V_NONE, V_LOG, V_INT, V_REAL, V_CMPLX, V_STR, V_PDG
    use eval_trees
    use polarizations
    use rt_data

    <Standard module head>

    <Commands: public>

    <Commands: types>

    <Commands: variables>

    <Commands: parameters>

    <Commands: interfaces>

    interface
    <Commands: sub interfaces>
    end interface

  contains

    <Commands: main procedures>

  end module commands

<commands_sub.f90>≡
  <File header>

  submodule (commands) commands_s

    <Use mpi f08>
    use io_units
    use string_utils, only: lower_case, split_string, str
    use format_utils, only: write_indent
    use format_defs, only: FMT_14, FMT_19
    use constants, only: one
    use physics_defs
```

```

use sorting
use sf_lhapdf, only: lhapdf_global_reset
use os_interface
use ifiles
use analysis
use pdg_arrays
use observables, only: var_list_check_observable
use observables, only: var_list_check_result_var
use models
use auto_components
use flavors
use particle_specifiers
use process_libraries
use process
use instances
use prclib_stacks
use slha_interface
use user_files
use eio_data
use process_configurations
use compilations, only: compile_library, compile_executable
use integrations, only: integrate_process
use restricted_subprocesses, only: get_libname_res
use restricted_subprocesses, only: spawn_resonant_subprocess_libraries
use event_streams
use radiation_generator
use simulations

implicit none

contains

<Commands: procedures>

end submodule commands_s

```

35.1.1 The command type

The command type is a generic type that holds any command, compiled for execution.

Each command may come with its own local environment. The command list that determines this environment is allocated as `options`, if necessary. (It has to be allocated as a pointer because the type definition is recursive.) The local environment is available as a pointer which either points to the global environment, or is explicitly allocated and initialized.

<Commands: types>≡

```

type, abstract :: command_t
  type(parse_node_t), pointer :: pn => null ()
  class(command_t), pointer :: next => null ()
  type(parse_node_t), pointer :: pn_opt => null ()
  type(command_list_t), pointer :: options => null ()
  type(rt_data_t), pointer :: local => null ()

```

```

contains
  <Commands: command: TBP>
end type command_t

```

Finalizer: If there is an option list, finalize the option list and deallocate. If not, the local environment is just a pointer.

```

<Commands: command: TBP>≡
  procedure :: final => command_final

<Commands: sub interfaces>≡
  recursive module subroutine command_final (cmd)
    class(command_t), intent(inout) :: cmd
  end subroutine command_final

<Commands: procedures>≡
  recursive module subroutine command_final (cmd)
    class(command_t), intent(inout) :: cmd
    if (associated (cmd%options)) then
      call cmd%options%final ()
      deallocate (cmd%options)
      call cmd%local%local_final ()
      deallocate (cmd%local)
    else
      cmd%local => null ()
    end if
  end subroutine command_final

```

Allocate a command with the appropriate concrete type. Store the parse node pointer in the command object, so we can reference to it when compiling. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Commands: main procedures>≡
  subroutine dispatch_command (command, pn)
    class(command_t), intent(inout), pointer :: command
    type(parse_node_t), intent(in), target :: pn
    select case (char (parse_node_get_rule_key (pn)))
    case ("cmd_model")
      allocate (cmd_model_t :: command)
    case ("cmd_library")
      allocate (cmd_library_t :: command)
    case ("cmd_process")
      allocate (cmd_process_t :: command)
    case ("cmd_nlo")
      allocate (cmd_nlo_t :: command)
    case ("cmd_compile")
      allocate (cmd_compile_t :: command)
    case ("cmd_exec")
      allocate (cmd_exec_t :: command)
    case ("cmd_num", "cmd_complex", "cmd_real", "cmd_int", &
          "cmd_log_decl", "cmd_log", "cmd_string", "cmd_string_decl", &
          "cmd_alias", "cmd_result")
      allocate (cmd_var_t :: command)
    case ("cmd_slha")
      allocate (cmd_slha_t :: command)
    case ("cmd_show")

```

```

        allocate (cmd_show_t :: command)
case ("cmd_clear")
        allocate (cmd_clear_t :: command)
case ("cmd_expect")
        allocate (cmd_expect_t :: command)
case ("cmd_beams")
        allocate (cmd_beams_t :: command)
case ("cmd_beams_pol_density")
        allocate (cmd_beams_pol_density_t :: command)
case ("cmd_beams_pol_fraction")
        allocate (cmd_beams_pol_fraction_t :: command)
case ("cmd_beams_momentum")
        allocate (cmd_beams_momentum_t :: command)
case ("cmd_beams_theta")
        allocate (cmd_beams_theta_t :: command)
case ("cmd_beams_phi")
        allocate (cmd_beams_phi_t :: command)
case ("cmd_cuts")
        allocate (cmd_cuts_t :: command)
case ("cmd_scale")
        allocate (cmd_scale_t :: command)
case ("cmd_fac_scale")
        allocate (cmd_fac_scale_t :: command)
case ("cmd_ren_scale")
        allocate (cmd_ren_scale_t :: command)
case ("cmd_weight")
        allocate (cmd_weight_t :: command)
case ("cmd_selection")
        allocate (cmd_selection_t :: command)
case ("cmd_reweight")
        allocate (cmd_reweight_t :: command)
case ("cmd_iterations")
        allocate (cmd_iterations_t :: command)
case ("cmd_integrate")
        allocate (cmd_integrate_t :: command)
case ("cmd_observable")
        allocate (cmd_observable_t :: command)
case ("cmd_histogram")
        allocate (cmd_histogram_t :: command)
case ("cmd_plot")
        allocate (cmd_plot_t :: command)
case ("cmd_graph")
        allocate (cmd_graph_t :: command)
case ("cmd_record")
        allocate (cmd_record_t :: command)
case ("cmd_analysis")
        allocate (cmd_analysis_t :: command)
case ("cmd_alt_setup")
        allocate (cmd_alt_setup_t :: command)
case ("cmd_unstable")
        allocate (cmd_unstable_t :: command)
case ("cmd_stable")
        allocate (cmd_stable_t :: command)
case ("cmd_polarized")

```

```

        allocate (cmd_polarized_t :: command)
case ("cmd_unpolarized")
    allocate (cmd_unpolarized_t :: command)
case ("cmd_sample_format")
    allocate (cmd_sample_format_t :: command)
case ("cmd_simulate")
    allocate (cmd_simulate_t :: command)
case ("cmd_rescan")
    allocate (cmd_rescan_t :: command)
case ("cmd_write_analysis")
    allocate (cmd_write_analysis_t :: command)
case ("cmd_compile_analysis")
    allocate (cmd_compile_analysis_t :: command)
case ("cmd_open_out")
    allocate (cmd_open_out_t :: command)
case ("cmd_close_out")
    allocate (cmd_close_out_t :: command)
case ("cmd_printf")
    allocate (cmd_printf_t :: command)
case ("cmd_scan")
    allocate (cmd_scan_t :: command)
case ("cmd_if")
    allocate (cmd_if_t :: command)
case ("cmd_include")
    allocate (cmd_include_t :: command)
case ("cmd_export")
    allocate (cmd_export_t :: command)
case ("cmd_quit")
    allocate (cmd_quit_t :: command)
case default
    print *, char (parse_node_get_rule_key (pn))
    call msg_bug ("Command not implemented")
end select
command%pn => pn
end subroutine dispatch_command

```

Output. We allow for indentation so we can display a command tree.

```

⟨Commands: command: TBP⟩+≡
    procedure (command_write), deferred :: write

⟨Commands: interfaces⟩≡
    abstract interface
        subroutine command_write (cmd, unit, indent)
            import
            class(command_t), intent(in) :: cmd
            integer, intent(in), optional :: unit, indent
        end subroutine command_write
    end interface

```

Compile a command. The command type is already fixed, so this is a deferred type-bound procedure.

```

⟨Commands: command: TBP⟩+≡
    procedure (command_compile), deferred :: compile

```

```

<Commands: interfaces>+≡
  abstract interface
    subroutine command_compile (cmd, global)
      import
      class(command_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
    end subroutine command_compile
  end interface

```

Execute a command. This will use and/or modify the runtime data set. If the `quit` flag is set, the caller should terminate command execution.

```

<Commands: command: TBP>+≡
  procedure (command_execute), deferred :: execute

```

```

<Commands: interfaces>+≡
  abstract interface
    subroutine command_execute (cmd, global)
      import
      class(command_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
    end subroutine command_execute
  end interface

```

35.1.2 Options

The `options` command list is allocated, initialized, and executed, if the command is associated with an option text in curly braces. If present, a separate local runtime data set `local` will be allocated and initialized; otherwise, `local` becomes a pointer to the global dataset.

For output, we indent the options list.

```

<Commands: command: TBP>+≡
  procedure :: write_options => command_write_options

<Commands: sub interfaces>+≡
  recursive module subroutine command_write_options (cmd, unit, indent)
    class(command_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine command_write_options

<Commands: procedures>+≡
  recursive module subroutine command_write_options (cmd, unit, indent)
    class(command_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: ind
    ind = 1; if (present (indent)) ind = indent + 1
    if (associated (cmd%options)) call cmd%options%write (unit, ind)
  end subroutine command_write_options

```

Compile the options list, if any. This implies initialization of the local environment. Should be done once the `pn_opt` node has been assigned (if applicable), but before the actual command compilation.

```

<Commands: command: TBP>+≡
  procedure :: compile_options => command_compile_options

```

```

<Commands: sub interfaces>+≡
    recursive module subroutine command_compile_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine command_compile_options

<Commands: procedures>+≡
    recursive module subroutine command_compile_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (associated (cmd%pn_opt)) then
            allocate (cmd%local)
            call cmd%local%local_init (global)
            call global%copy_globals (cmd%local)
            allocate (cmd%options)
            call cmd%options%compile (cmd%pn_opt, cmd%local)
            call global%restore_globals (cmd%local)
            call cmd%local%deactivate ()
        else
            cmd%local => global
        end if
    end subroutine command_compile_options

```

Execute options. First prepare the local environment, then execute the command list.

```

<Commands: command: TBP>+≡
    procedure :: execute_options => cmd_execute_options

<Commands: sub interfaces>+≡
    recursive module subroutine cmd_execute_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_execute_options

<Commands: procedures>+≡
    recursive module subroutine cmd_execute_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (associated (cmd%options)) then
            call cmd%local%activate ()
            call cmd%options%execute (cmd%local)
        end if
    end subroutine cmd_execute_options

```

This must be called after the parent command has been executed, to undo temporary modifications to the environment. Note that some modifications to global can become permanent.

```

<Commands: command: TBP>+≡
    procedure :: reset_options => cmd_reset_options

<Commands: sub interfaces>+≡
    module subroutine cmd_reset_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_reset_options

```



```

<Commands: procedures>+≡
module subroutine cmd_reset_options (cmd, global)
  class(command_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  if (associated (cmd%options)) then
    call cmd%local%deactivate (global)
  end if
end subroutine cmd_reset_options

```

35.1.3 Specific command types

Model configuration

The command declares a model, looks for the specified file and loads it.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_model_t
  private
  type(string_t) :: name
  type(string_t) :: scheme
  logical :: ufo_model = .false.
  logical :: ufo_path_set = .false.
  type(string_t) :: ufo_path
contains
  <Commands: cmd model: TBP>
end type cmd_model_t

```

Output

```

<Commands: cmd model: TBP>≡
  procedure :: write => cmd_model_write

<Commands: sub interfaces>+≡
  module subroutine cmd_model_write (cmd, unit, indent)
    class(cmd_model_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_model_write

<Commands: procedures>+≡
  module subroutine cmd_model_write (cmd, unit, indent)
    class(cmd_model_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,'"',A,'"',", advance='no") "model =", char (cmd%name)
    if (cmd%ufo_model) then
      if (cmd%ufo_path_set) then
        write (u, "(1x,A,A,A)") "(ufo (", char (cmd%ufo_path), ")")
      else
        write (u, "(1x,A)") "(ufo)"
      end if
    else if (cmd%scheme /= "") then
      write (u, "(1x,'(,A,')')") char (cmd%scheme)
    else

```

```

        write (u, *)
    end if
end subroutine cmd_model_write

```

Compile. Get the model name and read the model from file, so it is readily available when the command list is executed. If the model has a scheme argument, take this into account.

Assign the model pointer in the `global` record, so it can be used for (read-only) variable lookup while compiling further commands.

(Commands: cmd model: TBP)+≡

```

    procedure :: compile => cmd_model_compile

```

(Commands: sub interfaces)+≡

```

    module subroutine cmd_model_compile (cmd, global)
        class(cmd_model_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_model_compile

```

(Commands: procedures)+≡

```

    module subroutine cmd_model_compile (cmd, global)
        class(cmd_model_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_name, pn_arg, pn_scheme
        type(parse_node_t), pointer :: pn_ufo_arg, pn_path
        type(model_t), pointer :: model
        type(string_t) :: scheme
        pn_name => cmd%pn%get_sub_ptr (3)
        pn_arg => pn_name%get_next_ptr ()
        if (associated (pn_arg)) then
            pn_scheme => pn_arg%get_sub_ptr ()
        else
            pn_scheme => null ()
        end if
        cmd%name = pn_name%get_string ()
        if (associated (pn_scheme)) then
            select case (char (pn_scheme%get_rule_key ()))
            case ("ufo_spec")
                cmd%ufo_model = .true.
                pn_ufo_arg => pn_scheme%get_sub_ptr (2)
                if (associated (pn_ufo_arg)) then
                    pn_path => pn_ufo_arg%get_sub_ptr ()
                    cmd%ufo_path_set = .true.
                    cmd%ufo_path = pn_path%get_string ()
                end if
            case default
                scheme = pn_scheme%get_string ()
            end select
        end if
        select case (char (lower_case (scheme)))
        case ("ufo"); cmd%ufo_model = .true.
        case default; cmd%scheme = scheme
        end select
    end select
    if (cmd%ufo_model) then
        if (cmd%ufo_path_set) then
            call preload_ufo_model (model, cmd%name, cmd%ufo_path)
        end if
    end if
end subroutine cmd_model_compile

```

```

        else
            call preload_ufo_model (model, cmd%name)
        end if
    else
        call preload_model (model, cmd%name, cmd%scheme)
    end if
else
    cmd%scheme = ""
    call preload_model (model, cmd%name)
end if
global%model => model
if (associated (global%model)) then
    call global%model%link_var_list (global%var_list)
end if
contains
subroutine preload_model (model, name, scheme)
    type(model_t), pointer, intent(out) :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    model => null ()
    if (associated (global%model)) then
        if (global%model%matches (name, scheme)) then
            model => global%model
        end if
    end if
    if (.not. associated (model)) then
        if (global%model_list%model_exists (name, scheme)) then
            model => global%model_list%get_model_ptr (name, scheme)
        else
            call global%read_model (name, model, scheme)
        end if
    end if
end subroutine preload_model
subroutine preload_ufo_model (model, name, ufo_path)
    type(model_t), pointer, intent(out) :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: ufo_path
    model => null ()
    if (associated (global%model)) then
        if (global%model%matches (name, ufo=.true., ufo_path=ufo_path)) then
            model => global%model
        end if
    end if
    if (.not. associated (model)) then
        if (global%model_list%model_exists (name, &
            ufo=.true., ufo_path=ufo_path)) then
            model => global%model_list%get_model_ptr (name, &
                ufo=.true., ufo_path=ufo_path)
        else
            call global%read_ufo_model (name, model, ufo_path=ufo_path)
        end if
    end if
end subroutine preload_ufo_model
end subroutine cmd_model_compile

```

Execute: Insert a pointer into the global data record and reassign the variable list.

```

⟨Commands: cmd model: TBP⟩+=
    procedure :: execute => cmd_model_execute

⟨Commands: sub interfaces⟩+=
    module subroutine cmd_model_execute (cmd, global)
        class(cmd_model_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_model_execute

⟨Commands: procedures⟩+=
    module subroutine cmd_model_execute (cmd, global)
        class(cmd_model_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (cmd%ufo_model) then
            if (cmd%ufo_path_set) then
                call global%select_model (cmd%name, ufo=.true., ufo_path=cmd%ufo_path)
            else
                call global%select_model (cmd%name, ufo=.true.)
            end if
        else if (cmd%scheme /= "") then
            call global%select_model (cmd%name, cmd%scheme)
        else
            call global%select_model (cmd%name)
        end if
        if (.not. associated (global%model)) &
            call msg_fatal ("Switching to model '" &
                // char (cmd%name) // "': model not found")
    end subroutine cmd_model_execute

```

Library configuration

We configure a process library that should hold the subsequently defined processes. If the referenced library exists already, just make it the currently active one.

```

⟨Commands: types⟩+=
    type, extends (command_t) :: cmd_library_t
        private
        type(string_t) :: name
    contains
        ⟨Commands: cmd library: TBP⟩
    end type cmd_library_t

```

Output.

```

⟨Commands: cmd library: TBP⟩=
    procedure :: write => cmd_library_write

⟨Commands: sub interfaces⟩+=
    module subroutine cmd_library_write (cmd, unit, indent)
        class(cmd_library_t), intent(in) :: cmd

```

```

integer, intent(in), optional :: unit, indent
end subroutine cmd_library_write

```

<Commands: procedures>+≡

```

module subroutine cmd_library_write (cmd, unit, indent)
  class(cmd_library_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit)
  call write_indent (u, indent)
  write (u, "(1x,A,1x,'"',A,'\"') "library =", char (cmd%name)
end subroutine cmd_library_write

```

Compile. Get the library name.

<Commands: cmd library: TBP>+≡

```

procedure :: compile => cmd_library_compile

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_library_compile (cmd, global)
  class(cmd_library_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_library_compile

```

<Commands: procedures>+≡

```

module subroutine cmd_library_compile (cmd, global)
  class(cmd_library_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_name
  pn_name => parse_node_get_sub_ptr (cmd%pn, 3)
  cmd%name = parse_node_get_string (pn_name)
end subroutine cmd_library_compile

```

Execute: Initialize a new library and push it on the library stack (if it does not yet exist). Insert a pointer to the library into the global data record. Then, try to load the library unless the **rebuild** flag is set.

<Commands: cmd library: TBP>+≡

```

procedure :: execute => cmd_library_execute

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_library_execute (cmd, global)
  class(cmd_library_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_library_execute

```

<Commands: procedures>+≡

```

module subroutine cmd_library_execute (cmd, global)
  class(cmd_library_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(prclib_entry_t), pointer :: lib_entry
  type(process_library_t), pointer :: lib
  logical :: rebuild_library
  lib => global%prclib_stack%get_library_ptr (cmd%name)
  rebuild_library = &
    global%var_list%get_lval (var_str ("?rebuild_library"))
  if (.not. (associated (lib))) then

```

```

        allocate (lib_entry)
        call lib_entry%init (cmd%name)
        lib => lib_entry%process_library_t
        call global%add_prclib (lib_entry)
    else
        call global%update_prclib (lib)
    end if
    if (associated (lib) .and. .not. rebuild_library) then
        call lib%update_status (global%os_data)
    end if
end subroutine cmd_library_execute

```

Process configuration

We define a process-configuration command as a specific type. The incoming and outgoing particles are given evaluation-trees which we transform to PDG-code arrays. For transferring to O'MEGA, they are reconverted to strings.

For the incoming particles, we store parse nodes individually. We do not yet resolve the outgoing state, so we store just a single parse node.

This also includes the choice of method for the corresponding process: `omega` for O'MEGA matrix elements as Fortran code, `ovm` for O'MEGA matrix elements as a bytecode virtual machine, `test` for special processes, `unit_test` for internal test matrix elements generated by WHIZARD, `template` and `template_unity` for test matrix elements generated by WHIZARD as Fortran code similar to the O'MEGA code. If the one-loop program (OLP) GoSam is linked, also matrix elements from there (at leading and next-to-leading order) can be generated via `gosam`.

```

<Commands: types>+=
    type, extends (command_t) :: cmd_process_t
    private
    type(string_t) :: id
    integer :: n_in = 0
    type(parse_node_p), dimension(:), allocatable :: pn_pdg_in
    type(parse_node_t), pointer :: pn_out => null ()
    contains
    <Commands: cmd process: TBP>
end type cmd_process_t

```

Output. The particle expressions are not resolved, so we just list the number of incoming particles.

```

<Commands: cmd process: TBP>=
    procedure :: write => cmd_process_write

<Commands: sub interfaces>+=
    module subroutine cmd_process_write (cmd, unit, indent)
        class(cmd_process_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_process_write

<Commands: procedures>+=
    module subroutine cmd_process_write (cmd, unit, indent)
        class(cmd_process_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_process_write

```

```

integer :: u
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A,A,A,I0,A)") "process: ", char (cmd%id), " (", &
      size (cmd%pn_pdg_in), " -> X)"
call cmd%write_options (u, indent)
end subroutine cmd_process_write

```

Compile. Find and assign the parse nodes.

```

⟨Commands: cmd process: TBP⟩+≡
  procedure :: compile => cmd_process_compile

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_process_compile (cmd, global)
    class(cmd_process_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_process_compile

⟨Commands: procedures⟩+≡
  module subroutine cmd_process_compile (cmd, global)
    class(cmd_process_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_id, pn_in, pn_codes
    integer :: i
    pn_id => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_in => parse_node_get_next_ptr (pn_id, 2)
    cmd%pn_out => parse_node_get_next_ptr (pn_in, 2)
    cmd%pn_opt => parse_node_get_next_ptr (cmd%pn_out)
    call cmd%compile_options (global)
    cmd%id = parse_node_get_string (pn_id)
    cmd%n_in = parse_node_get_n_sub (pn_in)
    pn_codes => parse_node_get_sub_ptr (pn_in)
    allocate (cmd%pn_pdg_in (cmd%n_in))
    do i = 1, cmd%n_in
      cmd%pn_pdg_in(i)%ptr => pn_codes
      pn_codes => parse_node_get_next_ptr (pn_codes)
    end do
  end subroutine cmd_process_compile

```

Command execution. Evaluate the subevents, transform PDG codes into strings, and add the current process configuration to the process library.

The initial state will be unique (one or two particles). For the final state, we allow for expressions. The expressions will be expanded until we have a sum of final states. Each distinct final state will get its own process component.

To identify equivalent final states, we transform the final state into an array of PDG codes, which we sort and compare. If a particle entry is actually a PDG array, only the first entry in the array is used for the comparison. The user should make sure that there is no overlap between different particles or arrays which would make the expansion ambiguous.

There are two possibilities that a process contains more than one component: by an explicit component statement by the user for inclusive processes, or by having one process at NLO level. The first option is determined in the chunk

scan components, and determines n_components.

(Commands: cmd process: TBP)+≡

```
procedure :: execute => cmd_process_execute
```

(Commands: sub interfaces)+≡

```
module subroutine cmd_process_execute (cmd, global)
  class(cmd_process_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_process_execute
```

(Commands: procedures)+≡

```
module subroutine cmd_process_execute (cmd, global)
  class(cmd_process_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(pdg_array_t) :: pdg_in, pdg_out
  type(pdg_array_t), dimension(:), allocatable :: pdg_out_tab
  type(string_t), dimension(:), allocatable :: prt_in
  type(string_t) :: prt_out, prt_out1
  type(process_configuration_t) :: prc_config
  type(prt_expr_t) :: prt_expr_out
  type(prt_spec_t), dimension(:), allocatable :: prt_spec_in
  type(prt_spec_t), dimension(:), allocatable :: prt_spec_out
  type(var_list_t), pointer :: var_list
  integer, dimension(:), allocatable :: ipdg
  integer, dimension(:), allocatable :: i_term
  integer, dimension(:), allocatable :: nlo_comp
  integer :: i, j, n_in, n_out, n_terms, n_components
  logical :: nlo_fixed_order
  logical :: qcd_corr, qed_corr
  type(string_t), dimension(:), allocatable :: prt_in_nlo, prt_out_nlo
  type(radiation_generator_t) :: radiation_generator
  type(pdg_list_t) :: pl_in, pl_out, pl_excluded_gaugeSplittings
  type(string_t) :: method, born_me_method, loop_me_method, &
    correlation_me_method, real_tree_me_method, dglap_me_method
  integer, dimension(:), allocatable :: i_list
  logical :: use_real_finite
  logical :: gks_active
  logical :: initial_state_colored
  logical :: neg_sf
  integer :: comp_mult
  integer :: gks_multiplicity
  integer :: n_components_init
  integer :: alpha_power, alphas_power
  logical :: requires_soft_mismatch, requires_dglap_remnants
  type(string_t) :: nlo_correction_type
  type(pdg_array_t), dimension(:), allocatable :: pdg
  if (debug_on) call msg_debug (D_CORE, "cmd_process_execute")
  var_list => cmd%local%get_var_list_ptr ()

  n_in = size (cmd%pn_pdg_in)
  allocate (prt_in (n_in), prt_spec_in (n_in))
  do i = 1, n_in
    pdg_in = &
      eval_pdg_array (cmd%pn_pdg_in(i)%ptr, var_list)
    prt_in(i) = make_flavor_string (pdg_in, cmd%local%model)
```



```

        prt_spec_in(i) = new_prt_spec (prt_in(i))
    end do
    call compile_prt_expr &
        (prt_expr_out, cmd%pn_out, var_list, cmd%local%model)
    call prt_expr_out%expand ()
    <Commands: cmd process execute: scan components>
    allocate (nlo_comp (n_components))

    nlo_fixed_order = cmd%local%nlo_fixed_order
    gks_multiplicity = var_list%get_ival (var_str ("gks_multiplicity"))
    gks_active = gks_multiplicity > 2
    neg_sf = .false.
    select case (char (var_list%get_sval (var_str ("negative_sf"))))
    case ("default")
        neg_sf = nlo_fixed_order
    case ("negative")
        neg_sf = .true.
    case ("positive")
        neg_sf = .false.
    case default
        call msg_fatal ("Negative PDF handling can only be " // &
            "default, negative or positive.")
    end select
    <Commands: cmd process execute: check for nlo corrections>

    method = var_list%get_sval (var_str ("method"))
    born_me_method = var_list%get_sval (var_str ("born_me_method"))
    if (born_me_method == var_str ("")) born_me_method = method
    select case (char (var_list%get_sval (var_str ("real_partition_mode"))))
    case ("default", "off", "singular")
        use_real_finite = .false.
    case ("all", "on", "finite")
        use_real_finite = .true.
    case default
        call msg_fatal ("The real partition mode can only be " // &
            "default, off, all, on, singular or finite.")
    end select
    if (nlo_fixed_order) then
        real_tree_me_method = &
            var_list%get_sval (var_str ("real_tree_me_method"))
        if (real_tree_me_method == var_str ("")) &
            real_tree_me_method = method
        loop_me_method = var_list%get_sval (var_str ("loop_me_method"))
        if (loop_me_method == var_str ("")) &
            loop_me_method = method
        correlation_me_method = &
            var_list%get_sval (var_str ("correlation_me_method"))
        if (correlation_me_method == var_str ("")) &
            correlation_me_method = method
        dglap_me_method = var_list%get_sval (var_str ("dglap_me_method"))
        if (dglap_me_method == var_str ("")) &
            dglap_me_method = method
        call check_nlo_options (cmd%local)
    end if

```

```

call determine_needed_components ()
call prc_config%init (cmd%id, n_in, n_components_init, &
  cmd%local%model, cmd%local%var_list, &
  nlo_process = nlo_fixed_order, &
  negative_sf = neg_sf)

alpha_power = var_list%get_ival (var_str ("alpha_power"))
alphas_power = var_list%get_ival (var_str ("alphas_power"))
call prc_config%set_coupling_powers (alpha_power, alphas_power)

call setup_components ()
call prc_config%record (cmd%local)

contains

<Commands: cmd process execute procedures>

end subroutine cmd_process_execute

<Commands: cmd process execute procedures>≡
elemental function is_threshold (method)
  logical :: is_threshold
  type(string_t), intent(in) :: method
  is_threshold = method == var_str ("threshold")
end function is_threshold

subroutine check_threshold_consistency ()
  if (nlo_fixed_order .and. is_threshold (born_me_method)) then
    if (.not. (is_threshold (real_tree_me_method) .and. is_threshold (loop_me_method) &
      .and. is_threshold (correlation_me_method))) then
      print *, 'born: ', char (born_me_method)
      print *, 'real: ', char (real_tree_me_method)
      print *, 'loop: ', char (loop_me_method)
      print *, 'correlation: ', char (correlation_me_method)
      call msg_fatal ("Inconsistent methods: All components need to be threshold")
    end if
  end if
end subroutine check_threshold_consistency

<Commands: cmd process execute: check for nlo corrections>≡
if (nlo_fixed_order .or. gks_active) then
  nlo_correction_type = &
    var_list%get_sval (var_str ('$nlo_correction_type'))
  select case (char (nlo_correction_type))
  case ("QCD")
    qcd_corr = .true.; qed_corr = .false.
  case ("EW")
    qcd_corr = .false.; qed_corr = .true.
  case ("Full")
    qcd_corr = .true.; qed_corr = .true.
  case default
    call msg_fatal ("Invalid NLO correction type. " // &

```

```

        "Valid inputs are: QCD, EW, Full (default: QCD)")
    end select
    call check_for_excluded_gauge_boson_splitting_partners ()
    call setup_radiation_generator ()
end if
if (nlo_fixed_order) then
    call radiation_generator%findSplittings ()
    if (debug2_active (D_CORE)) then
        print *, ""
        print *, 'Found (pdg) splittings: '
        do i = 1, radiation_generator%if_table%get_length ()
            call radiation_generator%if_table%get_pdg_out (i, pdg)
            call pdg_array_write_set (pdg)
            print *, '-----'
        end do
    end if

    nlo_fixed_order = radiation_generator%contains_emissions ()
    if (.not. nlo_fixed_order) call msg_warning &
        (arr = [var_str ("No NLO corrections found for process ") // &
        cmd%id // var_str("."), var_str ("Proceed with usual " // &
        "leading-order integration and simulation")])
end if

```

(Commands: cmd process execute procedures)+≡

```

subroutine check_for_excluded_gauge_boson_splitting_partners ()
    type(string_t) :: str_excluded_partners
    type(string_t), dimension(:), allocatable :: excluded_partners
    type(pdg_list_t) :: pl_tmp, pl_anti
    integer :: i, n_anti
    str_excluded_partners = var_list%get_sval &
        (var_str ("exclude_gauge_splittings"))
    if (str_excluded_partners == "") then
        return
    else
        call split_string (str_excluded_partners, &
            var_str (":"), excluded_partners)
        call pl_tmp%init (size (excluded_partners))
        do i = 1, size (excluded_partners)
            call pl_tmp%set (i, &
                cmd%local%model%get_pdg (excluded_partners(i), .true.))
        end do
        call pl_tmp%create_antiparticles (pl_anti, n_anti)
        call pl_excluded_gauge_splittings%init (pl_tmp%get_size () + n_anti)
        do i = 1, pl_tmp%get_size ()
            call pl_excluded_gauge_splittings%set (i, pl_tmp%get(i))
        end do
        do i = 1, n_anti
            j = i + pl_tmp%get_size ()
            call pl_excluded_gauge_splittings%set (j, pl_anti%get(i))
        end do
    end if
end subroutine check_for_excluded_gauge_boson_splitting_partners

```

<Commands: cmd process execute procedures>+≡

```
subroutine determine_needed_components ()
  type(string_t) :: fks_method
  comp_mult = 1
  if (nlo_fixed_order) then
    fks_method = var_list%get_sval (var_str ('$fks_mapping_type'))
    call check_threshold_consistency ()
    requires_soft_mismatch = fks_method == var_str ('resonances')
    comp_mult = needed_extra_components (requires_dglap_remnants, &
      use_real_finite, requires_soft_mismatch)
    allocate (i_list (comp_mult))
  else if (gks_active) then
    call radiation_generator%generate_multiple &
      (gks_multiplicity, cmd%local%model)
    comp_mult = radiation_generator%get_n_gks_states () + 1
  end if
  n_components_init = n_components * comp_mult
end subroutine determine_needed_components
```

<Commands: cmd process execute procedures>+≡

```
subroutine setup_radiation_generator ()
  call split_prt (prt_spec_in, n_in, pl_in)
  call split_prt (prt_spec_out, n_out, pl_out)
  call radiation_generator%init (pl_in, pl_out, &
    pl_excluded_gaugeSplittings, qcd = qcd_corr, qed = qed_corr)
  call radiation_generator%set_n (n_in, n_out, 0)
  initial_state_colored = pdg_in%has_colored_particles ()
  if ((n_in == 2 .and. initial_state_colored) .or. qed_corr) then
    requires_dglap_remnants = n_in == 2 .and. initial_state_colored
    call radiation_generator%set_initial_state_emissions ()
  else
    requires_dglap_remnants = .false.
  end if
  call radiation_generator%set_constraints (.false., .false., .true., .true.)
  call radiation_generator%setup_if_table (cmd%local%model)
end subroutine setup_radiation_generator
```

<Commands: cmd process execute: scan components>≡

```
n_terms = prt_expr_out%get_n_terms ()
allocate (pdg_out_tab (n_terms))
allocate (i_term (n_terms), source = 0)
n_components = 0
SCAN: do i = 1, n_terms
  if (allocated (ipdg)) deallocate (ipdg)
  call prt_expr_out%term_to_array (prt_spec_out, i)
  n_out = size (prt_spec_out)
  allocate (ipdg (n_out))
  do j = 1, n_out
    prt_out = prt_spec_out(j)%to_string ()
    call split (prt_out, prt_out1, ":")
    ipdg(j) = cmd%local%model%get_pdg (prt_out1)
  end do
  pdg_out = sort (ipdg)
```

```

do j = 1, n_components
  if (pdg_out == pdg_out_tab(j)) cycle SCAN
end do
n_components = n_components + 1
i_term(n_components) = i
pdg_out_tab(n_components) = pdg_out
end do SCAN

```

(Commands: cmd process execute procedures)+≡

```

subroutine split_prt (prt, n_out, pl)
  type(prt_spec_t), intent(in), dimension(:), allocatable :: prt
  integer, intent(in) :: n_out
  type(pdg_list_t), intent(out) :: pl
  type(pdg_array_t) :: pdg
  type(string_t) :: prt_string, prt_tmp
  integer, parameter :: max_particle_number = 25
  integer, dimension(max_particle_number) :: i_particle
  integer :: i, j, n
  i_particle = 0
  call pl%init (n_out)
  do i = 1, n_out
    n = 1
    prt_string = prt(i)%to_string ()
    do
      call split (prt_string, prt_tmp, ":")
      if (prt_tmp /= "") then
        i_particle(n) = cmd%local%model%get_pdg (prt_tmp)
        n = n + 1
      else
        exit
      end if
    end do
    call pdg%init (n - 1)
    do j = 1, n - 1
      call pdg%set (j, i_particle(j))
    end do
    call pl%set (i, pdg)
    call pdg%delete ()
  end do
end subroutine split_prt

```

(Commands: cmd process execute procedures)+≡

```

subroutine setup_components()
  integer :: k, i_comp, add_index
  i_comp = 0
  add_index = 0
  if (debug_on) call msg_debug (D_CORE, "setup_components")
  do i = 1, n_components
    call prt_expr_out%term_to_array (prt_spec_out, i_term(i))
    if (nlo_fixed_order) then
      associate (selected_nlo_parts => cmd%local%selected_nlo_parts)
        if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
          i_comp + 1)
      end associate
    end if
  end do

```

```

call prc_config%setup_component (i_comp + 1, &
    prt_spec_in, prt_spec_out, &
    cmd%local%model, var_list, BORN, &
    can_be_integrated = selected_nlo_parts (BORN))
call radiation_generator%generate_real_particle_strings &
    (prt_in_nlo, prt_out_nlo)
if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
    i_comp + 2)
call prc_config%setup_component (i_comp + 2, &
    new_prt_spec (prt_in_nlo), new_prt_spec (prt_out_nlo), &
    cmd%local%model, var_list, NLO_REAL, &
    can_be_integrated = selected_nlo_parts (NLO_REAL))
if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
    i_comp + 3)
call prc_config%setup_component (i_comp + 3, &
    prt_spec_in, prt_spec_out, &
    cmd%local%model, var_list, NLO_VIRTUAL, &
    can_be_integrated = selected_nlo_parts (NLO_VIRTUAL))
if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
    i_comp + 4)
call prc_config%setup_component (i_comp + 4, &
    prt_spec_in, prt_spec_out, &
    cmd%local%model, var_list, NLO_SUBTRACTION, &
    can_be_integrated = selected_nlo_parts (NLO_SUBTRACTION))
do k = 1, 4
    i_list(k) = i_comp + k
end do
if (requires_dglap_remnants) then
    if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
        i_comp + 5)
    call prc_config%setup_component (i_comp + 5, &
        prt_spec_in, prt_spec_out, &
        cmd%local%model, var_list, NLO_DGLAP, &
        can_be_integrated = selected_nlo_parts (NLO_DGLAP))
    i_list(5) = i_comp + 5
    add_index = add_index + 1
end if
if (use_real_finite) then
    if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
        i_comp + 5 + add_index)
    call prc_config%setup_component (i_comp + 5 + add_index, &
        new_prt_spec (prt_in_nlo), new_prt_spec (prt_out_nlo), &
        cmd%local%model, var_list, NLO_REAL, &
        can_be_integrated = selected_nlo_parts (NLO_REAL))
    i_list(5 + add_index) = i_comp + 5 + add_index
    add_index = add_index + 1
end if
if (requires_soft_mismatch) then
    if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
        i_comp + 5 + add_index)
    call prc_config%setup_component (i_comp + 5 + add_index, &
        prt_spec_in, prt_spec_out, &
        cmd%local%model, var_list, NLO_MISMATCH, &
        can_be_integrated = selected_nlo_parts (NLO_MISMATCH))

```

```

        i_list(5 + add_index) = i_comp + 5 + add_index
    end if
    call prc_config%set_component_associations (i_list, &
        requires_dglap_remnants, use_real_finite, &
        requires_soft_mismatch)
    end associate
else if (gks_active) then
    call prc_config%setup_component (i_comp + 1, prt_spec_in, &
        prt_spec_out, cmd%local%model, var_list, BORN, &
        can_be_integrated = .true.)
    call radiation_generator%reset_queue ()
    do j = 1, comp_mult
        prt_out_nlo = radiation_generator%get_next_state ()
        call prc_config%setup_component (i_comp + 1 + j, &
            new_prt_spec (prt_in), new_prt_spec (prt_out_nlo), &
            cmd%local%model, var_list, GKS, can_be_integrated = .false.)
    end do
else
    call prc_config%setup_component (i, &
        prt_spec_in, prt_spec_out, &
        cmd%local%model, var_list, can_be_integrated = .true.)
end if
i_comp = i_comp + comp_mult
end do
end subroutine setup_components

```

These three functions should be bundled with the logicals they depend on into an object (the pcm?).

(*Commands: procedures*) +=

```

subroutine check_nlo_options (local)
    type(rt_data_t), intent(in) :: local
    type(var_list_t), pointer :: var_list => null ()
    real :: mult_real, mult_virt, mult_dglap
    logical :: combined, powheg
    logical :: case_lo_but_any_other
    logical :: fixed_order_nlo_events
    logical :: real_finite_only
    var_list => local%get_var_list_ptr ()
    combined = var_list%get_lval (var_str ('?combined_nlo_integration'))
    powheg = var_list%get_lval (var_str ('?powheg_matching'))
    if (powheg .and. .not. combined) then
        call msg_fatal ("POWHEG matching requires the 'combined_nlo_integration' &
            &-option to be set to true.")
    end if
    fixed_order_nlo_events = &
        var_list%get_lval (var_str ('?fixed_order_nlo_events'))
    if (fixed_order_nlo_events .and. .not. combined .and. &
        count (local%selected_nlo_parts) > 1) &
        call msg_fatal ("Option mismatch: Fixed order NLO events of multiple ", &
            [var_str ("components are requested, but ?combined_nlo_integration "), &
            var_str ("is false. You can either switch to the combined NLO "), &
            var_str ("integration mode for the full process or choose one "), &
            var_str ("individual NLO component to generate events with.")])

```

```

real_finite_only = local%var_list%get_sval (var_str ("$real_partition_mode")) == "finite"
associate (nlo_parts => local%selected_nlo_parts)
  ! TODO (PS-2020-03-26): This technically leaves the possibility to skip this
  ! message by deactivating the dglap component for a proton collider process.
  ! To circumvent this, the selected_nlo_parts should be refactored.
  if (combined .and. .not. (nlo_parts(BORN) &
    .and. nlo_parts(NLO_VIRTUAL) .and. nlo_parts(NLO_REAL))) then
    call msg_fatal ("A combined integration of anything else than", &
      [var_str ("all NLO components together is not supported.")])
  end if
  if (real_finite_only .and. combined) then
    call msg_fatal ("You cannot do a combined integration without", &
      [var_str ("the real singular component.")])
  end if
  if (real_finite_only .and. count(nlo_parts([BORN,NLO_VIRTUAL,NLO_DGLAP])) > 1) then
    call msg_fatal ("You cannot do a full NLO integration without", &
      [var_str ("the real singular component.")])
  end if
end associate
mult_real = local%var_list%get_rval (var_str ("mult_call_real"))
mult_virt = local%var_list%get_rval (var_str ("mult_call_virt"))
mult_dglap = local%var_list%get_rval (var_str ("mult_call_dglap"))
if (combined .and. (mult_real /= one .or. mult_virt /= one .or. mult_dglap /= one)) then
  call msg_warning ("mult_call_real, mult_call_virt and mult_call_dglap", &
    [var_str (" will be ignored because of ?combined_nlo_integration = true. ")])
end if
end subroutine check_nlo_options

```

There are four components for a general NLO process, namely Born, real, virtual and subtraction. There will be additional components for DGLAP remnant, in case real contributions are split into singular and finite pieces, and for resonance-aware FKS subtraction for the needed soft mismatch component.

```

<Commands: procedures>+≡
pure function needed_extra_components (requires_dglap_remnant, &
  use_real_finite, requires_soft_mismatch) result (n)
  integer :: n
  logical, intent(in) :: requires_dglap_remnant, &
    use_real_finite, requires_soft_mismatch
  n = 4
  if (requires_dglap_remnant) n = n + 1
  if (use_real_finite) n = n + 1
  if (requires_soft_mismatch) n = n + 1
end function needed_extra_components

```

This is a method of the eval tree, but cannot be coded inside the `expressions` module since it uses the `model` and `flv` types which are not available there.

```

<Commands: procedures>+≡
function make_flavor_string (aval, model) result (prt)
  type(string_t) :: prt
  type(pdg_array_t), intent(in) :: aval
  type(model_t), intent(in), target :: model
  integer, dimension(:), allocatable :: pdg
  type(flavor_t), dimension(:), allocatable :: flv

```



```

integer :: i
pdg = aval
allocate (flv (size (pdg)))
call flv%init (pdg, model)
if (size (pdg) /= 0) then
  prt = flv(1)%get_name ()
  do i = 2, size (flv)
    prt = prt // ":" // flv(i)%get_name ()
  end do
else
  prt = "?"
end if
end function make_flavor_string

```

Create a pdg array from a particle-specification array

(Commands: procedures)+≡

```

function make_pdg_array (prt, model) result (pdg_array)
  type(prt_spec_t), intent(in), dimension(:) :: prt
  type(model_t), intent(in) :: model
  integer, dimension(:), allocatable :: aval
  type(pdg_array_t) :: pdg_array
  type(flavor_t) :: flv
  integer :: k
  allocate (aval (size (prt)))
  do k = 1, size (prt)
    call flv%init (prt(k)%to_string (), model)
    aval (k) = flv%get_pdg ()
  end do
  pdg_array = aval
end function make_pdg_array

```

Compile a (possible nested) expression, to obtain a particle-specifier expression which we can process further.

(Commands: procedures)+≡

```

recursive subroutine compile_prt_expr (prt_expr, pn, var_list, model)
  type(prt_expr_t), intent(out) :: prt_expr
  type(parse_node_t), intent(in), target :: pn
  type(var_list_t), intent(in), target :: var_list
  type(model_t), intent(in), target :: model
  type(parse_node_t), pointer :: pn_entry, pn_term, pn_addition
  type(pdg_array_t) :: pdg
  type(string_t) :: prt_string
  integer :: n_entry, n_term, i
  select case (char (parse_node_get_rule_key (pn)))
  case ("prt_state_list")
    n_entry = parse_node_get_n_sub (pn)
    pn_entry => parse_node_get_sub_ptr (pn)
    if (n_entry == 1) then
      call compile_prt_expr (prt_expr, pn_entry, var_list, model)
    else
      call prt_expr%init_list (n_entry)
      select type (x => prt_expr%x)
      type is (prt_spec_list_t)

```

```

        do i = 1, n_entry
            call compile_prt_expr (x%expr(i), pn_entry, var_list, model)
            pn_entry => parse_node_get_next_ptr (pn_entry)
        end do
    end select
end if
case ("prt_state_sum")
    n_term = parse_node_get_n_sub (pn)
    pn_term => parse_node_get_sub_ptr (pn)
    pn_addition => pn_term
    if (n_term == 1) then
        call compile_prt_expr (prt_expr, pn_term, var_list, model)
    else
        call prt_expr%init_sum (n_term)
        select type (x => prt_expr%x)
        type is (prt_spec_sum_t)
            do i = 1, n_term
                call compile_prt_expr (x%expr(i), pn_term, var_list, model)
                pn_addition => parse_node_get_next_ptr (pn_addition)
                if (associated (pn_addition)) &
                    pn_term => parse_node_get_sub_ptr (pn_addition, 2)
            end do
        end select
    end if
case ("cexpr")
    pdg = eval_pdg_array (pn, var_list)
    prt_string = make_flavor_string (pdg, model)
    call prt_expr%init_spec (new_prt_spec (prt_string))
case default
    call parse_node_write_rec (pn)
    call msg_bug ("compile prt expr: impossible syntax rule")
end select
end subroutine compile_prt_expr

```

Initiating a NLO calculation

```

<Commands: types>+≡
type, extends (command_t) :: cmd_nlo_t
private
integer, dimension(:), allocatable :: nlo_component
contains
    <Commands: cmd nlo: TBP>
end type cmd_nlo_t

```

Incomplete.

```

<Commands: cmd nlo: TBP>≡
procedure :: write => cmd_nlo_write

<Commands: sub interfaces>+≡
module subroutine cmd_nlo_write (cmd, unit, indent)
    class(cmd_nlo_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
end subroutine cmd_nlo_write

```

```

<Commands: procedures>+≡
  module subroutine cmd_nlo_write (cmd, unit, indent)
    class(cmd_nlo_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_nlo_write

```

As it is, the NLO calculation is switched on by putting nlo behind the process definition. This should be made nicer in the future.

```

<Commands: cmd nlo: TBP>+≡
  procedure :: compile => cmd_nlo_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_nlo_compile (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_nlo_compile

<Commands: procedures>+≡
  module subroutine cmd_nlo_compile (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg, pn_comp
    integer :: i, n_comp
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)
    if (associated (pn_arg)) then
      n_comp = parse_node_get_n_sub (pn_arg)
      allocate (cmd%nlo_component (n_comp))
      pn_comp => parse_node_get_sub_ptr (pn_arg)
      i = 0
      do while (associated (pn_comp))
        i = i + 1
        cmd%nlo_component(i) = component_status &
          (parse_node_get_rule_key (pn_comp))
        pn_comp => parse_node_get_next_ptr (pn_comp)
      end do
    else
      allocate (cmd%nlo_component (0))
    end if
  end subroutine cmd_nlo_compile

```

```

<Commands: cmd nlo: TBP>+≡
  procedure :: execute => cmd_nlo_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_nlo_execute (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_nlo_execute

<Commands: procedures>+≡
  module subroutine cmd_nlo_execute (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(string_t) :: string
    integer :: n, i, j

```

```

logical, dimension(0:5) :: selected_nlo_parts
if (debug_on) call msg_debug (D_CORE, "cmd_nlo_execute")
selected_nlo_parts = .false.
if (allocated (cmd%nlo_component)) then
    n = size (cmd%nlo_component)
else
    n = 0
end if
do i = 1, n
    select case (cmd%nlo_component (i))
    case (BORN, NLO_VIRTUAL, NLO_MISMATCH, NLO_DGLAP, NLO_REAL)
        selected_nlo_parts(cmd%nlo_component (i)) = .true.
    case (NLO_FULL)
        selected_nlo_parts = .true.
        selected_nlo_parts (NLO_SUBTRACTION) = .false.
    case default
        string = var_str ("")
        do j = BORN, NLO_DGLAP
            string = string // component_status (j) // ", "
        end do
        string = string // component_status (NLO_FULL)
        call msg_fatal ("Invalid NLO mode. Valid modes are: " // &
            char (string))
    end select
end do
global%nlo_fixed_order = any (selected_nlo_parts)
global%selected_nlo_parts = selected_nlo_parts
allocate (global%nlo_component (size (cmd%nlo_component)))
global%nlo_component = cmd%nlo_component
end subroutine cmd_nlo_execute

```

Process compilation

```

<Commands: types>+≡
type, extends (command_t) :: cmd_compile_t
private
type(string_t), dimension(:), allocatable :: libname
logical :: make_executable = .false.
type(string_t) :: exec_name
contains
<Commands: cmd compile: TBP>
end type cmd_compile_t

```

Output: list all libraries to be compiled.

```

<Commands: cmd compile: TBP>≡
procedure :: write => cmd_compile_write

<Commands: sub interfaces>+≡
module subroutine cmd_compile_write (cmd, unit, indent)
    class(cmd_compile_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
end subroutine cmd_compile_write

```

<Commands: procedures>+≡

```

module subroutine cmd_compile_write (cmd, unit, indent)
  class(cmd_compile_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A)", advance="no") "compile ("
  if (allocated (cmd%libname)) then
    do i = 1, size (cmd%libname)
      if (i > 1) write (u, "(A,1x)", advance="no") " ,"
      write (u, "(',' ", A, "',')", advance="no") char (cmd%libname(i))
    end do
  end if
  write (u, "(A)") ")"
end subroutine cmd_compile_write

```

Compile the libraries specified in the argument. If the argument is empty, compile all libraries which can be found in the process library stack.

<Commands: cmd compile: TBP>+≡

```

procedure :: compile => cmd_compile_compile

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_compile_compile (cmd, global)
  class(cmd_compile_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_compile_compile

```

<Commands: procedures>+≡

```

module subroutine cmd_compile_compile (cmd, global)
  class(cmd_compile_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_cmd, pn_clause, pn_arg, pn_lib
  type(parse_node_t), pointer :: pn_exec_name_spec, pn_exec_name
  integer :: n_lib, i
  pn_cmd => parse_node_get_sub_ptr (cmd%pn)
  pn_clause => parse_node_get_sub_ptr (pn_cmd)
  pn_exec_name_spec => parse_node_get_sub_ptr (pn_clause, 2)
  if (associated (pn_exec_name_spec)) then
    pn_exec_name => parse_node_get_sub_ptr (pn_exec_name_spec, 2)
  else
    pn_exec_name => null ()
  end if
  pn_arg => parse_node_get_next_ptr (pn_clause)
  cmd%pn_opt => parse_node_get_next_ptr (pn_cmd)
  call cmd%compile_options (global)
  if (associated (pn_arg)) then
    n_lib = parse_node_get_n_sub (pn_arg)
  else
    n_lib = 0
  end if
  if (n_lib > 0) then
    allocate (cmd%libname (n_lib))
    pn_lib => parse_node_get_sub_ptr (pn_arg)
    do i = 1, n_lib

```

```

        cmd%libname(i) = parse_node_get_string (pn_lib)
        pn_lib => parse_node_get_next_ptr (pn_lib)
    end do
end if
if (associated (pn_exec_name)) then
    cmd%make_executable = .true.
    cmd%exec_name = parse_node_get_string (pn_exec_name)
end if
end subroutine cmd_compile_compile

```

Command execution. Generate code, write driver, compile and link. Do this for all libraries in the list.

If no library names have been given and stored while compiling this command, we collect all libraries from the current stack and compile those.

As a bonus, a compiled library may be able to spawn new process libraries. For instance, a processes may ask for a set of resonant subprocesses which go into their own library, but this can be determined only after the process is available as a compiled object. Therefore, the compilation loop is implemented as a recursive internal subroutine.

We can compile static libraries (which actually just loads them). However, we can't incorporate in a generated executable.

(Commands: cmd compile: TBP)+≡

```

    procedure :: execute => cmd_compile_execute

```

(Commands: sub interfaces)+≡

```

    module subroutine cmd_compile_execute (cmd, global)
        class(cmd_compile_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_compile_execute

```

(Commands: procedures)+≡

```

    module subroutine cmd_compile_execute (cmd, global)
        class(cmd_compile_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(string_t), dimension(:), allocatable :: libname, libname_static
        integer :: i, n_lib
        (Commands: cmd compile execute: extra variables)
        (Commands: cmd compile execute: extra init)
        if (allocated (cmd%libname)) then
            allocate (libname (size (cmd%libname)))
            libname = cmd%libname
        else
            call cmd%local%prclib_stack%get_names (libname)
        end if
        n_lib = size (libname)
        if (cmd%make_executable) then
            call get_prclib_static (libname_static)
            do i = 1, n_lib
                if (any (libname_static == libname(i))) then
                    call msg_fatal ("Compile: can't include static library '" &
                                   // char (libname(i)) // "'")
                end if
            end do
        end if
        call compile_executable (cmd%exec_name, libname, cmd%local)
    end subroutine cmd_compile_execute

```

```

else
  call compile_libraries (libname)
  call global%update_prclib &
    (global%prclib_stack%get_library_ptr (libname(n_lib)))
end if
<Commands: cmd compile execute: extra end init>
contains
  recursive subroutine compile_libraries (libname)
    type(string_t), dimension(:), intent(in) :: libname
    integer :: i
    type(string_t), dimension(:), allocatable :: libname_extra
    type(process_library_t), pointer :: lib_saved
    do i = 1, size (libname)
      call compile_library (libname(i), cmd%local)
      lib_saved => global%prclib
      call spawn_extra_libraries &
        (libname(i), cmd%local, global, libname_extra)
      call compile_libraries (libname_extra)
      call global%update_prclib (lib_saved)
    end do
  end subroutine compile_libraries
end subroutine cmd_compile_execute

```

<Commands: cmd compile execute: extra variables>≡

<Commands: cmd compile execute: extra init>≡

<Commands: cmd compile execute: extra end init>≡

The parallelization leads to undefined behavior while writing simultaneously to one file. The master worker has to initialize single-handed the corresponding library files. The slave worker will wait with a blocking MPI_BCAST until they receive a logical flag.

<MPI: Commands: cmd compile execute: extra variables>≡

```

logical :: compile_init
integer :: rank, n_size

```

<MPI: Commands: cmd compile execute: extra init>≡

```

if (debug_on) call msg_debug (D_MPI, "cmd_compile_execute")
compile_init = .false.
call mpi_get_comm_id (n_size, rank)
if (debug_on) call msg_debug (D_MPI, "n_size", rank)
if (debug_on) call msg_debug (D_MPI, "rank", rank)
if (rank /= 0) then
  if (debug_on) call msg_debug (D_MPI, "wait for master")
  call MPI_bcast (compile_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
else
  compile_init = .true.
end if

```

```

if (compile_init) then

```

<MPI: Commands: cmd compile execute: extra end init>≡

```

if (rank == 0) then
  if (debug_on) call msg_debug (D_MPI, "load slaves")
  call MPI_bcast (compile_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)

```

```

    end if
  end if
  call MPI_barrier (MPI_COMM_WORLD)

```

This is the interface to the external procedure which returns the names of all static libraries which are part of the executable. (The default is none.) The routine must allocate the array.

```

<Commands: public>≡
  public :: get_prclib_static

<Commands: interfaces>+≡
  interface
    subroutine get_prclib_static (libname)
      import
      type(string_t), dimension(:), intent(inout), allocatable :: libname
    end subroutine get_prclib_static
  end interface

```

Spawn extra libraries. We can ask the processes within a compiled library, which we have available at this point, whether they need additional processes which should go into their own libraries.

The current implementation only concerns resonant subprocesses.

Note that the libraries should be created (source code), but not be compiled here. This is done afterwards.

```

<Commands: procedures>+≡
  subroutine spawn_extra_libraries (libname, local, global, libname_extra)
    type(string_t), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), target :: global
    type(string_t), dimension(:), allocatable, intent(out) :: libname_extra
    type(string_t), dimension(:), allocatable :: libname_res
    allocate (libname_extra (0))
    call spawn_resonant_subprocess_libraries &
      (libname, local, global, libname_res)
    if (allocated (libname_res)) libname_extra = [libname_extra, libname_res]
  end subroutine spawn_extra_libraries

```

Execute a shell command

The argument is a string expression.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_exec_t
    private
    type(parse_node_t), pointer :: pn_command => null ()
  contains
    <Commands: cmd exec: TBP>
  end type cmd_exec_t

```

Simply tell the status.

```

<Commands: cmd exec: TBP>≡
  procedure :: write => cmd_exec_write

```



```

<Commands: sub interfaces>+≡
    module subroutine cmd_exec_write (cmd, unit, indent)
        class(cmd_exec_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_exec_write

```

```

<Commands: procedures>+≡
    module subroutine cmd_exec_write (cmd, unit, indent)
        class(cmd_exec_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        if (associated (cmd%pn_command)) then
            write (u, "(1x,A)") "exec: [command associated]"
        else
            write (u, "(1x,A)") "exec: [undefined]"
        end if
    end subroutine cmd_exec_write

```

Compile the exec command.

```

<Commands: cmd exec: TBP>+≡
    procedure :: compile => cmd_exec_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_exec_compile (cmd, global)
        class(cmd_exec_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_exec_compile

<Commands: procedures>+≡
    module subroutine cmd_exec_compile (cmd, global)
        class(cmd_exec_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_arg, pn_command
        pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
        pn_command => parse_node_get_sub_ptr (pn_arg)
        cmd%pn_command => pn_command
    end subroutine cmd_exec_compile

```

Execute the specified shell command.

```

<Commands: cmd exec: TBP>+≡
    procedure :: execute => cmd_exec_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_exec_execute (cmd, global)
        class(cmd_exec_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_exec_execute

<Commands: procedures>+≡
    module subroutine cmd_exec_execute (cmd, global)
        class(cmd_exec_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(string_t) :: command

```

```

logical :: is_known
integer :: status
command = eval_string (cmd%pn_command, global%var_list, is_known=is_known)
if (is_known) then
  if (command /= "") then
    call os_system_call (command, status, verbose=.true.)
    if (status /= 0) then
      write (msg_buffer, "(A,I0)") "Return code = ", status
      call msg_message ()
      call msg_error ("System command returned with nonzero status code")
    end if
  end if
end if
end subroutine cmd_exec_execute

```

Variable declaration

A variable can have various types. Hold the definition as an eval tree.

There are intrinsic variables, user variables, and model variables. The latter are further divided in independent variables and dependent variables.

Regarding model variables: When dealing with them, we always look at two variable lists in parallel. The global (or local) variable list contains the user-visible values. It includes variables that correspond to variables in the current model's list. These, in turn, are pointers to the model's parameter list, so the model is always in sync, internally. To keep the global variable list in sync with the model, the global variables carry the `is_copy` property and contain a separate pointer to the model variable. (The pointer is reassigned whenever the model changes.) Modifying the global variable changes two values simultaneously: the visible value and the model variable, via this extra pointer. After each modification, we update dependent parameters in the model variable list and re-synchronize the global variable list (again, using these pointers) with the model variable this. In the last step, modifications in the derived parameters become visible.

When we integrate a process, we capture the current variable list of the current model in a separate model instance, which is stored in the process object. Thus, the model parameters associated to this process at this time are preserved for the lifetime of the process object.

When we generate or rescan events, we can again capture a local model variable list in a model instance. This allows us to reweight event by event with different parameter sets simultaneously.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_var_t
  private
  type(string_t) :: name
  integer :: type = V_NONE
  type(parse_node_t), pointer :: pn_value => null ()
  logical :: is_intrinsic = .false.
  logical :: is_model_var = .false.
  contains
  ⟨Commands: cmd var: TBP⟩

```

```
end type cmd_var_t
```

Output. We know name, type, and properties, but not the value.

<Commands: cmd var: TBP>≡

```
procedure :: write => cmd_var_write
```

<Commands: sub interfaces>+≡

```
module subroutine cmd_var_write (cmd, unit, indent)
  class(cmd_var_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
end subroutine cmd_var_write
```

<Commands: procedures>+≡

```
module subroutine cmd_var_write (cmd, unit, indent)
  class(cmd_var_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A,A,A)", advance="no") "var: ", char (cmd%name), " ("
  select case (cmd%type)
  case (V_NONE)
    write (u, "(A)", advance="no") "[unknown]"
  case (V_LOG)
    write (u, "(A)", advance="no") "logical"
  case (V_INT)
    write (u, "(A)", advance="no") "int"
  case (V_REAL)
    write (u, "(A)", advance="no") "real"
  case (V_CMPLX)
    write (u, "(A)", advance="no") "complex"
  case (V_STR)
    write (u, "(A)", advance="no") "string"
  case (V_PDG)
    write (u, "(A)", advance="no") "alias"
  end select
  if (cmd%is_intrinsic) then
    write (u, "(A)", advance="no") ", intrinsic"
  end if
  if (cmd%is_model_var) then
    write (u, "(A)", advance="no") ", model"
  end if
  write (u, "(A)") ")"
end subroutine cmd_var_write
```

Compile the lhs and determine the variable name and type. Check whether this variable can be created or modified as requested, and append the value to the variable list, if appropriate. The value is initially undefined. The rhs is assigned to a pointer, to be compiled and evaluated when the command is executed.

<Commands: cmd var: TBP>+≡

```
procedure :: compile => cmd_var_compile
```

<Commands: sub interfaces>+≡

```
module subroutine cmd_var_compile (cmd, global)
```

```

        class(cmd_var_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_var_compile

```

(Commands: procedures)+≡

```

module subroutine cmd_var_compile (cmd, global)
    class(cmd_var_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_var, pn_name
    type(parse_node_t), pointer :: pn_result, pn_proc
    type(string_t) :: var_name
    type(var_list_t), pointer :: model_vars
    integer :: type
    logical :: new
    pn_result => null ()
    new = .false.
    select case (char (parse_node_get_rule_key (cmd%pn)))
    case ("cmd_log_decl");      type = V_LOG
        pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
        if (.not. associated (pn_var)) then    ! handle masked syntax error
            cmd%type = V_NONE; return
        end if
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        new = .true.
    case ("cmd_log");           type = V_LOG
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
    case ("cmd_int");           type = V_INT
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
        new = .true.
    case ("cmd_real");          type = V_REAL
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
        new = .true.
    case ("cmd_complex");       type = V_CMPLX
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
        new = .true.
    case ("cmd_num");           type = V_NONE
        pn_name => parse_node_get_sub_ptr (cmd%pn)
    case ("cmd_string_decl");   type = V_STR
        pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
        if (.not. associated (pn_var)) then    ! handle masked syntax error
            cmd%type = V_NONE; return
        end if
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        new = .true.
    case ("cmd_string");        type = V_STR
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
    case ("cmd_alias");         type = V_PDG
        pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
        new = .true.
    case ("cmd_result");        type = V_REAL
        pn_name => parse_node_get_sub_ptr (cmd%pn)
        pn_result => parse_node_get_sub_ptr (pn_name)
        pn_proc => parse_node_get_next_ptr (pn_result)
    case default
        call parse_node_mismatch &

```

```

        ("logical|int|real|complex|?|$$|alias|var_name", cmd%pn) ! $
end select
if (.not. associated (pn_name)) then ! handle masked syntax error
    cmd%type = V_NONE; return
end if
if (.not. associated (pn_result)) then
    var_name = parse_node_get_string (pn_name)
else
    var_name = parse_node_get_key (pn_result) &
        // "(" // parse_node_get_string (pn_proc) // ")"
end if
select case (type)
case (V_LOG); var_name = "?" // var_name
case (V_STR); var_name = "$" // var_name ! $
end select
if (associated (global%model)) then
    model_vars => global%model%get_var_list_ptr ()
else
    model_vars => null ()
end if
call var_list_check_observable (global%var_list, var_name, type)
call var_list_check_result_var (global%var_list, var_name, type)
call global%var_list%check_user_var (var_name, type, new)
cmd%name = var_name
cmd%pn_value => parse_node_get_next_ptr (pn_name, 2)
if (global%var_list%contains (cmd%name, follow_link = .false.)) then
    ! local variable
    cmd%is_intrinsic = &
        global%var_list%is_intrinsic (cmd%name, follow_link = .false.)
    cmd%type = &
        global%var_list%get_type (cmd%name, follow_link = .false.)
else
    if (new) cmd%type = type
    if (global%var_list%contains (cmd%name, follow_link = .true.)) then
        ! global variable
        cmd%is_intrinsic = &
            global%var_list%is_intrinsic (cmd%name, follow_link = .true.)
        if (cmd%type == V_NONE) then
            cmd%type = &
                global%var_list%get_type (cmd%name, follow_link = .true.)
        end if
    else if (associated (model_vars)) then ! check model variable
        cmd%is_model_var = &
            model_vars%contains (cmd%name)
        if (cmd%type == V_NONE) then
            cmd%type = &
                model_vars%get_type (cmd%name)
        end if
    end if
    if (cmd%type == V_NONE) then
        call msg_fatal ("Variable '" // char (cmd%name) // "' " &
            // "set without declaration")
        cmd%type = V_NONE; return
    end if
end if

```

```

    if (cmd%is_model_var) then
    if (new) then
        call msg_fatal ("Model variable '" // char (cmd%name) // "' " &
            // "redeclared")
    else if (model_vars%is_locked (cmd%name)) then
        call msg_fatal ("Model variable '" // char (cmd%name) // "' " &
            // "is locked")
    end if
else
    select case (cmd%type)
    case (V_LOG)
        call global%var_list%append_log (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_INT)
        call global%var_list%append_int (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_REAL)
        call global%var_list%append_real (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_CMPLX)
        call global%var_list%append_cmplx (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_PDG)
        call global%var_list%append_pdg_array (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_STR)
        call global%var_list%append_string (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    end select
    end if
end if
end subroutine cmd_var_compile

```

Execute. Evaluate the definition and assign the variable value. If the variable is a model variable, take a snapshot of the model if necessary and set the variable in the local model.

```

<Commands: cmd var: TBP>+=
    procedure :: execute => cmd_var_execute

<Commands: sub interfaces>+=
    module subroutine cmd_var_execute (cmd, global)
        class(cmd_var_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_var_execute

<Commands: procedures>+=
    module subroutine cmd_var_execute (cmd, global)
        class(cmd_var_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        real(default) :: rval
        logical :: is_known, pacified
        var_list => global%get_var_list_ptr ()
        if (cmd%is_model_var) then

```

```

        pacified = var_list%get_lval (var_str ("?pacify"))
        rval = eval_real (cmd%pn_value, var_list, is_known=is_known)
        call global%model_set_real &
            (cmd%name, rval, verbose=.true., pacified=pacified)
    else if (cmd%type /= V_NONE) then
        call cmd%set_value (var_list, verbose=.true.)
    end if
end subroutine cmd_var_execute

```

Copy the value to the variable list, where the variable should already exist.

(Commands: cmd var: TBP)+≡

```

    procedure :: set_value => cmd_var_set_value

```

(Commands: sub interfaces)+≡

```

    module subroutine cmd_var_set_value (var, var_list, verbose, model_name)
        class(cmd_var_t), intent(inout) :: var
        type(var_list_t), intent(inout), target :: var_list
        logical, intent(in), optional :: verbose
        type(string_t), intent(in), optional :: model_name
    end subroutine cmd_var_set_value

```

(Commands: procedures)+≡

```

    module subroutine cmd_var_set_value (var, var_list, verbose, model_name)
        class(cmd_var_t), intent(inout) :: var
        type(var_list_t), intent(inout), target :: var_list
        logical, intent(in), optional :: verbose
        type(string_t), intent(in), optional :: model_name
        logical :: lval, pacified
        integer :: ival
        real(default) :: rval
        complex(default) :: cval
        type(pdg_array_t) :: aval
        type(string_t) :: sval
        logical :: is_known
        pacified = var_list%get_lval (var_str ("?pacify"))
        select case (var%type)
        case (V_LOG)
            lval = eval_log (var%pn_value, var_list, is_known=is_known)
            call var_list%set_log (var%name, &
                lval, is_known, verbose=verbose, model_name=model_name)
        case (V_INT)
            ival = eval_int (var%pn_value, var_list, is_known=is_known)
            call var_list%set_int (var%name, &
                ival, is_known, verbose=verbose, model_name=model_name)
        case (V_REAL)
            rval = eval_real (var%pn_value, var_list, is_known=is_known)
            call var_list%set_real (var%name, &
                rval, is_known, verbose=verbose, &
                model_name=model_name, pacified = pacified)
        case (V_CMPLX)
            cval = eval_cmplx (var%pn_value, var_list, is_known=is_known)
            call var_list%set_cmplx (var%name, &
                cval, is_known, verbose=verbose, &
                model_name=model_name, pacified = pacified)
        case (V_PDG)

```

```

        aval = eval_pdg_array (var%pn_value, var_list, is_known=is_known)
        call var_list%set_pdg_array (var%name, &
            aval, is_known, verbose=verbose, model_name=model_name)
    case (V_STR)
        sval = eval_string (var%pn_value, var_list, is_known=is_known)
        call var_list%set_string (var%name, &
            sval, is_known, verbose=verbose, model_name=model_name)
    end select
end subroutine cmd_var_set_value

```

SLHA

Read a SLHA (SUSY Les Houches Accord) file to fill the appropriate model parameters. We do not access the current variable record, but directly work on the appropriate SUSY model, which is loaded if necessary.

We may be in read or write mode. In the latter case, we may write just input parameters, or the complete spectrum, or the spectrum with all decays.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_slha_t
    private
    type(string_t) :: file
    logical :: write_mode = .false.
    contains
    <Commands: cmd slha: TBP>
end type cmd_slha_t

```

Output.

```

<Commands: cmd slha: TBP>≡
    procedure :: write => cmd_slha_write

<Commands: sub interfaces>+≡
    module subroutine cmd_slha_write (cmd, unit, indent)
        class(cmd_slha_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_slha_write

<Commands: procedures>+≡
    module subroutine cmd_slha_write (cmd, unit, indent)
        class(cmd_slha_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,A)") "slha: file name = ", char (cmd%file)
        write (u, "(1x,A,L1)") "slha: write mode = ", cmd%write_mode
    end subroutine cmd_slha_write

```

Compile. Read the filename and store it.

```

<Commands: cmd slha: TBP>+≡
    procedure :: compile => cmd_slha_compile

```



```

<Commands: sub interfaces>+≡
    module subroutine cmd_slha_compile (cmd, global)
        class(cmd_slha_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_slha_compile

<Commands: procedures>+≡
    module subroutine cmd_slha_compile (cmd, global)
        class(cmd_slha_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_key, pn_arg, pn_file
        pn_key => parse_node_get_sub_ptr (cmd%pn)
        pn_arg => parse_node_get_next_ptr (pn_key)
        pn_file => parse_node_get_sub_ptr (pn_arg)
        call cmd%compile_options (global)
        cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
        select case (char (parse_node_get_key (pn_key)))
        case ("read_slha")
            cmd%write_mode = .false.
        case ("write_slha")
            cmd%write_mode = .true.
        case default
            call parse_node_mismatch ("read_slha|write_slha", cmd%pn)
        end select
        cmd%file = parse_node_get_string (pn_file)
    end subroutine cmd_slha_compile

```

Execute. Read or write the specified SLHA file. Behind the scenes, this will first read the WHIZARD model file, then read the SLHA file and assign the SLHA parameters as far as determined by `dispatch_slha`. Finally, the global variables are synchronized with the model. This is similar to executing `cmd_model`.

```

<Commands: cmd slha: TBP>+≡
    procedure :: execute => cmd_slha_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_slha_execute (cmd, global)
        class(cmd_slha_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_slha_execute

<Commands: procedures>+≡
    module subroutine cmd_slha_execute (cmd, global)
        class(cmd_slha_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        logical :: input, spectrum, decays
        if (cmd%write_mode) then
            input = .true.
            spectrum = .false.
            decays = .false.
            if (.not. associated (cmd%local%model)) then
                call msg_fatal ("SLHA: local model not associated")
                return
            end if
            call slha_write_file &
                (cmd%file, cmd%local%model, &

```

```

        input = input, spectrum = spectrum, decays = decays)
else
    if (.not. associated (global%model)) then
        call msg_fatal ("SLHA: global model not associated")
        return
    end if
    call dispatch_slha (cmd%local%var_list, &
        input = input, spectrum = spectrum, decays = decays)
    call global%ensure_model_copy ()
    call slha_read_file &
        (cmd%file, cmd%local%os_data, global%model, &
        input = input, spectrum = spectrum, decays = decays)
end if
end subroutine cmd_slha_execute

```

Show values

This command shows the current values of variables or other objects, in a suitably condensed form.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_show_t
private
    type(string_t), dimension(:), allocatable :: name
contains
    <Commands: cmd show: TBP>
end type cmd_show_t

```

Output: list the object names, not values.

```

<Commands: cmd show: TBP>≡
    procedure :: write => cmd_show_write

<Commands: sub interfaces>+≡
    module subroutine cmd_show_write (cmd, unit, indent)
        class(cmd_show_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_show_write

<Commands: procedures>+≡
    module subroutine cmd_show_write (cmd, unit, indent)
        class(cmd_show_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)", advance="no") "show: "
        if (allocated (cmd%name)) then
            do i = 1, size (cmd%name)
                write (u, "(1x,A)", advance="no") char (cmd%name(i))
            end do
            write (u, *)
        else
            write (u, "(5x,A)") "[undefined]"
        end if
    end subroutine cmd_show_write

```

```
end subroutine cmd_show_write
```

Compile. Allocate an array which is filled with the names of the variables to show.

```
<Commands: cmd show: TBP>+≡
```

```
procedure :: compile => cmd_show_compile
```

```
<Commands: sub interfaces>+≡
```

```
module subroutine cmd_show_compile (cmd, global)
  class(cmd_show_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_show_compile
```

```
<Commands: procedures>+≡
```

```
module subroutine cmd_show_compile (cmd, global)
  class(cmd_show_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name
  type(string_t) :: key
  integer :: i, n_args
  pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
  if (associated (pn_arg)) then
    select case (char (parse_node_get_rule_key (pn_arg)))
    case ("show_arg")
      cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
    case default
      cmd%pn_opt => pn_arg
      pn_arg => null ()
    end select
  end if
  call cmd%compile_options (global)
  if (associated (pn_arg)) then
    n_args = parse_node_get_n_sub (pn_arg)
    allocate (cmd%name (n_args))
    pn_var => parse_node_get_sub_ptr (pn_arg)
    i = 0
    do while (associated (pn_var))
      i = i + 1
      select case (char (parse_node_get_rule_key (pn_var)))
      case ("model", "library", "beams", "iterations", &
            "cuts", "weight", "int", "real", "complex", &
            "scale", "factorization_scale", "renormalization_scale", &
            "selection", "reweight", "analysis", "pdg", &
            "stable", "unstable", "polarized", "unpolarized", &
            "results", "expect", "intrinsic", "string", "logical")
        cmd%name(i) = parse_node_get_key (pn_var)
      case ("result_var")
        pn_prefix => parse_node_get_sub_ptr (pn_var)
        pn_name => parse_node_get_next_ptr (pn_prefix)
        if (associated (pn_name)) then
          cmd%name(i) = parse_node_get_key (pn_prefix) &
            // "(" // parse_node_get_string (pn_name) // ")"
        else
          cmd%name(i) = parse_node_get_key (pn_prefix)
        end if
      end select
    end do
  end if
```

```

case ("log_var", "string_var", "alias_var")
  pn_prefix => parse_node_get_sub_ptr (pn_var)
  pn_name => parse_node_get_next_ptr (pn_prefix)
  key = parse_node_get_key (pn_prefix)
  if (associated (pn_name)) then
    select case (char (parse_node_get_rule_key (pn_name)))
    case ("var_name")
      select case (char (key))
      case ("?", "$") ! $ sign
        cmd%name(i) = key // parse_node_get_string (pn_name)
      case ("alias")
        cmd%name(i) = parse_node_get_string (pn_name)
      end select
    case default
      call parse_node_mismatch &
        ("var_name", pn_name)
    end select
  else
    cmd%name(i) = key
  end if
case default
  cmd%name(i) = parse_node_get_string (pn_var)
end select
pn_var => parse_node_get_next_ptr (pn_var)
end do
else
  allocate (cmd%name (0))
end if
end subroutine cmd_show_compile

```

Execute. Scan the list of objects to show.

```

<Commands: parameters>≡
  integer, parameter, public :: SHOW_BUFFER_SIZE = 4096

<Commands: cmd show: TBP>+≡
  procedure :: execute => cmd_show_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_show_execute (cmd, global)
    class(cmd_show_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_show_execute

<Commands: procedures>+≡
  module subroutine cmd_show_execute (cmd, global)
    class(cmd_show_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list, model_vars
    type(model_t), pointer :: model
    type(string_t) :: name
    integer :: n, pdg
    type(flavor_t) :: flv
    type(process_library_t), pointer :: prc_lib
    type(process_t), pointer :: process
    logical :: pacified

```

```

character(SHOW_BUFFER_SIZE) :: buffer
type(string_t) :: out_file
integer :: i, j, u, u_log, u_out, u_ext
u = free_unit ()
var_list => cmd%local%var_list
if (associated (cmd%local%model)) then
    model_vars => cmd%local%model%get_var_list_ptr ()
else
    model_vars => null ()
end if
pacified = var_list%get_lval (var_str ("?pacify"))
out_file = var_list%get_sval (var_str ("out_file"))
if (file_list_is_open (global%out_files, out_file, action="write")) then
    call msg_message ("show: copying output to file '" &
        // char (out_file) // "'")
    u_ext = file_list_get_unit (global%out_files, out_file)
else
    u_ext = -1
end if
open (u, status = "scratch", action = "readwrite")
if (associated (cmd%local%model)) then
    name = cmd%local%model%get_name ()
end if
if (size (cmd%name) == 0) then
    if (associated (model_vars)) then
        call model_vars%write (model_name = name, &
            unit = u, pacified = pacified, follow_link = .false.)
    end if
    call var_list%write (unit = u, pacified = pacified)
else
    do i = 1, size (cmd%name)
        select case (char (cmd%name(i)))
        case ("model")
            if (associated (cmd%local%model)) then
                call cmd%local%model%show (u)
            else
                write (u, "(A)") "Model: [undefined]"
            end if
        case ("library")
            if (associated (cmd%local%prclib)) then
                call cmd%local%prclib%show (u)
            else
                write (u, "(A)") "Process library: [undefined]"
            end if
        case ("beams")
            call cmd%local%show_beams (u)
        case ("iterations")
            call cmd%local%it_list%write (u)
        case ("results")
            call cmd%local%process_stack%show (u, fifo=.true.)
        case ("stable")
            call cmd%local%model%show_stable (u)
        case ("polarized")
            call cmd%local%model%show_polarized (u)
        end select
    end do

```

```

case ("unpolarized")
  call cmd%local%model%show_unpolarized (u)
case ("unstable")
  model => cmd%local%model
  call model%show_unstable (u)
  n = model%get_n_field ()
  do j = 1, n
    pdg = model%get_pdg (j)
    call flv%init (pdg, model)
    if (.not. flv%is_stable ()) &
      call show_unstable (cmd%local, pdg, u)
    if (flv%has_antiparticle ()) then
      associate (anti => flv%anti ())
        if (.not. anti%is_stable ()) &
          call show_unstable (cmd%local, -pdg, u)
      end associate
    end if
  end do
case ("cuts", "weight", "scale", &
  "factorization_scale", "renormalization_scale", &
  "selection", "reweight", "analysis")
  call cmd%local%pn%show (cmd%name(i), u)
case ("expect")
  call expect_summary (force = .true.)
case ("intrinsic")
  call var_list%write (intrinsic=.true., unit=u, &
    pacified = pacified)
case ("logical")
  if (associated (model_vars)) then
    call model_vars%write (only_type=V_LOG, &
      model_name = name, unit=u, pacified = pacified, &
      follow_link=.false.)
  end if
  call var_list%write (&
    only_type=V_LOG, unit=u, pacified = pacified)
case ("int")
  if (associated (model_vars)) then
    call model_vars%write (only_type=V_INT, &
      model_name = name, unit=u, pacified = pacified, &
      follow_link=.false.)
  end if
  call var_list%write (only_type=V_INT, &
    unit=u, pacified = pacified)
case ("real")
  if (associated (model_vars)) then
    call model_vars%write (only_type=V_REAL, &
      model_name = name, unit=u, pacified = pacified, &
      follow_link=.false.)
  end if
  call var_list%write (only_type=V_REAL, &
    unit=u, pacified = pacified)
case ("complex")
  if (associated (model_vars)) then
    call model_vars%write (only_type=V_CMPLX, &

```

```

        model_name = name, unit=u, pacified = pacified, &
        follow_link=.false.)
    end if
    call var_list%write (only_type=V_CMPLX, &
        unit=u, pacified = pacified)
case ("pdg")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_PDG, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_PDG, &
        unit=u, pacified = pacified)
case ("string")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_STR, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_STR, &
        unit=u, pacified = pacified)
case default
    if (analysis_exists (cmd%name(i))) then
        call analysis_write (cmd%name(i), u)
    else if (cmd%local%process_stack%exists (cmd%name(i))) then
        process => cmd%local%process_stack%get_process_ptr (cmd%name(i))
        call process%show (u)
    else if (associated (cmd%local%prclib_stack%get_library_ptr &
        (cmd%name(i)))) then
        prc_lib => cmd%local%prclib_stack%get_library_ptr (cmd%name(i))
        call prc_lib%show (u)
    else if (associated (model_vars)) then
        if (model_vars%contains (cmd%name(i), follow_link=.false.)) then
            call model_vars%write_var (cmd%name(i), &
                unit = u, model_name = name, pacified = pacified)
        else if (var_list%contains (cmd%name(i))) then
            call var_list%write_var (cmd%name(i), &
                unit = u, pacified = pacified)
        else
            call msg_error ("show: object '" // char (cmd%name(i)) &
                // "' not found")
        end if
    else if (var_list%contains (cmd%name(i))) then
        call var_list%write_var (cmd%name(i), &
            unit = u, pacified = pacified)
    else
        call msg_error ("show: object '" // char (cmd%name(i)) &
            // "' not found")
    end if
end select
end do
end if
rewind (u)
u_log = logfile_unit ()

```

```

u_out = given_output_unit ()
do
  read (u, "(A)", end = 1) buffer
  if (u_log > 0) write (u_log, "(A)") trim (buffer)
  if (u_out > 0) write (u_out, "(A)") trim (buffer)
  if (u_ext > 0) write (u_ext, "(A)") trim (buffer)
end do
1 close (u)
if (u_log > 0) flush (u_log)
if (u_out > 0) flush (u_out)
if (u_ext > 0) flush (u_ext)
end subroutine cmd_show_execute

```

Clear values

This command clears the current values of variables or other objects, where this makes sense. It parallels the `show` command. The objects are cleared, but not deleted.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_clear_t
  private
  type(string_t), dimension(:), allocatable :: name
  contains
  ⟨Commands: cmd clear: TBP⟩
end type cmd_clear_t

```

Output: list the names of the objects to be cleared.

```

⟨Commands: cmd clear: TBP⟩≡
  procedure :: write => cmd_clear_write

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_clear_write (cmd, unit, indent)
    class(cmd_clear_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_clear_write

⟨Commands: procedures⟩+≡
  module subroutine cmd_clear_write (cmd, unit, indent)
    class(cmd_clear_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "clear: "
    if (allocated (cmd%name)) then
      do i = 1, size (cmd%name)
        write (u, "(1x,A)", advance="no") char (cmd%name(i))
      end do
      write (u, *)
    else
      write (u, "(5x,A)") "[undefined]"
    end if
  end subroutine cmd_clear_write

```


Compile. Allocate an array which is filled with the names of the objects to be cleared.

Note: there is currently no need to account for options, but we prepare for that possibility.

```

<Commands: cmd clear: TBP>+≡
    procedure :: compile => cmd_clear_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_clear_compile (cmd, global)
        class(cmd_clear_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_clear_compile

<Commands: procedures>+≡
    module subroutine cmd_clear_compile (cmd, global)
        class(cmd_clear_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name
        type(string_t) :: key
        integer :: i, n_args
        pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
        if (associated (pn_arg)) then
            select case (char (parse_node_get_rule_key (pn_arg)))
            case ("clear_arg")
                cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
            case default
                cmd%pn_opt => pn_arg
                pn_arg => null ()
            end select
        end if
        call cmd%compile_options (global)
        if (associated (pn_arg)) then
            n_args = parse_node_get_n_sub (pn_arg)
            allocate (cmd%name (n_args))
            pn_var => parse_node_get_sub_ptr (pn_arg)
            i = 0
            do while (associated (pn_var))
                i = i + 1
                select case (char (parse_node_get_rule_key (pn_var)))
                case ("beams", "iterations", &
                    "cuts", "weight", &
                    "scale", "factorization_scale", "renormalization_scale", &
                    "selection", "reweight", "analysis", &
                    "unstable", "polarized", &
                    "expect")
                    cmd%name(i) = parse_node_get_key (pn_var)
                case ("log_var", "string_var")
                    pn_prefix => parse_node_get_sub_ptr (pn_var)
                    pn_name => parse_node_get_next_ptr (pn_prefix)
                    key = parse_node_get_key (pn_prefix)
                    if (associated (pn_name)) then
                        select case (char (parse_node_get_rule_key (pn_name)))
                        case ("var_name")

```

```

        select case (char (key))
        case ("?", "$") ! $ sign
            cmd%name(i) = key // parse_node_get_string (pn_name)
        end select
        case default
            call parse_node_mismatch &
                ("var_name", pn_name)
        end select
    else
        cmd%name(i) = key
    end if
case default
    cmd%name(i) = parse_node_get_string (pn_var)
end select
pn_var => parse_node_get_next_ptr (pn_var)
end do
else
    allocate (cmd%name (0))
end if
end subroutine cmd_clear_compile

```

Execute. Scan the list of objects to clear.

Objects that can be shown but not cleared: model, library, results

(Commands: cmd clear: TBP)+≡

```

    procedure :: execute => cmd_clear_execute

```

(Commands: sub interfaces)+≡

```

    module subroutine cmd_clear_execute (cmd, global)
        class(cmd_clear_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_clear_execute

```

(Commands: procedures)+≡

```

    module subroutine cmd_clear_execute (cmd, global)
        class(cmd_clear_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        integer :: i
        logical :: success
        type(var_list_t), pointer :: model_vars
        if (size (cmd%name) == 0) then
            call msg_warning ("clear: no object specified")
        else
            do i = 1, size (cmd%name)
                success = .true.
                select case (char (cmd%name(i)))
                case ("beams")
                    call cmd%local%clear_beams ()
                case ("iterations")
                    call cmd%local%it_list%clear ()
                case ("polarized")
                    call cmd%local%model%clear_polarized ()
                case ("unstable")
                    call cmd%local%model%clear_unstable ()
                case ("cuts", "weight", "scale", &
                    "factorization_scale", "renormalization_scale", &

```

```

        "selection", "reweight", "analysis")
    call cmd%local%pn%clear (cmd%name(i))
case ("expect")
    call expect_clear ()
case default
    if (analysis_exists (cmd%name(i))) then
        call analysis_clear (cmd%name(i))
    else if (cmd%local%var_list%contains (cmd%name(i))) then
        if (.not. cmd%local%var_list%is_locked (cmd%name(i))) then
            call cmd%local%var_list%unset (cmd%name(i))
        else
            call msg_error ("clear: variable '" // char (cmd%name(i)) &
                // "' is locked and can't be cleared")
            success = .false.
        end if
    else if (associated (cmd%local%model)) then
        model_vars => cmd%local%model%get_var_list_ptr ()
        if (model_vars%contains (cmd%name(i), follow_link=.false.)) then
            call msg_error ("clear: variable '" // char (cmd%name(i)) &
                // "' is a model variable and can't be cleared")
        else
            call msg_error ("clear: object '" // char (cmd%name(i)) &
                // "' not found")
        end if
        success = .false.
    else
        call msg_error ("clear: object '" // char (cmd%name(i)) &
            // "' not found")
        success = .false.
    end if
end select
if (success) call msg_message ("cleared: " // char (cmd%name(i)))
end do
end if
end subroutine cmd_clear_execute

```

Compare values of variables to expectation

The implementation is similar to the `show` command. There are just two arguments: two values that should be compared. For providing local values for the numerical tolerance, the command has a local argument list.

If the expectation fails, an error condition is recorded.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_expect_t
        private
            type(parse_node_t), pointer :: pn_lexpr => null ()
        contains
            <Commands: cmd expect: TBP>
        end type cmd_expect_t

```

Simply tell the status.

```

<Commands: cmd expect: TBP>≡

```

```

    procedure :: write => cmd_expect_write
  <Commands: sub interfaces>+≡
    module subroutine cmd_expect_write (cmd, unit, indent)
      class(cmd_expect_t), intent(in) :: cmd
      integer, intent(in), optional :: unit, indent
    end subroutine cmd_expect_write
  <Commands: procedures>+≡
    module subroutine cmd_expect_write (cmd, unit, indent)
      class(cmd_expect_t), intent(in) :: cmd
      integer, intent(in), optional :: unit, indent
      integer :: u
      u = given_output_unit (unit); if (u < 0) return
      call write_indent (u, indent)
      if (associated (cmd%pn_lexpr)) then
        write (u, "(1x,A)") "expect: [expression associated]"
      else
        write (u, "(1x,A)") "expect: [undefined]"
      end if
    end subroutine cmd_expect_write

```

Compile. This merely assigns the parse node, the actual compilation is done at execution. This is necessary because the origin of variables (local/global) may change during execution.

```

  <Commands: cmd expect: TBP>+≡
    procedure :: compile => cmd_expect_compile
  <Commands: sub interfaces>+≡
    module subroutine cmd_expect_compile (cmd, global)
      class(cmd_expect_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_expect_compile
  <Commands: procedures>+≡
    module subroutine cmd_expect_compile (cmd, global)
      class(cmd_expect_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
      type(parse_node_t), pointer :: pn_arg
      pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
      cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
      cmd%pn_lexpr => parse_node_get_sub_ptr (pn_arg)
      call cmd%compile_options (global)
    end subroutine cmd_expect_compile

```

Execute. Evaluate both arguments, print them and their difference (if numerical), and whether they agree. Record the result.

```

  <Commands: cmd expect: TBP>+≡
    procedure :: execute => cmd_expect_execute
  <Commands: sub interfaces>+≡
    module subroutine cmd_expect_execute (cmd, global)
      class(cmd_expect_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_expect_execute

```

```

⟨Commands: procedures⟩+≡
module subroutine cmd_expect_execute (cmd, global)
  class(cmd_expect_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  logical :: success, is_known
  var_list => cmd%local%get_var_list_ptr ()
  success = eval_log (cmd%pn_lexpr, var_list, is_known=is_known)
  if (is_known) then
    if (success) then
      call msg_message ("expect: success")
    else
      call msg_error ("expect: failure")
    end if
  else
    call msg_error ("expect: undefined result")
    success = .false.
  end if
  call expect_record (success)
end subroutine cmd_expect_execute

```

Beams

The beam command includes both beam and structure-function definition.

```

⟨Commands: types⟩+≡
type, extends (command_t) :: cmd_beams_t
  private
  integer :: n_in = 0
  type(parse_node_p), dimension(:), allocatable :: pn_pdg
  integer :: n_sf_record = 0
  integer, dimension(:), allocatable :: n_entry
  type(parse_node_p), dimension(:, :), allocatable :: pn_sf_entry
contains
  ⟨Commands: cmd beams: TBP⟩
end type cmd_beams_t

```

Output. The particle expressions are not resolved.

```

⟨Commands: cmd beams: TBP⟩≡
  procedure :: write => cmd_beams_write

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_beams_write (cmd, unit, indent)
    class(cmd_beams_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_beams_write

⟨Commands: procedures⟩+≡
  module subroutine cmd_beams_write (cmd, unit, indent)
    class(cmd_beams_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
  end subroutine cmd_beams_write

```

```

select case (cmd%n_in)
case (1)
  write (u, "(1x,A)") "beams: 1 [decay]"
case (2)
  write (u, "(1x,A)") "beams: 2 [scattering]"
case default
  write (u, "(1x,A)") "beams: [undefined]"
end select
if (allocated (cmd%n_entry)) then
  if (cmd%n_sf_record > 0) then
    write (u, "(1x,A,99(1x,I0))") "structure function entries:", &
      cmd%n_entry
  end if
end if
end subroutine cmd_beams_write

```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```

<Commands: cmd beams: TBP>+≡
  procedure :: compile => cmd_beams_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_beams_compile (cmd, global)
    class(cmd_beams_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_compile

<Commands: procedures>+≡
  module subroutine cmd_beams_compile (cmd, global)
    class(cmd_beams_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_beam_def, pn_beam_spec
    type(parse_node_t), pointer :: pn_beam_list
    type(parse_node_t), pointer :: pn_codes
    type(parse_node_t), pointer :: pn_strfun_seq, pn_strfun_pair
    type(parse_node_t), pointer :: pn_strfun_def
    integer :: i
    pn_beam_def => parse_node_get_sub_ptr (cmd%pn, 3)
    pn_beam_spec => parse_node_get_sub_ptr (pn_beam_def)
    pn_strfun_seq => parse_node_get_next_ptr (pn_beam_spec)
    pn_beam_list => parse_node_get_sub_ptr (pn_beam_spec)
    call cmd%compile_options (global)
    cmd%n_in = parse_node_get_n_sub (pn_beam_list)
    allocate (cmd%pn_pdg (cmd%n_in))
    pn_codes => parse_node_get_sub_ptr (pn_beam_list)
    do i = 1, cmd%n_in
      cmd%pn_pdg(i)%ptr => pn_codes
      pn_codes => parse_node_get_next_ptr (pn_codes)
    end do
    if (associated (pn_strfun_seq)) then
      cmd%n_sf_record = parse_node_get_n_sub (pn_beam_def) - 1
      allocate (cmd%n_entry (cmd%n_sf_record), source = 1)
      allocate (cmd%pn_sf_entry (2, cmd%n_sf_record))
      do i = 1, cmd%n_sf_record
        pn_strfun_pair => parse_node_get_sub_ptr (pn_strfun_seq, 2)

```

```

        pn_strfun_def => parse_node_get_sub_ptr (pn_strfun_pair)
        cmd%pn_sf_entry(1,i)%ptr => pn_strfun_def
        pn_strfun_def => parse_node_get_next_ptr (pn_strfun_def)
        cmd%pn_sf_entry(2,i)%ptr => pn_strfun_def
        if (associated (pn_strfun_def)) cmd%n_entry(i) = 2
        pn_strfun_seq => parse_node_get_next_ptr (pn_strfun_seq)
    end do
else
    allocate (cmd%n_entry (0))
    allocate (cmd%pn_sf_entry (0, 0))
end if
end subroutine cmd_beams_compile

```

Command execution: Determine beam particles and structure-function names, if any. The results are stored in the `beam_structure` component of the `global` data block.

(Commands: cmd beams: TBP)+≡

```

    procedure :: execute => cmd_beams_execute

```

(Commands: sub interfaces)+≡

```

    module subroutine cmd_beams_execute (cmd, global)
        class(cmd_beams_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_execute

```

(Commands: procedures)+≡

```

    module subroutine cmd_beams_execute (cmd, global)
        class(cmd_beams_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(pdg_array_t) :: pdg_array
        integer, dimension(:), allocatable :: pdg
        type(flavor_t), dimension(:), allocatable :: flv
        type(parse_node_t), pointer :: pn_key
        type(string_t) :: sf_name
        integer :: i, j
        call lhpdf_global_reset ()
        var_list => cmd%local%get_var_list_ptr ()
        allocate (flv (cmd%n_in))
        do i = 1, cmd%n_in
            pdg_array = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
            pdg = pdg_array
            select case (size (pdg))
            case (1)
                call flv(i)%init ( pdg(1), cmd%local%model)
            case default
                call msg_fatal ("Beams: beam particles must be unique")
            end select
        end do
        select case (cmd%n_in)
        case (1)
            if (cmd%n_sf_record > 0) then
                call msg_fatal ("Beam setup: no structure functions allowed &
                                &for decay")
            end if
        end case
    end subroutine cmd_beams_execute

```

```

        end if
        call global%beam_structure%init_sf (flv%get_name ())
    case (2)
        call global%beam_structure%init_sf (flv%get_name (), cmd%n_entry)
        do i = 1, cmd%n_sf_record
            do j = 1, cmd%n_entry(i)
                pn_key => parse_node_get_sub_ptr (cmd%pn_sf_entry(j,i)%ptr)
                sf_name = parse_node_get_key (pn_key)
                call global%beam_structure%set_sf (i, j, sf_name)
            end do
        end do
    end select
end subroutine cmd_beams_execute

```

Density matrices for beam polarization

For holding beam polarization, we define a notation and a data structure for sparse matrices. The entries (and the index expressions) are numerical expressions, so we use evaluation trees.

Each entry in the sparse matrix is an n-tuple of expressions. The first tuple elements represent index values, the last one is an arbitrary (complex) number. Absent expressions are replaced by default-value rules.

Note: Here, and in some other commands, we would like to store an evaluation tree, not just a parse node pointer. However, the current expression handler wants all variables defined, so the evaluation tree can only be built by `evaluate`, i.e., compiled just-in-time and evaluated immediately.

```

<Commands: types>+≡
    type :: sentry_expr_t
        type(parse_node_p), dimension(:), allocatable :: expr
        contains
        <Commands: sentry expr: TBP>
    end type sentry_expr_t

```

Compile parse nodes into evaluation trees.

```

<Commands: sentry expr: TBP>≡
    procedure :: compile => sentry_expr_compile

<Commands: sub interfaces>+≡
    module subroutine sentry_expr_compile (sentry, pn)
        class(sentry_expr_t), intent(out) :: sentry
        type(parse_node_t), intent(in), target :: pn
    end subroutine sentry_expr_compile

<Commands: procedures>+≡
    module subroutine sentry_expr_compile (sentry, pn)
        class(sentry_expr_t), intent(out) :: sentry
        type(parse_node_t), intent(in), target :: pn
        type(parse_node_t), pointer :: pn_expr, pn_extra
        integer :: n_expr, i
        n_expr = parse_node_get_n_sub (pn)
        allocate (sentry%expr (n_expr))
        if (n_expr > 0) then

```



```

i = 0
pn_expr => parse_node_get_sub_ptr (pn)
pn_extra => parse_node_get_next_ptr (pn_expr)
do i = 1, n_expr
  sentry%expr(i)%ptr => pn_expr
  if (associated (pn_extra)) then
    pn_expr => parse_node_get_sub_ptr (pn_extra, 2)
    pn_extra => parse_node_get_next_ptr (pn_extra)
  end if
end do
end if
end subroutine sentry_expr_compile

```

Evaluate the expressions and return an index array of predefined length together with a complex value. If the value (as the last expression) is undefined, set it to unity. If index values are undefined, repeat the previous index value.

<Commands: sentry expr: TBP>+≡

```

procedure :: evaluate => sentry_expr_evaluate

```

<Commands: sub interfaces>+≡

```

module subroutine sentry_expr_evaluate (sentry, index, value, global)
  class(sentry_expr_t), intent(inout) :: sentry
  integer, dimension(:), intent(out) :: index
  complex(default), intent(out) :: value
  type(rt_data_t), intent(in), target :: global
end subroutine sentry_expr_evaluate

```

<Commands: procedures>+≡

```

module subroutine sentry_expr_evaluate (sentry, index, value, global)
  class(sentry_expr_t), intent(inout) :: sentry
  integer, dimension(:), intent(out) :: index
  complex(default), intent(out) :: value
  type(rt_data_t), intent(in), target :: global
  type(var_list_t), pointer :: var_list
  integer :: i, n_expr, n_index
  type(eval_tree_t) :: eval_tree
  var_list => global%get_var_list_ptr ()
  n_expr = size (sentry%expr)
  n_index = size (index)
  if (n_expr <= n_index + 1) then
    do i = 1, min (n_expr, n_index)
      associate (expr => sentry%expr(i))
        call eval_tree%init_expr (expr%ptr, var_list)
        call eval_tree%evaluate ()
        if (eval_tree%is_known ()) then
          index(i) = eval_tree%get_int ()
        else
          call msg_fatal ("Evaluating density matrix: undefined index")
        end if
      end associate
    end do
    do i = n_expr + 1, n_index
      index(i) = index(n_expr)
    end do
  end if
end subroutine

```

```

    if (n_expr == n_index + 1) then
        associate (expr => sentry%expr(n_expr))
            call eval_tree%init_expr (expr%ptr, var_list)
            call eval_tree%evaluate ()
            if (eval_tree%is_known ()) then
                value = eval_tree%get_cmplx ()
            else
                call msg_fatal ("Evaluating density matrix: undefined index")
            end if
            call eval_tree%final ()
        end associate
    else
        value = 1
    end if
else
    call msg_fatal ("Evaluating density matrix: index expression too long")
end if
end subroutine sentry_expr_evaluate

```

The sparse matrix itself consists of an arbitrary number of entries.

```

<Commands: types>+≡
    type :: smatrix_expr_t
        type(sentry_expr_t), dimension(:), allocatable :: entry
        contains
        <Commands: smatrix_expr: TBP>
    end type smatrix_expr_t

```

Compile: assign sub-nodes to sentry-expressions and compile those.

```

<Commands: smatrix_expr: TBP>≡
    procedure :: compile => smatrix_expr_compile

<Commands: sub interfaces>+≡
    module subroutine smatrix_expr_compile (smatrix_expr, pn)
        class(smatrix_expr_t), intent(out) :: smatrix_expr
        type(parse_node_t), intent(in), target :: pn
    end subroutine smatrix_expr_compile

<Commands: procedures>+≡
    module subroutine smatrix_expr_compile (smatrix_expr, pn)
        class(smatrix_expr_t), intent(out) :: smatrix_expr
        type(parse_node_t), intent(in), target :: pn
        type(parse_node_t), pointer :: pn_arg, pn_entry
        integer :: n_entry, i
        pn_arg => parse_node_get_sub_ptr (pn, 2)
        if (associated (pn_arg)) then
            n_entry = parse_node_get_n_sub (pn_arg)
            allocate (smatrix_expr%entry (n_entry))
            pn_entry => parse_node_get_sub_ptr (pn_arg)
            do i = 1, n_entry
                call smatrix_expr%entry(i)%compile (pn_entry)
            end do
            pn_entry => parse_node_get_next_ptr (pn_arg)
        else
            allocate (smatrix_expr%entry (0))
        end if
    end subroutine smatrix_expr_compile

```

```

    end if
end subroutine smatrix_expr_compile

```

Evaluate the entries and build a new `smatrix` object, which contains just the numerical results.

```

<Commands: smatrix expr: TBP>+≡
    procedure :: evaluate => smatrix_expr_evaluate

<Commands: sub interfaces>+≡
    module subroutine smatrix_expr_evaluate (smatrix_expr, smatrix, global)
        class(smatrix_expr_t), intent(inout) :: smatrix_expr
        type(smatrix_t), intent(out) :: smatrix
        type(rt_data_t), intent(in), target :: global
    end subroutine smatrix_expr_evaluate

<Commands: procedures>+≡
    module subroutine smatrix_expr_evaluate (smatrix_expr, smatrix, global)
        class(smatrix_expr_t), intent(inout) :: smatrix_expr
        type(smatrix_t), intent(out) :: smatrix
        type(rt_data_t), intent(in), target :: global
        integer, dimension(2) :: idx
        complex(default) :: value
        integer :: i, n_entry
        n_entry = size (smatrix_expr%entry)
        call smatrix%init (2, n_entry)
        do i = 1, n_entry
            call smatrix_expr%entry(i)%evaluate (idx, value, global)
            call smatrix%set_entry (i, idx, value)
        end do
    end subroutine smatrix_expr_evaluate

```

Beam polarization density

The beam polarization command defines spin density matrix for one or two beams (scattering or decay).

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_beams_pol_density_t
        private
        integer :: n_in = 0
        type(smatrix_expr_t), dimension(:), allocatable :: smatrix
    contains
        <Commands: cmd beams pol density: TBP>
    end type cmd_beams_pol_density_t

```

Output.

```

<Commands: cmd beams pol density: TBP>≡
    procedure :: write => cmd_beams_pol_density_write

<Commands: sub interfaces>+≡
    module subroutine cmd_beams_pol_density_write (cmd, unit, indent)
        class(cmd_beams_pol_density_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_beams_pol_density_write

```

```

<Commands: procedures>+≡
module subroutine cmd_beams_pol_density_write (cmd, unit, indent)
  class(cmd_beams_pol_density_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  select case (cmd%n_in)
  case (1)
    write (u, "(1x,A)") "beams polarization setup: 1 [decay]"
  case (2)
    write (u, "(1x,A)") "beams polarization setup: 2 [scattering]"
  case default
    write (u, "(1x,A)") "beams polarization setup: [undefined]"
  end select
end subroutine cmd_beams_pol_density_write

```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```

<Commands: cmd beams pol density: TBP>+≡
  procedure :: compile => cmd_beams_pol_density_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_beams_pol_density_compile (cmd, global)
    class(cmd_beams_pol_density_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_beams_pol_density_compile

<Commands: procedures>+≡
module subroutine cmd_beams_pol_density_compile (cmd, global)
  class(cmd_beams_pol_density_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_pol_spec, pn_smatrix
  integer :: i
  pn_pol_spec => parse_node_get_sub_ptr (cmd%pn, 3)
  call cmd%compile_options (global)
  cmd%n_in = parse_node_get_n_sub (pn_pol_spec)
  allocate (cmd%smatrix (cmd%n_in))
  pn_smatrix => parse_node_get_sub_ptr (pn_pol_spec)
  do i = 1, cmd%n_in
    call cmd%smatrix(i)%compile (pn_smatrix)
    pn_smatrix => parse_node_get_next_ptr (pn_smatrix)
  end do
end subroutine cmd_beams_pol_density_compile

```

Command execution: Fill polarization density matrices. No check yet, the matrices are checked and normalized when the actual beam object is created, just before integration. For intermediate storage, we use the `beam_structure` object in the `global` data set.

```

<Commands: cmd beams pol density: TBP>+≡
  procedure :: execute => cmd_beams_pol_density_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_beams_pol_density_execute (cmd, global)

```

```

        class(cmd_beams_pol_density_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_pol_density_execute
<Commands: procedures>+≡
module subroutine cmd_beams_pol_density_execute (cmd, global)
    class(cmd_beams_pol_density_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(smatrix_t) :: smatrix
    integer :: i
    call global%beam_structure%init_pol (cmd%n_in)
    do i = 1, cmd%n_in
        call cmd%smatrix(i)%evaluate (smatrix, global)
        call global%beam_structure%set_smatrix (i, smatrix)
    end do
end subroutine cmd_beams_pol_density_execute

```

Beam polarization fraction

In addition to the polarization density matrix, we can independently specify the polarization fraction for one or both beams.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_beams_pol_fraction_t
    private
    integer :: n_in = 0
    type(parse_node_p), dimension(:), allocatable :: expr
contains
    <Commands: cmd beams pol fraction: TBP>
end type cmd_beams_pol_fraction_t

```

Output.

```

<Commands: cmd beams pol fraction: TBP>≡
    procedure :: write => cmd_beams_pol_fraction_write
<Commands: sub interfaces>+≡
    module subroutine cmd_beams_pol_fraction_write (cmd, unit, indent)
        class(cmd_beams_pol_fraction_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_beams_pol_fraction_write
<Commands: procedures>+≡
module subroutine cmd_beams_pol_fraction_write (cmd, unit, indent)
    class(cmd_beams_pol_fraction_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    select case (cmd%n_in)
    case (1)
        write (u, "(1x,A)") "beams polarization fraction: 1 [decay]"
    case (2)
        write (u, "(1x,A)") "beams polarization fraction: 2 [scattering]"
    case default

```

```

        write (u, "(1x,A)") "beams polarization fraction: [undefined]"
    end select
end subroutine cmd_beams_pol_fraction_write

```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```

<Commands: cmd beams pol fraction: TBP>+≡
    procedure :: compile => cmd_beams_pol_fraction_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_beams_pol_fraction_compile (cmd, global)
        class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_pol_fraction_compile

<Commands: procedures>+≡
    module subroutine cmd_beams_pol_fraction_compile (cmd, global)
        class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_frac_spec, pn_expr
        integer :: i
        pn_frac_spec => parse_node_get_sub_ptr (cmd%pn, 3)
        call cmd%compile_options (global)
        cmd%n_in = parse_node_get_n_sub (pn_frac_spec)
        allocate (cmd%expr (cmd%n_in))
        pn_expr => parse_node_get_sub_ptr (pn_frac_spec)
        do i = 1, cmd%n_in
            cmd%expr(i)%ptr => pn_expr
            pn_expr => parse_node_get_next_ptr (pn_expr)
        end do
    end subroutine cmd_beams_pol_fraction_compile

```

Command execution: Retrieve the numerical values of the beam polarization fractions. The results are stored in the `beam_structure` component of the global data block.

```

<Commands: cmd beams pol fraction: TBP>+≡
    procedure :: execute => cmd_beams_pol_fraction_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_beams_pol_fraction_execute (cmd, global)
        class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_pol_fraction_execute

<Commands: procedures>+≡
    module subroutine cmd_beams_pol_fraction_execute (cmd, global)
        class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        real(default), dimension(:), allocatable :: pol_f
        type(eval_tree_t) :: expr
        integer :: i
        var_list => global%get_var_list_ptr ()
        allocate (pol_f (cmd%n_in))
        do i = 1, cmd%n_in

```

```

        call expr%init_expr (cmd%expr(i)%ptr, var_list)
        call expr%evaluate ()
        if (expr%is_known ()) then
            pol_f(i) = expr%get_real ()
        else
            call msg_fatal ("beams polarization fraction: undefined value")
        end if
        call expr%final ()
    end do
    call global%beam_structure%set_pol_f (pol_f)
end subroutine cmd_beams_pol_fraction_execute

```

Beam momentum

This is completely analogous to the previous command, hence we can use inheritance.

```

⟨Commands: types⟩+≡
    type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_momentum_t
    contains
    ⟨Commands: cmd beams momentum: TBP⟩
end type cmd_beams_momentum_t

```

Output.

```

⟨Commands: cmd beams momentum: TBP⟩≡
    procedure :: write => cmd_beams_momentum_write

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_beams_momentum_write (cmd, unit, indent)
        class(cmd_beams_momentum_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_beams_momentum_write

⟨Commands: procedures⟩+≡
    module subroutine cmd_beams_momentum_write (cmd, unit, indent)
        class(cmd_beams_momentum_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        select case (cmd%n_in)
        case (1)
            write (u, "(1x,A)") "beams momentum: 1 [decay]"
        case (2)
            write (u, "(1x,A)") "beams momentum: 2 [scattering]"
        case default
            write (u, "(1x,A)") "beams momentum: [undefined]"
        end select
    end subroutine cmd_beams_momentum_write

```

Compile: inherited.

Command execution: Not inherited, but just the error string and the final command are changed.

```

⟨Commands: cmd beams momentum: TBP⟩+≡

```

```

    procedure :: execute => cmd_beams_momentum_execute
  <Commands: sub interfaces>+≡
    module subroutine cmd_beams_momentum_execute (cmd, global)
      class(cmd_beams_momentum_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_beams_momentum_execute
  <Commands: procedures>+≡
    module subroutine cmd_beams_momentum_execute (cmd, global)
      class(cmd_beams_momentum_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
      type(var_list_t), pointer :: var_list
      real(default), dimension(:), allocatable :: p
      type(eval_tree_t) :: expr
      integer :: i
      var_list => global%get_var_list_ptr ()
      allocate (p (cmd%n_in))
      do i = 1, cmd%n_in
        call expr%init_expr (cmd%expr(i)%ptr, var_list)
        call expr%evaluate ()
        if (expr%is_known ()) then
          p(i) = expr%get_real ()
        else
          call msg_fatal ("beams momentum: undefined value")
        end if
        call expr%final ()
      end do
      call global%beam_structure%set_momentum (p)
    end subroutine cmd_beams_momentum_execute

```

Beam angles

Again, this is analogous. There are two angles, polar angle θ and azimuthal angle ϕ , which can be set independently for both beams.

```

  <Commands: types>+≡
    type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_theta_t
      contains
      <Commands: cmd beams theta: TBP>
    end type cmd_beams_theta_t

    type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_phi_t
      contains
      <Commands: cmd beams phi: TBP>
    end type cmd_beams_phi_t

```

Output.

```

  <Commands: cmd beams theta: TBP>≡
    procedure :: write => cmd_beams_theta_write

  <Commands: cmd beams phi: TBP>≡
    procedure :: write => cmd_beams_phi_write

```



```

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_beams_theta_write (cmd, unit, indent)
        class(cmd_beams_theta_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_beams_theta_write
    module subroutine cmd_beams_phi_write (cmd, unit, indent)
        class(cmd_beams_phi_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_beams_phi_write

```

```

⟨Commands: procedures⟩+≡
    module subroutine cmd_beams_theta_write (cmd, unit, indent)
        class(cmd_beams_theta_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        select case (cmd%n_in)
            case (1)
                write (u, "(1x,A)") "beams theta: 1 [decay]"
            case (2)
                write (u, "(1x,A)") "beams theta: 2 [scattering]"
            case default
                write (u, "(1x,A)") "beams theta: [undefined]"
        end select
    end subroutine cmd_beams_theta_write

    module subroutine cmd_beams_phi_write (cmd, unit, indent)
        class(cmd_beams_phi_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        select case (cmd%n_in)
            case (1)
                write (u, "(1x,A)") "beams phi: 1 [decay]"
            case (2)
                write (u, "(1x,A)") "beams phi: 2 [scattering]"
            case default
                write (u, "(1x,A)") "beams phi: [undefined]"
        end select
    end subroutine cmd_beams_phi_write

```

Compile: inherited.

Command execution: Not inherited, but just the error string and the final command are changed.

```

⟨Commands: cmd beams theta: TBP⟩+≡
    procedure :: execute => cmd_beams_theta_execute

```

```

⟨Commands: cmd beams phi: TBP⟩+≡
    procedure :: execute => cmd_beams_phi_execute

```

```

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_beams_theta_execute (cmd, global)
        class(cmd_beams_theta_t), intent(inout) :: cmd

```

```

    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_beams_theta_execute
module subroutine cmd_beams_phi_execute (cmd, global)
    class(cmd_beams_phi_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_beams_phi_execute

```

(Commands: procedures)+≡

```

module subroutine cmd_beams_theta_execute (cmd, global)
    class(cmd_beams_theta_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    real(default), dimension(:), allocatable :: theta
    type(eval_tree_t) :: expr
    integer :: i
    var_list => global%get_var_list_ptr ()
    allocate (theta (cmd%n_in))
    do i = 1, cmd%n_in
        call expr%init_expr (cmd%expr(i)%ptr, var_list)
        call expr%evaluate ()
        if (expr%is_known ()) then
            theta(i) = expr%get_real ()
        else
            call msg_fatal ("beams theta: undefined value")
        end if
        call expr%final ()
    end do
    call global%beam_structure%set_theta (theta)
end subroutine cmd_beams_theta_execute

```

```

module subroutine cmd_beams_phi_execute (cmd, global)
    class(cmd_beams_phi_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    real(default), dimension(:), allocatable :: phi
    type(eval_tree_t) :: expr
    integer :: i
    var_list => global%get_var_list_ptr ()
    allocate (phi (cmd%n_in))
    do i = 1, cmd%n_in
        call expr%init_expr (cmd%expr(i)%ptr, var_list)
        call expr%evaluate ()
        if (expr%is_known ()) then
            phi(i) = expr%get_real ()
        else
            call msg_fatal ("beams phi: undefined value")
        end if
        call expr%final ()
    end do
    call global%beam_structure%set_phi (phi)
end subroutine cmd_beams_phi_execute

```

Cuts

Define a cut expression. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the cut expression is used.

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_cuts_t
  private
  type(parse_node_t), pointer :: pn_lexpr => null ()
  contains
  <Commands: cmd cuts: TBP>
end type cmd_cuts_t
```

Output. Do not print the parse tree, since this may get cluttered. Just a message that cuts have been defined.

```
<Commands: cmd cuts: TBP>≡
  procedure :: write => cmd_cuts_write

<Commands: sub interfaces>+≡
  module subroutine cmd_cuts_write (cmd, unit, indent)
    class(cmd_cuts_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_cuts_write

<Commands: procedures>+≡
  module subroutine cmd_cuts_write (cmd, unit, indent)
    class(cmd_cuts_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "cuts: [defined]"
  end subroutine cmd_cuts_write
```

Compile. Simply store the parse (sub)tree.

```
<Commands: cmd cuts: TBP>+≡
  procedure :: compile => cmd_cuts_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_cuts_compile (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_cuts_compile

<Commands: procedures>+≡
  module subroutine cmd_cuts_compile (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_cuts_compile
```

Instead of evaluating the cut expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```
<Commands: cmd cuts: TBP>+≡
  procedure :: execute => cmd_cuts_execute
```

```

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_cuts_execute (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_cuts_execute

```

```

⟨Commands: procedures⟩+≡
  module subroutine cmd_cuts_execute (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%cuts_lexpr => cmd%pn_lexpr
  end subroutine cmd_cuts_execute

```

General, Factorization and Renormalization Scales

Define a scale expression for either the renormalization or the factorization scale. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the expression is used.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_scale_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
  contains
  ⟨Commands: cmd scale: TBP⟩
end type cmd_scale_t

```

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_fac_scale_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
  contains
  ⟨Commands: cmd fac scale: TBP⟩
end type cmd_fac_scale_t

```

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_ren_scale_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
  contains
  ⟨Commands: cmd ren scale: TBP⟩
end type cmd_ren_scale_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

⟨Commands: cmd scale: TBP⟩≡
  procedure :: write => cmd_scale_write

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_scale_write (cmd, unit, indent)
    class(cmd_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_scale_write

```

```

<Commands: procedures>+≡
  module subroutine cmd_scale_write (cmd, unit, indent)
    class(cmd_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "scale: [defined]"
  end subroutine cmd_scale_write

<Commands: cmd fac scale: TBP>≡
  procedure :: write => cmd_fac_scale_write

<Commands: sub interfaces>+≡
  module subroutine cmd_fac_scale_write (cmd, unit, indent)
    class(cmd_fac_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_fac_scale_write

<Commands: procedures>+≡
  module subroutine cmd_fac_scale_write (cmd, unit, indent)
    class(cmd_fac_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "factorization scale: [defined]"
  end subroutine cmd_fac_scale_write

<Commands: cmd ren scale: TBP>≡
  procedure :: write => cmd_ren_scale_write

<Commands: sub interfaces>+≡
  module subroutine cmd_ren_scale_write (cmd, unit, indent)
    class(cmd_ren_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_ren_scale_write

<Commands: procedures>+≡
  module subroutine cmd_ren_scale_write (cmd, unit, indent)
    class(cmd_ren_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "renormalization scale: [defined]"
  end subroutine cmd_ren_scale_write

```

Compile. Simply store the parse (sub)tree.

```

<Commands: cmd scale: TBP>+≡
  procedure :: compile => cmd_scale_compile

```

```

<Commands: sub interfaces>+≡
    module subroutine cmd_scale_compile (cmd, global)
        class(cmd_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_scale_compile

<Commands: procedures>+≡
    module subroutine cmd_scale_compile (cmd, global)
        class(cmd_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
    end subroutine cmd_scale_compile

<Commands: cmd fac scale: TBP>+≡
    procedure :: compile => cmd_fac_scale_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_fac_scale_compile (cmd, global)
        class(cmd_fac_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_fac_scale_compile

<Commands: procedures>+≡
    module subroutine cmd_fac_scale_compile (cmd, global)
        class(cmd_fac_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
    end subroutine cmd_fac_scale_compile

<Commands: cmd ren scale: TBP>+≡
    procedure :: compile => cmd_ren_scale_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_ren_scale_compile (cmd, global)
        class(cmd_ren_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_ren_scale_compile

<Commands: procedures>+≡
    module subroutine cmd_ren_scale_compile (cmd, global)
        class(cmd_ren_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
    end subroutine cmd_ren_scale_compile

```

Instead of evaluating the scale expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

<Commands: cmd scale: TBP>+≡
    procedure :: execute => cmd_scale_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_scale_execute (cmd, global)
        class(cmd_scale_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_scale_execute

```

```

<Commands: procedures>+≡
module subroutine cmd_scale_execute (cmd, global)
  class(cmd_scale_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  global%pn%scale_expr => cmd%pn_expr
end subroutine cmd_scale_execute

<Commands: cmd fac scale: TBP>+≡
procedure :: execute => cmd_fac_scale_execute

<Commands: sub interfaces>+≡
module subroutine cmd_fac_scale_execute (cmd, global)
  class(cmd_fac_scale_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_fac_scale_execute

<Commands: procedures>+≡
module subroutine cmd_fac_scale_execute (cmd, global)
  class(cmd_fac_scale_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  global%pn%fac_scale_expr => cmd%pn_expr
end subroutine cmd_fac_scale_execute

<Commands: cmd ren scale: TBP>+≡
procedure :: execute => cmd_ren_scale_execute

<Commands: sub interfaces>+≡
module subroutine cmd_ren_scale_execute (cmd, global)
  class(cmd_ren_scale_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_ren_scale_execute

<Commands: procedures>+≡
module subroutine cmd_ren_scale_execute (cmd, global)
  class(cmd_ren_scale_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  global%pn%ren_scale_expr => cmd%pn_expr
end subroutine cmd_ren_scale_execute

```

Weight

Define a weight expression. The weight is applied to a process to be integrated, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the expression is used.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_weight_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
contains
  <Commands: cmd weight: TBP>
end type cmd_weight_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

⟨Commands: cmd weight: TBP⟩≡
  procedure :: write => cmd_weight_write

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_weight_write (cmd, unit, indent)
    class(cmd_weight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_weight_write

⟨Commands: procedures⟩+≡
  module subroutine cmd_weight_write (cmd, unit, indent)
    class(cmd_weight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "weight expression: [defined]"
  end subroutine cmd_weight_write

```

Compile. Simply store the parse (sub)tree.

```

⟨Commands: cmd weight: TBP⟩+≡
  procedure :: compile => cmd_weight_compile

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_weight_compile (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_weight_compile

⟨Commands: procedures⟩+≡
  module subroutine cmd_weight_compile (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_weight_compile

```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

⟨Commands: cmd weight: TBP⟩+≡
  procedure :: execute => cmd_weight_execute

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_weight_execute (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_weight_execute

⟨Commands: procedures⟩+≡
  module subroutine cmd_weight_execute (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%weight_expr => cmd%pn_expr
  end subroutine cmd_weight_execute

```


Selection

Define a selection expression. This is to be applied upon simulation or event-file rescanning, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the environment where the expression is used.

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_selection_t
  private
    type(parse_node_t), pointer :: pn_expr => null ()
  contains
    <Commands: cmd selection: TBP>
  end type cmd_selection_t

<Commands: cmd selection: TBP>≡
  procedure :: write => cmd_selection_write

<Commands: sub interfaces>+≡
  module subroutine cmd_selection_write (cmd, unit, indent)
    class(cmd_selection_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_selection_write

<Commands: procedures>+≡
  module subroutine cmd_selection_write (cmd, unit, indent)
    class(cmd_selection_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "selection expression: [defined]"
  end subroutine cmd_selection_write
```

Compile. Simply store the parse (sub)tree.

```
<Commands: cmd selection: TBP>+≡
  procedure :: compile => cmd_selection_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_selection_compile (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_selection_compile

<Commands: procedures>+≡
  module subroutine cmd_selection_compile (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_selection_compile
```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

<Commands: cmd selection: TBP>+≡
  procedure :: execute => cmd_selection_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_selection_execute (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_selection_execute

<Commands: procedures>+≡
  module subroutine cmd_selection_execute (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%selection_lexpr => cmd%pn_expr
  end subroutine cmd_selection_execute

```

Reweight

Define a reweight expression. This is to be applied upon simulation or event-file rescanning, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the environment where the expression is used.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_reweight_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
  contains
  <Commands: cmd reweight: TBP>
  end type cmd_reweight_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

<Commands: cmd reweight: TBP>≡
  procedure :: write => cmd_reweight_write

<Commands: sub interfaces>+≡
  module subroutine cmd_reweight_write (cmd, unit, indent)
    class(cmd_reweight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_reweight_write

<Commands: procedures>+≡
  module subroutine cmd_reweight_write (cmd, unit, indent)
    class(cmd_reweight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "reweight expression: [defined]"
  end subroutine cmd_reweight_write

```

Compile. Simply store the parse (sub)tree.

```

⟨Commands: cmd reweight: TBP⟩+≡
  procedure :: compile => cmd_reweight_compile

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_reweight_compile (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_reweight_compile

⟨Commands: procedures⟩+≡
  module subroutine cmd_reweight_compile (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_reweight_compile

```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

⟨Commands: cmd reweight: TBP⟩+≡
  procedure :: execute => cmd_reweight_execute

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_reweight_execute (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_reweight_execute

⟨Commands: procedures⟩+≡
  module subroutine cmd_reweight_execute (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%reweight_expr => cmd%pn_expr
  end subroutine cmd_reweight_execute

```

Alternative Simulation Setups

Together with simulation, we can re-evaluate event weights in the context of alternative setups. The `cmd_alt_setup_t` object is designed to hold these setups, which are brace-enclosed command lists. Compilation is deferred to the simulation environment where the setup expression is used.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_alt_setup_t
  private
  type(parse_node_p), dimension(:), allocatable :: setup
  contains
  ⟨Commands: cmd alt setup: TBP⟩
  end type cmd_alt_setup_t

```

Output. Print just a message that the alternative setup list has been defined.

```

⟨Commands: cmd alt setup: TBP⟩≡
  procedure :: write => cmd_alt_setup_write

```

```

<Commands: sub interfaces>+≡
    module subroutine cmd_alt_setup_write (cmd, unit, indent)
        class(cmd_alt_setup_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_alt_setup_write

<Commands: procedures>+≡
    module subroutine cmd_alt_setup_write (cmd, unit, indent)
        class(cmd_alt_setup_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,I0,A)") "alt_setup: ", size (cmd%setup), " entries"
    end subroutine cmd_alt_setup_write

```

Compile. Store the parse sub-trees in an array.

```

<Commands: cmd alt setup: TBP>+≡
    procedure :: compile => cmd_alt_setup_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_alt_setup_compile (cmd, global)
        class(cmd_alt_setup_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_alt_setup_compile

<Commands: procedures>+≡
    module subroutine cmd_alt_setup_compile (cmd, global)
        class(cmd_alt_setup_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_list, pn_setup
        integer :: i
        pn_list => parse_node_get_sub_ptr (cmd%pn, 3)
        if (associated (pn_list)) then
            allocate (cmd%setup (parse_node_get_n_sub (pn_list)))
            i = 1
            pn_setup => parse_node_get_sub_ptr (pn_list)
            do while (associated (pn_setup))
                cmd%setup(i)%ptr => pn_setup
                i = i + 1
                pn_setup => parse_node_get_next_ptr (pn_setup)
            end do
        else
            allocate (cmd%setup (0))
        end if
    end subroutine cmd_alt_setup_compile

```

Execute. Transfer the array of command lists to the global environment.

```

<Commands: cmd alt setup: TBP>+≡
    procedure :: execute => cmd_alt_setup_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_alt_setup_execute (cmd, global)
        class(cmd_alt_setup_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_alt_setup_execute

```

```

<Commands: procedures>+≡
module subroutine cmd_alt_setup_execute (cmd, global)
  class(cmd_alt_setup_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  if (allocated (global%pn%alt_setup)) deallocate (global%pn%alt_setup)
  allocate (global%pn%alt_setup (size (cmd%setup)))
  global%pn%alt_setup = cmd%setup
end subroutine cmd_alt_setup_execute

```

Integration

Integrate several processes, consecutively with identical parameters.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_integrate_t
  private
  integer :: n_proc = 0
  type(string_t), dimension(:), allocatable :: process_id
contains
  <Commands: cmd integrate: TBP>
end type cmd_integrate_t

```

Output: we know the process IDs.

```

<Commands: cmd integrate: TBP>≡
procedure :: write => cmd_integrate_write

<Commands: sub interfaces>+≡
module subroutine cmd_integrate_write (cmd, unit, indent)
  class(cmd_integrate_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
end subroutine cmd_integrate_write

<Commands: procedures>+≡
module subroutine cmd_integrate_write (cmd, unit, indent)
  class(cmd_integrate_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A)", advance="no") "integrate ("
  do i = 1, cmd%n_proc
    if (i > 1) write (u, "(A,1x)", advance="no") " ,"
    write (u, "(A)", advance="no") char (cmd%process_id(i))
  end do
  write (u, "(A)") ")"
end subroutine cmd_integrate_write

```

Compile.

```

<Commands: cmd integrate: TBP>+≡
procedure :: compile => cmd_integrate_compile

```

<Commands: sub interfaces>+≡

```
module subroutine cmd_integrate_compile (cmd, global)
  class(cmd_integrate_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_integrate_compile
```

<Commands: procedures>+≡

```
module subroutine cmd_integrate_compile (cmd, global)
  class(cmd_integrate_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_proclist, pn_proc
  integer :: i
  pn_proclist => parse_node_get_sub_ptr (cmd%pn, 2)
  cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
  call cmd%compile_options (global)
  cmd%n_proc = parse_node_get_n_sub (pn_proclist)
  allocate (cmd%process_id (cmd%n_proc))
  pn_proc => parse_node_get_sub_ptr (pn_proclist)
  do i = 1, cmd%n_proc
    cmd%process_id(i) = parse_node_get_string (pn_proc)
    call global%process_stack%init_result_vars (cmd%process_id(i))
    pn_proc => parse_node_get_next_ptr (pn_proc)
  end do
end subroutine cmd_integrate_compile
```

Command execution. Integrate the process(es) with the predefined number of passes, iterations and calls. For structure functions, cuts, weight and scale, use local definitions if present; by default, the local definitions are initialized with the global ones.

The `integrate` procedure should take its input from the currently active local environment, but produce a process record in the stack of the global environment.

Since the process acquires a snapshot of the variable list, so if the global list (or the local one) is deleted, this does no harm. This implies that later changes of the variable list do not affect the stored process.

<Commands: cmd integrate: TBP>+≡

```
procedure :: execute => cmd_integrate_execute
```

<Commands: sub interfaces>+≡

```
module subroutine cmd_integrate_execute (cmd, global)
  class(cmd_integrate_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_integrate_execute
```

<Commands: procedures>+≡

```
module subroutine cmd_integrate_execute (cmd, global)
  class(cmd_integrate_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  integer :: i
  if (debug_on) call msg_debug (D_CORE, "cmd_integrate_execute")
  do i = 1, cmd%n_proc
    if (debug_on) call msg_debug &
      (D_CORE, "cmd%process_id(i) ", cmd%process_id(i))
    call integrate_process (cmd%process_id(i), cmd%local, global)
  end do
end subroutine cmd_integrate_execute
```

```

        call global%process_stack%fill_result_vars (cmd%process_id(i))
        call global%process_stack%update_result_vars &
            (cmd%process_id(i), global%var_list)
        if (signal_is_pending ()) return
    end do
end subroutine cmd_integrate_execute

```

Observables

Declare an observable. After the declaration, it can be used to record data, and at the end one can retrieve average and error.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_observable_t
    private
    type(string_t) :: id
    contains
    ⟨Commands: cmd observable: TBP⟩
end type cmd_observable_t

```

Output. We know the ID.

```

⟨Commands: cmd observable: TBP⟩≡
    procedure :: write => cmd_observable_write

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_observable_write (cmd, unit, indent)
        class(cmd_observable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_observable_write

⟨Commands: procedures⟩+≡
    module subroutine cmd_observable_write (cmd, unit, indent)
        class(cmd_observable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,A)" "observable: ", char (cmd%id)
    end subroutine cmd_observable_write

```

Compile. Just record the observable ID.

```

⟨Commands: cmd observable: TBP⟩+≡
    procedure :: compile => cmd_observable_compile

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_observable_compile (cmd, global)
        class(cmd_observable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_observable_compile

⟨Commands: procedures⟩+≡
    module subroutine cmd_observable_compile (cmd, global)
        class(cmd_observable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global

```

```

type(parse_node_t), pointer :: pn_tag
pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
if (associated (pn_tag)) then
    cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
end if
call cmd%compile_options (global)
select case (char (parse_node_get_rule_key (pn_tag)))
case ("analysis_id")
    cmd%id = parse_node_get_string (pn_tag)
case default
    call msg_bug ("observable: name expression not implemented (yet)")
end select
end subroutine cmd_observable_compile

```

Command execution. This declares the observable and allocates it in the analysis store.

```

⟨Commands: cmd observable: TBP⟩+≡
    procedure :: execute => cmd_observable_execute

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_observable_execute (cmd, global)
        class(cmd_observable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_observable_execute

⟨Commands: procedures⟩+≡
    module subroutine cmd_observable_execute (cmd, global)
        class(cmd_observable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(graph_options_t) :: graph_options
        type(string_t) :: label, unit
        var_list => cmd%local%get_var_list_ptr ()
        label = var_list%get_sval (var_str ("obs_label"))
        unit = var_list%get_sval (var_str ("obs_unit"))
        call graph_options%init ()
        call set_graph_options (graph_options, var_list)
        call analysis_init_observable (cmd%id, label, unit, graph_options)
    end subroutine cmd_observable_execute

```

Histograms

Declare a histogram. At minimum, we have to set lower and upper bound and bin width.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_histogram_t
    private
    type(string_t) :: id
    type(parse_node_t), pointer :: pn_lower_bound => null ()
    type(parse_node_t), pointer :: pn_upper_bound => null ()
    type(parse_node_t), pointer :: pn_bin_width => null ()
contains
    ⟨Commands: cmd histogram: TBP⟩

```



```
end type cmd_histogram_t
```

Output. Just print the ID.

```
<Commands: cmd histogram: TBP>≡
  procedure :: write => cmd_histogram_write

<Commands: sub interfaces>+≡
  module subroutine cmd_histogram_write (cmd, unit, indent)
    class(cmd_histogram_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_histogram_write

<Commands: procedures>+≡
  module subroutine cmd_histogram_write (cmd, unit, indent)
    class(cmd_histogram_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,A)") "histogram: ", char (cmd%id)
  end subroutine cmd_histogram_write
```

Compile. Record the histogram ID and initialize lower, upper bound and bin width.

```
<Commands: cmd histogram: TBP>+≡
  procedure :: compile => cmd_histogram_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_histogram_compile (cmd, global)
    class(cmd_histogram_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_histogram_compile

<Commands: procedures>+≡
  module subroutine cmd_histogram_compile (cmd, global)
    class(cmd_histogram_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_tag, pn_args, pn_arg1, pn_arg2, pn_arg3
    character(*), parameter :: e_illegal_use = &
      "illegal usage of 'histogram': insufficient number of arguments"
    pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_args => parse_node_get_next_ptr (pn_tag)
    if (associated (pn_args)) then
      pn_arg1 => parse_node_get_sub_ptr (pn_args)
      if (.not. associated (pn_arg1)) call msg_fatal (e_illegal_use)
      pn_arg2 => parse_node_get_next_ptr (pn_arg1)
      if (.not. associated (pn_arg2)) call msg_fatal (e_illegal_use)
      pn_arg3 => parse_node_get_next_ptr (pn_arg2)
      cmd%pn_opt => parse_node_get_next_ptr (pn_args)
    end if
    call cmd%compile_options (global)
    select case (char (parse_node_get_rule_key (pn_tag)))
    case ("analysis_id")
      cmd%id = parse_node_get_string (pn_tag)
    case default
```

```

        call msg_bug ("histogram: name expression not implemented (yet)")
    end select
    cmd%pn_lower_bound => pn_arg1
    cmd%pn_upper_bound => pn_arg2
    cmd%pn_bin_width => pn_arg3
end subroutine cmd_histogram_compile

```

Command execution. This declares the histogram and allocates it in the analysis store.

```

<Commands: cmd histogram: TBP>+≡
    procedure :: execute => cmd_histogram_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_histogram_execute (cmd, global)
        class(cmd_histogram_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_histogram_execute

<Commands: procedures>+≡
    module subroutine cmd_histogram_execute (cmd, global)
        class(cmd_histogram_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        real(default) :: lower_bound, upper_bound, bin_width
        integer :: bin_number
        logical :: bin_width_is_used, normalize_bins
        type(string_t) :: obs_label, obs_unit
        type(graph_options_t) :: graph_options
        type(drawing_options_t) :: drawing_options

        var_list => cmd%local%get_var_list_ptr ()
        lower_bound = eval_real (cmd%pn_lower_bound, var_list)
        upper_bound = eval_real (cmd%pn_upper_bound, var_list)
        if (associated (cmd%pn_bin_width)) then
            bin_width = eval_real (cmd%pn_bin_width, var_list)
            bin_width_is_used = .true.
        else if (var_list%is_known (var_str ("n_bins"))) then
            bin_number = &
                var_list%get_ival (var_str ("n_bins"))
            bin_width_is_used = .false.
        else
            call msg_error ("Cmd '" // char (cmd%id) // &
                "' : neither bin width nor number is defined")
        end if
        normalize_bins = &
            var_list%get_lval (var_str ("?normalize_bins"))
        obs_label = &
            var_list%get_sval (var_str ("$obs_label"))
        obs_unit = &
            var_list%get_sval (var_str ("$obs_unit"))

        call graph_options%init ()
        call set_graph_options (graph_options, var_list)
        call drawing_options%init_histogram ()
        call set_drawing_options (drawing_options, var_list)
    end subroutine cmd_histogram_execute

```

```

if (bin_width_is_used) then
  call analysis_init_histogram &
    (cmd%id, lower_bound, upper_bound, bin_width, &
     normalize_bins, &
     obs_label, obs_unit, &
     graph_options, drawing_options)
else
  call analysis_init_histogram &
    (cmd%id, lower_bound, upper_bound, bin_number, &
     normalize_bins, &
     obs_label, obs_unit, &
     graph_options, drawing_options)
end if
end subroutine cmd_histogram_execute

```

Set the graph options from a variable list.

(Commands: procedures)+≡

```

subroutine set_graph_options (gro, var_list)
  type(graph_options_t), intent(inout) :: gro
  type(var_list_t), intent(in) :: var_list
  call gro%set (title = var_list%get_sval (var_str ("title")))
  call gro%set (description = var_list%get_sval (var_str ("description")))
  call gro%set (x_label = var_list%get_sval (var_str ("x_label")))
  call gro%set (y_label = var_list%get_sval (var_str ("y_label")))
  call gro%set (width_mm = var_list%get_ival (var_str ("graph_width_mm")))
  call gro%set (height_mm = var_list%get_ival (var_str ("graph_height_mm")))
  call gro%set (x_log = var_list%get_lval (var_str ("x_log")))
  call gro%set (y_log = var_list%get_lval (var_str ("y_log")))
  if (var_list%is_known (var_str ("x_min"))) &
    call gro%set (x_min = var_list%get_rval (var_str ("x_min")))
  if (var_list%is_known (var_str ("x_max"))) &
    call gro%set (x_max = var_list%get_rval (var_str ("x_max")))
  if (var_list%is_known (var_str ("y_min"))) &
    call gro%set (y_min = var_list%get_rval (var_str ("y_min")))
  if (var_list%is_known (var_str ("y_max"))) &
    call gro%set (y_max = var_list%get_rval (var_str ("y_max")))
  call gro%set (gmlcode_bg = var_list%get_sval (var_str ("gmlcode_bg")))
  call gro%set (gmlcode_fg = var_list%get_sval (var_str ("gmlcode_fg")))
end subroutine set_graph_options

```

Set the drawing options from a variable list.

(Commands: procedures)+≡

```

subroutine set_drawing_options (dro, var_list)
  type(drawing_options_t), intent(inout) :: dro
  type(var_list_t), intent(in) :: var_list
  if (var_list%is_known (var_str ("draw_histogram"))) then
    if (var_list%get_lval (var_str ("draw_histogram"))) then
      call dro%set (with_hbars = .true.)
    else
      call dro%set (with_hbars = .false., &
                    with_base = .false., fill = .false., piecewise = .false.)
    end if
  end if

```

```

end if
if (var_list%is_known (var_str ("?draw_base"))) then
  if (var_list%get_lval (var_str ("?draw_base"))) then
    call dro%set (with_base = .true.)
  else
    call dro%set (with_base = .false., fill = .false.)
  end if
end if
if (var_list%is_known (var_str ("?draw_pieewise"))) then
  if (var_list%get_lval (var_str ("?draw_pieewise"))) then
    call dro%set (pieewise = .true.)
  else
    call dro%set (pieewise = .false.)
  end if
end if
if (var_list%is_known (var_str ("?fill_curve"))) then
  if (var_list%get_lval (var_str ("?fill_curve"))) then
    call dro%set (fill = .true., with_base = .true.)
  else
    call dro%set (fill = .false.)
  end if
end if
if (var_list%is_known (var_str ("?draw_curve"))) then
  if (var_list%get_lval (var_str ("?draw_curve"))) then
    call dro%set (draw = .true.)
  else
    call dro%set (draw = .false.)
  end if
end if
if (var_list%is_known (var_str ("?draw_errors"))) then
  if (var_list%get_lval (var_str ("?draw_errors"))) then
    call dro%set (err = .true.)
  else
    call dro%set (err = .false.)
  end if
end if
if (var_list%is_known (var_str ("?draw_symbols"))) then
  if (var_list%get_lval (var_str ("?draw_symbols"))) then
    call dro%set (symbols = .true.)
  else
    call dro%set (symbols = .false.)
  end if
end if
if (var_list%is_known (var_str ("$fill_options"))) then
  call dro%set (fill_options = &
    var_list%get_sval (var_str ("$fill_options")))
end if
if (var_list%is_known (var_str ("$draw_options"))) then
  call dro%set (draw_options = &
    var_list%get_sval (var_str ("$draw_options")))
end if
if (var_list%is_known (var_str ("$err_options"))) then
  call dro%set (err_options = &
    var_list%get_sval (var_str ("$err_options")))

```

```

end if
if (var_list%is_known (var_str ("symbol"))) then
    call dro%set (symbol = &
        var_list%get_sval (var_str ("symbol")))
end if
if (var_list%is_known (var_str ("gmlcode_bg"))) then
    call dro%set (gmlcode_bg = &
        var_list%get_sval (var_str ("gmlcode_bg")))
end if
if (var_list%is_known (var_str ("gmlcode_fg"))) then
    call dro%set (gmlcode_fg = &
        var_list%get_sval (var_str ("gmlcode_fg")))
end if
end subroutine set_drawing_options

```

Plots

Declare a plot. No mandatory arguments, just options.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_plot_t
    private
    type(string_t) :: id
    contains
    ⟨Commands: cmd plot: TBP⟩
end type cmd_plot_t

```

Output. Just print the ID.

```

⟨Commands: cmd plot: TBP⟩≡
    procedure :: write => cmd_plot_write

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_plot_write (cmd, unit, indent)
        class(cmd_plot_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_plot_write

⟨Commands: procedures⟩+≡
    module subroutine cmd_plot_write (cmd, unit, indent)
        class(cmd_plot_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,A)" "plot: ", char (cmd%id)
    end subroutine cmd_plot_write

```

Compile. Record the plot ID and initialize lower, upper bound and bin width.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: compile => cmd_plot_compile

```

```

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_plot_compile (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_plot_compile

```

```

⟨Commands: procedures⟩+≡
    module subroutine cmd_plot_compile (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_tag
        pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
        cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
        call cmd%init (pn_tag, global)
    end subroutine cmd_plot_compile

```

This init routine is separated because it is reused below for graph initialization.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: init => cmd_plot_init

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_plot_init (plot, pn_tag, global)
        class(cmd_plot_t), intent(inout) :: plot
        type(parse_node_t), intent(in), pointer :: pn_tag
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_plot_init

⟨Commands: procedures⟩+≡
    module subroutine cmd_plot_init (plot, pn_tag, global)
        class(cmd_plot_t), intent(inout) :: plot
        type(parse_node_t), intent(in), pointer :: pn_tag
        type(rt_data_t), intent(inout), target :: global
        call plot%compile_options (global)
        select case (char (parse_node_get_rule_key (pn_tag)))
        case ("analysis_id")
            plot%id = parse_node_get_string (pn_tag)
        case default
            call msg_bug ("plot: name expression not implemented (yet)")
        end select
    end subroutine cmd_plot_init

```

Command execution. This declares the plot and allocates it in the analysis store.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: execute => cmd_plot_execute

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_plot_execute (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_plot_execute

⟨Commands: procedures⟩+≡
    module subroutine cmd_plot_execute (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd

```

```

type(rt_data_t), intent(inout), target :: global
type(var_list_t), pointer :: var_list
type(graph_options_t) :: graph_options
type(drawing_options_t) :: drawing_options

var_list => cmd%local%get_var_list_ptr ()
call graph_options%init ()
call set_graph_options (graph_options, var_list)
call drawing_options%init_plot ()
call set_drawing_options (drawing_options, var_list)

call analysis_init_plot (cmd%id, graph_options, drawing_options)
end subroutine cmd_plot_execute

```

Graphs

Declare a graph. The graph is defined in terms of its contents. Both the graph and its contents may carry options.

The graph object contains its own ID as well as the IDs of its elements. For the elements, we reuse the `cmd_plot_t` defined above.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_graph_t
  private
  type(string_t) :: id
  integer :: n_elements = 0
  type(cmd_plot_t), dimension(:), allocatable :: el
  type(string_t), dimension(:), allocatable :: element_id
contains
  <Commands: cmd graph: TBP>
end type cmd_graph_t

```

Output. Just print the ID.

```

<Commands: cmd graph: TBP>≡
  procedure :: write => cmd_graph_write

<Commands: sub interfaces>+≡
  module subroutine cmd_graph_write (cmd, unit, indent)
    class(cmd_graph_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_graph_write

<Commands: procedures>+≡
  module subroutine cmd_graph_write (cmd, unit, indent)
    class(cmd_graph_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,A,A,A,I0,A)" "graph: ", char (cmd%id), &
      " (", cmd%n_elements, " entries)"
  end subroutine cmd_graph_write

```

Compile. Record the graph ID and initialize lower, upper bound and bin width. For compiling the graph element syntax, we use part of the `cmd_plot_t` compiler.

Note: currently, we do not respect options, therefore just IDs on the RHS.

```

⟨Commands: cmd graph: TBP⟩+≡
    procedure :: compile => cmd_graph_compile

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_graph_compile (cmd, global)
        class(cmd_graph_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_graph_compile

⟨Commands: procedures⟩+≡
    module subroutine cmd_graph_compile (cmd, global)
        class(cmd_graph_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_term, pn_tag, pn_def, pn_app
        integer :: i

        pn_term => parse_node_get_sub_ptr (cmd%pn, 2)
        pn_tag => parse_node_get_sub_ptr (pn_term)
        cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
        call cmd%compile_options (global)
        select case (char (parse_node_get_rule_key (pn_tag)))
        case ("analysis_id")
            cmd%id = parse_node_get_string (pn_tag)
        case default
            call msg_bug ("graph: name expression not implemented (yet)")
        end select
        pn_def => parse_node_get_next_ptr (pn_term, 2)
        cmd%n_elements = parse_node_get_n_sub (pn_def)
        allocate (cmd%element_id (cmd%n_elements))
        allocate (cmd%el (cmd%n_elements))
        pn_term => parse_node_get_sub_ptr (pn_def)
        pn_tag => parse_node_get_sub_ptr (pn_term)
        cmd%el(1)%pn_opt => parse_node_get_next_ptr (pn_tag)
        call cmd%el(1)%init (pn_tag, global)
        cmd%element_id(1) = parse_node_get_string (pn_tag)
        pn_app => parse_node_get_next_ptr (pn_term)
        do i = 2, cmd%n_elements
            pn_term => parse_node_get_sub_ptr (pn_app, 2)
            pn_tag => parse_node_get_sub_ptr (pn_term)
            cmd%el(i)%pn_opt => parse_node_get_next_ptr (pn_tag)
            call cmd%el(i)%init (pn_tag, global)
            cmd%element_id(i) = parse_node_get_string (pn_tag)
            pn_app => parse_node_get_next_ptr (pn_app)
        end do

    end subroutine cmd_graph_compile

```

Command execution. This declares the graph, allocates it in the analysis store, and copies the graph elements.

For the graph, we set graph and default drawing options. For the elements, we reset individual drawing options.

This accesses internals of the contained elements of type `cmd_plot_t`, see above. We might disentangle such an interdependency when this code is rewritten using proper type extension.

```

⟨Commands: cmd graph: TBP⟩+≡
    procedure :: execute => cmd_graph_execute

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_graph_execute (cmd, global)
        class(cmd_graph_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_graph_execute

⟨Commands: procedures⟩+≡
    module subroutine cmd_graph_execute (cmd, global)
        class(cmd_graph_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(graph_options_t) :: graph_options
        type(drawing_options_t) :: drawing_options
        integer :: i, type

        var_list => cmd%local%get_var_list_ptr ()
        call graph_options%init ()
        call set_graph_options (graph_options, var_list)
        call analysis_init_graph (cmd%id, cmd%n_elements, graph_options)

        do i = 1, cmd%n_elements
            if (associated (cmd%el(i)%options)) then
                call cmd%el(i)%options%execute (cmd%el(i)%local)
            end if
            type = analysis_store_get_object_type (cmd%element_id(i))
            select case (type)
            case (AN_HISTOGRAM)
                call drawing_options%init_histogram ()
            case (AN_PLOT)
                call drawing_options%init_plot ()
            end select
            call set_drawing_options (drawing_options, var_list)
            if (associated (cmd%el(i)%options)) then
                call set_drawing_options (drawing_options, cmd%el(i)%local%var_list)
            end if
            call analysis_fill_graph (cmd%id, i, cmd%element_id(i), drawing_options)
        end do
    end subroutine cmd_graph_execute

```

Analysis

Hold the analysis ID either as a string or as an expression:

```

⟨Commands: types⟩+≡
    type :: analysis_id_t
        type(string_t) :: tag

```

```

    type(parse_node_t), pointer :: pn_sexpr => null ()
end type analysis_id_t

```

Define the analysis expression. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the analysis expression is used.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_analysis_t
    private
    type(parse_node_t), pointer :: pn_lexpr => null ()
    contains
    ⟨Commands: cmd analysis: TBP⟩
end type cmd_analysis_t

```

Output. Print just a message that analysis has been defined.

```

⟨Commands: cmd analysis: TBP⟩≡
    procedure :: write => cmd_analysis_write

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_analysis_write (cmd, unit, indent)
        class(cmd_analysis_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_analysis_write

⟨Commands: procedures⟩+≡
    module subroutine cmd_analysis_write (cmd, unit, indent)
        class(cmd_analysis_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)") "analysis: [defined]"
    end subroutine cmd_analysis_write

```

Compile. Simply store the parse (sub)tree.

```

⟨Commands: cmd analysis: TBP⟩+≡
    procedure :: compile => cmd_analysis_compile

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_analysis_compile (cmd, global)
        class(cmd_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_analysis_compile

⟨Commands: procedures⟩+≡
    module subroutine cmd_analysis_compile (cmd, global)
        class(cmd_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        cmd%pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 3)
    end subroutine cmd_analysis_compile

```

Instead of evaluating the cut expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

⟨Commands: cmd analysis: TBP⟩+≡
    procedure :: execute => cmd_analysis_execute

```

```

<Commands: sub interfaces>+≡
    module subroutine cmd_analysis_execute (cmd, global)
        class(cmd_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_analysis_execute

```

```

<Commands: procedures>+≡
    module subroutine cmd_analysis_execute (cmd, global)
        class(cmd_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        global%pn%analysis_lexpr => cmd%pn_lexpr
    end subroutine cmd_analysis_execute

```

Write histograms and plots

The data type encapsulating the command:

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_write_analysis_t
    private
    type(analysis_id_t), dimension(:), allocatable :: id
    type(string_t), dimension(:), allocatable :: tag
    contains
    <Commands: cmd write analysis: TBP>
end type cmd_write_analysis_t

```

Output. Just the keyword.

```

<Commands: cmd write analysis: TBP>≡
    procedure :: write => cmd_write_analysis_write

<Commands: sub interfaces>+≡
    module subroutine cmd_write_analysis_write (cmd, unit, indent)
        class(cmd_write_analysis_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_write_analysis_write

<Commands: procedures>+≡
    module subroutine cmd_write_analysis_write (cmd, unit, indent)
        class(cmd_write_analysis_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)" ) "write_analysis"
    end subroutine cmd_write_analysis_write

```

Compile.

```

<Commands: cmd write analysis: TBP>+≡
    procedure :: compile => cmd_write_analysis_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_write_analysis_compile (cmd, global)
        class(cmd_write_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_write_analysis_compile

```

```

<Commands: procedures>+≡
module subroutine cmd_write_analysis_compile (cmd, global)
  class(cmd_write_analysis_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_clause, pn_args, pn_id
  integer :: n, i
  pn_clause => parse_node_get_sub_ptr (cmd%pn)
  pn_args => parse_node_get_sub_ptr (pn_clause, 2)
  cmd%pn_opt => parse_node_get_next_ptr (pn_clause)
  call cmd%compile_options (global)
  if (associated (pn_args)) then
    n = parse_node_get_n_sub (pn_args)
    allocate (cmd%id (n))
    do i = 1, n
      pn_id => parse_node_get_sub_ptr (pn_args, i)
      if (char (parse_node_get_rule_key (pn_id)) == "analysis_id") then
        cmd%id(i)%tag = parse_node_get_string (pn_id)
      else
        cmd%id(i)%pn_sexpr => pn_id
      end if
    end do
  else
    allocate (cmd%id (0))
  end if
end subroutine cmd_write_analysis_compile

```

The output format for real data values:

```

<Commands: parameters>+≡
character(*), parameter, public :: &
  DEFAULT_ANALYSIS_FILENAME = "whizard_analysis.dat"
character(len=1), dimension(2), parameter, public :: &
  FORBIDDEN_ENDINGS1 = [ "o", "a" ]
character(len=2), dimension(6), parameter, public :: &
  FORBIDDEN_ENDINGS2 = [ "mp", "ps", "vg", "pg", "lo", "la" ]
character(len=3), dimension(20), parameter, public :: &
  FORBIDDEN_ENDINGS3 = [ "aux", "dvi", "evt", "evx", "f03", "f90", &
    "f95", "log", "ltp", "mod", "mpx", "olc", "olp", "pdf", "phs", &
    "sin", "sub", "tex", "vg2", "vgx" ]

```

As this contains a lot of similar code to `cmd_compile_analysis_execute` we outsource the main code to a subroutine.

```

<Commands: cmd write analysis: TBP>+≡
  procedure :: execute => cmd_write_analysis_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_write_analysis_execute (cmd, global)
    class(cmd_write_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_write_analysis_execute

<Commands: procedures>+≡
  module subroutine cmd_write_analysis_execute (cmd, global)
    class(cmd_write_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global

```

```

type(var_list_t), pointer :: var_list
var_list => cmd%local%get_var_list_ptr ()
call write_analysis_wrap (var_list, global%out_files, &
    cmd%id, tag = cmd%tag)
end subroutine cmd_write_analysis_execute

```

If the `data_file` optional argument is present, this is called from `cmd_compile_analysis_execute`, which needs the file name for further processing, and requires the default format. For the moment, parameters and macros for custom data processing are disabled.

(Commands: procedures)+≡

```

subroutine write_analysis_wrap (var_list, out_files, id, tag, data_file)
type(var_list_t), intent(inout), target :: var_list
type(file_list_t), intent(inout), target :: out_files
type(analysis_id_t), dimension(:), intent(in), target :: id
type(string_t), dimension(:), allocatable, intent(out) :: tag
type(string_t), intent(out), optional :: data_file
type(string_t) :: defaultfile, file
integer :: i
logical :: keep_open
type(string_t) :: extension
logical :: one_file
defaultfile = var_list%get_sval (var_str ("out_file"))
if (present (data_file)) then
    if (defaultfile == "" .or. defaultfile == ".") then
        defaultfile = DEFAULT_ANALYSIS_FILENAME
    else
        if (scan(".", defaultfile) > 0) then
            call split (defaultfile, extension, ".", back=.true.)
            if (any (lower_case (char(extension)) == FORBIDDEN_ENDINGS1) .or. &
                any (lower_case (char(extension)) == FORBIDDEN_ENDINGS2) .or. &
                any (lower_case (char(extension)) == FORBIDDEN_ENDINGS3)) &
                call msg_fatal ("The ending " // char(extension) // &
                    " is internal and not allowed as data file.")
            if (extension /= "") then
                if (defaultfile /= "") then
                    defaultfile = defaultfile // "." // extension
                else
                    defaultfile = "whizard_analysis." // extension
                end if
            else
                defaultfile = defaultfile // ".dat"
            endif
        else
            defaultfile = defaultfile // ".dat"
        end if
    end if
    data_file = defaultfile
end if
one_file = defaultfile /= ""
if (one_file) then
    file = defaultfile
    keep_open = file_list_is_open (out_files, file, &

```

```

        action = "write")
    if (keep_open) then
        if (present (data_file)) then
            call msg_fatal ("Compiling analysis: File '" &
                // char (data_file) &
                // "' can't be used, it is already open.")
        else
            call msg_message ("Appending analysis data to file '" &
                // char (file) // "'")
        end if
    else
        call file_list_open (out_files, file, &
            action = "write", status = "replace", position = "asis")
        call msg_message ("Writing analysis data to file '" &
            // char (file) // "'")
    end if
end if

call get_analysis_tags (tag, id, var_list)
do i = 1, size (tag)
    call file_list_write_analysis &
        (out_files, file, tag(i))
end do
if (one_file .and. .not. keep_open) then
    call file_list_close (out_files, file)
end if

contains

subroutine get_analysis_tags (analysis_tag, id, var_list)
    type(string_t), dimension(:), intent(out), allocatable :: analysis_tag
    type(analysis_id_t), dimension(:), intent(in) :: id
    type(var_list_t), intent(in), target :: var_list
    if (size (id) /= 0) then
        allocate (analysis_tag (size (id)))
        do i = 1, size (id)
            if (associated (id(i)%pn_sexpr)) then
                analysis_tag(i) = eval_string (id(i)%pn_sexpr, var_list)
            else
                analysis_tag(i) = id(i)%tag
            end if
        end do
    else
        call analysis_store_get_ids (tag)
    end if
end subroutine get_analysis_tags

end subroutine write_analysis_wrap

```

Compile analysis results

This command writes files in a form suitable for GAMELAN and executes the appropriate commands to compile them. The first part is identical to

```

cmd_write_analysis.
<Commands: types>+≡
  type, extends (command_t) :: cmd_compile_analysis_t
  private
  type(analysis_id_t), dimension(:), allocatable :: id
  type(string_t), dimension(:), allocatable :: tag
  contains
  <Commands: cmd compile analysis: TBP>
end type cmd_compile_analysis_t

```

Output. Just the keyword.

```

<Commands: cmd compile analysis: TBP>≡
  procedure :: write => cmd_compile_analysis_write

<Commands: sub interfaces>+≡
  module subroutine cmd_compile_analysis_write (cmd, unit, indent)
    class(cmd_compile_analysis_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_compile_analysis_write

<Commands: procedures>+≡
  module subroutine cmd_compile_analysis_write (cmd, unit, indent)
    class(cmd_compile_analysis_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "compile_analysis"
  end subroutine cmd_compile_analysis_write

```

Compile.

```

<Commands: cmd compile analysis: TBP>+≡
  procedure :: compile => cmd_compile_analysis_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_compile_analysis_compile (cmd, global)
    class(cmd_compile_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_compile_analysis_compile

<Commands: procedures>+≡
  module subroutine cmd_compile_analysis_compile (cmd, global)
    class(cmd_compile_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_clause, pn_args, pn_id
    integer :: n, i
    pn_clause => parse_node_get_sub_ptr (cmd%pn)
    pn_args => parse_node_get_sub_ptr (pn_clause, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_clause)
    call cmd%compile_options (global)
    if (associated (pn_args)) then
      n = parse_node_get_n_sub (pn_args)
      allocate (cmd%id (n))
      do i = 1, n
        pn_id => parse_node_get_sub_ptr (pn_args, i)

```

```

        if (char (parse_node_get_rule_key (pn_id)) == "analysis_id") then
            cmd%id(i)%tag = parse_node_get_string (pn_id)
        else
            cmd%id(i)%pn_sexpr => pn_id
        end if
    end do
else
    allocate (cmd%id (0))
end if
end subroutine cmd_compile_analysis_compile

```

First write the analysis data to file, then write a GAMELAN driver and produce MetaPost and T_EX output.

```

⟨Commands: cmd compile analysis: TBP⟩+≡
    procedure :: execute => cmd_compile_analysis_execute

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_compile_analysis_execute (cmd, global)
        class(cmd_compile_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_compile_analysis_execute

⟨Commands: procedures⟩+≡
    module subroutine cmd_compile_analysis_execute (cmd, global)
        class(cmd_compile_analysis_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(string_t) :: file, basename, extension, driver_file, &
            makefile
        integer :: u_driver, u_makefile
        logical :: has_gmlcode, only_file
        var_list => cmd%local%get_var_list_ptr ()
        call write_analysis_wrap (var_list, &
            global%out_files, cmd%id, tag = cmd%tag, &
            data_file = file)
        basename = file
        if (scan (".", basename) > 0) then
            call split (basename, extension, ".", back=.true.)
        else
            extension = ""
        end if
        driver_file = basename // ".tex"
        makefile = basename // "_ana.makefile"
        u_driver = free_unit ()
        open (unit=u_driver, file=char(driver_file), &
            action="write", status="replace")
        if (allocated (cmd%tag)) then
            call analysis_write_driver (file, cmd%tag, unit=u_driver)
            has_gmlcode = analysis_has_plots (cmd%tag)
        else
            call analysis_write_driver (file, unit=u_driver)
            has_gmlcode = analysis_has_plots ()
        end if
        close (u_driver)
        u_makefile = free_unit ()
    end subroutine cmd_compile_analysis_execute

```



```

open (unit=u_makefile, file=char(makefile), &
      action="write", status="replace")
call analysis_write_makefile (basename, u_makefile, &
      has_gmlcode, global%os_data)
close (u_makefile)
call msg_message ("Compiling analysis results display in '" &
      // char (driver_file) // "'")
call msg_message ("Providing analysis steering makefile '" &
      // char (makefile) // "'")
only_file = global%var_list%get_lval &
      (var_str ("?analysis_file_only"))
if (.not. only_file) call analysis_compile_tex &
      (basename, has_gmlcode, global%os_data)
end subroutine cmd_compile_analysis_execute

```

35.1.4 User-controlled output to data files

Open file (output)

Open a file for output.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_open_out_t
  private
  type(parse_node_t), pointer :: file_expr => null ()
  contains
  <Commands: cmd open out: TBP>
  end type cmd_open_out_t

```

Finalizer for the embedded eval tree.

```

<Commands: procedures>+≡
  subroutine cmd_open_out_final (object)
  class(cmd_open_out_t), intent(inout) :: object
  end subroutine cmd_open_out_final

```

Output (trivial here).

```

<Commands: cmd open out: TBP>≡
  procedure :: write => cmd_open_out_write

<Commands: sub interfaces>+≡
  module subroutine cmd_open_out_write (cmd, unit, indent)
  class(cmd_open_out_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  end subroutine cmd_open_out_write

<Commands: procedures>+≡
  module subroutine cmd_open_out_write (cmd, unit, indent)
  class(cmd_open_out_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A)", advance="no") "open_out: <filename>"

```

```
end subroutine cmd_open_out_write
```

Compile: create an eval tree for the filename expression.

<Commands: cmd open out: TBP>+≡

```
procedure :: compile => cmd_open_out_compile
```

<Commands: sub interfaces>+≡

```
module subroutine cmd_open_out_compile (cmd, global)
  class(cmd_open_out_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_open_out_compile
```

<Commands: procedures>+≡

```
module subroutine cmd_open_out_compile (cmd, global)
  class(cmd_open_out_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  cmd%file_expr => parse_node_get_sub_ptr (cmd%pn, 2)
  if (associated (cmd%file_expr)) then
    cmd%pn_opt => parse_node_get_next_ptr (cmd%file_expr)
  end if
  call cmd%compile_options (global)
end subroutine cmd_open_out_compile
```

Execute: append the file to the global list of open files.

<Commands: cmd open out: TBP>+≡

```
procedure :: execute => cmd_open_out_execute
```

<Commands: sub interfaces>+≡

```
module subroutine cmd_open_out_execute (cmd, global)
  class(cmd_open_out_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_open_out_execute
```

<Commands: procedures>+≡

```
module subroutine cmd_open_out_execute (cmd, global)
  class(cmd_open_out_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(eval_tree_t) :: file_expr
  type(string_t) :: file
  var_list => cmd%local%get_var_list_ptr ()
  call file_expr%init_sexpr (cmd%file_expr, var_list)
  call file_expr%evaluate ()
  if (file_expr%is_known ()) then
    file = file_expr%get_string ()
    call file_list_open (global%out_files, file, &
      action = "write", status = "replace", position = "asis")
  else
    call msg_fatal ("open_out: file name argument evaluates to unknown")
  end if
  call file_expr%final ()
end subroutine cmd_open_out_execute
```

Open file (output)

Close an output file. Except for the `execute` method, everything is analogous to the open command, so we can just inherit.

```
<Commands: types>+≡
  type, extends (cmd_open_out_t) :: cmd_close_out_t
  private
  contains
  <Commands: cmd close out: TBP>
end type cmd_close_out_t
```

Execute: remove the file from the global list of output files.

```
<Commands: cmd close out: TBP>≡
  procedure :: execute => cmd_close_out_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_close_out_execute (cmd, global)
    class(cmd_close_out_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_close_out_execute

<Commands: procedures>+≡
  module subroutine cmd_close_out_execute (cmd, global)
    class(cmd_close_out_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    type(eval_tree_t) :: file_expr
    type(string_t) :: file
    var_list => cmd%local%var_list
    call file_expr%init_sexpr (cmd%file_expr, var_list)
    call file_expr%evaluate ()
    if (file_expr%is_known ()) then
      file = file_expr%get_string ()
      call file_list_close (global%out_files, file)
    else
      call msg_fatal ("close_out: file name argument evaluates to unknown")
    end if
    call file_expr%final ()
  end subroutine cmd_close_out_execute
```

35.1.5 Print custom-formatted values

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_printf_t
  private
  type(parse_node_t), pointer :: sexpr => null ()
  type(parse_node_t), pointer :: sprintf_fun => null ()
  type(parse_node_t), pointer :: sprintf_clause => null ()
  type(parse_node_t), pointer :: sprintf => null ()
  contains
  <Commands: cmd printf: TBP>
end type cmd_printf_t
```

Finalize.

```

<Commands: cmd printf: TBP>≡
    procedure :: final => cmd_printf_final

<Commands: sub interfaces>+≡
    module subroutine cmd_printf_final (cmd)
        class(cmd_printf_t), intent(inout) :: cmd
    end subroutine cmd_printf_final

<Commands: procedures>+≡
    module subroutine cmd_printf_final (cmd)
        class(cmd_printf_t), intent(inout) :: cmd
        call parse_node_final (cmd%sexpr, recursive = .false.)
        deallocate (cmd%sexpr)
        call parse_node_final (cmd%sprintf_fun, recursive = .false.)
        deallocate (cmd%sprintf_fun)
        call parse_node_final (cmd%sprintf_clause, recursive = .false.)
        deallocate (cmd%sprintf_clause)
        call parse_node_final (cmd%sprintf, recursive = .false.)
        deallocate (cmd%sprintf)
    end subroutine cmd_printf_final

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that cuts have been defined.

```

<Commands: cmd printf: TBP>+≡
    procedure :: write => cmd_printf_write

<Commands: sub interfaces>+≡
    module subroutine cmd_printf_write (cmd, unit, indent)
        class(cmd_printf_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_printf_write

<Commands: procedures>+≡
    module subroutine cmd_printf_write (cmd, unit, indent)
        class(cmd_printf_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)") "printf:"
    end subroutine cmd_printf_write

```

Compile. We create a fake parse node (subtree) with a `sprintf` command with identical arguments which can then be handled by the corresponding evaluation procedure.

```

<Commands: cmd printf: TBP>+≡
    procedure :: compile => cmd_printf_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_printf_compile (cmd, global)
        class(cmd_printf_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_printf_compile

```

<Commands: procedures>+≡

```

module subroutine cmd_printf_compile (cmd, global)
  class(cmd_printf_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_cmd, pn_clause, pn_args, pn_format
  pn_cmd => parse_node_get_sub_ptr (cmd%pn)
  pn_clause => parse_node_get_sub_ptr (pn_cmd)
  pn_format => parse_node_get_sub_ptr (pn_clause, 2)
  pn_args => parse_node_get_next_ptr (pn_clause)
  cmd%pn_opt => parse_node_get_next_ptr (pn_cmd)
  call cmd%compile_options (global)
  allocate (cmd%sexpr)
  call parse_node_create_branch (cmd%sexpr, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("sexpr")))
  allocate (cmd%sprintf_fun)
  call parse_node_create_branch (cmd%sprintf_fun, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf_fun")))
  allocate (cmd%sprintf_clause)
  call parse_node_create_branch (cmd%sprintf_clause, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf_clause")))
  allocate (cmd%sprintf)
  call parse_node_create_key (cmd%sprintf, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf")))
  call parse_node_append_sub (cmd%sprintf_clause, cmd%sprintf)
  call parse_node_append_sub (cmd%sprintf_clause, pn_format)
  call parse_node_freeze_branch (cmd%sprintf_clause)
  call parse_node_append_sub (cmd%sprintf_fun, cmd%sprintf_clause)
  if (associated (pn_args)) then
    call parse_node_append_sub (cmd%sprintf_fun, pn_args)
  end if
  call parse_node_freeze_branch (cmd%sprintf_fun)
  call parse_node_append_sub (cmd%sexpr, cmd%sprintf_fun)
  call parse_node_freeze_branch (cmd%sexpr)
end subroutine cmd_printf_compile

```

Execute. Evaluate the string (pretending this is a `sprintf` expression) and print it.

<Commands: cmd printf: TBP>+≡

```

procedure :: execute => cmd_printf_execute

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_printf_execute (cmd, global)
  class(cmd_printf_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_printf_execute

```

<Commands: procedures>+≡

```

module subroutine cmd_printf_execute (cmd, global)
  class(cmd_printf_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(string_t) :: string, file
  type(eval_tree_t) :: sprintf_expr
  logical :: advance
  var_list => cmd%local%get_var_list_ptr ()

```

```

advance = var_list%get_lval (&
    var_str ("?out_advance"))
file = var_list%get_sval (&
    var_str ("out_file"))
call sprintf_expr%init_sexpr (cmd%sexpr, var_list)
call sprintf_expr%evaluate ()
if (sprintf_expr%is_known ()) then
    string = sprintf_expr%get_string ()
    if (len (file) == 0) then
        call msg_result (char (string))
    else
        call file_list_write (global%out_files, file, string, advance)
    end if
end if
end subroutine cmd_printf_execute

```

Record data

The expression syntax already contains a **record** keyword; this evaluates to a logical which is always true, but it has the side-effect of recording data into analysis objects. Here we define a command as an interface to this construct.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_record_t
    private
        type(parse_node_t), pointer :: pn_lexpr => null ()
    contains
        ⟨Commands: cmd record: TBP⟩
    end type cmd_record_t

```

Output. With the compile hack below, there is nothing of interest to print here.

```

⟨Commands: cmd record: TBP⟩≡
    procedure :: write => cmd_record_write

⟨Commands: sub interfaces⟩+≡
    module subroutine cmd_record_write (cmd, unit, indent)
        class(cmd_record_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_record_write

⟨Commands: procedures⟩+≡
    module subroutine cmd_record_write (cmd, unit, indent)
        class(cmd_record_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)") "record"
    end subroutine cmd_record_write

```

Compile. This is a hack which transforms the **record** command into a **record** expression, which we handle in the **expressions** module.

```

⟨Commands: cmd record: TBP⟩+≡
    procedure :: compile => cmd_record_compile

```

```

<Commands: sub interfaces>+≡
  module subroutine cmd_record_compile (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_record_compile

<Commands: procedures>+≡
  module subroutine cmd_record_compile (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_lexpr, pn_lsinglet, pn_lterm, pn_record
    call parse_node_create_branch (pn_lexpr, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lexpr")))
    call parse_node_create_branch (pn_lsinglet, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lsinglet")))
    call parse_node_append_sub (pn_lexpr, pn_lsinglet)
    call parse_node_create_branch (pn_lterm, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lterm")))
    call parse_node_append_sub (pn_lsinglet, pn_lterm)
    pn_record => parse_node_get_sub_ptr (cmd%pn)
    call parse_node_append_sub (pn_lterm, pn_record)
    cmd%pn_lexpr => pn_lexpr
  end subroutine cmd_record_compile

```

Command execution. Again, transfer this to the embedded expression and just forget the logical result.

```

<Commands: cmd record: TBP>+≡
  procedure :: execute => cmd_record_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_record_execute (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_record_execute

<Commands: procedures>+≡
  module subroutine cmd_record_execute (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    logical :: lval
    var_list => global%get_var_list_ptr ()
    lval = eval_log (cmd%pn_lexpr, var_list)
  end subroutine cmd_record_execute

```

Unstable particles

Mark a particle as unstable. For each unstable particle, we store a number of decay channels and compute their respective BRs.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_unstable_t
  private
  integer :: n_proc = 0

```

```

        type(string_t), dimension(:), allocatable :: process_id
        type(parse_node_t), pointer :: pn_prt_in => null ()
contains
    <Commands: cmd unstable: TBP>
end type cmd_unstable_t

```

Output: we know the process IDs.

```

<Commands: cmd unstable: TBP>≡
    procedure :: write => cmd_unstable_write

<Commands: sub interfaces>+≡
    module subroutine cmd_unstable_write (cmd, unit, indent)
        class(cmd_unstable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_unstable_write

<Commands: procedures>+≡
    module subroutine cmd_unstable_write (cmd, unit, indent)
        class(cmd_unstable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,1x,I0,1x,A)", advance="no") &
            "unstable:", 1, "("
        do i = 1, cmd%n_proc
            if (i > 1) write (u, "(A,1x)", advance="no") " ,"
            write (u, "(A)", advance="no") char (cmd%process_id(i))
        end do
        write (u, "(A)") ")"
    end subroutine cmd_unstable_write

```

Compile. Initiate an eval tree for the decaying particle and determine the decay channel process IDs.

```

<Commands: cmd unstable: TBP>+≡
    procedure :: compile => cmd_unstable_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_unstable_compile (cmd, global)
        class(cmd_unstable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_unstable_compile

<Commands: procedures>+≡
    module subroutine cmd_unstable_compile (cmd, global)
        class(cmd_unstable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_list, pn_proc
        integer :: i
        cmd%pn_prt_in => parse_node_get_sub_ptr (cmd%pn, 2)
        pn_list => parse_node_get_next_ptr (cmd%pn_prt_in)
        if (associated (pn_list)) then
            select case (char (parse_node_get_rule_key (pn_list)))
            case ("unstable_arg")
                cmd%n_proc = parse_node_get_n_sub (pn_list)

```



```

        cmd%pn_opt => parse_node_get_next_ptr (pn_list)
    case default
        cmd%n_proc = 0
        cmd%pn_opt => pn_list
        pn_list => null ()
    end select
end if
call cmd%compile_options (global)
if (associated (pn_list)) then
    allocate (cmd%process_id (cmd%n_proc))
    pn_proc => parse_node_get_sub_ptr (pn_list)
    do i = 1, cmd%n_proc
        cmd%process_id(i) = parse_node_get_string (pn_proc)
        call cmd%local%process_stack%init_result_vars (cmd%process_id(i))
        pn_proc => parse_node_get_next_ptr (pn_proc)
    end do
else
    allocate (cmd%process_id (0))
end if
end if
end subroutine cmd_unstable_compile

```

Command execution. Evaluate the decaying particle and mark the decays in the current model object.

<Commands: cmd unstable: TBP>+≡

```

    procedure :: execute => cmd_unstable_execute

```

<Commands: sub interfaces>+≡

```

    module subroutine cmd_unstable_execute (cmd, global)
        class(cmd_unstable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_unstable_execute

```

<Commands: procedures>+≡

```

    module subroutine cmd_unstable_execute (cmd, global)
        class(cmd_unstable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        logical :: auto_decays, auto_decays_radiative
        integer :: auto_decays_multiplicity
        logical :: isotropic_decay, diagonal_decay, polarized_decay
        integer :: decay_helicity
        type(pdg_array_t) :: pa_in
        integer :: pdg_in
        type(string_t) :: libname_cur, libname_dec
        type(string_t), dimension(:), allocatable :: auto_id, tmp_id
        integer :: n_proc_user
        integer :: i, u_tmp
        character(80) :: buffer
        var_list => cmd%local%get_var_list_ptr ()
        auto_decays = &
            var_list%get_lval (var_str ("?auto_decays"))
        if (auto_decays) then
            auto_decays_multiplicity = &
                var_list%get_ival (var_str ("auto_decays_multiplicity"))
            auto_decays_radiative = &

```

```

        var_list%get_lval (var_str ("?auto_decays_radiative"))
end if
isotropic_decay = &
    var_list%get_lval (var_str ("?isotropic_decay"))
if (isotropic_decay) then
    diagonal_decay = .false.
    polarized_decay = .false.
else
    diagonal_decay = &
        var_list%get_lval (var_str ("?diagonal_decay"))
    if (diagonal_decay) then
        polarized_decay = .false.
    else
        polarized_decay = &
            var_list%is_known (var_str ("decay_helicity"))
        if (polarized_decay) then
            decay_helicity = var_list%get_lval (var_str ("decay_helicity"))
        end if
    end if
end if
end if
pa_in = eval_pdg_array (cmd%pn_prt_in, var_list)
if (pa_in%get_length () /= 1) &
    call msg_fatal ("Unstable: decaying particle must be unique")
pdg_in = pa_in%get (1)
n_proc_user = cmd%n_proc
if (auto_decays) then
    call create_auto_decays (pdg_in, &
        auto_decays_multiplicity, auto_decays_radiative, &
        libname_dec, auto_id, cmd%local)
    allocate (tmp_id (cmd%n_proc + size (auto_id)))
    tmp_id (:cmd%n_proc) = cmd%process_id
    tmp_id (cmd%n_proc+1:) = auto_id
    call move_alloc (from = tmp_id, to = cmd%process_id)
    cmd%n_proc = size (cmd%process_id)
end if
libname_cur = cmd%local%prclib%get_name ()
do i = 1, cmd%n_proc
    if (i == n_proc_user + 1) then
        call cmd%local%update_prclib &
            (cmd%local%prclib_stack%get_library_ptr (libname_dec))
    end if
    if (.not. global%process_stack%exists (cmd%process_id(i))) then
        call var_list%set_log &
            (var_str ("?decay_rest_frame"), .false., is_known = .true.)
        call integrate_process (cmd%process_id(i), cmd%local, global)
        call global%process_stack%fill_result_vars (cmd%process_id(i))
    end if
end do
end do
call cmd%local%update_prclib &
    (cmd%local%prclib_stack%get_library_ptr (libname_cur))
if (cmd%n_proc > 0) then
    if (polarized_decay) then
        call global%modify_particle (pdg_in, stable = .false., &
            decay = cmd%process_id, &

```

```

        isotropic_decay = .false., &
        diagonal_decay = .false., &
        decay_helicity = decay_helicity, &
        polarized = .false.)
    else
        call global%modify_particle (pdg_in, stable = .false., &
            decay = cmd%process_id, &
            isotropic_decay = isotropic_decay, &
            diagonal_decay = diagonal_decay, &
            polarized = .false.)
    end if
    u_tmp = free_unit ()
    open (u_tmp, status = "scratch", action = "readwrite")
    call show_unstable (global, pdg_in, u_tmp)
    rewind (u_tmp)
    do
        read (u_tmp, "(A)", end = 1) buffer
        write (msg_buffer, "(A)" trim (buffer))
        call msg_message ()
    end do
1    continue
    close (u_tmp)
else
    call err_unstable (global, pdg_in)
end if
end subroutine cmd_unstable_execute

```

Show data for the current unstable particle. This is called both by the `unstable` and by the `show` command.

To determine decay branching ratios, we look at the decay process IDs and inspect the corresponding `integral()` result variables.

(Commands: procedures)+≡

```

subroutine show_unstable (global, pdg, u)
    type(rt_data_t), intent(in), target :: global
    integer, intent(in) :: pdg, u
    type(flavor_t) :: flv
    type(string_t), dimension(:), allocatable :: decay
    real(default), dimension(:), allocatable :: br
    real(default) :: width
    type(process_t), pointer :: process
    type(process_component_def_t), pointer :: prc_def
    type(string_t), dimension(:), allocatable :: prt_out, prt_out_str
    integer :: i, j
    logical :: opened
    call flv%init (pdg, global%model)
    call flv%get_decays (decay)
    if (.not. allocated (decay)) return
    allocate (prt_out_str (size (decay)))
    allocate (br (size (decay)))
    do i = 1, size (br)
        process => global%process_stack%get_process_ptr (decay(i))
        prc_def => process%get_component_def_ptr (1)
        call prc_def%get_prt_out (prt_out)
    end do
end subroutine show_unstable

```

```

    prt_out_str(i) = prt_out(1)
    do j = 2, size (prt_out)
        prt_out_str(i) = prt_out_str(i) // ", " // prt_out(j)
    end do
    br(i) = global%get_rval ("integral(" // decay(i) // ")")
end do
if (all (br >= 0)) then
    if (any (br > 0)) then
        width = sum (br)
        br = br / sum (br)
        write (u, "(A)") "Unstable particle " &
            // char (flv%get_name ()) &
            // ": computed branching ratios:"
        do i = 1, size (br)
            write (u, "(2x,A,':'," // FMT_14 // ",3x,A)") &
                char (decay(i)), br(i), char (prt_out_str(i))
        end do
        write (u, "(2x,'Total width ='," // FMT_14 // ", ' GeV (computed)')") width
        write (u, "(2x,'          ='," // FMT_14 // ", ' GeV (preset)')") &
            flv%get_width ()
        if (flv%decays_isotropically ()) then
            write (u, "(2x,A)") "Decay options: isotropic"
        else if (flv%decays_diagonal ()) then
            write (u, "(2x,A)") "Decay options: &
                &projection on diagonal helicity states"
        else if (flv%has_decay_helicity ()) then
            write (u, "(2x,A,1x,I0)") "Decay options: projection onto helicity =", &
                flv%get_decay_helicity ()
        else
            write (u, "(2x,A)") "Decay options: helicity treated exactly"
        end if
    else
        inquire (unit = u, opened = opened)
        if (opened .and. .not. mask_fatal_errors) close (u)
        call msg_fatal ("Unstable particle " &
            // char (flv%get_name ()) &
            // ": partial width vanishes for all decay channels")
    end if
else
    inquire (unit = u, opened = opened)
    if (opened .and. .not. mask_fatal_errors) close (u)
    call msg_fatal ("Unstable particle " &
        // char (flv%get_name ()) &
        // ": partial width is negative")
end if
end subroutine show_unstable

```

If no decays have been found, issue a non-fatal error.

```

<Commands: procedures>+≡
subroutine err_unstable (global, pdg)
    type(rt_data_t), intent(in), target :: global
    integer, intent(in) :: pdg
    type(flavor_t) :: flv
    call flv%init (pdg, global%model)

```

```

        call msg_error ("Unstable: no allowed decays found for particle " &
            // char (flv%get_name ()) // ", keeping as stable")
    end subroutine err_unstable

```

Auto decays: create process IDs and make up process configurations, using the PDG codes generated by the `ds_table` make method.

We allocate and use a self-contained process library that contains only the decay processes of the current particle. When done, we revert the global library pointer to the original library but return the name of the new one. The new library becomes part of the global library stack and can thus be referred to at any time.

```

<Commands: procedures>+≡
subroutine create_auto_decays &
    (pdg_in, mult, rad, libname_dec, process_id, global)
    integer, intent(in) :: pdg_in
    integer, intent(in) :: mult
    logical, intent(in) :: rad
    type(string_t), intent(out) :: libname_dec
    type(string_t), dimension(:), allocatable, intent(out) :: process_id
    type(rt_data_t), intent(inout) :: global
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    type(ds_table_t) :: ds_table
    type(split_constraints_t) :: constraints
    type(pdg_array_t), dimension(:), allocatable :: pa_out
    character(80) :: buffer
    character :: p_or_a
    type(string_t) :: process_string, libname_cur
    type(flavor_t) :: flv_in, flv_out
    type(string_t) :: prt_in
    type(string_t), dimension(:), allocatable :: prt_out
    type(process_configuration_t) :: prc_config
    integer :: i, j, k
    call flv_in%init (pdg_in, global%model)
    if (rad) then
        call constraints%init (2)
    else
        call constraints%init (3)
        call constraints%set (3, constrain_radiation ())
    end if
    call constraints%set (1, constrain_n_tot (mult))
    call constraints%set (2, &
        constrain_mass_sum (flv_in%get_mass (), margin = 0._default))
    call ds_table%make (global%model, pdg_in, constraints)
    prt_in = flv_in%get_name ()
    if (pdg_in > 0) then
        p_or_a = "p"
    else
        p_or_a = "a"
    end if
    if (ds_table%get_length () == 0) then
        call msg_warning ("Auto-decays: Particle " // char (prt_in) // ": " &
            // "no decays found")
    end if
end subroutine create_auto_decays

```

```

libname_dec = ""
allocate (process_id (0))
else
  call msg_message ("Creating decay process library for particle " &
    // char (prt_in))
  libname_cur = global%prclib%get_name ()
  write (buffer, "(A,A,I0)" " _d", p_or_a, abs (pdg_in)
  libname_dec = libname_cur // trim (buffer)
  lib => global%prclib_stack%get_library_ptr (libname_dec)
  if (.not. (associated (lib))) then
    allocate (lib_entry)
    call lib_entry%init (libname_dec)
    lib => lib_entry%process_library_t
    call global%add_prclib (lib_entry)
  else
    call global%update_prclib (lib)
  end if
  allocate (process_id (ds_table%get_length ()))
  do i = 1, size (process_id)
    write (buffer, "(A,'_',A,I0,'_',I0)" &
      "decay", p_or_a, abs (pdg_in), i
    process_id(i) = trim (buffer)
    process_string = process_id(i) // ": " // prt_in // " =>"
    call ds_table%get_pdg_out (i, pa_out)
    allocate (prt_out (size (pa_out)))
    do j = 1, size (pa_out)
      do k = 1, pa_out(j)%get_length ()
        call flv_out%init (pa_out(j)%get (k), global%model)
        if (k == 1) then
          prt_out(j) = flv_out%get_name ()
        else
          prt_out(j) = prt_out(j) // ":" // flv_out%get_name ()
        end if
      end do
      process_string = process_string // " " // prt_out(j)
    end do
    call msg_message (char (process_string))
    call prc_config%init (process_id(i), 1, 1, &
      global%model, global%var_list, &
      nlo_process = global%nlo_fixed_order)
    call prc_config%setup_component (1, new_prt_spec ([prt_in]), &
      new_prt_spec (prt_out), global%model, global%var_list)
    call prc_config%record (global)
    deallocate (prt_out)
    deallocate (pa_out)
  end do
  lib => global%prclib_stack%get_library_ptr (libname_cur)
  call global%update_prclib (lib)
end if
call ds_table%final ()
end subroutine create_auto_decays

```

(Stable particles

Revert the unstable declaration for a list of particles.

```
<Commands: types>+≡
    type, extends (command_t) :: cmd_stable_t
        private
            type(parse_node_p), dimension(:), allocatable :: pn_pdg
        contains
            <Commands: cmd stable: TBP>
        end type cmd_stable_t
```

Output: we know only the number of particles.

```
<Commands: cmd stable: TBP>≡
    procedure :: write => cmd_stable_write

<Commands: sub interfaces>+≡
    module subroutine cmd_stable_write (cmd, unit, indent)
        class(cmd_stable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_stable_write

<Commands: procedures>+≡
    module subroutine cmd_stable_write (cmd, unit, indent)
        class(cmd_stable_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,1x,I0)") "stable:", size (cmd%pn_pdg)
    end subroutine cmd_stable_write
```

Compile. Assign parse nodes for the particle IDs.

```
<Commands: cmd stable: TBP>+≡
    procedure :: compile => cmd_stable_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_stable_compile (cmd, global)
        class(cmd_stable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_stable_compile

<Commands: procedures>+≡
    module subroutine cmd_stable_compile (cmd, global)
        class(cmd_stable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_list, pn_prt
        integer :: n, i
        pn_list => parse_node_get_sub_ptr (cmd%pn, 2)
        cmd%pn_opt => parse_node_get_next_ptr (pn_list)
        call cmd%compile_options (global)
        n = parse_node_get_n_sub (pn_list)
        allocate (cmd%pn_pdg (n))
        pn_prt => parse_node_get_sub_ptr (pn_list)
        i = 1
        do while (associated (pn_prt))
```

```

        cmd%pn_pdg(i)%ptr => pn_prt
        pn_prt => parse_node_get_next_ptr (pn_prt)
        i = i + 1
    end do
end subroutine cmd_stable_compile

```

Execute: apply the modifications to the current model.

```

<Commands: cmd stable: TBP>+≡
    procedure :: execute => cmd_stable_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_stable_execute (cmd, global)
        class(cmd_stable_t), intent(inout) :: cmd
        type(rt_data_t), target, intent(inout) :: global
    end subroutine cmd_stable_execute

<Commands: procedures>+≡
    module subroutine cmd_stable_execute (cmd, global)
        class(cmd_stable_t), intent(inout) :: cmd
        type(rt_data_t), target, intent(inout) :: global
        type(var_list_t), pointer :: var_list
        type(pdg_array_t) :: pa
        integer :: pdg
        type(flavor_t) :: flv
        integer :: i
        var_list => cmd%local%get_var_list_ptr ()
        do i = 1, size (cmd%pn_pdg)
            pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
            if (pa%get_length () /= 1) &
                call msg_fatal ("Stable: listed particles must be unique")
            pdg = pa%get (1)
            call global%modify_particle (pdg, stable = .true., &
                isotropic_decay = .false., &
                diagonal_decay = .false., &
                polarized = .false.)
            call flv%init (pdg, cmd%local%model)
            call msg_message ("Particle " &
                // char (flv%get_name ()) &
                // " declared as stable")
        end do
    end subroutine cmd_stable_execute

```

Polarized particles

These commands mark particles as (un)polarized, to be applied in subsequent simulation passes. Since this is technically the same as the `stable` command, we take a shortcut and make this an extension, just overriding methods.

```

<Commands: types>+≡
    type, extends (cmd_stable_t) :: cmd_polarized_t
    contains
    <Commands: cmd polarized: TBP>
end type cmd_polarized_t

```



```

type, extends (cmd_stable_t) :: cmd_unpolarized_t
contains
  <Commands: cmd unpolarized: TBP>≡
end type cmd_unpolarized_t

```

Output: we know only the number of particles.

```

<Commands: cmd polarized: TBP>≡
  procedure :: write => cmd_polarized_write

<Commands: cmd unpolarized: TBP>≡
  procedure :: write => cmd_unpolarized_write

<Commands: sub interfaces>+≡
  module subroutine cmd_polarized_write (cmd, unit, indent)
    class(cmd_polarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_polarized_write
  module subroutine cmd_unpolarized_write (cmd, unit, indent)
    class(cmd_unpolarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_unpolarized_write

<Commands: procedures>+≡
  module subroutine cmd_polarized_write (cmd, unit, indent)
    class(cmd_polarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,I0)") "polarized:", size (cmd%pn_pdg)
  end subroutine cmd_polarized_write

  module subroutine cmd_unpolarized_write (cmd, unit, indent)
    class(cmd_unpolarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,I0)") "unpolarized:", size (cmd%pn_pdg)
  end subroutine cmd_unpolarized_write

```

Compile: accounted for by the base command.

Execute: apply the modifications to the current model.

```

<Commands: cmd polarized: TBP>+≡
  procedure :: execute => cmd_polarized_execute

<Commands: cmd unpolarized: TBP>+≡
  procedure :: execute => cmd_unpolarized_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_polarized_execute (cmd, global)
    class(cmd_polarized_t), intent(inout) :: cmd
    type(rt_data_t), target, intent(inout) :: global
  end subroutine cmd_polarized_execute
  module subroutine cmd_unpolarized_execute (cmd, global)
    class(cmd_unpolarized_t), intent(inout) :: cmd

```

```

        type(rt_data_t), target, intent(inout) :: global
    end subroutine cmd_unpolarized_execute

    {Commands: procedures}+≡
    module subroutine cmd_polarized_execute (cmd, global)
        class(cmd_polarized_t), intent(inout) :: cmd
        type(rt_data_t), target, intent(inout) :: global
        type(var_list_t), pointer :: var_list
        type(pdg_array_t) :: pa
        integer :: pdg
        type(flavor_t) :: flv
        integer :: i
        var_list => cmd%local%get_var_list_ptr ()
        do i = 1, size (cmd%pn_pdg)
            pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
            if (pa%get_length () /= 1) &
                call msg_fatal ("Polarized: listed particles must be unique")
            pdg = pa%get (1)
            call global%modify_particle (pdg, polarized = .true., &
                stable = .true., &
                isotropic_decay = .false., &
                diagonal_decay = .false.)
            call flv%init (pdg, cmd%local%model)
            call msg_message ("Particle " &
                // char (flv%get_name ()) &
                // " declared as polarized")
        end do
    end subroutine cmd_polarized_execute

    module subroutine cmd_unpolarized_execute (cmd, global)
        class(cmd_unpolarized_t), intent(inout) :: cmd
        type(rt_data_t), target, intent(inout) :: global
        type(var_list_t), pointer :: var_list
        type(pdg_array_t) :: pa
        integer :: pdg
        type(flavor_t) :: flv
        integer :: i
        var_list => cmd%local%get_var_list_ptr ()
        do i = 1, size (cmd%pn_pdg)
            pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
            if (pa%get_length () /= 1) &
                call msg_fatal ("Unpolarized: listed particles must be unique")
            pdg = pa%get (1)
            call global%modify_particle (pdg, polarized = .false., &
                stable = .true., &
                isotropic_decay = .false., &
                diagonal_decay = .false.)
            call flv%init (pdg, cmd%local%model)
            call msg_message ("Particle " &
                // char (flv%get_name ()) &
                // " declared as unpolarized")
        end do
    end subroutine cmd_unpolarized_execute

```

Parameters: formats for event-sample output

Specify all event formats that are to be used for output files in the subsequent simulation run. (The raw format is on by default and can be turned off here.)

```
<Commands: types>+≡
    type, extends (command_t) :: cmd_sample_format_t
        private
        type(string_t), dimension(:), allocatable :: format
    contains
        <Commands: cmd sample format: TBP>
    end type cmd_sample_format_t
```

Output: here, everything is known.

```
<Commands: cmd sample format: TBP>≡
    procedure :: write => cmd_sample_format_write

<Commands: sub interfaces>+≡
    module subroutine cmd_sample_format_write (cmd, unit, indent)
        class(cmd_sample_format_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_sample_format_write

<Commands: procedures>+≡
    module subroutine cmd_sample_format_write (cmd, unit, indent)
        class(cmd_sample_format_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)", advance="no") "sample_format = "
        do i = 1, size (cmd%format)
            if (i > 1) write (u, "(A,1x)", advance="no") " ,"
            write (u, "(A)", advance="no") char (cmd%format(i))
        end do
        write (u, "(A)")
    end subroutine cmd_sample_format_write
```

Compile. Initialize evaluation trees.

```
<Commands: cmd sample format: TBP>+≡
    procedure :: compile => cmd_sample_format_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_sample_format_compile (cmd, global)
        class(cmd_sample_format_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_sample_format_compile

<Commands: procedures>+≡
    module subroutine cmd_sample_format_compile (cmd, global)
        class(cmd_sample_format_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_arg
        type(parse_node_t), pointer :: pn_format
        integer :: i, n_format
        pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)
```

```

if (associated (pn_arg)) then
  n_format = parse_node_get_n_sub (pn_arg)
  allocate (cmd%format (n_format))
  pn_format => parse_node_get_sub_ptr (pn_arg)
  i = 0
  do while (associated (pn_format))
    i = i + 1
    cmd%format(i) = parse_node_get_string (pn_format)
    pn_format => parse_node_get_next_ptr (pn_format)
  end do
else
  allocate (cmd%format (0))
end if
end subroutine cmd_sample_format_compile

```

Execute. Transfer the list of format specifications to the corresponding array in the runtime data set.

```

<Commands: cmd sample format: TBP>+≡
  procedure :: execute => cmd_sample_format_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_sample_format_execute (cmd, global)
    class(cmd_sample_format_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_sample_format_execute

<Commands: procedures>+≡
  module subroutine cmd_sample_format_execute (cmd, global)
    class(cmd_sample_format_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    if (allocated (global%sample_fmt)) deallocate (global%sample_fmt)
    allocate (global%sample_fmt (size (cmd%format)), source = cmd%format)
  end subroutine cmd_sample_format_execute

```

The simulate command

This is the actual SINDARIN command.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_simulate_t
    ! not private anymore as required by the whizard-c-interface
    integer :: n_proc = 0
    type(string_t), dimension(:), allocatable :: process_id
  contains
    <Commands: cmd simulate: TBP>
  end type cmd_simulate_t

```

Output: we know the process IDs.

```

<Commands: cmd simulate: TBP>≡
  procedure :: write => cmd_simulate_write

```

```

<Commands: sub interfaces>+≡
    module subroutine cmd_simulate_write (cmd, unit, indent)
        class(cmd_simulate_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_simulate_write

<Commands: procedures>+≡
    module subroutine cmd_simulate_write (cmd, unit, indent)
        class(cmd_simulate_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)", advance="no") "simulate ("
        do i = 1, cmd%n_proc
            if (i > 1) write (u, "(A,1x)", advance="no") ", "
            write (u, "(A)", advance="no") char (cmd%process_id(i))
        end do
        write (u, "(A)") ")"
    end subroutine cmd_simulate_write

```

Compile. In contrast to WHIZARD 1 the confusing option to give the number of unweighted events for weighted events as if unweighting were to take place has been abandoned. (We both use `n_events` for weighted and unweighted events, the variable `n_calls` from WHIZARD 1 has been discarded.

```

<Commands: cmd simulate: TBP>+≡
    procedure :: compile => cmd_simulate_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_simulate_compile (cmd, global)
        class(cmd_simulate_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_simulate_compile

<Commands: procedures>+≡
    module subroutine cmd_simulate_compile (cmd, global)
        class(cmd_simulate_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_proclist, pn_proc
        integer :: i
        pn_proclist => parse_node_get_sub_ptr (cmd%pn, 2)
        cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
        call cmd%compile_options (global)
        cmd%n_proc = parse_node_get_n_sub (pn_proclist)
        allocate (cmd%process_id (cmd%n_proc))
        pn_proc => parse_node_get_sub_ptr (pn_proclist)
        do i = 1, cmd%n_proc
            cmd%process_id(i) = parse_node_get_string (pn_proc)
            call global%process_stack%init_result_vars (cmd%process_id(i))
            pn_proc => parse_node_get_next_ptr (pn_proc)
        end do
    end subroutine cmd_simulate_compile

```

Execute command: Simulate events. This is done via a `simulation_t` object and its associated methods.

Signal handling: the `generate` method may exit abnormally if there is a pending signal. The current logic ensures that the `es_array` output channels are closed before the `execute` routine returns. The program will terminate then in `command_list_execute`.

```

<Commands: cmd simulate: TBP>+≡
    procedure :: execute => cmd_simulate_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_simulate_execute (cmd, global)
        class(cmd_simulate_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_simulate_execute

<Commands: procedures>+≡
    module subroutine cmd_simulate_execute (cmd, global)
        class(cmd_simulate_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(rt_data_t), dimension(:), allocatable, target :: alt_env
        integer :: n_events
        type(simulation_t), target :: sim
        type(event_stream_array_t) :: es_array
        integer :: i, checkpoint, callback
        var_list => cmd%local%var_list
        if (cmd%local%nlo_fixed_order) then
            call check_nlo_options (cmd%local)
        end if
        if (allocated (cmd%local%pn%alt_setup)) then
            allocate (alt_env (size (cmd%local%pn%alt_setup)))
            do i = 1, size (alt_env)
                call build_alt_setup (alt_env(i), cmd%local, &
                    cmd%local%pn%alt_setup(i)%ptr)
            end do
            call sim%init (cmd%process_id, .true., .true., cmd%local, global, &
                alt_env)
        else
            call sim%init (cmd%process_id, .true., .true., cmd%local, global)
        end if
        if (signal_is_pending ()) return
        if (sim%is_valid ()) then
            call sim%init_process_selector ()
            call sim%setup_openmp ()
            call sim%compute_n_events (n_events)
            call sim%set_n_events_requested (n_events)
            call sim%activate_extra_logging ()
            call sim%prepare_event_streams (es_array)
            if (es_array%is_valid ()) then
                call sim%generate (es_array)
            else
                call sim%generate ()
            end if
            call es_array%final ()
            if (allocated (alt_env)) then
                do i = 1, size (alt_env)
                    call alt_env(i)%local_final ()
                end do
            end if
        end if
    end subroutine cmd_simulate_execute

```

```

        end do
      end if
    end if
    call sim%final ()
  end subroutine cmd_simulate_execute

```

Build an alternative setup: the parse tree is stored in the global environment. We create a temporary command list to compile and execute this; the result is an alternative local environment `alt_env` which we can hand over to the `simulate` command.

```

<Commands: procedures>+=
  recursive subroutine build_alt_setup (alt_env, global, pn)
    type(rt_data_t), intent(inout), target :: alt_env
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), intent(in), target :: pn
    type(command_list_t), allocatable :: alt_options
    allocate (alt_options)
    call alt_env%local_init (global)
    call alt_env%activate ()
    call alt_options%compile (pn, alt_env)
    call alt_options%execute (alt_env)
    call alt_env%deactivate (global, keep_local = .true.)
    call alt_options%final ()
  end subroutine build_alt_setup

```

The rescan command

This is the actual SINDARIN command.

```

<Commands: types>+=
  type, extends (command_t) :: cmd_rescan_t
    ! private
    type(parse_node_t), pointer :: pn_filename => null ()
    integer :: n_proc = 0
    type(string_t), dimension(:), allocatable :: process_id
  contains
    <Commands: cmd rescan: TBP>
  end type cmd_rescan_t

```

Output: we know the process IDs.

```

<Commands: cmd rescan: TBP>=
  procedure :: write => cmd_rescan_write

<Commands: sub interfaces>+=
  module subroutine cmd_rescan_write (cmd, unit, indent)
    class(cmd_rescan_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_rescan_write

<Commands: procedures>+=
  module subroutine cmd_rescan_write (cmd, unit, indent)
    class(cmd_rescan_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent

```

```

integer :: u, i
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A)", advance="no") "rescan ("
do i = 1, cmd%n_proc
    if (i > 1) write (u, "(A,1x)", advance="no") ", "
    write (u, "(A)", advance="no") char (cmd%process_id(i))
end do
write (u, "(A)") ")"
end subroutine cmd_rescan_write

```

Compile. The command takes a suffix argument, namely the file name of requested event file.

<Commands: cmd rescan: TBP>+≡

```
procedure :: compile => cmd_rescan_compile
```

<Commands: sub interfaces>+≡

```

module subroutine cmd_rescan_compile (cmd, global)
    class(cmd_rescan_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_rescan_compile

```

<Commands: procedures>+≡

```

module subroutine cmd_rescan_compile (cmd, global)
    class(cmd_rescan_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_filename, pn_proclist, pn_proc
    integer :: i
    pn_filename => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_proclist => parse_node_get_next_ptr (pn_filename)
    cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
    call cmd%compile_options (global)
    cmd%pn_filename => pn_filename
    cmd%n_proc = parse_node_get_n_sub (pn_proclist)
    allocate (cmd%process_id (cmd%n_proc))
    pn_proc => parse_node_get_sub_ptr (pn_proclist)
    do i = 1, cmd%n_proc
        cmd%process_id(i) = parse_node_get_string (pn_proc)
        pn_proc => parse_node_get_next_ptr (pn_proc)
    end do
end subroutine cmd_rescan_compile

```

Execute command: Rescan events. This is done via a `simulation_t` object and its associated methods.

<Commands: cmd rescan: TBP>+≡

```
procedure :: execute => cmd_rescan_execute
```

<Commands: sub interfaces>+≡

```

module subroutine cmd_rescan_execute (cmd, global)
    class(cmd_rescan_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_rescan_execute

```


<Commands: procedures>+≡

```

module subroutine cmd_rescan_execute (cmd, global)
  class(cmd_rescan_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(rt_data_t), dimension(:), allocatable, target :: alt_env
  type(string_t) :: sample, sample_suffix
  logical :: exist, write_raw, update_event, update_sqme
  type(simulation_t), target :: sim
  type(event_sample_data_t) :: input_data, data
  type(string_t) :: input_sample
  integer :: n_fmt
  type(string_t), dimension(:), allocatable :: sample_fmt
  type(string_t) :: input_format, input_ext, input_file
  type(string_t) :: lhef_extension, extension_hepmc, extension_lcio
  type(event_stream_array_t) :: es_array
  integer :: i, n_events
<Commands: cmd rescan execute: extra variables>
  var_list => cmd%local%var_list
  if (allocated (cmd%local%pn%alt_setup)) then
    allocate (alt_env (size (cmd%local%pn%alt_setup)))
    do i = 1, size (alt_env)
      call build_alt_setup (alt_env(i), cmd%local, &
        cmd%local%pn%alt_setup(i)%ptr)
    end do
    call sim%init (cmd%process_id, .false., .false., cmd%local, global, &
      alt_env)
  else
    call sim%init (cmd%process_id, .false., .false., cmd%local, global)
  end if
  call sim%compute_n_events (n_events)
  input_sample = eval_string (cmd%pn_filename, var_list)
  input_format = var_list%get_sval (&
    var_str ("$_rescan_input_format"))
  sample_suffix = ""
<Commands: cmd rescan execute: extra init>
  sample = var_list%get_sval (var_str ("$_sample"))
  if (sample == "") then
    sample = sim%get_default_sample_name () // sample_suffix
  else
    sample = var_list%get_sval (var_str ("$_sample")) // sample_suffix
  end if
  write_raw = var_list%get_lval (var_str ("?write_raw"))
  if (allocated (cmd%local%sample_fmt)) then
    n_fmt = size (cmd%local%sample_fmt)
  else
    n_fmt = 0
  end if
  if (write_raw) then
    if (sample == input_sample) then
      call msg_error ("Rescan: ?write_raw = true: " &
        // "suppressing raw event output (filename clashes with input)")
      allocate (sample_fmt (n_fmt))
      if (n_fmt > 0) sample_fmt = cmd%local%sample_fmt
    end if
  end if

```

```

else
    allocate (sample_fmt (n_fmt + 1))
    if (n_fmt > 0) sample_fmt(:n_fmt) = cmd%local%sample_fmt
    sample_fmt(n_fmt+1) = var_str ("raw")
end if
else
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = cmd%local%sample_fmt
end if
update_event = &
    var_list%get_lval (var_str ("?update_event"))
update_sqme = &
    var_list%get_lval (var_str ("?update_sqme"))
if (update_event .or. update_sqme) then
    call msg_message ("Recalculating observables")
    if (update_sqme) then
        call msg_message ("Recalculating squared matrix elements")
    end if
end if
lhef_extension = &
    var_list%get_sval (var_str ("$lhef_extension"))
extension_hepmc = &
    var_list%get_sval (var_str ("$extension_hepmc"))
extension_lcio = &
    var_list%get_sval (var_str ("$extension_lcio"))
select case (input_format)
case ("raw"); input_ext = "evx"
    call cmd%local%set_log &
        (var_str ("?recover_beams"), .false., is_known=.true.)
case ("lhef"); input_ext = lhef_extension
case ("hepmc"); input_ext = extension_hepmc
case ("lcio"); input_ext = extension_lcio
case default
    call msg_fatal ("rescan: input sample format '" // char (input_format) &
        // "' not supported")
end select
input_file = input_sample // "." // input_ext
inquire (file = char (input_file), exist = exist)
if (exist) then
    input_data = sim%get_data (alt = .false.)
    input_data%n_evt = n_events
    data = sim%get_data ()
    data%n_evt = n_events
    input_data%md5sum_cfg = ""
    call es_array%init (sample, &
        sample_fmt, cmd%local, data, &
        input = input_format, input_sample = input_sample, &
        input_data = input_data, &
        allow_switch = .false.)
    call sim%rescan (n_events, es_array, global = cmd%local)
    call es_array%final ()
else
    call msg_fatal ("Rescan: event file '" &
        // char (input_file) // "' not found")

```

```

end if
if (allocated (alt_env)) then
  do i = 1, size (alt_env)
    call alt_env(i)%local_final ()
  end do
end if
call sim%final ()
end subroutine cmd_rescan_execute

```

MPI: Append rank id to sample name.

<Commands: cmd rescan execute: extra variables>≡

<MPI: Commands: cmd rescan execute: extra variables>≡

```

logical :: mpi_logging
integer :: rank, n_size

```

<Commands: cmd rescan execute: extra init>≡

<MPI: Commands: cmd rescan execute: extra init>≡

```

call mpi_get_comm_id (n_size, rank)
if (n_size > 1) then
  sample_suffix = var_str ("-") // str (rank)
end if
mpi_logging = (("vamp2" == char (var_list%get_sval (var_str ("integration_method")))) &
  & .and. (n_size > 1)) &
  & .or. var_list%get_lval (var_str ("mpi_logging")))
call mpi_set_logging (mpi_logging)

```

Parameters: number of iterations

Specify number of iterations and number of calls for one integration pass.

<Commands: types>+≡

```

type, extends (command_t) :: cmd_iterations_t
  private
  integer :: n_pass = 0
  type(parse_node_p), dimension(:), allocatable :: pn_expr_n_it
  type(parse_node_p), dimension(:), allocatable :: pn_expr_n_calls
  type(parse_node_p), dimension(:), allocatable :: pn_sexpr_adapt
contains
  <Commands: cmd iterations: TBP>
end type cmd_iterations_t

```

Output. Display the number of passes, which is known after compilation.

<Commands: cmd iterations: TBP>≡

```

procedure :: write => cmd_iterations_write

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_iterations_write (cmd, unit, indent)
  class(cmd_iterations_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
end subroutine cmd_iterations_write

```

<Commands: procedures>+≡

```

module subroutine cmd_iterations_write (cmd, unit, indent)
  class(cmd_iterations_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  select case (cmd%n_pass)
  case (0)
    write (u, "(1x,A)") "iterations: [empty]"
  case (1)
    write (u, "(1x,A,I0,A)") "iterations: ", cmd%n_pass, " pass"
  case default
    write (u, "(1x,A,I0,A)") "iterations: ", cmd%n_pass, " passes"
  end select
end subroutine cmd_iterations_write

```

Compile. Initialize evaluation trees.

<Commands: cmd iterations: TBP>+≡

```

procedure :: compile => cmd_iterations_compile

```

<Commands: sub interfaces>+≡

```

module subroutine cmd_iterations_compile (cmd, global)
  class(cmd_iterations_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
end subroutine cmd_iterations_compile

```

<Commands: procedures>+≡

```

module subroutine cmd_iterations_compile (cmd, global)
  class(cmd_iterations_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_arg, pn_n_it, pn_n_calls, pn_adapt
  type(parse_node_t), pointer :: pn_it_spec, pn_calls_spec, pn_adapt_spec
  integer :: i
  pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)
  if (associated (pn_arg)) then
    cmd%n_pass = parse_node_get_n_sub (pn_arg)
    allocate (cmd%pn_expr_n_it (cmd%n_pass))
    allocate (cmd%pn_expr_n_calls (cmd%n_pass))
    allocate (cmd%pn_sexpr_adapt (cmd%n_pass))
    pn_it_spec => parse_node_get_sub_ptr (pn_arg)
    i = 1
    do while (associated (pn_it_spec))
      pn_n_it => parse_node_get_sub_ptr (pn_it_spec)
      pn_calls_spec => parse_node_get_next_ptr (pn_n_it)
      pn_n_calls => parse_node_get_sub_ptr (pn_calls_spec, 2)
      pn_adapt_spec => parse_node_get_next_ptr (pn_calls_spec)
      if (associated (pn_adapt_spec)) then
        pn_adapt => parse_node_get_sub_ptr (pn_adapt_spec, 2)
      else
        pn_adapt => null ()
      end if
      cmd%pn_expr_n_it(i)%ptr => pn_n_it
      cmd%pn_expr_n_calls(i)%ptr => pn_n_calls
      cmd%pn_sexpr_adapt(i)%ptr => pn_adapt
    end do
  end if
end subroutine cmd_iterations_compile

```

```

        i = i + 1
        pn_it_spec => parse_node_get_next_ptr (pn_it_spec)
    end do
else
    allocate (cmd%pn_expr_n_it (0))
    allocate (cmd%pn_expr_n_calls (0))
end if
end subroutine cmd_iterations_compile

```

Execute. Evaluate the trees and transfer the results to the iteration list in the runtime data set.

<Commands: cmd iterations: TBP>+≡

```

    procedure :: execute => cmd_iterations_execute

```

<Commands: sub interfaces>+≡

```

    module subroutine cmd_iterations_execute (cmd, global)
        class(cmd_iterations_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_iterations_execute

```

<Commands: procedures>+≡

```

    module subroutine cmd_iterations_execute (cmd, global)
        class(cmd_iterations_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        integer, dimension(cmd%n_pass) :: n_it, n_calls
        logical, dimension(cmd%n_pass) :: custom_adapt
        type(string_t), dimension(cmd%n_pass) :: adapt_code
        integer :: i
        var_list => global%get_var_list_ptr ()
        do i = 1, cmd%n_pass
            n_it(i) = eval_int (cmd%pn_expr_n_it(i)%ptr, var_list)
            n_calls(i) = &
                eval_int (cmd%pn_expr_n_calls(i)%ptr, var_list)
            if (associated (cmd%pn_sexpr_adapt(i)%ptr)) then
                adapt_code(i) = &
                    eval_string (cmd%pn_sexpr_adapt(i)%ptr, &
                        var_list, is_known = custom_adapt(i))
            else
                custom_adapt(i) = .false.
            end if
        end do
        call global%it_list%init (n_it, n_calls, custom_adapt, adapt_code)
    end subroutine cmd_iterations_execute

```

Range expressions

We need a special type for storing and evaluating range expressions.

<Commands: parameters>+≡

```

    integer, parameter :: STEP_NONE = 0
    integer, parameter :: STEP_ADD = 1
    integer, parameter :: STEP_SUB = 2
    integer, parameter :: STEP_MUL = 3

```

```

integer, parameter :: STEP_DIV = 4
integer, parameter :: STEP_COMP_ADD = 11
integer, parameter :: STEP_COMP_MUL = 13

```

There is an abstract base type and two implementations: scan over integers and scan over reals.

```

⟨Commands: types⟩+=
  type, abstract :: range_t
    type(parse_node_t), pointer :: pn_expr => null ()
    type(parse_node_t), pointer :: pn_term => null ()
    type(parse_node_t), pointer :: pn_factor => null ()
    type(parse_node_t), pointer :: pn_value => null ()
    type(parse_node_t), pointer :: pn_literal => null ()
    type(parse_node_t), pointer :: pn_beg => null ()
    type(parse_node_t), pointer :: pn_end => null ()
    type(parse_node_t), pointer :: pn_step => null ()
    type(eval_tree_t) :: expr_beg
    type(eval_tree_t) :: expr_end
    type(eval_tree_t) :: expr_step
    integer :: step_mode = 0
    integer :: n_step = 0
  contains
    ⟨Commands: range: TBP⟩
  end type range_t

```

These are the implementations:

```

⟨Commands: types⟩+=
  type, extends (range_t) :: range_int_t
    integer :: i_beg = 0
    integer :: i_end = 0
    integer :: i_step = 0
  contains
    ⟨Commands: range int: TBP⟩
  end type range_int_t

  type, extends (range_t) :: range_real_t
    real(default) :: r_beg = 0
    real(default) :: r_end = 0
    real(default) :: r_step = 0
    real(default) :: lr_beg = 0
    real(default) :: lr_end = 0
    real(default) :: lr_step = 0
  contains
    ⟨Commands: range real: TBP⟩
  end type range_real_t

```

Finalize the allocated dummy node. The other nodes are just pointers.

```

⟨Commands: range: TBP⟩=
  procedure :: final => range_final

⟨Commands: sub interfaces⟩+=
  module subroutine range_final (object)
    class(range_t), intent(inout) :: object
  end subroutine range_final

```

```

<Commands: procedures>+≡
module subroutine range_final (object)
  class(range_t), intent(inout) :: object
  if (associated (object%pn_expr)) then
    call parse_node_final (object%pn_expr, recursive = .false.)
    call parse_node_final (object%pn_term, recursive = .false.)
    call parse_node_final (object%pn_factor, recursive = .false.)
    call parse_node_final (object%pn_value, recursive = .false.)
    call parse_node_final (object%pn_literal, recursive = .false.)
    deallocate (object%pn_expr)
    deallocate (object%pn_term)
    deallocate (object%pn_factor)
    deallocate (object%pn_value)
    deallocate (object%pn_literal)
  end if
end subroutine range_final

```

Output.

```

<Commands: range: TBP>+≡
  procedure (range_write), deferred :: write
  procedure :: base_write => range_write

<Commands: range int: TBP>≡
  procedure :: write => range_int_write

<Commands: range real: TBP>≡
  procedure :: write => range_real_write

<Commands: sub interfaces>+≡
  module subroutine range_write (object, unit)
    class(range_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine range_write
  module subroutine range_int_write (object, unit)
    class(range_int_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine range_int_write
  module subroutine range_real_write (object, unit)
    class(range_real_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine range_real_write

<Commands: procedures>+≡
module subroutine range_write (object, unit)
  class(range_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Range specification:"
  if (associated (object%pn_expr)) then
    write (u, "(1x,A)") "Dummy value:"
    call parse_node_write_rec (object%pn_expr, u)
  end if
  if (associated (object%pn_beg)) then
    write (u, "(1x,A)") "Initial value:"
    call parse_node_write_rec (object%pn_beg, u)
  end if
end subroutine range_write

```

```

call object%expr_beg%write (u)
if (associated (object%pn_end)) then
  write (u, "(1x,A)") "Final value:"
  call parse_node_write_rec (object%pn_end, u)
  call object%expr_end%write (u)
  if (associated (object%pn_step)) then
    write (u, "(1x,A)") "Step value:"
    call parse_node_write_rec (object%pn_step, u)
    select case (object%step_mode)
      case (STEP_ADD); write (u, "(1x,A)") "Step mode: +"
      case (STEP_SUB); write (u, "(1x,A)") "Step mode: -"
      case (STEP_MUL); write (u, "(1x,A)") "Step mode: *"
      case (STEP_DIV); write (u, "(1x,A)") "Step mode: /"
      case (STEP_COMP_ADD); write (u, "(1x,A)") "Division mode: +"
      case (STEP_COMP_MUL); write (u, "(1x,A)") "Division mode: *"
    end select
  end if
end if
else
  write (u, "(1x,A)") "Expressions: [undefined]"
end if
end subroutine range_write

module subroutine range_int_write (object, unit)
  class(range_int_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  call object%base_write (unit)
  write (u, "(1x,A)") "Range parameters:"
  write (u, "(3x,A,I0)") "i_beg = ", object%i_beg
  write (u, "(3x,A,I0)") "i_end = ", object%i_end
  write (u, "(3x,A,I0)") "i_step = ", object%i_step
  write (u, "(3x,A,I0)") "n_step = ", object%n_step
end subroutine range_int_write

module subroutine range_real_write (object, unit)
  class(range_real_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  call object%base_write (unit)
  write (u, "(1x,A)") "Range parameters:"
  write (u, "(3x,A," // FMT_19 // ")") "r_beg = ", object%r_beg
  write (u, "(3x,A," // FMT_19 // ")") "r_end = ", object%r_end
  write (u, "(3x,A," // FMT_19 // ")") "r_step = ", object%r_end
  write (u, "(3x,A,I0)") "n_step = ", object%n_step
end subroutine range_real_write

```

Initialize, given a range expression parse node. This is common to the implementations.

```

⟨Commands: range: TBP⟩+≡
  procedure :: init => range_init

```


<Commands: sub interfaces>+≡

```

module subroutine range_init (range, pn)
  class(range_t), intent(out) :: range
  type(parse_node_t), intent(in), target :: pn
end subroutine range_init

```

<Commands: procedures>+≡

```

module subroutine range_init (range, pn)
  class(range_t), intent(out) :: range
  type(parse_node_t), intent(in), target :: pn
  type(parse_node_t), pointer :: pn_spec, pn_end, pn_step_spec, pn_op
  select case (char (parse_node_get_rule_key (pn)))
  case ("expr")
  case ("range_expr")
    range%pn_beg => parse_node_get_sub_ptr (pn)
    pn_spec => parse_node_get_next_ptr (range%pn_beg)
    if (associated (pn_spec)) then
      pn_end => parse_node_get_sub_ptr (pn_spec, 2)
      range%pn_end => pn_end
      pn_step_spec => parse_node_get_next_ptr (pn_end)
      if (associated (pn_step_spec)) then
        pn_op => parse_node_get_sub_ptr (pn_step_spec)
        range%pn_step => parse_node_get_next_ptr (pn_op)
        select case (char (parse_node_get_rule_key (pn_op)))
        case ("/+"); range%step_mode = STEP_ADD
        case ("/-"); range%step_mode = STEP_SUB
        case ("/*"); range%step_mode = STEP_MUL
        case ("//"); range%step_mode = STEP_DIV
        case ("/+"); range%step_mode = STEP_COMP_ADD
        case ("/*"); range%step_mode = STEP_COMP_MUL
        case default
          call range%write ()
          call msg_bug ("Range: step mode not implemented")
        end select
      else
        range%step_mode = STEP_ADD
      end if
    else
      range%step_mode = STEP_NONE
    end if
    call range%create_value_node ()
  case default
    call msg_bug ("range expression: node type '" &
      // char (parse_node_get_rule_key (pn)) &
      // "' not implemented")
  end select
end subroutine range_init

```

This method manually creates a parse node (actually, a cascade of parse nodes) that hold a constant value as a literal. The idea is that this node is inserted as the right-hand side of a fake variable assignment, which is prepended to each scan iteration. Before the variable assignment is compiled and executed, we can manually reset the value of the literal and thus pretend that the loop variable is assigned this value.

```

{Commands: range: TBP}+≡
    procedure :: create_value_node => range_create_value_node

{Commands: sub interfaces}+≡
    module subroutine range_create_value_node (range)
        class(range_t), intent(inout) :: range
    end subroutine range_create_value_node

{Commands: procedures}+≡
    module subroutine range_create_value_node (range)
        class(range_t), intent(inout) :: range
        allocate (range%pn_literal)
        allocate (range%pn_value)
        select type (range)
        type is (range_int_t)
            call parse_node_create_value (range%pn_literal, &
                syntax_get_rule_ptr (syntax_cmd_list, var_str ("integer_literal")), &
                ival = 0)
            call parse_node_create_branch (range%pn_value, &
                syntax_get_rule_ptr (syntax_cmd_list, var_str ("integer_value")))
        type is (range_real_t)
            call parse_node_create_value (range%pn_literal, &
                syntax_get_rule_ptr (syntax_cmd_list, var_str ("real_literal")), &
                rval = 0._default)
            call parse_node_create_branch (range%pn_value, &
                syntax_get_rule_ptr (syntax_cmd_list, var_str ("real_value")))
        class default
            call msg_bug ("range: create value node: type not implemented")
        end select
        call parse_node_append_sub (range%pn_value, range%pn_literal)
        call parse_node_freeze_branch (range%pn_value)
        allocate (range%pn_factor)
        call parse_node_create_branch (range%pn_factor, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("factor")))
        call parse_node_append_sub (range%pn_factor, range%pn_value)
        call parse_node_freeze_branch (range%pn_factor)
        allocate (range%pn_term)
        call parse_node_create_branch (range%pn_term, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("term")))
        call parse_node_append_sub (range%pn_term, range%pn_factor)
        call parse_node_freeze_branch (range%pn_term)
        allocate (range%pn_expr)
        call parse_node_create_branch (range%pn_expr, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("expr")))
        call parse_node_append_sub (range%pn_expr, range%pn_term)
        call parse_node_freeze_branch (range%pn_expr)
    end subroutine range_create_value_node

```

Compile, given an environment.

```

{Commands: range: TBP}+≡
    procedure :: compile => range_compile

{Commands: sub interfaces}+≡
    module subroutine range_compile (range, global)
        class(range_t), intent(inout) :: range

```

```

        type(rt_data_t), intent(in), target :: global
    end subroutine range_compile

<Commands: procedures>+≡
    module subroutine range_compile (range, global)
        class(range_t), intent(inout) :: range
        type(rt_data_t), intent(in), target :: global
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        if (associated (range%pn_beg)) then
            call range%expr_beg%init_expr (range%pn_beg, var_list)
            if (associated (range%pn_end)) then
                call range%expr_end%init_expr (range%pn_end, var_list)
                if (associated (range%pn_step)) then
                    call range%expr_step%init_expr (range%pn_step, var_list)
                end if
            end if
        end if
    end if
end subroutine range_compile

```

Evaluate: compute the actual bounds and parameters that determine the values that we can iterate.

This is implementation-specific.

```

<Commands: range: TBP>+≡
    procedure (range_evaluate), deferred :: evaluate

<Commands: interfaces>+≡
    abstract interface
        subroutine range_evaluate (range)
            import
            class(range_t), intent(inout) :: range
        end subroutine range_evaluate
    end interface

```

The version for an integer variable. If the step is subtractive, we invert the sign and treat it as an additive step. For a multiplicative step, the step must be greater than one, and the initial and final values must be of same sign and strictly ordered. Analogously for a division step.

```

<Commands: range int: TBP>+≡
    procedure :: evaluate => range_int_evaluate

<Commands: sub interfaces>+≡
    module subroutine range_int_evaluate (range)
        class(range_int_t), intent(inout) :: range
    end subroutine range_int_evaluate

<Commands: procedures>+≡
    module subroutine range_int_evaluate (range)
        class(range_int_t), intent(inout) :: range
        integer :: ival
        if (associated (range%pn_beg)) then
            call range%expr_beg%evaluate ()
            if (range%expr_beg%is_known ()) then
                range%i_beg = range%expr_beg%get_int ()
            end if
        end if
    end subroutine range_int_evaluate

```

```

else
    call range%write ()
    call msg_fatal &
        ("Range expression: initial value evaluates to unknown")
end if
if (associated (range%pn_end)) then
    call range%expr_end%evaluate ()
    if (range%expr_end%is_known ()) then
        range%i_end = range%expr_end%get_int ()
        if (associated (range%pn_step)) then
            call range%expr_step%evaluate ()
            if (range%expr_step%is_known ()) then
                range%i_step = range%expr_step%get_int ()
                select case (range%step_mode)
                case (STEP_SUB); range%i_step = - range%i_step
                end select
            else
                call range%write ()
                call msg_fatal &
                    ("Range expression: step value evaluates to unknown")
            end if
        else
            range%i_step = 1
        end if
    else
        call range%write ()
        call msg_fatal &
            ("Range expression: final value evaluates to unknown")
    end if
else
    range%i_end = range%i_beg
    range%i_step = 1
end if
select case (range%step_mode)
case (STEP_NONE)
    range%n_step = 1
case (STEP_ADD, STEP_SUB)
    if (range%i_step /= 0) then
        if (range%i_beg == range%i_end) then
            range%n_step = 1
        else if (sign (1, range%i_end - range%i_beg) &
            == sign (1, range%i_step)) then
            range%n_step = (range%i_end - range%i_beg) / range%i_step + 1
        else
            range%n_step = 0
        end if
    else
        call msg_fatal ("range evaluation (add): step value is zero")
    end if
case (STEP_MUL)
    if (range%i_step > 1) then
        if (range%i_beg == range%i_end) then
            range%n_step = 1
        else if (range%i_beg == 0) then

```

```

        call msg_fatal ("range evaluation (mul): initial value is zero")
    else if (sign (1, range%i_beg) == sign (1, range%i_end) &
        .and. abs (range%i_beg) < abs (range%i_end)) then
        range%n_step = 0
        ival = range%i_beg
        do while (abs (ival) <= abs (range%i_end))
            range%n_step = range%n_step + 1
            ival = ival * range%i_step
        end do
    else
        range%n_step = 0
    end if
else
    call msg_fatal &
        ("range evaluation (mult): step value is one or less")
end if
case (STEP_DIV)
    if (range%i_step > 1) then
        if (range%i_beg == range%i_end) then
            range%n_step = 1
        else if (sign (1, range%i_beg) == sign (1, range%i_end) &
            .and. abs (range%i_beg) > abs (range%i_end)) then
            range%n_step = 0
            ival = range%i_beg
            do while (abs (ival) >= abs (range%i_end))
                range%n_step = range%n_step + 1
                if (ival == 0) exit
                ival = ival / range%i_step
            end do
        else
            range%n_step = 0
        end if
    else
        call msg_fatal &
            ("range evaluation (div): step value is one or less")
    end if
case (STEP_COMP_ADD)
    call msg_fatal ("range evaluation: &
        &step mode /+ not allowed for integer variable")
case (STEP_COMP_MUL)
    call msg_fatal ("range evaluation: &
        &step mode /* not allowed for integer variable")
case default
    call range%write ()
    call msg_bug ("range evaluation: step mode not implemented")
end select
end if
end subroutine range_int_evaluate

```

The version for a real variable.

```

<Commands: range real: TBP>+≡
    procedure :: evaluate => range_real_evaluate
<Commands: sub interfaces>+≡

```

```

module subroutine range_real_evaluate (range)
  class(range_real_t), intent(inout) :: range
end subroutine range_real_evaluate

(Commands: procedures) +=
module subroutine range_real_evaluate (range)
  class(range_real_t), intent(inout) :: range
  if (associated (range%pn_beg)) then
    call range%expr_beg%evaluate ()
    if (range%expr_beg%is_known ()) then
      range%r_beg = range%expr_beg%get_real ()
    else
      call range%write ()
      call msg_fatal &
        ("Range expression: initial value evaluates to unknown")
    end if
  if (associated (range%pn_end)) then
    call range%expr_end%evaluate ()
    if (range%expr_end%is_known ()) then
      range%r_end = range%expr_end%get_real ()
      if (associated (range%pn_step)) then
        if (range%expr_step%is_known ()) then
          select case (range%step_mode)
            case (STEP_ADD, STEP_SUB, STEP_MUL, STEP_DIV)
              call range%expr_step%evaluate ()
              range%r_step = range%expr_step%get_real ()
              select case (range%step_mode)
                case (STEP_SUB); range%r_step = - range%r_step
              end select
            case (STEP_COMP_ADD, STEP_COMP_MUL)
              range%n_step = &
                max (range%expr_step%get_int (), 0)
          end select
        else
          call range%write ()
          call msg_fatal &
            ("Range expression: step value evaluates to unknown")
        end if
      else
        call range%write ()
        call msg_fatal &
          ("Range expression (real): step value must be provided")
        end if
      else
        call range%write ()
        call msg_fatal &
          ("Range expression: final value evaluates to unknown")
        end if
      else
        range%r_end = range%r_beg
        range%r_step = 1
      end if
      select case (range%step_mode)
        case (STEP_NONE)
          range%n_step = 1

```

```

case (STEP_ADD, STEP_SUB)
  if (range%r_step /= 0) then
    if (sign (1._default, range%r_end - range%r_beg) &
      == sign (1._default, range%r_step)) then
      range%n_step = &
        nint ((range%r_end - range%r_beg) / range%r_step + 1)
    else
      range%n_step = 0
    end if
  else
    call msg_fatal ("range evaluation (add): step value is zero")
  end if
case (STEP_MUL)
  if (range%r_step > 1) then
    if (range%r_beg == 0 .or. range%r_end == 0) then
      call msg_fatal ("range evaluation (mul): bound is zero")
    else if (sign (1._default, range%r_beg) &
      == sign (1._default, range%r_end) &
      .and. abs (range%r_beg) <= abs (range%r_end)) then
      range%lr_beg = log (abs (range%r_beg))
      range%lr_end = log (abs (range%r_end))
      range%lr_step = log (range%r_step)
      range%n_step = nint &
        (abs ((range%lr_end - range%lr_beg) / range%lr_step) + 1)
    else
      range%n_step = 0
    end if
  else
    call msg_fatal &
      ("range evaluation (mult): step value is one or less")
  end if
case (STEP_DIV)
  if (range%r_step > 1) then
    if (range%r_beg == 0 .or. range%r_end == 0) then
      call msg_fatal ("range evaluation (div): bound is zero")
    else if (sign (1._default, range%r_beg) &
      == sign (1._default, range%r_end) &
      .and. abs (range%r_beg) >= abs (range%r_end)) then
      range%lr_beg = log (abs (range%r_beg))
      range%lr_end = log (abs (range%r_end))
      range%lr_step = -log (range%r_step)
      range%n_step = nint &
        (abs ((range%lr_end - range%lr_beg) / range%lr_step) + 1)
    else
      range%n_step = 0
    end if
  else
    call msg_fatal &
      ("range evaluation (mult): step value is one or less")
  end if
case (STEP_COMP_ADD)
  ! Number of steps already known
case (STEP_COMP_MUL)
  ! Number of steps already known

```

```

        if (range%r_beg == 0 .or. range%r_end == 0) then
            call msg_fatal ("range evaluation (mul): bound is zero")
        else if (sign (1._default, range%r_beg) &
            == sign (1._default, range%r_end)) then
            range%lr_beg = log (abs (range%r_beg))
            range%lr_end = log (abs (range%r_end))
        else
            range%n_step = 0
        end if
    case default
        call range%write ()
        call msg_bug ("range evaluation: step mode not implemented")
    end select
end if
end subroutine range_real_evaluate

```

Return the number of iterations:

```

<Commands: range: TBP>+≡
    procedure :: get_n_iterations => range_get_n_iterations

<Commands: sub interfaces>+≡
    module function range_get_n_iterations (range) result (n)
        class(range_t), intent(in) :: range
        integer :: n
    end function range_get_n_iterations

<Commands: procedures>+≡
    module function range_get_n_iterations (range) result (n)
        class(range_t), intent(in) :: range
        integer :: n
        n = range%n_step
    end function range_get_n_iterations

```

Compute the value for iteration i and store it in the embedded token.

```

<Commands: range: TBP>+≡
    procedure (range_set_value), deferred :: set_value

<Commands: interfaces>+≡
    abstract interface
        subroutine range_set_value (range, i)
            import
            class(range_t), intent(inout) :: range
            integer, intent(in) :: i
        end subroutine range_set_value
    end interface

```

In the integer case, we compute the value directly for additive step. For multiplicative step, we perform a loop in the same way as above, where the number of iteration was determined.

```

<Commands: range int: TBP>+≡
    procedure :: set_value => range_int_set_value

```



```

<Commands: sub interfaces>+≡
    module subroutine range_int_set_value (range, i)
        class(range_int_t), intent(inout) :: range
        integer, intent(in) :: i
    end subroutine range_int_set_value

<Commands: procedures>+≡
    module subroutine range_int_set_value (range, i)
        class(range_int_t), intent(inout) :: range
        integer, intent(in) :: i
        integer :: k, ival
        select case (range%step_mode)
        case (STEP_NONE)
            ival = range%i_beg
        case (STEP_ADD, STEP_SUB)
            ival = range%i_beg + (i - 1) * range%i_step
        case (STEP_MUL)
            ival = range%i_beg
            do k = 1, i - 1
                ival = ival * range%i_step
            end do
        case (STEP_DIV)
            ival = range%i_beg
            do k = 1, i - 1
                ival = ival / range%i_step
            end do
        case default
            call range%write ()
            call msg_bug ("range iteration: step mode not implemented")
        end select
        call parse_node_set_value (range%pn_literal, ival = ival)
    end subroutine range_int_set_value

```

In the integer case, we compute the value directly for additive step. For multiplicative step, we perform a loop in the same way as above, where the number of iteration was determined.

```

<Commands: range real: TBP>+≡
    procedure :: set_value => range_real_set_value

<Commands: sub interfaces>+≡
    module subroutine range_real_set_value (range, i)
        class(range_real_t), intent(inout) :: range
        integer, intent(in) :: i
    end subroutine range_real_set_value

<Commands: procedures>+≡
    module subroutine range_real_set_value (range, i)
        class(range_real_t), intent(inout) :: range
        integer, intent(in) :: i
        real(default) :: rval, x
        select case (range%step_mode)
        case (STEP_NONE)
            rval = range%r_beg
        case (STEP_ADD, STEP_SUB, STEP_COMP_ADD)
            if (range%n_step > 1) then

```

```

        x = real (i - 1, default) / (range%n_step - 1)
    else
        x = 1._default / 2
    end if
    rval = x * range%r_end + (1 - x) * range%r_beg
case (STEP_MUL, STEP_DIV, STEP_COMP_MUL)
    if (range%n_step > 1) then
        x = real (i - 1, default) / (range%n_step - 1)
    else
        x = 1._default / 2
    end if
    rval = sign &
        (exp (x * range%lr_end + (1 - x) * range%lr_beg), range%r_beg)
case default
    call range%write ()
    call msg_bug ("range iteration: step mode not implemented")
end select
call parse_node_set_value (range%pn_literal, rval = rval)
end subroutine range_real_set_value

```

Scan over parameters and other objects

The scan command allocates a new parse node for the variable assignment (the lhs). The rhs of this parse node is assigned from the available rhs expressions in the scan list, one at a time, so the compiled parse node can be prepended to the scan body.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_scan_t
private
type(string_t) :: name
integer :: n_values = 0
type(parse_node_p), dimension(:), allocatable :: scan_cmd
class(range_t), dimension(:), allocatable :: range
contains
<Commands: cmd scan: TBP>
end type cmd_scan_t

```

Finalizer.

The auxiliary parse nodes that we have constructed have to be treated carefully: the embedded pointers all point to persistent objects somewhere else and should not be finalized, so we should not call the finalizer recursively.

```

<Commands: cmd scan: TBP>≡
procedure :: final => cmd_scan_final

<Commands: sub interfaces>+≡
recursive module subroutine cmd_scan_final (cmd)
    class(cmd_scan_t), intent(inout) :: cmd
end subroutine cmd_scan_final

<Commands: procedures>+≡
recursive module subroutine cmd_scan_final (cmd)
    class(cmd_scan_t), intent(inout) :: cmd

```

```

type(parse_node_t), pointer :: pn_var_single, pn_decl_single
type(string_t) :: key
integer :: i
if (allocated (cmd%scan_cmd)) then
  do i = 1, size (cmd%scan_cmd)
    pn_var_single => parse_node_get_sub_ptr (cmd%scan_cmd(i)%ptr)
    key = parse_node_get_rule_key (pn_var_single)
    select case (char (key))
    case ("scan_string_decl", "scan_log_decl")
      pn_decl_single => parse_node_get_sub_ptr (pn_var_single, 2)
      call parse_node_final (pn_decl_single, recursive=.false.)
      deallocate (pn_decl_single)
    end select
    call parse_node_final (pn_var_single, recursive=.false.)
    deallocate (pn_var_single)
  end do
  deallocate (cmd%scan_cmd)
end if
if (allocated (cmd%range)) then
  do i = 1, size (cmd%range)
    call cmd%range(i)%final ()
  end do
end if
end subroutine cmd_scan_final

```

Output.

```

<Commands: cmd scan: TBP>+≡
  procedure :: write => cmd_scan_write

<Commands: sub interfaces>+≡
  module subroutine cmd_scan_write (cmd, unit, indent)
    class(cmd_scan_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_scan_write

<Commands: procedures>+≡
  module subroutine cmd_scan_write (cmd, unit, indent)
    class(cmd_scan_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,A,1x,'(',I0,')')") "scan:", char (cmd%name), &
      cmd%n_values
  end subroutine cmd_scan_write

```

Compile the scan command. We construct a new parse node that implements the variable assignment for a single element on the rhs, instead of the whole list that we get from the original parse tree. By simply copying the node, we copy all pointers and inherit the targets from the original. During execution, we should replace the rhs by the stored rhs pointers (the list elements), one by one, then (re)compile the redefined node. Gfortran 7/8/9 bug, has to remain in the main module:

```

<Commands: cmd scan: TBP>+≡

```

```

procedure :: compile => cmd_scan_compile

(Commands: main procedures)+≡
recursive subroutine cmd_scan_compile (cmd, global)
  class(cmd_scan_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(parse_node_t), pointer :: pn_var, pn_body, pn_body_first
  type(parse_node_t), pointer :: pn_decl, pn_name
  type(parse_node_t), pointer :: pn_arg, pn_scan_cmd, pn_rhs
  type(parse_node_t), pointer :: pn_decl_single, pn_var_single
  type(syntax_rule_t), pointer :: var_rule_decl, var_rule
  type(string_t) :: key
  integer :: var_type
  integer :: i
  if (debug_on) call msg_debug (D_CORE, "cmd_scan_compile")
  if (debug_active (D_CORE)) call parse_node_write_rec (cmd%pn)
  pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
  pn_body => parse_node_get_next_ptr (pn_var)
  if (associated (pn_body)) then
    pn_body_first => parse_node_get_sub_ptr (pn_body)
  else
    pn_body_first => null ()
  end if
  key = parse_node_get_rule_key (pn_var)
  select case (char (key))
  case ("scan_num")
    pn_name => parse_node_get_sub_ptr (pn_var)
    cmd%name = parse_node_get_string (pn_name)
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_num"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
  case ("scan_int")
    pn_name => parse_node_get_sub_ptr (pn_var, 2)
    cmd%name = parse_node_get_string (pn_name)
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_int"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
  case ("scan_real")
    pn_name => parse_node_get_sub_ptr (pn_var, 2)
    cmd%name = parse_node_get_string (pn_name)
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_real"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
  case ("scan_complex")
    pn_name => parse_node_get_sub_ptr (pn_var, 2)
    cmd%name = parse_node_get_string (pn_name)
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_complex"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
  case ("scan_alias")
    pn_name => parse_node_get_sub_ptr (pn_var, 2)
    cmd%name = parse_node_get_string (pn_name)
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_alias"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
  case ("scan_string_decl")
    pn_decl => parse_node_get_sub_ptr (pn_var, 2)
    pn_name => parse_node_get_sub_ptr (pn_decl, 2)
    cmd%name = parse_node_get_string (pn_name)

```

```

var_rule_decl => syntax_get_rule_ptr (syntax_cmd_list, &
    var_str ("cmd_string"))
var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
    var_str ("cmd_string_decl"))
pn_arg => parse_node_get_next_ptr (pn_name, 2)
case ("scan_log_decl")
    pn_decl => parse_node_get_sub_ptr (pn_var, 2)
    pn_name => parse_node_get_sub_ptr (pn_decl, 2)
    cmd%name = parse_node_get_string (pn_name)
    var_rule_decl => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_log"))
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_log_decl"))
    pn_arg => parse_node_get_next_ptr (pn_name, 2)
case ("scan_cuts")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_cuts"))
    cmd%name = "cuts"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_weight")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_weight"))
    cmd%name = "weight"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_scale"))
    cmd%name = "scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_ren_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_ren_scale"))
    cmd%name = "renormalization_scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_fac_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_fac_scale"))
    cmd%name = "factorization_scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_selection")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_selection"))
    cmd%name = "selection"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_reweight")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_reweight"))
    cmd%name = "reweight"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_analysis")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_analysis"))
    cmd%name = "analysis"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)

```

```

case ("scan_model")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_model"))
    cmd%name = "model"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_library")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_library"))
    cmd%name = "library"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case default
    call msg_bug ("scan: case ' ' // char (key) // ' ' not implemented")
end select
if (associated (pn_arg)) then
    cmd%n_values = parse_node_get_n_sub (pn_arg)
end if
var_list => global%get_var_list_ptr ()
allocate (cmd%scan_cmd (cmd%n_values))
select case (char (key))
case ("scan_num")
    var_type = &
        var_list%get_type (cmd%name)
    select case (var_type)
    case (V_INT)
        allocate (range_int_t :: cmd%range (cmd%n_values))
    case (V_REAL)
        allocate (range_real_t :: cmd%range (cmd%n_values))
    case (V_CMPLX)
        call msg_fatal ("scan over complex variable not implemented")
    case (V_NONE)
        call msg_fatal ("scan: variable ' ' // char (cmd%name) // ' ' undefined")
    case default
        call msg_bug ("scan: impossible variable type")
    end select
case ("scan_int")
    allocate (range_int_t :: cmd%range (cmd%n_values))
case ("scan_real")
    allocate (range_real_t :: cmd%range (cmd%n_values))
case ("scan_complex")
    call msg_fatal ("scan over complex variable not implemented")
end select
i = 1
if (associated (pn_arg)) then
    pn_rhs => parse_node_get_sub_ptr (pn_arg)
else
    pn_rhs => null ()
end if
do while (associated (pn_rhs))
    allocate (pn_scan_cmd)
    call parse_node_create_branch (pn_scan_cmd, &
        syntax_get_rule_ptr (syntax_cmd_list, var_str ("command_list")))
    allocate (pn_var_single)
    pn_var_single = pn_var
    call parse_node_replace_rule (pn_var_single, var_rule)

```

```

select case (char (key))
case ("scan_num", "scan_int", "scan_real", &
      "scan_complex", "scan_alias", &
      "scan_cuts", "scan_weight", &
      "scan_scale", "scan_ren_scale", "scan_fac_scale", &
      "scan_selection", "scan_reweight", "scan_analysis", &
      "scan_model", "scan_library")
  if (allocated (cmd%range)) then
    call cmd%range(i)%init (pn_rhs)
    call parse_node_replace_last_sub &
      (pn_var_single, cmd%range(i)%pn_expr)
  else
    call parse_node_replace_last_sub (pn_var_single, pn_rhs)
  end if
case ("scan_string_decl", "scan_log_decl")
  allocate (pn_decl_single)
  pn_decl_single = pn_decl
  call parse_node_replace_rule (pn_decl_single, var_rule_decl)
  call parse_node_replace_last_sub (pn_decl_single, pn_rhs)
  call parse_node_freeze_branch (pn_decl_single)
  call parse_node_replace_last_sub (pn_var_single, pn_decl_single)
case default
  call msg_bug ("scan: case '" // char (key) &
    // "' broken")
end select
call parse_node_freeze_branch (pn_var_single)
call parse_node_append_sub (pn_scan_cmd, pn_var_single)
call parse_node_append_sub (pn_scan_cmd, pn_body_first)
call parse_node_freeze_branch (pn_scan_cmd)
cmd%scan_cmd(i)%ptr => pn_scan_cmd
i = i + 1
pn_rhs => parse_node_get_next_ptr (pn_rhs)
end do
if (debug_active (D_CORE)) then
  do i = 1, cmd%n_values
    print *, "scan command ", i
    call parse_node_write_rec (cmd%scan_cmd(i)%ptr)
    if (allocated (cmd%range)) call cmd%range(i)%write ()
  end do
  print *, "original"
  call parse_node_write_rec (cmd%pn)
end if
end subroutine cmd_scan_compile

```

Execute the loop for all values in the step list. We use the parse trees with single variable assignment that we have stored, to iteratively create a local environment, execute the stored commands, and destroy it again. When we encounter a range object, we execute the commands for each value that this object provides. Computing this value has the side effect of modifying the rhs of the variable assignment that heads the local command list, directly in the local parse tree.

<Commands: cmd scan: TBP>+≡
 procedure :: execute => cmd_scan_execute

```

<Commands: sub interfaces>+≡
    recursive module subroutine cmd_scan_execute (cmd, global)
        class(cmd_scan_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_scan_execute

<Commands: procedures>+≡
    recursive module subroutine cmd_scan_execute (cmd, global)
        class(cmd_scan_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(rt_data_t), allocatable :: local
        integer :: i, j
        do i = 1, cmd%n_values
            if (allocated (cmd%range)) then
                call cmd%range(i)%compile (global)
                call cmd%range(i)%evaluate ()
                do j = 1, cmd%range(i)%get_n_iterations ()
                    call cmd%range(i)%set_value (j)
                    allocate (local)
                    call build_alt_setup (local, global, cmd%scan_cmd(i)%ptr)
                    call local%local_final ()
                    deallocate (local)
                end do
            else
                allocate (local)
                call build_alt_setup (local, global, cmd%scan_cmd(i)%ptr)
                call local%local_final ()
                deallocate (local)
            end if
        end do
    end subroutine cmd_scan_execute

```

Conditionals

Conditionals are implemented as a list that is compiled and evaluated recursively; this allows for a straightforward representation of **else if** constructs. A `cmd_if_t` object can hold either an **else_if** clause which is another object of this type, or an **else_body**, but not both.

If- or else-bodies are no scoping units, so all data remain global and no copy-in copy-out is needed.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_if_t
    private
        type(parse_node_t), pointer :: pn_if_lexpr => null ()
        type(command_list_t), pointer :: if_body => null ()
        type(cmd_if_t), dimension(:), pointer :: elsif_cmd => null ()
        type(command_list_t), pointer :: else_body => null ()
    contains
        <Commands: cmd if: TBP>
    end type cmd_if_t

```


Finalizer. There are no local options, therefore we can simply override the default finalizer.

```

<Commands: cmd if: TBP>≡
    procedure :: final => cmd_if_final

<Commands: sub interfaces>+≡
    recursive module subroutine cmd_if_final (cmd)
        class(cmd_if_t), intent(inout) :: cmd
    end subroutine cmd_if_final

<Commands: procedures>+≡
    recursive module subroutine cmd_if_final (cmd)
        class(cmd_if_t), intent(inout) :: cmd
        integer :: i
        if (associated (cmd%if_body)) then
            call command_list_final (cmd%if_body)
            deallocate (cmd%if_body)
        end if
        if (associated (cmd%elsif_cmd)) then
            do i = 1, size (cmd%elsif_cmd)
                call cmd_if_final (cmd%elsif_cmd(i))
            end do
            deallocate (cmd%elsif_cmd)
        end if
        if (associated (cmd%else_body)) then
            call command_list_final (cmd%else_body)
            deallocate (cmd%else_body)
        end if
    end subroutine cmd_if_final

```

Output. Recursively write the command lists.

```

<Commands: cmd if: TBP>+≡
    procedure :: write => cmd_if_write

<Commands: sub interfaces>+≡
    module subroutine cmd_if_write (cmd, unit, indent)
        class(cmd_if_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_if_write

<Commands: procedures>+≡
    module subroutine cmd_if_write (cmd, unit, indent)
        class(cmd_if_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, ind, i
        u = given_output_unit (unit); if (u < 0) return
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, indent)
        write (u, "(A)") "if <expr> then"
        if (associated (cmd%if_body)) then
            call cmd%if_body%write (unit, ind + 1)
        end if
        if (associated (cmd%elsif_cmd)) then
            do i = 1, size (cmd%elsif_cmd)
                call write_indent (u, indent)

```

```

        write (u, "(A)") "elseif <expr> then"
        if (associated (cmd%elseif_cmd(i)%if_body)) then
            call cmd%elseif_cmd(i)%if_body%write (unit, ind + 1)
        end if
    end do
end if
if (associated (cmd%else_body)) then
    call write_indent (u, indent)
    write (u, "(A)") "else"
    call cmd%else_body%write (unit, ind + 1)
end if
end subroutine cmd_if_write

```

Compile the conditional.

<Commands: cmd if: TBP>+≡

```

procedure :: compile => cmd_if_compile

```

<Commands: sub interfaces>+≡

```

recursive module subroutine cmd_if_compile (cmd, global)
    class(cmd_if_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_if_compile

```

<Commands: procedures>+≡

```

recursive module subroutine cmd_if_compile (cmd, global)
    class(cmd_if_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_lexpr, pn_body
    type(parse_node_t), pointer :: pn_elseif_clauses, pn_cmd_elseif
    type(parse_node_t), pointer :: pn_else_clause, pn_cmd_else
    integer :: i, n_elseif
    pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 2)
    cmd%pn_if_lexpr => pn_lexpr
    pn_body => parse_node_get_next_ptr (pn_lexpr, 2)
    select case (char (parse_node_get_rule_key (pn_body)))
    case ("command_list")
        allocate (cmd%if_body)
        call cmd%if_body%compile (pn_body, global)
        pn_elseif_clauses => parse_node_get_next_ptr (pn_body)
    case default
        pn_elseif_clauses => pn_body
    end select
    select case (char (parse_node_get_rule_key (pn_elseif_clauses)))
    case ("elseif_clauses")
        n_elseif = parse_node_get_n_sub (pn_elseif_clauses)
        allocate (cmd%elseif_cmd (n_elseif))
        pn_cmd_elseif => parse_node_get_sub_ptr (pn_elseif_clauses)
        do i = 1, n_elseif
            pn_lexpr => parse_node_get_sub_ptr (pn_cmd_elseif, 2)
            cmd%elseif_cmd(i)%pn_if_lexpr => pn_lexpr
            pn_body => parse_node_get_next_ptr (pn_lexpr, 2)
            if (associated (pn_body)) then
                allocate (cmd%elseif_cmd(i)%if_body)
                call cmd%elseif_cmd(i)%if_body%compile (pn_body, global)
            end if
        end do
    end select
end subroutine cmd_if_compile

```

```

        pn_cmd_elsif => parse_node_get_next_ptr (pn_cmd_elsif)
    end do
    pn_else_clause => parse_node_get_next_ptr (pn_elsif_clauses)
case default
    pn_else_clause => pn_elsif_clauses
end select
select case (char (parse_node_get_rule_key (pn_else_clause)))
case ("else_clause")
    pn_cmd_else => parse_node_get_sub_ptr (pn_else_clause)
    pn_body => parse_node_get_sub_ptr (pn_cmd_else, 2)
    if (associated (pn_body)) then
        allocate (cmd%else_body)
        call cmd%else_body%compile (pn_body, global)
    end if
end select
end subroutine cmd_if_compile

```

(Recursively) execute the condition. Context remains global in all cases.

(Commands: cmd if: TBP)+≡

```

procedure :: execute => cmd_if_execute

```

(Commands: sub interfaces)+≡

```

recursive module subroutine cmd_if_execute (cmd, global)
    class(cmd_if_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
end subroutine cmd_if_execute

```

(Commands: procedures)+≡

```

recursive module subroutine cmd_if_execute (cmd, global)
    class(cmd_if_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    logical :: lval, is_known
    integer :: i
    var_list => global%get_var_list_ptr ()
    lval = eval_log (cmd%pn_if_lexpr, var_list, is_known=is_known)
    if (is_known) then
        if (lval) then
            if (associated (cmd%if_body)) then
                call cmd%if_body%execute (global)
            end if
            return
        end if
    else
        call error_undecided ()
        return
    end if
    if (associated (cmd%elsif_cmd)) then
        SCAN_ELSEIF: do i = 1, size (cmd%elsif_cmd)
            lval = eval_log (cmd%elsif_cmd(i)%pn_if_lexpr, var_list, &
                is_known=is_known)
            if (is_known) then
                if (lval) then
                    if (associated (cmd%elsif_cmd(i)%if_body)) then
                        call cmd%elsif_cmd(i)%if_body%execute (global)

```

```

        end if
        return
    end if
    else
        call error_undecided ()
        return
    end if
end do SCAN_ELSEIF
end if
if (associated (cmd%else_body)) then
    call cmd%else_body%execute (global)
end if
contains
    subroutine error_undecided ()
        call msg_error ("Undefined result of cmditional expression: " &
            // "neither branch will be executed")
    end subroutine error_undecided
end subroutine cmd_if_execute

```

Include another command-list file

The include command allocates a local parse tree. This must not be deleted before the command object itself is deleted, since pointers may point to subobjects of it.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_include_t
    private
    type(string_t) :: file
    type(command_list_t), pointer :: command_list => null ()
    type(parse_tree_t) :: parse_tree
    contains
    <Commands: cmd include: TBP>
end type cmd_include_t

```

Finalizer: delete the command list. No options, so we can simply override the default finalizer.

```

<Commands: cmd include: TBP>≡
    procedure :: final => cmd_include_final

<Commands: sub interfaces>+≡
    module subroutine cmd_include_final (cmd)
        class(cmd_include_t), intent(inout) :: cmd
    end subroutine cmd_include_final

<Commands: procedures>+≡
    module subroutine cmd_include_final (cmd)
        class(cmd_include_t), intent(inout) :: cmd
        call parse_tree_final (cmd%parse_tree)
        if (associated (cmd%command_list)) then
            call cmd%command_list%final ()
            deallocate (cmd%command_list)
        end if
    end subroutine cmd_include_final

```

Write: display the command list as-is, if allocated.

```

<Commands: cmd include: TBP>+≡
    procedure :: write => cmd_include_write

<Commands: sub interfaces>+≡
    module subroutine cmd_include_write (cmd, unit, indent)
        class(cmd_include_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_include_write

<Commands: procedures>+≡
    module subroutine cmd_include_write (cmd, unit, indent)
        class(cmd_include_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, indent)
        write (u, "(A,A,A,A)") "include ", "'", char (cmd%file), "'"
        if (associated (cmd%command_list)) then
            call cmd%command_list%write (u, ind + 1)
        end if
    end subroutine cmd_include_write

```

Compile file contents: First parse the file, then immediately compile its contents.
Use the global data set.

```

<Commands: cmd include: TBP>+≡
    procedure :: compile => cmd_include_compile

<Commands: sub interfaces>+≡
    module subroutine cmd_include_compile (cmd, global)
        class(cmd_include_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_include_compile

<Commands: procedures>+≡
    module subroutine cmd_include_compile (cmd, global)
        class(cmd_include_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_arg, pn_file
        type(string_t) :: file
        logical :: exist
        integer :: u
        type(stream_t), target :: stream
        type(lexer_t) :: lexer
        pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
        pn_file => parse_node_get_sub_ptr (pn_arg)
        file = parse_node_get_string (pn_file)
        inquire (file=char(file), exist=exist)
        if (exist) then
            cmd%file = file
        else
            cmd%file = global%os_data%whizard_cutspath // "/" // file
            inquire (file=char(cmd%file), exist=exist)
        end if
    end subroutine cmd_include_compile

```

```

        if (.not. exist) then
            call msg_error ("Include file '" // char (file) // "' not found")
            return
        end if
    end if
end if
u = free_unit ()
call lexer_init_cmd_list (lexer, global%lexer)
call stream_init (stream, char (cmd%file))
call lexer_assign_stream (lexer, stream)
call parse_tree_init (cmd%parse_tree, syntax_cmd_list, lexer)
call stream_final (stream)
call lexer_final (lexer)
close (u)
allocate (cmd%command_list)
call cmd%command_list%compile (cmd%parse_tree%get_root_ptr (), &
    global)
end subroutine cmd_include_compile

```

Execute file contents in the global context.

```

<Commands: cmd include: TBP>+≡
    procedure :: execute => cmd_include_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_include_execute (cmd, global)
        class(cmd_include_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_include_execute

<Commands: procedures>+≡
    module subroutine cmd_include_execute (cmd, global)
        class(cmd_include_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (associated (cmd%command_list)) then
            call msg_message &
                ("Including Sindarin from '" // char (cmd%file) // "'")
            call cmd%command_list%execute (global)
            call msg_message &
                ("End of included '" // char (cmd%file) // "'")
        end if
    end subroutine cmd_include_execute

```

Export values

This command exports the current values of variables or other objects to the surrounding scope. By default, a scope enclosed by braces keeps all objects local to it. The `export` command exports the values that are generated within the scope to the corresponding object in the outer scope.

The allowed set of exportable objects is, in principle, the same as the set of objects that the `show` command supports. This includes some convenience abbreviations.

TODO: The initial implementation inherits syntax from `show`, but supports only the `results` pseudo-object. The results (i.e., the process stack) is appended to the outer process stack instead of being discarded. The behavior of

the `export` command for other object kinds is to be defined on a case-by-case basis. It may involve replacing the outer value or, instead, doing some sort of appending or reduction.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_export_t
    private
    type(string_t), dimension(:), allocatable :: name
    contains
    ⟨Commands: cmd export: TBP⟩
  end type cmd_export_t

```

Output: list the object names, not values.

```

⟨Commands: cmd export: TBP⟩≡
  procedure :: write => cmd_export_write

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_export_write (cmd, unit, indent)
    class(cmd_export_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_export_write

⟨Commands: procedures⟩+≡
  module subroutine cmd_export_write (cmd, unit, indent)
    class(cmd_export_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "export: "
    if (allocated (cmd%name)) then
      do i = 1, size (cmd%name)
        write (u, "(1x,A)", advance="no") char (cmd%name(i))
      end do
      write (u, *)
    else
      write (u, "(5x,A)") "[undefined]"
    end if
  end subroutine cmd_export_write

```

Compile. Allocate an array which is filled with the names of the variables to export.

```

⟨Commands: cmd export: TBP⟩+≡
  procedure :: compile => cmd_export_compile

⟨Commands: sub interfaces⟩+≡
  module subroutine cmd_export_compile (cmd, global)
    class(cmd_export_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_export_compile

⟨Commands: procedures⟩+≡
  module subroutine cmd_export_compile (cmd, global)
    class(cmd_export_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name

```

```

type(string_t) :: key
integer :: i, n_args
pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
if (associated (pn_arg)) then
  select case (char (parse_node_get_rule_key (pn_arg)))
  case ("show_arg")
    cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
  case default
    cmd%pn_opt => pn_arg
    pn_arg => null ()
  end select
end if
call cmd%compile_options (global)
if (associated (pn_arg)) then
  n_args = parse_node_get_n_sub (pn_arg)
  allocate (cmd%name (n_args))
  pn_var => parse_node_get_sub_ptr (pn_arg)
  i = 0
  do while (associated (pn_var))
    i = i + 1
    select case (char (parse_node_get_rule_key (pn_var)))
    case ("model", "library", "beams", "iterations", &
          "cuts", "weight", "int", "real", "complex", &
          "scale", "factorization_scale", "renormalization_scale", &
          "selection", "reweight", "analysis", "pdg", &
          "stable", "unstable", "polarized", "unpolarized", &
          "results", "expect", "intrinsic", "string", "logical")
      cmd%name(i) = parse_node_get_key (pn_var)
    case ("result_var")
      pn_prefix => parse_node_get_sub_ptr (pn_var)
      pn_name => parse_node_get_next_ptr (pn_prefix)
      if (associated (pn_name)) then
        cmd%name(i) = parse_node_get_key (pn_prefix) &
          // "(" // parse_node_get_string (pn_name) // ")"
      else
        cmd%name(i) = parse_node_get_key (pn_prefix)
      end if
    case ("log_var", "string_var", "alias_var")
      pn_prefix => parse_node_get_sub_ptr (pn_var)
      pn_name => parse_node_get_next_ptr (pn_prefix)
      key = parse_node_get_key (pn_prefix)
      if (associated (pn_name)) then
        select case (char (parse_node_get_rule_key (pn_name)))
        case ("var_name")
          select case (char (key))
          case ("?", "$") ! $ sign
            cmd%name(i) = key // parse_node_get_string (pn_name)
          case ("alias")
            cmd%name(i) = parse_node_get_string (pn_name)
          end select
        case default
          call parse_node_mismatch &
            ("var_name", pn_name)
        end select
      end if
    end select
  end while
end if

```



```

        else
            cmd%name(i) = key
        end if
    case default
        cmd%name(i) = parse_node_get_string (pn_var)
    end select
    !!! restriction imposed by current lack of implementation
    select case (char (parse_node_get_rule_key (pn_var)))
    case ("results")
    case default
        call msg_fatal ("export: object (type) '" &
            // char (parse_node_get_rule_key (pn_var)) &
            // "' not supported yet")
    end select
    pn_var => parse_node_get_next_ptr (pn_var)
end do
else
    allocate (cmd%name (0))
end if
end subroutine cmd_export_compile

```

Execute. Scan the list of objects to export.

```

<Commands: cmd export: TBP>+≡
    procedure :: execute => cmd_export_execute

<Commands: sub interfaces>+≡
    module subroutine cmd_export_execute (cmd, global)
        class(cmd_export_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine cmd_export_execute

<Commands: procedures>+≡
    module subroutine cmd_export_execute (cmd, global)
        class(cmd_export_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        call global%append_exports (cmd%name)
    end subroutine cmd_export_execute

```

Quit command execution

The code is the return code of the whole program if it is terminated by this command.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_quit_t
    private
    logical :: has_code = .false.
    type(parse_node_t), pointer :: pn_code_expr => null ()
    contains
    <Commands: cmd quit: TBP>
    end type cmd_quit_t

```

Output.

```
<Commands: cmd quit: TBP>≡
  procedure :: write => cmd_quit_write

<Commands: sub interfaces>+≡
  module subroutine cmd_quit_write (cmd, unit, indent)
    class(cmd_quit_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_quit_write

<Commands: procedures>+≡
  module subroutine cmd_quit_write (cmd, unit, indent)
    class(cmd_quit_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,L1)") "quit: has_code = ", cmd%has_code
  end subroutine cmd_quit_write
```

Compile: allocate a quit object which serves as a placeholder.

```
<Commands: cmd quit: TBP>+≡
  procedure :: compile => cmd_quit_compile

<Commands: sub interfaces>+≡
  module subroutine cmd_quit_compile (cmd, global)
    class(cmd_quit_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_quit_compile

<Commands: procedures>+≡
  module subroutine cmd_quit_compile (cmd, global)
    class(cmd_quit_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (pn_arg)) then
      cmd%pn_code_expr => parse_node_get_sub_ptr (pn_arg)
      cmd%has_code = .true.
    end if
  end subroutine cmd_quit_compile
```

Execute: The quit command does not execute anything, it just stops command execution. This is achieved by setting quit flag and quit code in the global variable list. However, the return code, if present, is an expression which has to be evaluated.

```
<Commands: cmd quit: TBP>+≡
  procedure :: execute => cmd_quit_execute

<Commands: sub interfaces>+≡
  module subroutine cmd_quit_execute (cmd, global)
    class(cmd_quit_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
  end subroutine cmd_quit_execute
```

```

<Commands: procedures>+≡
module subroutine cmd_quit_execute (cmd, global)
  class(cmd_quit_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  logical :: is_known
  var_list => global%get_var_list_ptr ()
  if (cmd%has_code) then
    global%quit_code = eval_int (cmd%pn_code_expr, var_list, &
      is_known=is_known)
    if (.not. is_known) then
      call msg_error ("Undefined return code of quit/exit command")
    end if
  end if
  global%quit = .true.
end subroutine cmd_quit_execute

```

35.1.6 The command list

The command list holds a list of commands and relevant global data.

```

<Commands: public>+≡
  public :: command_list_t

<Commands: types>+≡
  type :: command_list_t
    ! not private anymore as required by the whizard-c-interface
    class(command_t), pointer :: first => null ()
    class(command_t), pointer :: last => null ()
  contains
    <Commands: command list: TBP>
  end type command_list_t

```

Output.

```

<Commands: command list: TBP>≡
  procedure :: write => command_list_write

<Commands: sub interfaces>+≡
  recursive module subroutine command_list_write (cmd_list, unit, indent)
    class(command_list_t), intent(in) :: cmd_list
    integer, intent(in), optional :: unit, indent
  end subroutine command_list_write

<Commands: procedures>+≡
  recursive module subroutine command_list_write (cmd_list, unit, indent)
    class(command_list_t), intent(in) :: cmd_list
    integer, intent(in), optional :: unit, indent
    class(command_t), pointer :: cmd
    cmd => cmd_list%first
    do while (associated (cmd))
      call cmd%write (unit, indent)
      cmd => cmd%next
    end do
  end subroutine command_list_write

```

Append a new command to the list and free the original pointer.

```

<Commands: command list: TBP>+≡
    procedure :: append => command_list_append

<Commands: sub interfaces>+≡
    module subroutine command_list_append (cmd_list, command)
        class(command_list_t), intent(inout) :: cmd_list
        class(command_t), intent(inout), pointer :: command
    end subroutine command_list_append

<Commands: procedures>+≡
    module subroutine command_list_append (cmd_list, command)
        class(command_list_t), intent(inout) :: cmd_list
        class(command_t), intent(inout), pointer :: command
        if (associated (cmd_list%last)) then
            cmd_list%last%next => command
        else
            cmd_list%first => command
        end if
        cmd_list%last => command
        command => null ()
    end subroutine command_list_append

```

Finalize.

```

<Commands: command list: TBP>+≡
    procedure :: final => command_list_final

<Commands: sub interfaces>+≡
    recursive module subroutine command_list_final (cmd_list)
        class(command_list_t), intent(inout) :: cmd_list
    end subroutine command_list_final

<Commands: procedures>+≡
    recursive module subroutine command_list_final (cmd_list)
        class(command_list_t), intent(inout) :: cmd_list
        class(command_t), pointer :: command
        do while (associated (cmd_list%first))
            command => cmd_list%first
            cmd_list%first => cmd_list%first%next
            call command%final ()
            deallocate (command)
        end do
        cmd_list%last => null ()
    end subroutine command_list_final

```

35.1.7 Compiling the parse tree

Transform a parse tree into a command list. Initialization is assumed to be done.

After each command, we set a breakpoint. Gfortran 7/8/9 bug: has to remain in the main module:

```

<Commands: command list: TBP>+≡
    procedure :: compile => command_list_compile

```

```

<Commands: main procedures>+≡
recursive subroutine command_list_compile (cmd_list, pn, global)
  class(command_list_t), intent(inout), target :: cmd_list
  type(parse_node_t), intent(in), target :: pn
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_cmd
  class(command_t), pointer :: command
  integer :: i
  pn_cmd => parse_node_get_sub_ptr (pn)
  do i = 1, parse_node_get_n_sub (pn)
    call dispatch_command (command, pn_cmd)
    call command%compile (global)
    call cmd_list%append (command)
    call terminate_now_if_signal ()
    pn_cmd => parse_node_get_next_ptr (pn_cmd)
  end do
end subroutine command_list_compile

```

35.1.8 Executing the command list

Before executing a command we should execute its options (if any). After that, reset the options, i.e., remove temporary effects from the global state.

Also here, after each command we set a breakpoint.

```

<Commands: command list: TBP>+≡
procedure :: execute => command_list_execute

<Commands: sub interfaces>+≡
recursive module subroutine command_list_execute (cmd_list, global)
  class(command_list_t), intent(in) :: cmd_list
  type(rt_data_t), intent(inout), target :: global
end subroutine command_list_execute

<Commands: procedures>+≡
recursive module subroutine command_list_execute (cmd_list, global)
  class(command_list_t), intent(in) :: cmd_list
  type(rt_data_t), intent(inout), target :: global
  class(command_t), pointer :: command
  command => cmd_list%first
  COMMAND_COND: do while (associated (command))
    call command%execute_options (global)
    call command%execute (global)
    call command%reset_options (global)
    call terminate_now_if_signal ()
    if (global%quit) exit COMMAND_COND
    command => command%next
  end do COMMAND_COND
end subroutine command_list_execute

```

35.1.9 Command list syntax

```

<Commands: public>+≡
public :: syntax_cmd_list

```

```

<Commands: variables>+=
    type(syntax_t), target, save :: syntax_cmd_list

<Commands: public>+=
    public :: syntax_cmd_list_init

<Commands: sub interfaces>+=
    module subroutine syntax_cmd_list_init ()
    end subroutine syntax_cmd_list_init

<Commands: procedures>+=
    module subroutine syntax_cmd_list_init ()
    type(ifile_t) :: ifile
    call define_cmd_list_syntax (ifile)
    call syntax_init (syntax_cmd_list, ifile)
    call ifile_final (ifile)
    end subroutine syntax_cmd_list_init

<Commands: public>+=
    public :: syntax_cmd_list_final

<Commands: sub interfaces>+=
    module subroutine syntax_cmd_list_final ()
    end subroutine syntax_cmd_list_final

<Commands: procedures>+=
    module subroutine syntax_cmd_list_final ()
    call syntax_final (syntax_cmd_list)
    end subroutine syntax_cmd_list_final

<Commands: public>+=
    public :: syntax_cmd_list_write

<Commands: sub interfaces>+=
    module subroutine syntax_cmd_list_write (unit)
    integer, intent(in), optional :: unit
    end subroutine syntax_cmd_list_write

<Commands: procedures>+=
    module subroutine syntax_cmd_list_write (unit)
    integer, intent(in), optional :: unit
    call syntax_write (syntax_cmd_list, unit)
    end subroutine syntax_cmd_list_write

<Commands: procedures>+=
    subroutine define_cmd_list_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "SEQ command_list = command*")
    call ifile_append (ifile, "ALT command = " &
        // "cmd_model | cmd_library | cmd_iterations | cmd_sample_format | " &
        // "cmd_var | cmd_slha | " &
        // "cmd_show | cmd_clear | " &
        // "cmd_expect | " &
        // "cmd_cuts | cmd_scale | cmd_fac_scale | cmd_ren_scale | " &
        // "cmd_weight | cmd_selection | cmd_reweight | " &
        // "cmd_beams | cmd_beams_pol_density | cmd_beams_pol_fraction | " &

```

```

// "cmd_beams_momentum | cmd_beams_theta | cmd_beams_phi | " &
// "cmd_integrate | " &
// "cmd_observable | cmd_histogram | cmd_plot | cmd_graph | " &
// "cmd_record | " &
// "cmd_analysis | cmd_alt_setup | " &
// "cmd_unstable | cmd_stable | cmd_simulate | cmd_rescan | " &
// "cmd_process | cmd_compile | cmd_exec | " &
// "cmd_scan | cmd_if | cmd_include | cmd_quit | " &
// "cmd_export | " &
// "cmd_polarized | cmd_unpolarized | " &
// "cmd_open_out | cmd_close_out | cmd_printf | " &
// "cmd_write_analysis | cmd_compile_analysis | cmd_nlo | cmd_components")
call ifile_append (ifile, "GRO options = '{' local_command_list '}'")
call ifile_append (ifile, "SEQ local_command_list = local_command*")
call ifile_append (ifile, "ALT local_command = " &
// "cmd_model | cmd_library | cmd_iterations | cmd_sample_format | " &
// "cmd_var | cmd_slha | " &
// "cmd_show | " &
// "cmd_expect | " &
// "cmd_cuts | cmd_scale | cmd_fac_scale | cmd_ren_scale | " &
// "cmd_weight | cmd_selection | cmd_reweight | " &
// "cmd_beams | cmd_beams_pol_density | cmd_beams_pol_fraction | " &
// "cmd_beams_momentum | cmd_beams_theta | cmd_beams_phi | " &
// "cmd_observable | cmd_histogram | cmd_plot | cmd_graph | " &
// "cmd_clear | cmd_record | " &
// "cmd_analysis | cmd_alt_setup | " &
// "cmd_open_out | cmd_close_out | cmd_printf | " &
// "cmd_write_analysis | cmd_compile_analysis | cmd_nlo | cmd_components")
call ifile_append (ifile, "SEQ cmd_model = model '=' model_name model_arg?")
call ifile_append (ifile, "KEY model")
call ifile_append (ifile, "ALT model_name = model_id | string_literal")
call ifile_append (ifile, "IDE model_id")
call ifile_append (ifile, "ARG model_arg = ( model_scheme? )")
call ifile_append (ifile, "ALT model_scheme = " &
// "ufo_spec | scheme_id | string_literal")
call ifile_append (ifile, "SEQ ufo_spec = ufo ufo_arg?")
call ifile_append (ifile, "KEY ufo")
call ifile_append (ifile, "ARG ufo_arg = ( string_literal )")
call ifile_append (ifile, "IDE scheme_id")
call ifile_append (ifile, "SEQ cmd_library = library '=' lib_name")
call ifile_append (ifile, "KEY library")
call ifile_append (ifile, "ALT lib_name = lib_id | string_literal")
call ifile_append (ifile, "IDE lib_id")
call ifile_append (ifile, "ALT cmd_var = " &
// "cmd_log_decl | cmd_log | " &
// "cmd_int | cmd_real | cmd_complex | cmd_num | " &
// "cmd_string_decl | cmd_string | cmd_alias | " &
// "cmd_result")
call ifile_append (ifile, "SEQ cmd_log_decl = logical cmd_log")
call ifile_append (ifile, "SEQ cmd_log = '?' var_name '=' lexpr")
call ifile_append (ifile, "SEQ cmd_int = int var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_real = real var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_complex = complex var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_num = var_name '=' expr")

```

```

call ifile_append (ifile, "SEQ cmd_string_decl = string cmd_string")
call ifile_append (ifile, "SEQ cmd_string = " &
    // "'$' var_name '=' sexpr" ) ! $
call ifile_append (ifile, "SEQ cmd_alias = alias var_name '=' cexpr")
call ifile_append (ifile, "SEQ cmd_result = result '=' expr")
call ifile_append (ifile, "SEQ cmd_slha = slha_action slha_arg options?")
call ifile_append (ifile, "ALT slha_action = " &
    // "read_slha | write_slha")
call ifile_append (ifile, "KEY read_slha")
call ifile_append (ifile, "KEY write_slha")
call ifile_append (ifile, "ARG slha_arg = ( string_literal )")
call ifile_append (ifile, "SEQ cmd_show = show show_arg options?")
call ifile_append (ifile, "KEY show")
call ifile_append (ifile, "ARG show_arg = ( showable* )")
call ifile_append (ifile, "ALT showable = " &
    // "model | library | beams | iterations | " &
    // "cuts | weight | logical | string | pdg | " &
    // "scale | factorization_scale | renormalization_scale | " &
// "selection | reweight | analysis | " &
    // "stable | unstable | polarized | unpolarized | " &
    // "expect | intrinsic | int | real | complex | " &
    // "alias_var | string | results | result_var | " &
    // "log_var | string_var | var_name")
call ifile_append (ifile, "KEY results")
call ifile_append (ifile, "KEY intrinsic")
call ifile_append (ifile, "SEQ alias_var = alias var_name")
call ifile_append (ifile, "SEQ result_var = result_key result_arg?")
call ifile_append (ifile, "SEQ log_var = '?' var_name")
call ifile_append (ifile, "SEQ string_var = '$' var_name" ) ! $
call ifile_append (ifile, "SEQ cmd_clear = clear clear_arg options?")
call ifile_append (ifile, "KEY clear")
call ifile_append (ifile, "ARG clear_arg = ( clearable* )")
call ifile_append (ifile, "ALT clearable = " &
    // "beams | iterations | " &
    // "cuts | weight | " &
    // "scale | factorization_scale | renormalization_scale | " &
// "selection | reweight | analysis | " &
    // "unstable | polarized | " &
    // "expect | " &
    // "log_var | string_var | var_name")
call ifile_append (ifile, "SEQ cmd_expect = expect expect_arg options?")
call ifile_append (ifile, "KEY expect")
call ifile_append (ifile, "ARG expect_arg = ( lexpr )")
call ifile_append (ifile, "SEQ cmd_cuts = cuts '=' lexpr")
call ifile_append (ifile, "SEQ cmd_scale = scale '=' expr")
call ifile_append (ifile, "SEQ cmd_fac_scale = " &
    // "factorization_scale '=' expr")
call ifile_append (ifile, "SEQ cmd_ren_scale = " &
    // "renormalization_scale '=' expr")
call ifile_append (ifile, "SEQ cmd_weight = weight '=' expr")
call ifile_append (ifile, "SEQ cmd_selection = selection '=' lexpr")
call ifile_append (ifile, "SEQ cmd_reweight = reweight '=' expr")
call ifile_append (ifile, "KEY cuts")
call ifile_append (ifile, "KEY scale")

```



```

call ifile_append (ifile, "KEY factorization_scale")
call ifile_append (ifile, "KEY renormalization_scale")
call ifile_append (ifile, "KEY weight")
call ifile_append (ifile, "KEY selection")
call ifile_append (ifile, "KEY reweight")
call ifile_append (ifile, "SEQ cmd_process = process process_id '=' " &
// "process_prt '=>' prt_state_list options?")
call ifile_append (ifile, "KEY process")
call ifile_append (ifile, "KEY '=>'")
call ifile_append (ifile, "LIS process_prt = cexpr+")
call ifile_append (ifile, "LIS prt_state_list = prt_state_sum+")
call ifile_append (ifile, "SEQ prt_state_sum = " &
// "prt_state prt_state_addition*")
call ifile_append (ifile, "SEQ prt_state_addition = '+' prt_state")
call ifile_append (ifile, "ALT prt_state = grouped_prt_state_list | cexpr")
call ifile_append (ifile, "GRO grouped_prt_state_list = " &
// "( prt_state_list )")
call ifile_append (ifile, "SEQ cmd_compile = compile_cmd options?")
call ifile_append (ifile, "SEQ compile_cmd = compile_clause compile_arg?")
call ifile_append (ifile, "SEQ compile_clause = compile_exec_name_spec?")
call ifile_append (ifile, "KEY compile")
call ifile_append (ifile, "SEQ exec_name_spec = as exec_name")
call ifile_append (ifile, "KEY as")
call ifile_append (ifile, "ALT exec_name = exec_id | string_literal")
call ifile_append (ifile, "IDE exec_id")
call ifile_append (ifile, "ARG compile_arg = ( lib_name* )")
call ifile_append (ifile, "SEQ cmd_exec = exec exec_arg")
call ifile_append (ifile, "KEY exec")
call ifile_append (ifile, "ARG exec_arg = ( sexpr )")
call ifile_append (ifile, "SEQ cmd_beams = beams '=' beam_def")
call ifile_append (ifile, "KEY beams")
call ifile_append (ifile, "SEQ beam_def = beam_spec strfun_seq*")
call ifile_append (ifile, "SEQ beam_spec = beam_list")
call ifile_append (ifile, "LIS beam_list = cexpr, cexpr?")
call ifile_append (ifile, "SEQ cmd_beams_pol_density = " &
// "beams_pol_density '=' beams_pol_spec")
call ifile_append (ifile, "KEY beams_pol_density")
call ifile_append (ifile, "LIS beams_pol_spec = smatrix, smatrix?")
call ifile_append (ifile, "SEQ smatrix = '@' smatrix_arg")
! call ifile_append (ifile, "KEY '@'")      !!! Key already exists
call ifile_append (ifile, "ARG smatrix_arg = ( sentry* )")
call ifile_append (ifile, "SEQ sentry = expr extra_sentry*")
call ifile_append (ifile, "SEQ extra_sentry = ':' expr")
call ifile_append (ifile, "SEQ cmd_beams_pol_fraction = " &
// "beams_pol_fraction '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_pol_fraction")
call ifile_append (ifile, "SEQ cmd_beams_momentum = " &
// "beams_momentum '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_momentum")
call ifile_append (ifile, "SEQ cmd_beams_theta = " &
// "beams_theta '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_theta")
call ifile_append (ifile, "SEQ cmd_beams_phi = " &
// "beams_phi '=' beams_par_spec")

```

```

call ifile_append (ifile, "KEY beams_phi")
call ifile_append (ifile, "LIS beams_par_spec = expr, expr?")
call ifile_append (ifile, "SEQ strfun_seq = '=' strfun_pair")
call ifile_append (ifile, "LIS strfun_pair = strfun_def, strfun_def?")
call ifile_append (ifile, "SEQ strfun_def = strfun_id")
call ifile_append (ifile, "ALT strfun_id = " &
    // "none | lhpdf | lhpdf_photon | pdf_builtin | pdf_builtin_photon | " &
    // "isr | epa | ewa | circe1 | circe2 | energy_scan | " &
    // "gaussian | beam_events")
call ifile_append (ifile, "KEY none")
call ifile_append (ifile, "KEY lhpdf")
call ifile_append (ifile, "KEY lhpdf_photon")
call ifile_append (ifile, "KEY pdf_builtin")
call ifile_append (ifile, "KEY pdf_builtin_photon")
call ifile_append (ifile, "KEY isr")
call ifile_append (ifile, "KEY epa")
call ifile_append (ifile, "KEY ewa")
call ifile_append (ifile, "KEY circe1")
call ifile_append (ifile, "KEY circe2")
call ifile_append (ifile, "KEY energy_scan")
call ifile_append (ifile, "KEY gaussian")
call ifile_append (ifile, "KEY beam_events")
call ifile_append (ifile, "SEQ cmd_integrate = " &
    // "integrate proc_arg options?")
call ifile_append (ifile, "KEY integrate")
call ifile_append (ifile, "ARG proc_arg = ( proc_id* )")
call ifile_append (ifile, "IDE proc_id")
call ifile_append (ifile, "SEQ cmd_iterations = " &
    // "iterations '=' iterations_list")
call ifile_append (ifile, "KEY iterations")
call ifile_append (ifile, "LIS iterations_list = iterations_spec+")
call ifile_append (ifile, "ALT iterations_spec = it_spec")
call ifile_append (ifile, "SEQ it_spec = expr calls_spec adapt_spec?")
call ifile_append (ifile, "SEQ calls_spec = ':' expr")
call ifile_append (ifile, "SEQ adapt_spec = ':' sexpr")
call ifile_append (ifile, "SEQ cmd_components = " &
    // "active '=' component_list")
call ifile_append (ifile, "KEY active")
call ifile_append (ifile, "LIS component_list = sexpr+")
call ifile_append (ifile, "SEQ cmd_sample_format = " &
    // "sample_format '=' event_format_list")
call ifile_append (ifile, "KEY sample_format")
call ifile_append (ifile, "LIS event_format_list = event_format+")
call ifile_append (ifile, "IDE event_format")
call ifile_append (ifile, "SEQ cmd_observable = " &
    // "observable analysis_tag options?")
call ifile_append (ifile, "KEY observable")
call ifile_append (ifile, "SEQ cmd_histogram = " &
    // "histogram analysis_tag histogram_arg " &
    // "options?")
call ifile_append (ifile, "KEY histogram")
call ifile_append (ifile, "ARG histogram_arg = (expr, expr, expr?)")
call ifile_append (ifile, "SEQ cmd_plot = plot analysis_tag options?")
call ifile_append (ifile, "KEY plot")

```

```

call ifile_append (ifile, "SEQ cmd_graph = graph graph_term '=' graph_def")
call ifile_append (ifile, "KEY graph")
call ifile_append (ifile, "SEQ graph_term = analysis_tag options?")
call ifile_append (ifile, "SEQ graph_def = graph_term graph_append*")
call ifile_append (ifile, "SEQ graph_append = '&' graph_term")
call ifile_append (ifile, "SEQ cmd_analysis = analysis '=' lexpr")
call ifile_append (ifile, "KEY analysis")
call ifile_append (ifile, "SEQ cmd_alt_setup = " &
    // "alt_setup '=' option_list_expr")
call ifile_append (ifile, "KEY alt_setup")
call ifile_append (ifile, "ALT option_list_expr = " &
    // "grouped_option_list | option_list")
call ifile_append (ifile, "GRO grouped_option_list = ( option_list_expr )")
call ifile_append (ifile, "LIS option_list = options+")
call ifile_append (ifile, "SEQ cmd_open_out = open_out open_arg options?")
call ifile_append (ifile, "SEQ cmd_close_out = close_out open_arg options?")
call ifile_append (ifile, "KEY open_out")
call ifile_append (ifile, "KEY close_out")
call ifile_append (ifile, "ARG open_arg = (sexpr)")
call ifile_append (ifile, "SEQ cmd_printf = printf_cmd options?")
call ifile_append (ifile, "SEQ printf_cmd = printf_clause sprintf_args?")
call ifile_append (ifile, "SEQ printf_clause = printf sexpr")
call ifile_append (ifile, "KEY printf")
call ifile_append (ifile, "SEQ cmd_record = record_cmd")
call ifile_append (ifile, "SEQ cmd_unstable = " &
    // "unstable cexpr unstable_arg options?")
call ifile_append (ifile, "KEY unstable")
call ifile_append (ifile, "ARG unstable_arg = ( proc_id* )")
call ifile_append (ifile, "SEQ cmd_stable = stable stable_list options?")
call ifile_append (ifile, "KEY stable")
call ifile_append (ifile, "LIS stable_list = cexpr+")
call ifile_append (ifile, "KEY polarized")
call ifile_append (ifile, "SEQ cmd_polarized = polarized polarized_list options?")
call ifile_append (ifile, "LIS polarized_list = cexpr+")
call ifile_append (ifile, "KEY unpolarized")
call ifile_append (ifile, "SEQ cmd_unpolarized = unpolarized unpolarized_list options?")
call ifile_append (ifile, "LIS unpolarized_list = cexpr+")
call ifile_append (ifile, "SEQ cmd_simulate = " &
    // "simulate proc_arg options?")
call ifile_append (ifile, "KEY simulate")
call ifile_append (ifile, "SEQ cmd_rescan = " &
    // "rescan sexpr proc_arg options?")
call ifile_append (ifile, "KEY rescan")
call ifile_append (ifile, "SEQ cmd_scan = scan scan_var scan_body?")
call ifile_append (ifile, "KEY scan")
call ifile_append (ifile, "ALT scan_var = " &
    // "scan_log_decl | scan_log | " &
    // "scan_int | scan_real | scan_complex | scan_num | " &
    // "scan_string_decl | scan_string | scan_alias | " &
    // "scan_cuts | scan_weight | " &
    // "scan_scale | scan_ren_scale | scan_fac_scale | " &
    // "scan_selection | scan_reweight | scan_analysis | " &
    // "scan_model | scan_library")
call ifile_append (ifile, "SEQ scan_log_decl = logical scan_log")

```

```

call ifile_append (ifile, "SEQ scan_log = '?' var_name '=' scan_log_arg")
call ifile_append (ifile, "ARG scan_log_arg = ( lexpr* )")
call ifile_append (ifile, "SEQ scan_int = int var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_real = real var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_complex = " &
// "complex var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_num = var_name '=' scan_num_arg")
call ifile_append (ifile, "ARG scan_num_arg = ( range* )")
call ifile_append (ifile, "ALT range = grouped_range | range_expr")
call ifile_append (ifile, "GRO grouped_range = ( range_expr )")
call ifile_append (ifile, "SEQ range_expr = expr range_spec?")
call ifile_append (ifile, "SEQ range_spec = '=>' expr step_spec?")
call ifile_append (ifile, "SEQ step_spec = step_op expr")
call ifile_append (ifile, "ALT step_op = " &
// "'/' | '/'- | '/'* | '/'/' | '/+/' | '/*/'")
call ifile_append (ifile, "KEY '/'")
call ifile_append (ifile, "KEY '/'-")
call ifile_append (ifile, "KEY '/'*")
call ifile_append (ifile, "KEY '/'/'")
call ifile_append (ifile, "KEY '/+/'")
call ifile_append (ifile, "KEY '/*/'")
call ifile_append (ifile, "SEQ scan_string_decl = string scan_string")
call ifile_append (ifile, "SEQ scan_string = " &
// "'$' var_name '=' scan_string_arg")
call ifile_append (ifile, "ARG scan_string_arg = ( sexpr* )")
call ifile_append (ifile, "SEQ scan_alias = " &
// "alias var_name '=' scan_alias_arg")
call ifile_append (ifile, "ARG scan_alias_arg = ( cexpr* )")
call ifile_append (ifile, "SEQ scan_cuts = cuts '=' scan_lexpr_arg")
call ifile_append (ifile, "ARG scan_lexpr_arg = ( lexpr* )")
call ifile_append (ifile, "SEQ scan_scale = scale '=' scan_expr_arg")
call ifile_append (ifile, "ARG scan_expr_arg = ( expr* )")
call ifile_append (ifile, "SEQ scan_fac_scale = " &
// "factorization_scale '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_ren_scale = " &
// "renormalization_scale '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_weight = weight '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_selection = selection '=' scan_lexpr_arg")
call ifile_append (ifile, "SEQ scan_reweight = reweight '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_analysis = analysis '=' scan_lexpr_arg")
call ifile_append (ifile, "SEQ scan_model = model '=' scan_model_arg")
call ifile_append (ifile, "ARG scan_model_arg = ( model_name* )")
call ifile_append (ifile, "SEQ scan_library = library '=' scan_library_arg")
call ifile_append (ifile, "ARG scan_library_arg = ( lib_name* )")
call ifile_append (ifile, "GRO scan_body = '{' command_list '}'")
call ifile_append (ifile, "SEQ cmd_if = " &
// "if lexpr then command_list elsif_clauses else_clause endif")
call ifile_append (ifile, "SEQ elsif_clauses = cmd_elseif*")
call ifile_append (ifile, "SEQ cmd_elseif = elsif lexpr then command_list")
call ifile_append (ifile, "SEQ else_clause = cmd_else?")
call ifile_append (ifile, "SEQ cmd_else = else command_list")
call ifile_append (ifile, "SEQ cmd_include = include include_arg")
call ifile_append (ifile, "KEY include")
call ifile_append (ifile, "ARG include_arg = ( string_literal )")

```

```

call ifile_append (ifile, "SEQ cmd_quit = quit_cmd quit_arg?")
call ifile_append (ifile, "ALT quit_cmd = quit | exit")
call ifile_append (ifile, "KEY quit")
call ifile_append (ifile, "KEY exit")
call ifile_append (ifile, "ARG quit_arg = ( expr )")
call ifile_append (ifile, "SEQ cmd_export = export show_arg options?")
call ifile_append (ifile, "KEY export")
call ifile_append (ifile, "SEQ cmd_write_analysis = " &
// "write_analysis_clause options?")
call ifile_append (ifile, "SEQ cmd_compile_analysis = " &
// "compile_analysis_clause options?")
call ifile_append (ifile, "SEQ write_analysis_clause = " &
// "write_analysis write_analysis_arg?")
call ifile_append (ifile, "SEQ compile_analysis_clause = " &
// "compile_analysis write_analysis_arg?")
call ifile_append (ifile, "KEY write_analysis")
call ifile_append (ifile, "KEY compile_analysis")
call ifile_append (ifile, "ARG write_analysis_arg = ( analysis_tag* )")
call ifile_append (ifile, "SEQ cmd_nlo = " &
// "nlo_calculation '=' nlo_calculation_list")
call ifile_append (ifile, "KEY nlo_calculation")
call ifile_append (ifile, "LIS nlo_calculation_list = nlo_comp+")
call ifile_append (ifile, "ALT nlo_comp = " // &
"full | born | real | virtual | dglap | subtraction | " // &
"mismatch | GKS")
call ifile_append (ifile, "KEY full")
call ifile_append (ifile, "KEY born")
call ifile_append (ifile, "KEY virtual")
call ifile_append (ifile, "KEY dglap")
call ifile_append (ifile, "KEY subtraction")
call ifile_append (ifile, "KEY mismatch")
call ifile_append (ifile, "KEY GKS")
call define_expr_syntax (ifile, particles=.true., analysis=.true.)
end subroutine define_cmd_list_syntax

```

<Commands: public>+≡

```
public :: lexer_init_cmd_list
```

<Commands: sub interfaces>+≡

```

module subroutine lexer_init_cmd_list (lexer, parent_lexer)
  type(lexer_t), intent(out) :: lexer
  type(lexer_t), intent(in), optional, target :: parent_lexer
end subroutine lexer_init_cmd_list

```

<Commands: procedures>+≡

```

module subroutine lexer_init_cmd_list (lexer, parent_lexer)
  type(lexer_t), intent(out) :: lexer
  type(lexer_t), intent(in), optional, target :: parent_lexer
  call lexer_init (lexer, &
    comment_chars = "#!", &
    quote_chars = '"', &
    quote_match = '"', &
    single_chars = "()[]{};,:%?${}@", &
    special_class = [ "+-*/^", "<>=~ " ], &
    keyword_list = syntax_get_keyword_list_ptr (syntax_cmd_list), &

```

```

        parent = parent_lexer)
end subroutine lexer_init_cmd_list

```

35.1.10 Unit Tests

Test module, followed by the corresponding implementation module.

`<commands_ut.f90>`≡
<File header>

```

module commands_ut
  use unit_tests
  use system_dependencies, only: MPOST_AVAILABLE
  use commands_uti

```

<Standard module head>

<Commands: public test>

`contains`

<Commands: test driver>

```

end module commands_ut

```

`<commands_uti.f90>`≡
<File header>

```

module commands_uti

  <Use kinds>
  use kinds, only: i64
  <Use strings>
  use io_units
  use ifiles
  use parser
  use interactions, only: reset_interaction_counter
  use prclib_stacks
  use analysis
  use variables, only: var_list_t
  use models
  use slha_interface
  use rt_data
  use event_base, only: generic_event_t, event_callback_t
  use commands

```

<Standard module head>

<Commands: test declarations>

<Commands: test auxiliary types>

`contains`

<Commands: tests>

<Commands: test auxiliary>

end module commands_util

API: driver for the unit tests below.

<Commands: public test>≡

public :: commands_test

<Commands: test driver>≡

subroutine commands_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Commands: execute tests>

end subroutine commands_test

Prepare Sindarin code

This routine parses an internal file, prints the parse tree, and returns a parse node to the root. We use the routine in the tests below.

<Commands: public test auxiliary>≡

public :: parse_ifile

<Commands: test auxiliary>≡

subroutine parse_ifile (ifile, pn_root, u)

use ifiles

use lexers

use parser

use commands

type(ifile_t), intent(in) :: ifile

type(parse_node_t), pointer, intent(out) :: pn_root

integer, intent(in), optional :: u

type(stream_t), target :: stream

type(lexer_t), target :: lexer

type(parse_tree_t) :: parse_tree

call lexer_init_cmd_list (lexer)

call stream_init (stream, ifile)

call lexer_assign_stream (lexer, stream)

call parse_tree_init (parse_tree, syntax_cmd_list, lexer)

if (present (u)) call parse_tree_write (parse_tree, u)

pn_root => parse_tree%get_root_ptr ()

call stream_final (stream)

call lexer_final (lexer)

end subroutine parse_ifile

Empty command list

Compile and execute an empty command list. Should do nothing but test the integrity of the workflow.

```
(Commands: execute tests)≡
    call test (commands_1, "commands_1", &
               "empty command list", &
               u, results)

(Commands: test declarations)≡
    public :: commands_1

(Commands: tests)≡
    subroutine commands_1 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_1"
        write (u, "(A)")  "* Purpose: compile and execute empty command list"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "* Parse empty file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"

        if (associated (pn_root)) then
            call command_list%compile (pn_root, global)
        end if

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"

        call global%activate ()
        call command_list%execute (global)
        call global%deactivate ()

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call ifile_final (ifile)

        call command_list%final ()
```



```

call syntax_cmd_list_final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_1"

end subroutine commands_1

```

Read model

Execute a model assignment.

```

<Commands: execute tests>+≡
  call test (commands_2, "commands_2", &
    "model", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_2

<Commands: tests>+≡
  subroutine commands_2 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_2"
    write (u, "(A)")  "* Purpose: set model"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call syntax_model_file_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'model = "Test"')

    call ifile_write (ifile, u)

    write (u, "(A)")  "* Parse file"
    write (u, "(A)")

    call parse_ifile (ifile, pn_root, u)

    write (u, "(A)")
    write (u, "(A)")  "* Compile command list"
    write (u, "(A)")

```

```

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_2"

end subroutine commands_2

```

Declare Process

Read a model, then declare a process. The process library is allocated explicitly. For the process definition, We take the default (*omega*) method. Since we do not compile, O'MEGA is not actually called.

```

<Commands: execute tests>+≡
  call test (commands_3, "commands_3", &
    "process declaration", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_3

<Commands: tests>+≡
  subroutine commands_3 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_3"
    write (u, "(A)")  "* Purpose: define process"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()

```

```

call syntax_model_file_init ()
call global%global_init ()
call global%var_list%set_log (var_str ("?omega_omp"), &
    .false., is_known = .true.)

allocate (lib)
call lib%init (var_str ("lib_cmd3"))
call global%add_prclib (lib)

write (u, "(A)")  "*  Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process t3 = s, s => s, s')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*  Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "*  Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "*  Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "*  Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "*  Test output end: commands_3"

end subroutine commands_3

```

Compile Process

Read a model, then declare a process and compile the library. The process library is allocated explicitly. For the process definition, We take the default (`unit_test`) method. There is no external code, so compilation of the library is merely a formal status change.

```
(Commands: execute tests)+≡
    call test (commands_4, "commands_4", &
              "compilation", &
              u, results)

(Commands: test declarations)+≡
    public :: commands_4

(Commands: tests)+≡
    subroutine commands_4 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_4"
        write (u, "(A)")  "* Purpose: define process and compile library"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%var_list%set_string (var_str ("$method"), &
                                         var_str ("unit_test"), is_known=.true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd4"))
        call global%add_prclib (lib)

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'model = "Test"')
        call ifile_append (ifile, 'process t4 = s, s => s, s')
        call ifile_append (ifile, 'compile ("lib_cmd4")')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_4"

end subroutine commands_4

```

Integrate Process

Read a model, then declare a process, compile the library, and integrate over phase space. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration.

```

<Commands: execute tests>+≡
  call test (commands_5, "commands_5", &
    "integration", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_5

<Commands: tests>+≡
  subroutine commands_5 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_5"
  end subroutine

```

```

write (u, "(A)")  "*   Purpose: define process, iterations, and integrate"
write (u, "(A)")

write (u, "(A)")  "*   Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()
call global%var_list%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"), &
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)
call global%var_list%set_int (var_str ("seed"), 0, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd5"))
call global%add_prclib (lib)

write (u, "(A)")  "*   Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process t5 = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (t5)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*   Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "*   Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "*   Execute command list"
write (u, "(A)")

```

```

call reset_interaction_counter ()
call command_list%execute (global)

call global%it_list%write (u)
write (u, "(A)")
call global%process_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_5"

end subroutine commands_5

```

Variables

Set intrinsic and user-defined variables.

```

<Commands: execute tests>+≡
call test (commands_6, "commands_6", &
    "variables", &
    u, results)

<Commands: test declarations>+≡
public :: commands_6

<Commands: tests>+≡
subroutine commands_6 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_6"
    write (u, "(A)")  "* Purpose: define and set variables"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()
    call global%write_vars (u, [ &
        var_str ("$_run_id"), &
        var_str ("?unweighted"), &

```

```

var_str ("sqrts"]])

write (u, "(A)")
write (u, "(A)")  "*  Input file"
write (u, "(A)")

call ifile_append (ifile, '$run_id = "run1"')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'sqrts = 1000')
call ifile_append (ifile, 'int j = 10')
call ifile_append (ifile, 'real x = 1000.')
call ifile_append (ifile, 'complex z = 5')
call ifile_append (ifile, 'string $text = "abcd"')
call ifile_append (ifile, 'logical ?flag = true')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*  Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "*  Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "*  Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_vars (u, [ &
var_str ("run_id"), &
var_str ("unweighted"), &
var_str ("sqrts"), &
var_str ("j"), &
var_str ("x"), &
var_str ("z"), &
var_str ("text"), &
var_str ("flag"]])

write (u, "(A)")
write (u, "(A)")  "*  Cleanup"

call ifile_final (ifile)

call command_list%final ()
call syntax_cmd_list_final ()

```



```

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_6"

end subroutine commands_6

```

Process library

Open process libraries explicitly.

```

<Commands: execute tests>+≡
call test (commands_7, "commands_7", &
    "process library", &
    u, results)

<Commands: test declarations>+≡
public :: commands_7

<Commands: tests>+≡
subroutine commands_7 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_7"
    write (u, "(A)")  "* Purpose: declare process libraries"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()
    call global%var_list%set_log (var_str ("?omega_omp"), &
        .false., is_known = .true.)
    global%os_data%fc = "Fortran-compiler"
    global%os_data%fcflags = "Fortran-flags"
    global%os_data%fclibs = "Fortran-libs"

    write (u, "(A)")
    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'library = "lib_cmd7_1"')
    call ifile_append (ifile, 'library = "lib_cmd7_2"')
    call ifile_append (ifile, 'library = "lib_cmd7_1"')

    call ifile_write (ifile, u)

    write (u, "(A)")
    write (u, "(A)")  "* Parse file"
    write (u, "(A)")

```

```

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_libraries (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call syntax_cmd_list_final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_7"

end subroutine commands_7

```

Generate events

Read a model, then declare a process, compile the library, and generate weighted events. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration.

```

<Commands: execute tests>+≡
  call test (commands_8, "commands_8", &
    "event generation", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_8

<Commands: tests>+≡
  subroutine commands_8 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

```

```

write (u, "(A)")  "* Test output: commands_8"
write (u, "(A)")  "* Purpose: define process, integrate, generate events"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%var_list%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"), &
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd8"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_8_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_8_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'simulate (commands_8_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"

```

```

write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_8"

end subroutine commands_8

```

Define cuts

Declare a cut expression.

```

<Commands: execute tests>+≡
  call test (commands_9, "commands_9", &
    "cuts", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_9

<Commands: tests>+≡
  subroutine commands_9 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(string_t), dimension(0) :: no_vars

    write (u, "(A)")  "* Test output: commands_9"
    write (u, "(A)")  "* Purpose: define cuts"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

```

```

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'cuts = all Pt > 0 [particle]')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write (u, vars = no_vars)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_9"

end subroutine commands_9

```

Beams

Define beam setup.

```

<Commands: execute tests>+≡
  call test (commands_10, "commands_10", &
    "beams", &
    u, results)
<Commands: test declarations>+≡

```

```

public :: commands_10
<Commands: tests>+≡
subroutine commands_10 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_10"
  write (u, "(A)")  "* Purpose: define beams"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call syntax_model_file_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'model = QCD')
  call ifile_append (ifile, 'sqrts = 1000')
  call ifile_append (ifile, 'beams = p, p')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root, u)

  write (u, "(A)")
  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)
  call command_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Execute command list"
  write (u, "(A)")

  call command_list%execute (global)

  call global%write_beams (u)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call ifile_final (ifile)

```

```

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_10"

end subroutine commands_10

```

Structure functions

Define beam setup with structure functions

```

<Commands: execute tests>+≡
call test (commands_11, "commands_11", &
  "structure functions", &
  u, results)

<Commands: test declarations>+≡
public :: commands_11

<Commands: tests>+≡
subroutine commands_11 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_11"
  write (u, "(A)")  "* Purpose: define beams with structure functions"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call syntax_model_file_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'model = QCD')
  call ifile_append (ifile, 'sqrts = 1100')
  call ifile_append (ifile, 'beams = p, p => lhpdf => pdf_builtin, isr')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

```

```

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_beams (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_11"

end subroutine commands_11

```

Rescan events

Read a model, then declare a process, compile the library, and generate weighted events. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration. Then, rescan the generated event sample.

```

<Commands: execute tests>+≡
  call test (commands_12, "commands_12", &
    "event rescanning", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_12

<Commands: tests>+≡
  subroutine commands_12 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

```



```

type(prclib_entry_t), pointer :: lib

write (u, "(A)")  "* Test output: commands_12"
write (u, "(A)")  "* Purpose: generate events and rescan"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()

call global%global_init ()
call global%var_list%append_log (&
    var_str ("?rebuild_phase_space"), .false., &
    intrinsic=.true.)
call global%var_list%append_log (&
    var_str ("?rebuild_grids"), .false., &
    intrinsic=.true.)
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%var_list%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("$integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd12"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_12_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_12_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'simulate (commands_12_p)')
call ifile_append (ifile, '?write_raw = false')
call ifile_append (ifile, 'rescan "commands_12_p" (commands_12_p)')

```

```

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_12"

end subroutine commands_12

```

Event Files

Set output formats for event files.

```

<Commands: execute tests>+≡
  call test (commands_13, "commands_13", &
    "event output formats", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_13

<Commands: tests>+≡
  subroutine commands_13 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

```

```

logical :: exist

write (u, "(A)")  "* Test output: commands_13"
write (u, "(A)")  "* Purpose: generate events and rescan"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%var_list%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)

allocate (lib)
call lib%init (var_str ("lib_cmd13"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_13_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_13_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 1')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'sample_format = weight_stream')
call ifile_append (ifile, 'simulate (commands_13_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Verify output files"
write (u, "(A)")

inquire (file = "commands_13_p.evx", exist = exist)
if (exist) write (u, "(1x,A)") "raw"

inquire (file = "commands_13_p.weights.dat", exist = exist)
if (exist) write (u, "(1x,A)") "weight_stream"

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_13"

end subroutine commands_13

```

Compile Empty Libraries

(This is a regression test:) Declare two empty libraries and compile them.

```

<Commands: execute tests>+≡
  call test (commands_14, "commands_14", &
    "empty libraries", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_14

<Commands: tests>+≡
  subroutine commands_14 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global

```

```

type(parse_node_t), pointer :: pn_root

write (u, "(A)")  "* Test output: commands_14"
write (u, "(A)")  "* Purpose: define and compile empty libraries"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_cmd_list_init ()

call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'library = "lib1"')
call ifile_append (ifile, 'library = "lib2"')
call ifile_append (ifile, 'compile ()')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()

call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: commands_14"

    end subroutine commands_14

```

Compile Process

Read a model, then declare a process and compile the library. The process library is allocated explicitly. For the process definition, We take the default (`unit_test`) method. There is no external code, so compilation of the library is merely a formal status change.

```

<Commands: execute tests>+≡
    call test (commands_15, "commands_15", &
        "compilation", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_15

<Commands: tests>+≡
    subroutine commands_15 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_15"
        write (u, "(A)")  "* Purpose: define process and compile library"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%var_list%set_string (var_str ("$method"), &
            var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("$phs_method"), &
            var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("$integration_method"), &
            var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_real (var_str ("sqrts"), &
            1000._default, is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
            .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
            .false., is_known = .true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd15"))
        call global%add_prclib (lib)

```

```

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process t15 = s, s => s, s')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (t15)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_15"

end subroutine commands_15

```

Observable

Declare an observable, fill it and display.

```

<Commands: execute tests>+≡
  call test (commands_16, "commands_16", &
    "observables", &
    u, results)
<Commands: test declarations>+≡

```

```

public :: commands_16
<Commands: tests>+≡
subroutine commands_16 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_16"
  write (u, "(A)")  "*   Purpose: declare an observable"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, '$obs_label = "foo"')
  call ifile_append (ifile, '$obs_unit = "cm"')
  call ifile_append (ifile, '$title = "Observable foo"')
  call ifile_append (ifile, '$description = "This is observable foo"')
  call ifile_append (ifile, 'observable foo')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root)

  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)

  call command_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Execute command list"
  write (u, "(A)")

  call command_list%execute (global)

  write (u, "(A)")  "* Record two data items"
  write (u, "(A)")

  call analysis_record_data (var_str ("foo"), 1._default)
  call analysis_record_data (var_str ("foo"), 3._default)

```



```

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_16"

end subroutine commands_16

```

Histogram

Declare a histogram, fill it and display.

```

<Commands: execute tests>+≡
  call test (commands_17, "commands_17", &
    "histograms", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_17

<Commands: tests>+≡
  subroutine commands_17 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(string_t), dimension(3) :: name
    integer :: i

    write (u, "(A)")  "* Test output: commands_17"
    write (u, "(A)")  "* Purpose: declare histograms"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"

```

```

write (u, "(A)")

call ifile_append (ifile, '$obs_label = "foo"')
call ifile_append (ifile, '$obs_unit = "cm"')
call ifile_append (ifile, '$title = "Histogram foo"')
call ifile_append (ifile, '$description = "This is histogram foo"')
call ifile_append (ifile, 'histogram foo (0,5,1)')
call ifile_append (ifile, '$title = "Histogram bar"')
call ifile_append (ifile, '$description = "This is histogram bar"')
call ifile_append (ifile, 'n_bins = 2')
call ifile_append (ifile, 'histogram bar (0,5)')
call ifile_append (ifile, '$title = "Histogram gee"')
call ifile_append (ifile, '$description = "This is histogram gee"')
call ifile_append (ifile, '?normalize_bins = true')
call ifile_append (ifile, 'histogram gee (0,5)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Record two data items"
write (u, "(A)")

name(1) = "foo"
name(2) = "bar"
name(3) = "gee"

do i = 1, 3
  call analysis_record_data (name(i), 0.1_default, &
    weight = 0.25_default)
  call analysis_record_data (name(i), 3.1_default)
  call analysis_record_data (name(i), 4.1_default, &
    excess = 0.5_default)
  call analysis_record_data (name(i), 7.1_default)
end do

write (u, "(A)")  "* Display analysis store"

```

```

write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_17"

end subroutine commands_17

```

Plot

Declare a plot, fill it and display contents.

```

<Commands: execute tests>+≡
  call test (commands_18, "commands_18", &
    "plots", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_18

<Commands: tests>+≡
  subroutine commands_18 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_18"
    write (u, "(A)")  "* Purpose: declare a plot"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, '$obs_label = "foo"')
    call ifile_append (ifile, '$obs_unit = "cm"')

```

```

call ifile_append (ifile, '$title = "Plot foo"')
call ifile_append (ifile, '$description = "This is plot foo"')
call ifile_append (ifile, '$x_label = "x axis"')
call ifile_append (ifile, '$y_label = "y axis"')
call ifile_append (ifile, '?x_log = false')
call ifile_append (ifile, '?y_log = true')
call ifile_append (ifile, 'x_min = -1')
call ifile_append (ifile, 'x_max = 1')
call ifile_append (ifile, 'y_min = 0.1')
call ifile_append (ifile, 'y_max = 1000')
call ifile_append (ifile, 'plot foo')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Record two data items"
write (u, "(A)")

call analysis_record_data (var_str ("foo"), 0._default, 20._default, &
    xerr = 0.25_default)
call analysis_record_data (var_str ("foo"), 0.5_default, 0.2_default, &
    yerr = 0.07_default)
call analysis_record_data (var_str ("foo"), 3._default, 2._default)

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()

```

```

call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_18"

end subroutine commands_18

```

Graph

Combine two (empty) plots to a graph.

```

<Commands: execute tests>+≡
call test (commands_19, "commands_19", &
    "graphs", &
    u, results)

<Commands: test declarations>+≡
public :: commands_19

<Commands: tests>+≡
subroutine commands_19 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_19"
    write (u, "(A)")  "* Purpose: combine two plots to a graph"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'plot a')
    call ifile_append (ifile, 'plot b')
    call ifile_append (ifile, '$title = "Graph foo"')
    call ifile_append (ifile, '$description = "This is graph foo"')
    call ifile_append (ifile, 'graph foo = a & b')

    call ifile_write (ifile, u)

    write (u, "(A)")
    write (u, "(A)")  "* Parse file"
    write (u, "(A)")

    call parse_ifile (ifile, pn_root)

```

```

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (var_str ("foo"), u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_19"

end subroutine commands_19

```

Record Data

Record data in previously allocated analysis objects.

```

<Commands: execute tests>+≡
  call test (commands_20, "commands_20", &
    "record data", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_20

<Commands: tests>+≡
  subroutine commands_20 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

```

```

write (u, "(A)")  "* Test output: commands_20"
write (u, "(A)")  "* Purpose: record data"
write (u, "(A)")

write (u, "(A)")  "* Initialization: create observable, histogram, plot"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

call analysis_init_observable (var_str ("o"))
call analysis_init_histogram (var_str ("h"), 0._default, 1._default, 3, &
    normalize_bins = .false.)
call analysis_init_plot (var_str ("p"))

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'record o (1.234)')
call ifile_append (ifile, 'record h (0.5)')
call ifile_append (ifile, 'record p (1, 2)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (u, verbose = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()

```

```

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_20"

end subroutine commands_20

```

Analysis

Declare an analysis expression and use it to fill an observable during event generation.

```

<Commands: execute tests>+≡
  call test (commands_21, "commands_21", &
    "analysis expression", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_21

<Commands: tests>+≡
  subroutine commands_21 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_21"
    write (u, "(A)")  "* Purpose: create and use analysis expression"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create observable"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call syntax_model_file_init ()
    call global%global_init ()
    call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

    call global%var_list%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known=.true.)
    call global%var_list%set_string (var_str ("$phs_method"), &
      var_str ("single"), is_known=.true.)
    call global%var_list%set_string (var_str ("$integration_method"), &
      var_str ("midpoint"), is_known=.true.)
    call global%var_list%set_log (var_str ("?vis_history"), &
      .false., is_known=.true.)
    call global%var_list%set_log (var_str ("?integration_timer"), &

```



```

        .false., is_known = .true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd8"))
call global%add_prclib (lib)

call analysis_init_observable (var_str ("m"))

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_21_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:100')
call ifile_append (ifile, 'integrate (commands_21_p)')
call ifile_append (ifile, '?unweighted = true')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'observable m')
call ifile_append (ifile, 'analysis = record m (eval M [s])')
call ifile_append (ifile, 'simulate (commands_21_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_21"

end subroutine commands_21

```

Write Analysis

Write accumulated analysis data to file.

```

<Commands: execute tests>+≡
  call test (commands_22, "commands_22", &
    "write analysis", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_22

<Commands: tests>+≡
  subroutine commands_22 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    integer :: u_file, iostat
    logical :: exist
    character(80) :: buffer

    write (u, "(A)")  "* Test output: commands_22"
    write (u, "(A)")  "* Purpose: write analysis data"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create observable"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    call analysis_init_observable (var_str ("m"))
    call analysis_record_data (var_str ("m"), 125._default)

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, '$out_file = "commands_22.dat"')
    call ifile_append (ifile, 'write_analysis')

```

```

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis data"
write (u, "(A)")

inquire (file = "commands_22.dat", exist = exist)
if (.not. exist) then
    write (u, "(A)")  "ERROR: File commands_22.dat not found"
    return
end if

u_file = free_unit ()
open (u_file, file = "commands_22.dat", &
      action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat)  buffer
    if (iostat /= 0)  exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_22"

```

```
end subroutine commands_22
```

Compile Analysis

Write accumulated analysis data to file and compile.

```
<Commands: execute tests>+≡
  if (MPOST_AVAILABLE) then
    call test (commands_23, "commands_23", &
      "compile analysis", &
      u, results)
  end if

<Commands: test declarations>+≡
  public :: commands_23

<Commands: tests>+≡
  subroutine commands_23 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    integer :: u_file, iostat
    character(256) :: buffer
    logical :: exist
    type(graph_options_t) :: graph_options

    write (u, "(A)")  "* Test output: commands_23"
    write (u, "(A)")  "* Purpose: write and compile analysis data"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create and fill histogram"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    call graph_options%init ()
    call graph_options%set (title = var_str ("Histogram for test: commands 23"), &
      description = var_str ("This is a test."), &
      width_mm = 125, height_mm = 85)
    call analysis_init_histogram (var_str ("h"), &
      0._default, 10._default, 2._default, .false., &
      graph_options = graph_options)
    call analysis_record_data (var_str ("h"), 1._default)
    call analysis_record_data (var_str ("h"), 1._default)
    call analysis_record_data (var_str ("h"), 1._default)
    call analysis_record_data (var_str ("h"), 1._default)
    call analysis_record_data (var_str ("h"), 3._default)
    call analysis_record_data (var_str ("h"), 3._default)
    call analysis_record_data (var_str ("h"), 3._default)
    call analysis_record_data (var_str ("h"), 5._default)
    call analysis_record_data (var_str ("h"), 7._default)
    call analysis_record_data (var_str ("h"), 7._default)
```

```

call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, '$out_file = "commands_23.dat"')
call ifile_append (ifile, 'compile_analysis')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Delete Postscript output"
write (u, "(A)")

inquire (file = "commands_23.ps", exist = exist)
if (exist) then
  u_file = free_unit ()
  open (u_file, file = "commands_23.ps", action = "write", status = "old")
  close (u_file, status = "delete")
end if
inquire (file = "commands_23.ps", exist = exist)
write (u, "(1x,A,L1)")  "Postscript output exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* TeX file"
write (u, "(A)")

inquire (file = "commands_23.tex", exist = exist)

```

```

if (.not. exist) then
  write (u, "(A)") "ERROR: File commands_23.tex not found"
  return
end if

u_file = free_unit ()
open (u_file, file = "commands_23.tex", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)
write (u, *)

inquire (file = "commands_23.ps", exist = exist)
write (u, "(1x,A,L1)") "Postscript output exists = ", exist

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: commands_23"

end subroutine commands_23

```

Histogram

Declare a histogram, fill it and display.

```

<Commands: execute tests>+≡
  call test (commands_24, "commands_24", &
            "drawing options", &
            u, results)

<Commands: test declarations>+≡
  public :: commands_24

<Commands: tests>+≡
  subroutine commands_24 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

```

```

write (u, "(A)")  "* Test output: commands_24"
write (u, "(A)")  "* Purpose: check graph and drawing options"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, '$title = "Title"')
call ifile_append (ifile, '$description = "Description"')
call ifile_append (ifile, '$x_label = "X Label"')
call ifile_append (ifile, '$y_label = "Y Label"')
call ifile_append (ifile, 'graph_width_mm = 111')
call ifile_append (ifile, 'graph_height_mm = 222')
call ifile_append (ifile, 'x_min = -11')
call ifile_append (ifile, 'x_max = 22')
call ifile_append (ifile, 'y_min = -33')
call ifile_append (ifile, 'y_max = 44')
call ifile_append (ifile, '$gmlcode_bg = "GML Code BG"')
call ifile_append (ifile, '$gmlcode_fg = "GML Code FG"')
call ifile_append (ifile, '$fill_options = "Fill Options"')
call ifile_append (ifile, '$draw_options = "Draw Options"')
call ifile_append (ifile, '$err_options = "Error Options"')
call ifile_append (ifile, '$symbol = "Symbol"')
call ifile_append (ifile, 'histogram foo (0,1)')
call ifile_append (ifile, 'plot bar')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis store"

```

```

write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_24"

end subroutine commands_24

```

Local Environment

Declare a local environment.

```

<Commands: execute tests>+≡
  call test (commands_25, "commands_25", &
    "local process environment", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_25

<Commands: tests>+≡
  subroutine commands_25 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_25"
    write (u, "(A)")  "* Purpose: declare local environment for process"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_cmd_list_init ()
    call global%global_init ()
    call global%var_list%set_log (var_str ("?omega_omp"), &
      .false., is_known = .true.)

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'library = "commands_25_lib"')
    call ifile_append (ifile, 'model = "Test"')

```



```

call ifile_append (ifile, 'process commands_25_p1 = g, g => g, g &
    &{ model = "QCD" }')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)
call global%write_libraries (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_25"

end subroutine commands_25

```

Alternative Setups

Declare a list of alternative setups.

```

<Commands: execute tests>+≡
    call test (commands_26, "commands_26", &
        "alternative setups", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_26

<Commands: tests>+≡
    subroutine commands_26 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile

```

```

type(command_list_t), target :: command_list
type(rt_data_t), target :: global
type(parse_node_t), pointer :: pn_root

write (u, "(A)")  "* Test output: commands_26"
write (u, "(A)")  "* Purpose: declare alternative setups for simulation"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'int i = 0')
call ifile_append (ifile, 'alt_setup = ({ i = 1 }, { i = 2 })')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_26"

end subroutine commands_26

```

Unstable Particle

Define decay processes and declare a particle as unstable. Also check the commands stable, polarized, unpolarized.

```
<Commands: execute tests>+≡
    call test (commands_27, "commands_27", &
               "unstable and polarized particles", &
               u, results)

<Commands: test declarations>+≡
    public :: commands_27

<Commands: tests>+≡
    subroutine commands_27 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_27"
        write (u, "(A)")  "* Purpose: modify particle properties"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%var_list%set_string (var_str ("$method"), &
                                         var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("$phs_method"), &
                                         var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("$integration_method"), &
                                         var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
                                     .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
                                     .false., is_known = .true.)

        allocate (lib)
        call lib%init (var_str ("commands_27_lib"))
        call global%add_prclib (lib)

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'model = "Test"')
        call ifile_append (ifile, 'ff = 0.4')
        call ifile_append (ifile, 'process d1 = s => f, fbar')
        call ifile_append (ifile, 'unstable s (d1)')
        call ifile_append (ifile, 'polarized f, fbar')

        call ifile_write (ifile, u)

        write (u, "(A)")
```

```

write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, '?diagonal_decay = true')
call ifile_append (ifile, 'unstable s (d1)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

```

```

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, '?isotropic_decay = true')
call ifile_append (ifile, 'unstable s (d1)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, 'stable s')
call ifile_append (ifile, 'unpolarized f')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

```

```

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_model_file_init ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_27"

end subroutine commands_27

```

Quit the program

Quit the program.

```

<Commands: execute tests>+≡
call test (commands_28, "commands_28", &
    "quit", &
    u, results)

<Commands: test declarations>+≡
public :: commands_28

<Commands: tests>+≡
subroutine commands_28 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root1, pn_root2
    type(string_t), dimension(0) :: no_vars

    write (u, "(A)")  "* Test output: commands_28"
    write (u, "(A)")  "* Purpose: quit the program"
    write (u, "(A)")

```

```

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file: quit without code"
write (u, "(A)")

call ifile_append (ifile, 'quit')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root1, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root1, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write (u, vars = no_vars)

write (u, "(A)")
write (u, "(A)")  "* Input file: quit with code"
write (u, "(A)")

call ifile_final (ifile)
call command_list%final ()
call ifile_append (ifile, 'quit ( 3 + 4 )')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root2, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

```

```

call command_list%compile (pn_root2, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write (u, vars = no_vars)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_28"

end subroutine commands_28

```

SLHA interface

Testing commands steering the SLHA interface.

```

<Commands: execute tests>+≡
  call test (commands_29, "commands_29", &
    "SLHA interface", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_29

<Commands: tests>+≡
  subroutine commands_29 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(var_list_t), pointer :: model_vars
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_29"
    write (u, "(A)")  "* Purpose: test SLHA interface"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()

```



```

call syntax_model_file_init ()
call syntax_slha_init ()
call global%global_init ()

write (u, "(A)")  "* Model MSSM, read SLHA file"
write (u, "(A)")

call ifile_append (ifile, 'model = "MSSM"')
call ifile_append (ifile, '?slha_read_decays = true')
call ifile_append (ifile, 'read_slha ("spslap_decays.slha")')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Model MSSM, default values:"
write (u, "(A)")

call global%model%write (u, verbose = .false., &
    show_vertices = .false., show_particles = .false.)

write (u, "(A)")
write (u, "(A)")  "* Selected global variables"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%write_var (var_str ("mch1"), u)
call model_vars%write_var (var_str ("wch1"), u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Model MSSM, values from SLHA file"
write (u, "(A)")

call global%model%write (u, verbose = .false., &
    show_vertices = .false., show_particles = .false.)

```

```

write (u, "(A)")
write (u, "(A)")  "* Selected global variables"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%write_var (var_str ("mch1"), u)
call model_vars%write_var (var_str ("wch1"), u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_slha_final ()
call syntax_model_file_final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_29"

end subroutine commands_29

```

Expressions for scales

Declare a scale, factorization scale or factorization scale expression.

```

<Commands: execute tests>+≡
  call test (commands_30, "commands_30", &
    "scales", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_30

<Commands: tests>+≡
  subroutine commands_30 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_30"
    write (u, "(A)")  "* Purpose: define scales"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

```

```

write (u, "(A)")  "*  Input file"
write (u, "(A)")

call ifile_append (ifile, 'scale = 200 GeV')
call ifile_append (ifile, &
    'factorization_scale = eval Pt [particle]')
call ifile_append (ifile, &
    'renormalization_scale = eval E [particle]')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*  Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "*  Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "*  Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "*  Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "*  Test output end: commands_30"

end subroutine commands_30

```

Weight and reweight expressions

Declare an expression for event weights and reweighting.

```

(Commands: execute tests) +=
call test (commands_31, "commands_31", &
    "event weights/reweighting", &
    u, results)

```

```

<Commands: test declarations>+≡
    public :: commands_31

<Commands: tests>+≡
    subroutine commands_31 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_31"
        write (u, "(A)")  "*   Purpose: define weight/reweight"
        write (u, "(A)")

        write (u, "(A)")  "*   Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "*   Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'weight = eval Pz [particle]')
        call ifile_append (ifile, 'reweight = eval M2 [particle]')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "*   Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"
        write (u, "(A)")

        call command_list%execute (global)

        call global%write_expr (u)

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call ifile_final (ifile)

```

```

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_31"

end subroutine commands_31

```

Selecting events

Declare an expression for selecting events in an analysis.

```

<Commands: execute tests>+≡
call test (commands_32, "commands_32", &
  "event selection", &
  u, results)

<Commands: test declarations>+≡
public :: commands_32

<Commands: tests>+≡
subroutine commands_32 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_32"
  write (u, "(A)")  "* Purpose: define selection"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'selection = any PDG == 13 [particle]')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root, u)

  write (u, "(A)")
  write (u, "(A)")  "* Compile command list"

```

```

write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_32"

end subroutine commands_32

```

Executing shell commands

Execute a shell command.

```

<Commands: execute tests>+≡
  call test (commands_33, "commands_33", &
    "execute shell command", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_33

<Commands: tests>+≡
  subroutine commands_33 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    integer :: u_file, iostat
    character(3) :: buffer

    write (u, "(A)")  "* Test output: commands_33"
    write (u, "(A)")  "* Purpose: execute shell command"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

```

```

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'exec ("echo foo » bar"')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)
u_file = free_unit ()
open (u_file, file = "bar", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0) exit
end do
write (u, "(A,A)")  "should be 'foo': ", trim (buffer)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_33"

end subroutine commands_33

```

Callback

Instead of an explicit write, use the callback feature to write the analysis file during event generation. We generate 4 events and arrange that the callback is executed while writing the 3rd event.

```
(Commands: execute tests)+≡
    call test (commands_34, "commands_34", &
               "analysis via callback", &
               u, results)

(Commands: test declarations)+≡
    public :: commands_34

(Commands: tests)+≡
    subroutine commands_34 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib
        type(event_callback_34_t) :: event_callback

        write (u, "(A)")  "* Test output: commands_34"
        write (u, "(A)")  "* Purpose: write analysis data"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization: create observable"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        call syntax_model_file_init ()
        call global%global_init ()
        call global%init_fallback_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

        call global%var_list%set_string (var_str ("$method"), &
            var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("$phs_method"), &
            var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("$integration_method"), &
            var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_real (var_str ("sqrts"), &
            1000._default, is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
            .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
            .false., is_known=.true.)
        call global%var_list%set_int (var_str ("seed"), 0, is_known=.true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd34"))
        call global%add_prclib (lib)
```



```

write (u, "(A)")  "* Prepare callback for writing analysis to I/O unit"
write (u, "(A)")

event_callback%u = u
call global%set_event_callback (event_callback)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_34_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_34_p)')
call ifile_append (ifile, 'observable sq')
call ifile_append (ifile, 'analysis = record sq (sqrts)')
call ifile_append (ifile, 'n_events = 4')
call ifile_append (ifile, 'event_callback_interval = 3')
call ifile_append (ifile, 'simulate (commands_34_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: commands_34"

    end subroutine commands_34

```

For this test, we invent a callback object which simply writes the analysis file, using the standard call for this. Here we rely on the fact that the analysis data are stored as a global entity, otherwise we would have to access them via the event object.

```

<Commands: test auxiliary types>≡
    type, extends (event_callback_t) :: event_callback_34_t
    private
    integer :: u = 0
    contains
    procedure :: write => event_callback_34_write
    procedure :: proc => event_callback_34
    end type event_callback_34_t

```

The output routine is unused. The actual callback should write the analysis data to the output unit that we have injected into the callback object.

```

<Commands: test auxiliary>+≡
    subroutine event_callback_34_write (event_callback, unit)
    class(event_callback_34_t), intent(in) :: event_callback
    integer, intent(in), optional :: unit
    end subroutine event_callback_34_write

    subroutine event_callback_34 (event_callback, i, event)
    class(event_callback_34_t), intent(in) :: event_callback
    integer(i64), intent(in) :: i
    class(generic_event_t), intent(in) :: event
    call analysis_write (event_callback%u)
    end subroutine event_callback_34

```

35.2 Toplevel module WHIZARD

```
<whizard.f90>≡  
  <File header>  
  
  module whizard  
  
    use io_units  
    <Use strings>  
    use os_interface  
    use ifiles  
    use lexers  
    use parser  
    use rt_data  
  
    <Standard module head>  
  
    <WHIZARD: public>  
  
    <WHIZARD: types>  
  
    <WHIZARD: variables>  
  
    save  
  
    interface  
    <WHIZARD: sub interfaces>  
    end interface  
  
  end module whizard  
  
<whizard_sub.f90>≡  
  <File header>  
  
  submodule (whizard) whizard_s  
  
    use system_defs, only: VERSION_STRING  
    use system_defs, only: EOF, BACKSLASH  
    use diagnostics  
    use eval_trees  
    use models  
    use phs_forests  
    use prclib_stacks  
    use slha_interface  
    use commands  
  
    implicit none  
  
  contains  
  
    <WHIZARD: procedures>  
  
  end submodule whizard_s
```

35.2.1 Options

Here we introduce a wrapper that holds various user options, so they can transparently be passed from the main program to the `whizard` object. Most parameters are used for initializing the `global` state.

```
<WHIZARD: public>≡
    public :: whizard_options_t

<WHIZARD: types>≡
    type :: whizard_options_t
        type(string_t) :: job_id
        type(string_t), dimension(:), allocatable :: pack_args
        type(string_t), dimension(:), allocatable :: unpack_args
        type(string_t) :: preload_model
        type(string_t) :: default_lib
        type(string_t) :: preload_libraries
        logical :: rebuild_library = .false.
        logical :: recompile_library = .false.
        logical :: rebuild_phs = .false.
        logical :: rebuild_grids = .false.
        logical :: rebuild_events = .false.
    end type whizard_options_t
```

35.2.2 Parse tree stack

We collect all parse trees that we generate in the `whizard` object. To this end, we create a stack of parse trees. They must not be finalized before the `global` object is finalized, because items such as a cut definition may contain references to the parse tree from which they were generated.

```
<WHIZARD: types>+≡
    type, extends (parse_tree_t) :: pt_entry_t
        type(pt_entry_t), pointer :: previous => null ()
    end type pt_entry_t
```

This is the stack. Since we always prepend, we just need the `last` pointer.

```
<WHIZARD: types>+≡
    type :: pt_stack_t
        type(pt_entry_t), pointer :: last => null ()
        contains
            <WHIZARD: pt_stack: TBP>
    end type pt_stack_t
```

The finalizer is called at the very end.

```
<WHIZARD: pt_stack: TBP>≡
    procedure :: final => pt_stack_final

<WHIZARD: sub interfaces>≡
    module subroutine pt_stack_final (pt_stack)
        class(pt_stack_t), intent(inout) :: pt_stack
    end subroutine pt_stack_final
```

```

<WHIZARD: procedures>+=
module subroutine pt_stack_final (pt_stack)
  class(pt_stack_t), intent(inout) :: pt_stack
  type(pt_entry_t), pointer :: current
  do while (associated (pt_stack%last))
    current => pt_stack%last
    pt_stack%last => current%previous
    call parse_tree_final (current%parse_tree_t)
    deallocate (current)
  end do
end subroutine pt_stack_final

```

Create and push a new entry, keeping the previous ones.

```

<WHIZARD: pt_stack: TBP>+=
  procedure :: push => pt_stack_push

<WHIZARD: sub interfaces>+=
  module subroutine pt_stack_push (pt_stack, parse_tree)
    class(pt_stack_t), intent(inout) :: pt_stack
    type(parse_tree_t), intent(out), pointer :: parse_tree
  end subroutine pt_stack_push

<WHIZARD: procedures>+=
  module subroutine pt_stack_push (pt_stack, parse_tree)
    class(pt_stack_t), intent(inout) :: pt_stack
    type(parse_tree_t), intent(out), pointer :: parse_tree
    type(pt_entry_t), pointer :: current
    allocate (current)
    parse_tree => current%parse_tree_t
    current%previous => pt_stack%last
    pt_stack%last => current
  end subroutine pt_stack_push

```

35.2.3 The whizard object

An object of type `whizard_t` is the top-level wrapper for a WHIZARD instance. The object holds various default settings and the current state of the generator, the `global` object of type `rt_data_t`. This object contains, for instance, the list of variables and the process libraries.

Since components of the `global` subobject are frequently used as targets, the `whizard` object should also consistently carry the `target` attribute.

The various self-tests do not use this object. They initialize only specific subsets of the system, according to their needs.

Note: we intend to allow several concurrent instances. In the current implementation, there are still a few obstacles to this: the model library and the syntax tables are global variables, and the error handling uses global state. This should be improved.

```

<WHIZARD: public>+=
  public :: whizard_t

```

```

<WHIZARD: types>+=
  type :: whizard_t
    type(whizard_options_t) :: options
    type(rt_data_t) :: global
    type(pt_stack_t) :: pt_stack
  contains
    <WHIZARD: whizard: TBP>
  end type whizard_t

```

35.2.4 Initialization and finalization

```

<WHIZARD: whizard: TBP>=
  procedure :: init => whizard_init

<WHIZARD: sub interfaces>+=
  module subroutine whizard_init (whizard, options, paths, logfile)
    class(whizard_t), intent(out), target :: whizard
    type(whizard_options_t), intent(in) :: options
    type(paths_t), intent(in), optional :: paths
    type(string_t), intent(in), optional :: logfile
  end subroutine whizard_init

<WHIZARD: procedures>+=
  module subroutine whizard_init (whizard, options, paths, logfile)
    class(whizard_t), intent(out), target :: whizard
    type(whizard_options_t), intent(in) :: options
    type(paths_t), intent(in), optional :: paths
    type(string_t), intent(in), optional :: logfile
    call init_syntax_tables ()
    whizard%options = options
    call whizard%global%global_init (paths, logfile)
    call whizard%init_job_id ()
    call whizard%init_rebuild_flags ()
    call whizard%unpack_files ()
    call whizard%preload_model ()
    call whizard%preload_library ()
    call whizard%global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))
  end subroutine whizard_init

```

Apart from the global data which have been initialized above, the process and model lists need to be finalized.

```

<WHIZARD: whizard: TBP>+=
  procedure :: final => whizard_final

<WHIZARD: sub interfaces>+=
  module subroutine whizard_final (whizard)
    class(whizard_t), intent(inout), target :: whizard
  end subroutine whizard_final

<WHIZARD: procedures>+=
  module subroutine whizard_final (whizard)
    class(whizard_t), intent(inout), target :: whizard
    call whizard%global%final ()

```

```

    call whizard%pt_stack%final ()
    call whizard%pack_files ()
    call final_syntax_tables ()
end subroutine whizard_final

```

Set the job ID, if nonempty. If the ID string is empty, the value remains undefined.

```

<WHIZARD: whizard: TBP>+=
  procedure :: init_job_id => whizard_init_job_id

<WHIZARD: sub interfaces>+=
  module subroutine whizard_init_job_id (whizard)
    class(whizard_t), intent(inout), target :: whizard
  end subroutine whizard_init_job_id

<WHIZARD: procedures>+=
  module subroutine whizard_init_job_id (whizard)
    class(whizard_t), intent(inout), target :: whizard
    associate (var_list => whizard%global%var_list, options => whizard%options)
      if (options%job_id /= "") then
        call var_list%set_string (var_str ("$_job_id"), &
          options%job_id, is_known=.true.)
      end if
    end associate
  end subroutine whizard_init_job_id

```

Set the rebuild flags. They can be specified on the command line and set the initial value for the associated logical variables.

```

<WHIZARD: whizard: TBP>+=
  procedure :: init_rebuild_flags => whizard_init_rebuild_flags

<WHIZARD: sub interfaces>+=
  module subroutine whizard_init_rebuild_flags (whizard)
    class(whizard_t), intent(inout), target :: whizard
  end subroutine whizard_init_rebuild_flags

<WHIZARD: procedures>+=
  module subroutine whizard_init_rebuild_flags (whizard)
    class(whizard_t), intent(inout), target :: whizard
    associate (var_list => whizard%global%var_list, options => whizard%options)
      call var_list%append_log (var_str ("?rebuild_library"), &
        options%rebuild_library, intrinsic=.true.)
      call var_list%append_log (var_str ("?recompile_library"), &
        options%recompile_library, intrinsic=.true.)
      call var_list%append_log (var_str ("?rebuild_phase_space"), &
        options%rebuild_phs, intrinsic=.true.)
      call var_list%append_log (var_str ("?rebuild_grids"), &
        options%rebuild_grids, intrinsic=.true.)
      call var_list%append_log (var_str ("?rebuild_events"), &
        options%rebuild_events, intrinsic=.true.)
    end associate
  end subroutine whizard_init_rebuild_flags

```

Pack/unpack files in the working directory, if requested.

```
{WHIZARD: whizard: TBP}+=
  procedure :: pack_files => whizard_pack_files
  procedure :: unpack_files => whizard_unpack_files
{WHIZARD: sub interfaces}+=
  module subroutine whizard_pack_files (whizard)
    class(whizard_t), intent(in), target :: whizard
  end subroutine whizard_pack_files
  module subroutine whizard_unpack_files (whizard)
    class(whizard_t), intent(in), target :: whizard
  end subroutine whizard_unpack_files
{WHIZARD: procedures}+=
  module subroutine whizard_pack_files (whizard)
    class(whizard_t), intent(in), target :: whizard
    logical :: exist
    integer :: i
    type(string_t) :: file
    if (allocated (whizard%options%pack_args)) then
      do i = 1, size (whizard%options%pack_args)
        file = whizard%options%pack_args(i)
        call msg_message ("Packing file/dir '" // char (file) // "'")
        exist = os_file_exist (file) .or. os_dir_exist (file)
        if (exist) then
          call os_pack_file (whizard%options%pack_args(i), &
            whizard%global%os_data)
        else
          call msg_error ("File/dir '" // char (file) // "' not found")
        end if
      end do
    end if
  end subroutine whizard_pack_files

  module subroutine whizard_unpack_files (whizard)
    class(whizard_t), intent(in), target :: whizard
    logical :: exist
    integer :: i
    type(string_t) :: file
    if (allocated (whizard%options%unpack_args)) then
      do i = 1, size (whizard%options%unpack_args)
        file = whizard%options%unpack_args(i)
        call msg_message ("Unpacking file '" // char (file) // "'")
        exist = os_file_exist (file)
        if (exist) then
          call os_unpack_file (whizard%options%unpack_args(i), &
            whizard%global%os_data)
        else
          call msg_error ("File '" // char (file) // "' not found")
        end if
      end do
    end if
  end subroutine whizard_unpack_files
```

This procedure preloads a model, if a model name is given.


```

<WHIZARD: whizard: TBP>+=
  procedure :: preload_model => whizard_preload_model

<WHIZARD: sub interfaces>+=
  module subroutine whizard_preload_model (whizard)
    class(whizard_t), intent(inout), target :: whizard
    end subroutine whizard_preload_model

<WHIZARD: procedures>+=
  module subroutine whizard_preload_model (whizard)
    class(whizard_t), intent(inout), target :: whizard
    type(string_t) :: model_name
    model_name = whizard%options%preload_model
    if (model_name /= "") then
      call whizard%global%read_model (model_name, whizard%global%preload_model)
      whizard%global%model => whizard%global%preload_model
      if (associated (whizard%global%model)) then
        call whizard%global%model%link_var_list (whizard%global%var_list)
        call whizard%global%var_list%set_string (var_str ("$model_name"), &
          model_name, is_known = .true.)
        call msg_message ("Preloaded model: " &
          // char (model_name))
      else
        call msg_fatal ("Preloading model " // char (model_name) &
          // " failed")
      end if
    else
      call msg_message ("No model preloaded")
    end if
  end subroutine whizard_preload_model

```

This procedure preloads a library, if a library name is given.

Note: This version just opens a new library with that name. It does not load (yet) an existing library on file, as previous WHIZARD versions would do.

```

<WHIZARD: whizard: TBP>+=
  procedure :: preload_library => whizard_preload_library

<WHIZARD: sub interfaces>+=
  module subroutine whizard_preload_library (whizard)
    class(whizard_t), intent(inout), target :: whizard
    end subroutine whizard_preload_library

<WHIZARD: procedures>+=
  module subroutine whizard_preload_library (whizard)
    class(whizard_t), intent(inout), target :: whizard
    type(string_t) :: library_name, libs
    type(string_t), dimension(:), allocatable :: libname_static
    type(prclib_entry_t), pointer :: lib_entry
    integer :: i
    call get_prclib_static (libname_static)
    do i = 1, size (libname_static)
      allocate (lib_entry)
      call lib_entry%init_static (libname_static(i))
      call whizard%global%add_prclib (lib_entry)
    end do
    libs = adjustl (whizard%options%preload_libraries)

```

```

if (libs == "" .and. whizard%options%default_lib /= "") then
  allocate (lib_entry)
  call lib_entry%init (whizard%options%default_lib)
  call whizard%global%add_prclib (lib_entry)
  call msg_message ("Preloaded library: " // &
    char (whizard%options%default_lib))
end if
SCAN_LIBS: do while (libs /= "")
  call split (libs, library_name, " ")
  if (library_name /= "") then
    allocate (lib_entry)
    call lib_entry%init (library_name)
    call whizard%global%add_prclib (lib_entry)
    call msg_message ("Preloaded library: " // char (library_name))
  end if
end do SCAN_LIBS
end subroutine whizard_preload_library

```

35.2.5 Initialization and finalization: syntax tables

Initialize/finalize the syntax tables used by WHIZARD. These are effectively singleton objects. We introduce a module variable that tracks the initialization status.

Without syntax tables, essentially nothing will work. Any initializer has to call this.

```

<WHIZARD: variables>≡
  logical :: syntax_tables_exist = .false.

<WHIZARD: public>+≡
  public :: init_syntax_tables
  public :: final_syntax_tables

<WHIZARD: sub interfaces>+≡
  module subroutine init_syntax_tables ()
  end subroutine init_syntax_tables
  module subroutine final_syntax_tables ()
  end subroutine final_syntax_tables

<WHIZARD: procedures>+≡
  module subroutine init_syntax_tables ()
    if (.not. syntax_tables_exist) then
      call syntax_model_file_init ()
      call syntax_phs_forest_init ()
      call syntax_pexpr_init ()
      call syntax_slha_init ()
      call syntax_cmd_list_init ()
      syntax_tables_exist = .true.
    end if
  end subroutine init_syntax_tables

  module subroutine final_syntax_tables ()
    if (syntax_tables_exist) then
      call syntax_model_file_final ()
    end if
  end subroutine final_syntax_tables

```

```

        call syntax_phs_forest_final ()
        call syntax_pexpr_final ()
        call syntax_slha_final ()
        call syntax_cmd_list_final ()
        syntax_tables_exist = .false.
    end if
end subroutine final_syntax_tables

```

Write the syntax tables to external files.

```

<WHIZARD: public>+≡
    public :: write_syntax_tables

<WHIZARD: sub interfaces>+≡
    module subroutine write_syntax_tables ()
    end subroutine write_syntax_tables

<WHIZARD: procedures>+≡
    module subroutine write_syntax_tables ()
        integer :: unit
        character(*), parameter :: file_model = "whizard.model_file.syntax"
        character(*), parameter :: file_phs = "whizard.phase_space_file.syntax"
        character(*), parameter :: file_pexpr = "whizard.prt_expressions.syntax"
        character(*), parameter :: file_slha = "whizard.slha.syntax"
        character(*), parameter :: file_sindarin = "whizard.sindarin.syntax"
        if (.not. syntax_tables_exist) call init_syntax_tables ()
        unit = free_unit ()
        print *, "Writing file '" // file_model // "'"
        open (unit=unit, file=file_model, status="replace", action="write")
        write (unit, "(A)")  VERSION_STRING
        write (unit, "(A)")  "Syntax definition file: " // file_model
        call syntax_model_file_write (unit)
        close (unit)
        print *, "Writing file '" // file_phs // "'"
        open (unit=unit, file=file_phs, status="replace", action="write")
        write (unit, "(A)")  VERSION_STRING
        write (unit, "(A)")  "Syntax definition file: " // file_phs
        call syntax_phs_forest_write (unit)
        close (unit)
        print *, "Writing file '" // file_pexpr // "'"
        open (unit=unit, file=file_pexpr, status="replace", action="write")
        write (unit, "(A)")  VERSION_STRING
        write (unit, "(A)")  "Syntax definition file: " // file_pexpr
        call syntax_pexpr_write (unit)
        close (unit)
        print *, "Writing file '" // file_slha // "'"
        open (unit=unit, file=file_slha, status="replace", action="write")
        write (unit, "(A)")  VERSION_STRING
        write (unit, "(A)")  "Syntax definition file: " // file_slha
        call syntax_slha_write (unit)
        close (unit)
        print *, "Writing file '" // file_sindarin // "'"
        open (unit=unit, file=file_sindarin, status="replace", action="write")
        write (unit, "(A)")  VERSION_STRING
        write (unit, "(A)")  "Syntax definition file: " // file_sindarin
        call syntax_cmd_list_write (unit)
    end subroutine write_syntax_tables

```

```

        close (unit)
    end subroutine write_syntax_tables

```

35.2.6 Execute command lists

Process commands given on the command line, stored as an ifile. The whole input is read, compiled and executed as a whole.

```

<WHIZARD: whizard: TBP>+≡
    procedure :: process_ifile => whizard_process_ifile

<WHIZARD: sub interfaces>+≡
    module subroutine whizard_process_ifile (whizard, ifile, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(ifile_t), intent(in) :: ifile
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
    end subroutine whizard_process_ifile

<WHIZARD: procedures>+≡
    module subroutine whizard_process_ifile (whizard, ifile, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(ifile_t), intent(in) :: ifile
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
        type(lexer_t), target :: lexer
        type(stream_t), target :: stream
        call msg_message ("Reading commands given on the command line")
        call lexer_init_cmd_list (lexer)
        call stream_init (stream, ifile)
        call whizard%process_stream (stream, lexer, quit, quit_code)
        call stream_final (stream)
        call lexer_final (lexer)
    end subroutine whizard_process_ifile

```

Process standard input as a command list. The whole input is read, compiled and executed as a whole.

```

<WHIZARD: whizard: TBP>+≡
    procedure :: process_stdin => whizard_process_stdin

<WHIZARD: sub interfaces>+≡
    module subroutine whizard_process_stdin (whizard, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
    end subroutine whizard_process_stdin

<WHIZARD: procedures>+≡
    module subroutine whizard_process_stdin (whizard, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
        type(lexer_t), target :: lexer
        type(stream_t), target :: stream
        call msg_message ("Reading commands from standard input")
    end subroutine whizard_process_stdin

```

```

    call lexer_init_cmd_list (lexer)
    call stream_init (stream, 5)
    call whizard%process_stream (stream, lexer, quit, quit_code)
    call stream_final (stream)
    call lexer_final (lexer)
end subroutine whizard_process_stdin

```

Process a file as a command list.

```

<WHIZARD: whizard: TBP>+≡
    procedure :: process_file => whizard_process_file

<WHIZARD: sub interfaces>+≡
    module subroutine whizard_process_file (whizard, file, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(string_t), intent(in) :: file
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
    end subroutine whizard_process_file

<WHIZARD: procedures>+≡
    module subroutine whizard_process_file (whizard, file, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(string_t), intent(in) :: file
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
        type(lexer_t), target :: lexer
        type(stream_t), target :: stream
        logical :: exist
        call msg_message ("Reading commands from file '" // char (file) // "'")
        inquire (file=char(file), exist=exist)
        if (exist) then
            call lexer_init_cmd_list (lexer)
            call stream_init (stream, char (file))
            call whizard%process_stream (stream, lexer, quit, quit_code)
            call stream_final (stream)
            call lexer_final (lexer)
        else
            call msg_error ("File '" // char (file) // "' not found")
        end if
    end subroutine whizard_process_file

<WHIZARD: whizard: TBP>+≡
    procedure :: process_stream => whizard_process_stream

<WHIZARD: sub interfaces>+≡
    module subroutine whizard_process_stream &
        (whizard, stream, lexer, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(stream_t), intent(inout), target :: stream
        type(lexer_t), intent(inout), target :: lexer
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
    end subroutine whizard_process_stream

```

```

<WHIZARD: procedures>+≡
module subroutine whizard_process_stream &
    (whizard, stream, lexer, quit, quit_code)
    class(whizard_t), intent(inout), target :: whizard
    type(stream_t), intent(inout), target :: stream
    type(lexer_t), intent(inout), target :: lexer
    logical, intent(out) :: quit
    integer, intent(out) :: quit_code
    type(parse_tree_t), pointer :: parse_tree
    type(command_list_t), target :: command_list
    call lexer_assign_stream (lexer, stream)
    call whizard%pt_stack%push (parse_tree)
    call parse_tree_init (parse_tree, syntax_cmd_list, lexer)
    if (associated (parse_tree%get_root_ptr ())) then
        whizard%global%lexer => lexer
        call command_list%compile (parse_tree%get_root_ptr (), &
            whizard%global)
    end if
    call whizard%global%activate ()
    call command_list%execute (whizard%global)
    call command_list%final ()
    quit = whizard%global%quit
    quit_code = whizard%global%quit_code
end subroutine whizard_process_stream

```

35.2.7 The WHIZARD shell

This procedure implements interactive mode. One line is processed at a time.

```

<WHIZARD: whizard: TBP>+≡
procedure :: shell => whizard_shell

<WHIZARD: sub interfaces>+≡
module subroutine whizard_shell (whizard, quit_code)
    class(whizard_t), intent(inout), target :: whizard
    integer, intent(out) :: quit_code
end subroutine whizard_shell

<WHIZARD: procedures>+≡
module subroutine whizard_shell (whizard, quit_code)
    class(whizard_t), intent(inout), target :: whizard
    integer, intent(out) :: quit_code
    type(lexer_t), target :: lexer
    type(stream_t), target :: stream
    type(string_t) :: prompt1
    type(string_t) :: prompt2
    type(string_t) :: input
    type(string_t) :: extra
    integer :: last
    integer :: iostat
    logical :: mask_tmp
    logical :: quit
    call msg_message ("Launching interactive shell")
    call lexer_init_cmd_list (lexer)

```

```

prompt1 = "whish? "
prompt2 = "      > "
COMMAND_LOOP: do
  call put (6, prompt1)
  call get (5, input, iostat=iostat)
  if (iostat > 0 .or. iostat == EOF) exit COMMAND_LOOP
CONTINUE_INPUT: do
  last = len_trim (input)
  if (extract (input, last, last) /= BACKSLASH) exit CONTINUE_INPUT
  call put (6, prompt2)
  call get (5, extra, iostat=iostat)
  if (iostat > 0) exit COMMAND_LOOP
  input = replace (input, last, extra)
end do CONTINUE_INPUT
call stream_init (stream, input)
mask_tmp = mask_fatal_errors
mask_fatal_errors = .true.
call whizard%process_stream (stream, lexer, quit, quit_code)
msg_count = 0
mask_fatal_errors = mask_tmp
call stream_final (stream)
if (quit) exit COMMAND_LOOP
end do COMMAND_LOOP
print *
call lexer_final (lexer)
end subroutine whizard_shell

```

35.3 Query Feature Support

This module accesses the various optional features (modules) that WHIZARD can support and reports on their availability.

```
<features.f90>≡
  module features

    <Standard module head>

    <Features: public>

    interface
    <Features: sub interfaces>
    end interface

  end module features

<features_sub.f90>≡
  <File header>

  submodule (features) features_s

    use string_utils, only: lower_case
    use system_dependencies, only: WHIZARD_VERSION
    <Features: dependencies>

    implicit none

    contains

    <Features: procedures>

  end submodule features_s
```

35.3.1 Output

```
<Features: public>≡
  public :: print_features

<Features: sub interfaces>≡
  module subroutine print_features ()
    end subroutine print_features

<Features: procedures>≡
  module subroutine print_features ()
    print "(A)", "WHIZARD " // WHIZARD_VERSION
    print "(A)", "Build configuration:"
    <Features: config>
    print "(A)", "Optional features available in this build:"
    <Features: print>
  end subroutine print_features
```


35.3.2 Query function

```
<Features: procedures>+≡
  subroutine check (feature, recognized, result, help)
    character(*), intent(in) :: feature
    logical, intent(out) :: recognized
    character(*), intent(out) :: result, help
    recognized = .true.
    result = "no"
    select case (lower_case (trim (feature)))
<Features: cases>
      case default
        recognized = .false.
      end select
    end subroutine check
```

Print this result:

```
<Features: procedures>+≡
  subroutine print_check (feature)
    character(*), intent(in) :: feature
    character(16) :: f
    logical :: recognized
    character(10) :: result
    character(48) :: help
    call check (feature, recognized, result, help)
    if (.not. recognized) then
      result = "unknown"
      help = ""
    end if
    f = feature
    print "(2x,A,1x,A,'(',A,')')", f, result, trim (help)
  end subroutine print_check
```

35.3.3 Basic configuration

```
<Features: config>≡
  call print_check ("precision")

<Features: dependencies>≡
  use kinds, only: default

<Features: cases>≡
  case ("precision")
    write (result, "(I0)") precision (1._default)
    help = "significant decimals of real/complex numbers"
```

35.3.4 Optional features case by case

```
<Features: print>≡
  call print_check ("OpenMP")

<Features: dependencies>+≡
  use system_dependencies, only: openmp_is_active
```

```

<Features: cases>+=
  case ("openmp")
    if (openmp_is_active ()) then
      result = "yes"
    end if
    help = "OpenMP parallel execution"

<Features: print>+=
  call print_check ("GoSam")

<Features: dependencies>+=
  use system_dependencies, only: GOSAM_AVAILABLE

<Features: cases>+=
  case ("gosam")
    if (GOSAM_AVAILABLE) then
      result = "yes"
    end if
    help = "external NLO matrix element provider"

<Features: print>+=
  call print_check ("OpenLoops")

<Features: dependencies>+=
  use system_dependencies, only: OPENLOOPS_AVAILABLE

<Features: cases>+=
  case ("openloops")
    if (OPENLOOPS_AVAILABLE) then
      result = "yes"
    end if
    help = "external NLO matrix element provider"

<Features: print>+=
  call print_check ("Recola")

<Features: dependencies>+=
  use system_dependencies, only: RECOLA_AVAILABLE

<Features: cases>+=
  case ("recola")
    if (RECOLA_AVAILABLE) then
      result = "yes"
    end if
    help = "external NLO matrix element provider"

<Features: print>+=
  call print_check ("LHAPDF")

<Features: dependencies>+=
  use system_dependencies, only: LHAPDF5_AVAILABLE
  use system_dependencies, only: LHAPDF6_AVAILABLE

<Features: cases>+=
  case ("lhapdf")
    if (LHAPDF5_AVAILABLE) then
      result = "v5"
    else if (LHAPDF6_AVAILABLE) then
      result = "v6"
    end if
    help = "PDF library"

```

```

<Features: print>+≡
    call print_check ("HOPPET")

<Features: dependencies>+≡
    use system_dependencies, only: HOPPET_AVAILABLE

<Features: cases>+≡
    case ("hoppet")
        if (HOPPET_AVAILABLE) then
            result = "yes"
        end if
        help = "PDF evolution package"

<Features: print>+≡
    call print_check ("fastjet")

<Features: dependencies>+≡
    use jets, only: fastjet_available

<Features: cases>+≡
    case ("fastjet")
        if (fastjet_available ()) then
            result = "yes"
        end if
        help = "jet-clustering package"

<Features: print>+≡
    call print_check ("Pythia6")

<Features: dependencies>+≡
    use system_dependencies, only: PYTHIA6_AVAILABLE

<Features: cases>+≡
    case ("pythia6")
        if (PYTHIA6_AVAILABLE) then
            result = "yes"
        end if
        help = "direct access for shower/hadronization"

<Features: print>+≡
    call print_check ("Pythia8")

<Features: dependencies>+≡
    use system_dependencies, only: PYTHIA8_AVAILABLE

<Features: cases>+≡
    case ("pythia8")
        if (PYTHIA8_AVAILABLE) then
            result = "yes"
        end if
        help = "direct access for shower/hadronization"

<Features: print>+≡
    call print_check ("StdHEP")

<Features: cases>+≡
    case ("stdhep")
        result = "yes"
        help = "event I/O format"

```

```

<Features: print>+≡
    call print_check ("HepMC")

<Features: dependencies>+≡
    use hepmc_interface, only: hepmc_is_available

<Features: cases>+≡
    case ("hepmc")
        if (hepmc_is_available ()) then
            result = "yes"
        end if
        help = "event I/O format"

<Features: print>+≡
    call print_check ("LCIO")

<Features: dependencies>+≡
    use lcio_interface, only: lcio_is_available

<Features: cases>+≡
    case ("lcio")
        if (lcio_is_available ()) then
            result = "yes"
        end if
        help = "event I/O format"

<Features: print>+≡
    call print_check ("MetaPost")

<Features: dependencies>+≡
    use system_dependencies, only: EVENT_ANALYSIS

<Features: cases>+≡
    case ("metapost")
        result = EVENT_ANALYSIS
        help = "graphical event analysis via LaTeX/MetaPost"

```

Chapter 36

Cross References

36.1 Identifiers

36.2 Chunks